
DeePMD-kit

DeepModeling

Sep 01, 2023

GETTING STARTED

| | | |
|--------|---|----|
| 1 | Getting Started | 3 |
| 1.1 | Easy install | 3 |
| 1.1.1 | Install off-line packages | 3 |
| 1.1.2 | Install with conda | 4 |
| 1.1.3 | Install with docker | 4 |
| 1.1.4 | Install Python interface with pip | 5 |
| 1.2 | DeePMD-kit Quick Start Tutorial | 5 |
| 1.2.1 | Task | 5 |
| 1.2.2 | Table of contents | 6 |
| 1.2.3 | Get tutorial data via git | 6 |
| 1.2.4 | General Introduction | 6 |
| 1.2.5 | Data preparation | 7 |
| 1.2.6 | Prepare input script | 8 |
| 1.2.7 | Train a model | 10 |
| 1.2.8 | Freeze a model | 15 |
| 1.2.9 | Test a model | 16 |
| 1.2.10 | Run MD with LAMMPS | 20 |
| 2 | Installation | 25 |
| 2.1 | Easy install | 25 |
| 2.1.1 | Install off-line packages | 25 |
| 2.1.2 | Install with conda | 26 |
| 2.1.3 | Install with docker | 26 |
| 2.1.4 | Install Python interface with pip | 27 |
| 2.2 | Install from source code | 27 |
| 2.2.1 | Install the python interface | 28 |
| 2.2.2 | Install the C++ interface | 31 |
| 2.3 | Install from pre-compiled C library | 33 |
| 2.3.1 | Use Pre-compiled C Library to build the LAMMPS plugin and GROMACS patch | 33 |
| 2.4 | Install LAMMPS | 33 |
| 2.4.1 | Install LAMMPS's DeePMD-kit module (built-in mode) | 33 |
| 2.4.2 | Install LAMMPS (plugin mode) | 34 |
| 2.5 | Install i-PI | 35 |
| 2.6 | Install GROMACS with DeepMD | 35 |
| 2.6.1 | Patch source code of GROMACS | 35 |
| 2.6.2 | Compile GROMACS with deepmd-kit | 35 |
| 2.7 | Building conda packages | 36 |
| 2.8 | Install Node.js interface | 36 |
| 2.8.1 | Install from npm | 36 |
| 2.8.2 | Build from source | 37 |

| | | |
|--------|---|----|
| 3 | Data | 39 |
| 3.1 | System | 39 |
| 3.2 | Formats of a system | 41 |
| 3.2.1 | NumPy format | 41 |
| 3.2.2 | HDF5 format | 41 |
| 3.2.3 | Raw format and data conversion | 42 |
| 3.3 | Prepare data with dpdata | 42 |
| 4 | Model | 45 |
| 4.1 | Overall | 45 |
| 4.2 | Descriptor "se_e2_a" | 46 |
| 4.3 | Descriptor "se_e2_r" | 47 |
| 4.4 | Descriptor "se_e3" | 47 |
| 4.5 | Descriptor "se_atten" | 48 |
| 4.5.1 | DPA-1: Pretraining of Attention-based Deep Potential Model for Molecular Simulation | 48 |
| 4.5.2 | Installation | 48 |
| 4.5.3 | Introduction to new features of DPA-1 | 48 |
| 4.5.4 | Data format | 50 |
| 4.5.5 | Training example | 51 |
| 4.6 | Descriptor "hybrid" | 51 |
| 4.7 | Determine sel | 52 |
| 4.8 | Fit energy | 52 |
| 4.8.1 | The fitting network | 52 |
| 4.8.2 | Loss | 53 |
| 4.9 | Fit spin energy | 53 |
| 4.9.1 | Spin | 54 |
| 4.9.2 | Spin Loss | 54 |
| 4.10 | Fit tensor like Dipole and Polarizability | 55 |
| 4.10.1 | The fitting Network | 55 |
| 4.10.2 | Loss | 56 |
| 4.10.3 | Training Data Preparation | 56 |
| 4.10.4 | Train the Model | 56 |
| 4.11 | Fit electronic density of states (DOS) | 57 |
| 4.11.1 | The fitting Network | 58 |
| 4.11.2 | Loss | 58 |
| 4.11.3 | Training Data Preparation | 59 |
| 4.11.4 | Train the Model | 59 |
| 4.11.5 | Test the Model | 59 |
| 4.12 | Type embedding approach | 60 |
| 4.12.1 | Type embedding net | 60 |
| 4.13 | Descriptor "se_a_mask" | 61 |
| 4.14 | Deep potential long-range (DPLR) | 63 |
| 4.14.1 | Train a deep Wannier model for Wannier centroids | 63 |
| 4.14.2 | Train the DPLR model | 64 |
| 4.14.3 | Molecular dynamics simulation with DPLR | 64 |
| 4.15 | Deep Potential - Range Correction (DPRc) | 67 |
| 4.15.1 | Training data | 67 |
| 4.15.2 | Training the DPRc model | 67 |
| 4.15.3 | Run MD simulations | 69 |
| 4.15.4 | Pairwise DPRc | 69 |
| 5 | Training | 73 |
| 5.1 | Train a model | 73 |
| 5.2 | Advanced options | 74 |

| | | |
|--------|---|-----|
| 5.2.1 | Learning rate | 74 |
| 5.2.2 | Training parameters | 75 |
| 5.2.3 | Options and environment variables | 77 |
| 5.2.4 | Adjust <code>sel</code> of a frozen model | 78 |
| 5.3 | Training Parameters | 78 |
| 5.4 | Parallel training | 117 |
| 5.4.1 | Tuning learning rate | 117 |
| 5.4.2 | Scaling test | 117 |
| 5.4.3 | How to use | 118 |
| 5.4.4 | Logging | 118 |
| 5.5 | Multi-task training | 119 |
| 5.5.1 | Perform the multi-task training | 119 |
| 5.5.2 | Initialization from pretrained multi-task model | 120 |
| 5.5.3 | Share layers among energy fitting networks | 121 |
| 5.6 | TensorBoard Usage | 121 |
| 5.6.1 | Highlighted features | 121 |
| 5.6.2 | How to use Tensorboard with DeePMD-kit | 122 |
| 5.6.3 | Examples | 123 |
| 5.6.4 | Attention | 127 |
| 5.7 | Known limitations of using GPUs | 127 |
| 5.8 | Finetune the pretrained model | 128 |
| 6 | Freeze and Compress | 129 |
| 6.1 | Freeze a model | 129 |
| 6.2 | Compress a model | 129 |
| 7 | Test | 133 |
| 7.1 | Test a model | 133 |
| 7.2 | Calculate Model Deviation | 134 |
| 8 | Inference | 135 |
| 8.1 | Python interface | 135 |
| 8.2 | C/C++ interface | 136 |
| 8.2.1 | C++ interface | 136 |
| 8.2.2 | C interface | 136 |
| 8.2.3 | Header-only C++ library interface (recommended) | 137 |
| 8.3 | Node.js interface | 138 |
| 9 | Command line interface | 139 |
| 9.1 | Named Arguments | 139 |
| 9.2 | Valid subcommands | 139 |
| 9.3 | Sub-commands | 139 |
| 9.3.1 | transfer | 139 |
| 9.3.2 | train | 140 |
| 9.3.3 | freeze | 141 |
| 9.3.4 | test | 142 |
| 9.3.5 | compress | 143 |
| 9.3.6 | doc-train-input | 144 |
| 9.3.7 | model-devi | 144 |
| 9.3.8 | convert-from | 145 |
| 9.3.9 | neighbor-stat | 146 |
| 9.3.10 | train-nvnmd | 146 |
| 10 | Integrate with third-party packages | 149 |
| 10.1 | Use deep potential with ASE | 149 |

| | | |
|--------|---|-----|
| 10.2 | Run MD with LAMMPS | 149 |
| 10.3 | LAMMPS commands | 150 |
| 10.3.1 | Enable DeePMD-kit plugin (plugin mode) | 150 |
| 10.3.2 | pair_style deepmd | 150 |
| 10.3.3 | Compute tensorial properties | 151 |
| 10.3.4 | Long-range interaction | 152 |
| 10.3.5 | Use of the centroid/stress/atom to get the full 3x3 “atomic-virial” | 152 |
| 10.3.6 | Computation of heat flux | 153 |
| 10.4 | Run path-integral MD with i-PI | 153 |
| 10.5 | Running MD with GROMACS | 154 |
| 10.5.1 | DP/MM Simulation | 154 |
| 10.5.2 | All-atom DP Simulation | 156 |
| 10.6 | Interfaces out of DeePMD-kit | 157 |
| 10.6.1 | dpdata | 157 |
| 10.6.2 | OpenMM plugin for DeePMD-kit | 158 |
| 10.6.3 | AMBER interface to DeePMD-kit | 158 |
| 10.6.4 | DP-GEN | 158 |
| 10.6.5 | MLatom | 158 |
| 10.6.6 | ABACUS | 158 |
| 11 | Use NVNMD | 159 |
| 11.1 | Introduction | 159 |
| 11.2 | Training | 159 |
| 11.2.1 | Input script | 160 |
| 11.2.2 | Training | 162 |
| 11.3 | Testing | 162 |
| 11.4 | Running MD in Bohrium | 163 |
| 11.4.1 | Registration | 163 |
| 11.4.2 | Top-up and create a project | 163 |
| 11.4.3 | Run job | 164 |
| 11.4.4 | Check job status | 166 |
| 11.4.5 | Terminate and delete jobs | 166 |
| 11.4.6 | Download Results | 167 |
| 11.5 | Running MD in Nvnmd website | 167 |
| 11.5.1 | Account application | 168 |
| 11.5.2 | Adding task | 168 |
| 11.5.3 | Cancelling calculation | 170 |
| 11.5.4 | Downloading results | 170 |
| 11.5.5 | Deleting record | 171 |
| 11.5.6 | Clearing records | 171 |
| 12 | FAQs | 173 |
| 12.1 | How to tune Fitting/embedding-net size ? | 173 |
| 12.1.1 | Al2O3 | 173 |
| 12.1.2 | Cu | 174 |
| 12.1.3 | Water | 175 |
| 12.1.4 | Mg-Al | 176 |
| 12.2 | How to control the parallelism of a job? | 176 |
| 12.2.1 | MPI (optional) | 177 |
| 12.2.2 | Parallelism between independent operators | 177 |
| 12.2.3 | Parallelism within an individual operators | 177 |
| 12.2.4 | Tune the performance | 178 |
| 12.3 | Do we need to set rcut < half boxsize? | 178 |
| 12.4 | How to set sel? | 178 |

| | | |
|--------|--|-----|
| 12.5 | Installation | 179 |
| 12.5.1 | Inadequate versions of gcc/g++ | 179 |
| 12.5.2 | Build files left in DeePMD-kit | 179 |
| 12.6 | The temperature undulates violently during the early stages of MD | 179 |
| 12.7 | MD: cannot run LAMMPS after installing a new version of DeePMD-kit | 179 |
| 12.8 | Model compatibility | 180 |
| 12.9 | Why does a model have low precision? | 180 |
| 12.9.1 | Data | 180 |
| 12.9.2 | Model | 181 |
| 12.9.3 | Training | 181 |
| 13 | Find DeePMD-kit C/C++ library from CMake | 183 |
| 14 | Coding Conventions | 185 |
| 14.1 | Preface | 185 |
| 14.2 | Rules | 185 |
| 14.3 | Whitespace | 186 |
| 14.4 | General advice | 186 |
| 14.5 | Writing documentation in the code | 186 |
| 14.6 | Run pycodestyle on your code | 187 |
| 14.7 | Run mypy on your code | 187 |
| 14.8 | Run pydocstyle on your code | 187 |
| 14.9 | Run black on your code | 187 |
| 15 | Create a model | 189 |
| 15.1 | Design a new component | 189 |
| 15.2 | Register new arguments | 189 |
| 15.3 | Package new codes | 190 |
| 16 | Atom Type Embedding | 191 |
| 16.1 | Overview | 191 |
| 16.2 | Preliminary | 191 |
| 16.3 | How to use | 192 |
| 16.4 | Code Modification | 192 |
| 16.4.1 | trainer (train/trainer.py) | 192 |
| 16.4.2 | model (model/ener.py) | 192 |
| 16.4.3 | embedding net (descriptor/se*.py) | 193 |
| 16.4.4 | fitting net (fit/ener.py) | 193 |
| 17 | Python API | 195 |
| 17.1 | deepmd package | 195 |
| 17.1.1 | Subpackages | 200 |
| 17.1.2 | Submodules | 501 |
| 17.1.3 | deepmd.calculator module | 501 |
| 17.1.4 | deepmd.common module | 503 |
| 17.1.5 | deepmd.env module | 508 |
| 17.1.6 | deepmd.lmp module | 508 |
| 18 | OP API | 511 |
| 18.1 | op_module | 511 |
| 18.2 | op_grads_module | 560 |
| 19 | C++ API | 569 |
| 19.1 | Class Hierarchy | 569 |
| 19.2 | File Hierarchy | 569 |

| | | |
|--------|---------------------------------------|-----|
| 19.3 | Full API | 570 |
| 19.3.1 | Namespaces | 570 |
| 19.3.2 | Classes and Structs | 571 |
| 19.3.3 | Functions | 588 |
| 19.3.4 | Typedefs | 596 |
| 20 | C API | 599 |
| 20.1 | Class Hierarchy | 599 |
| 20.2 | File Hierarchy | 599 |
| 20.3 | Full API | 600 |
| 20.3.1 | Namespaces | 600 |
| 20.3.2 | Classes and Structs | 601 |
| 20.3.3 | Functions | 618 |
| 20.3.4 | Defines | 663 |
| 20.3.5 | Typedefs | 664 |
| 21 | Core API | 667 |
| 21.1 | Class Hierarchy | 667 |
| 21.2 | File Hierarchy | 668 |
| 21.3 | Full API | 669 |
| 21.3.1 | Namespaces | 669 |
| 21.3.2 | Classes and Structs | 673 |
| 21.3.3 | Unions | 683 |
| 21.3.4 | Functions | 683 |
| 21.3.5 | Variables | 723 |
| 21.3.6 | Defines | 723 |
| 21.3.7 | Typedefs | 726 |
| 22 | License | 727 |
| 23 | Authors and Credits | 729 |
| 23.1 | Cite DeePMD-kit and methods | 729 |
| 23.2 | Package Contributors | 729 |
| 23.3 | Other Credits | 731 |
| 24 | Logo | 733 |
| | Bibliography | 735 |
| | Python Module Index | 739 |
| | Index | 741 |

DeePMD-kit is a package written in Python/C++, designed to minimize the effort required to build deep learning-based models of interatomic potential energy and force field and to perform molecular dynamics (MD). This brings new hopes to addressing the accuracy-versus-efficiency dilemma in molecular simulations. Applications of DeePMD-kit span from finite molecules to extended systems and from metallic systems to chemically bonded systems.

Important: The project DeePMD-kit is licensed under [GNU LGPLv3.0](#). If you use this code in any future publications, please cite the following publications for general purpose:

- Han Wang, Linfeng Zhang, Jiequn Han, and Weinan E. “DeePMD-kit: A deep learning package for many-body potential energy representation and molecular dynamics.” *Computer Physics Communications* 228 (2018): 178-184.
- Jinzhe Zeng, Duo Zhang, Denghui Lu, Pinghui Mo, Zeyu Li, Yixiao Chen, Marián Rynik, Li’ang Huang, Ziyao Li, Shaochen Shi, Yingze Wang, Haotian Ye, Ping Tuo, Jiabin Yang, Ye Ding, Yifan Li, Davide Tisi, Qiyu Zeng, Han Bao, Yu Xia, Jiameng Huang, Koki Muraoka, Yibo Wang, Junhan Chang, Fengbo Yuan, Sigbjørn Løland Bore, Chun Cai, Yinnian Lin, Bo Wang, Jiayan Xu, Jia-Xin Zhu, Chenxing Luo, Yuzhi Zhang, Rhys E. A. Goodall, Wenshuo Liang, Anurag Kumar Singh, Sikai Yao, Jingchao Zhang, Renata Wentzcovitch, Jiequn Han, Jie Liu, Weile Jia, Darrin M. York, Weinan E, Roberto Car, Linfeng Zhang, Han Wang. “DeePMD-kit v2: A software package for Deep Potential models.” *J. Chem. Phys.*, 159, 054801 (2023).

In addition, please follow [this page](#) to cite the methods you used.

GETTING STARTED

In this text, we will call the deep neural network that is used to represent the interatomic interactions (Deep Potential) the model. The typical procedure of using DeePMD-kit is

1.1 Easy install

There are various easy methods to install DeePMD-kit. Choose one that you prefer. If you want to build by yourself, jump to the next two sections.

After your easy installation, DeePMD-kit (`dp`) and LAMMPS (`lmp`) will be available to execute. You can try `dp -h` and `lmp -h` to see the help. `mpirun` is also available considering you may want to train models or run LAMMPS in parallel.

Note: Note: The off-line packages and conda packages require the [GNU C Library 2.17](#) or above. The GPU version requires [compatible NVIDIA driver](#) to be installed in advance. It is possible to force conda to [override detection](#) when installation, but these requirements are still necessary during runtime.

- [Install off-line packages](#)
- [Install with conda](#)
- [Install with docker](#)
- [Install Python interface with pip](#)

1.1.1 Install off-line packages

Both CPU and GPU version offline packages are available in [the Releases page](#).

Some packages are splited into two files due to size limit of GitHub. One may merge them into one after downloading:

```
cat deepmd-kit-2.1.1-cuda11.6_gpu-Linux-x86_64.sh.0 deepmd-kit-2.1.1-cuda11.6_gpu-Linux-x86_64.sh.  
↪ 1 > deepmd-kit-2.1.1-cuda11.6_gpu-Linux-x86_64.sh
```

One may enable the environment using

```
conda activate /path/to/deepmd-kit
```

1.1.2 Install with conda

DeePMD-kit is available with [conda](#). Install [Anaconda](#) or [Miniconda](#) first.

Official channel

One may create an environment that contains the CPU version of DeePMD-kit and LAMMPS:

```
conda create -n deepmd deepmd-kit==*cpu libdeepmd==*cpu lammps -c https://conda.deepmodeling.com
↪ -c defaults
```

Or one may want to create a GPU environment containing [CUDA Toolkit](#):

```
conda create -n deepmd deepmd-kit==*gpu libdeepmd==*gpu lammps cudatoolkit=11.6 horovod -c
↪ https://conda.deepmodeling.com -c defaults
```

One could change the CUDA Toolkit version from 10.2 or 11.6.

One may specify the DeePMD-kit version such as 2.1.1 using

```
conda create -n deepmd deepmd-kit=2.1.1=*cpu libdeepmd=2.1.1=*cpu lammps horovod -c https://conda.
↪ deepmodeling.com -c defaults
```

One may enable the environment using

```
conda activate deepmd
```

conda-forge channel

DeePMD-kit is also available on the [conda-forge](#) channel:

```
conda create -n deepmd deepmd-kit lammps -c conda-forge
```

The supported platform includes Linux x86-64, macOS x86-64, and macOS arm64. Read [conda-forge FAQ](#) to learn how to install CUDA-enabled packages.

1.1.3 Install with docker

A docker for installing the DeePMD-kit is available [here](#).

To pull the CPU version:

```
docker pull ghcr.io/deepmodeling/deepmd-kit:2.1.1_cpu
```

To pull the GPU version:

```
docker pull ghcr.io/deepmodeling/deepmd-kit:2.1.1_cuda11.6_gpu
```

To pull the ROCm version:

```
docker pull deepmodeling/dpmdkit-rocm:dp2.0.3-rocm4.5.2-tf2.6-lmp29Sep2021
```

1.1.4 Install Python interface with pip

If you have no existing TensorFlow installed, you can use `pip` to install the pre-built package of the Python interface with CUDA 11 supported:

```
pip install deepmd-kit[gpu,cu11]
```

`cu11` is required only when CUDA Toolkit and cuDNN were not installed.

Or install the CPU version without CUDA supported:

```
pip install deepmd-kit[cpu]
```

The LAMMPS module and the i-Pi driver are only provided on Linux and macOS. To install LAMMPS and/or i-Pi, add `lmp` and/or `ipi` to extras:

```
pip install deepmd-kit[gpu,cu11,lmp,ipi]
```

MPICH is required for parallel running. (The macOS arm64 package doesn't support MPI yet.)

It is suggested to install the package into an isolated environment. The supported platform includes Linux x86-64 and aarch64 with GNU C Library 2.28 or above, macOS x86-64 and arm64, and Windows x86-64. A specific version of TensorFlow which is compatible with DeePMD-kit will be also installed.

Warning: If your platform is not supported, or want to build against the installed TensorFlow, or want to enable ROCm support, please build from source.

1.2 DeePMD-kit Quick Start Tutorial

DeePMD-kit is a deep learning package for many-body potential energy representation and molecular dynamics.

This tutorial can be directly run on Bohrium Notebook, you can click the **Open in Bohrium** button above to quickly run this document in Bohrium.

After opening Bohrium Notebook, click the button **connect**, and choose `deepmd-kit:2.2.1-cuda11.6-notebook` as image and `c4_m8_cpu` as computing resources. Wait a minute and you can get started.

1.2.1 Task

Mastering the paradigm cycle of using DeePMD-kit to establish deep potential molecular dynamics models, and following a complete case to learn how to apply it to molecular dynamics tasks.

By the end of this tutorial, you will be able to:

- Prepare the formative dataset and running scripts for training with DeePMD-kit;
- Train, freeze, and test DeePMD-kit models;
- Use DeePMD-kit in LAMMPS for calculations;

Work through this tutorial. It will take you 20 minutes, max!

1.2.2 Table of contents

- Get tutorial data via git
- General Introduction
- Data preparation
- Prepare input script
- Train a model
- Freeze a model
- Test a model
- Run MD with LAMMPS

1.2.3 Get tutorial data via git

```
! if ! [ -e colombo-academy-tutorials ];then git clone https://gitee.com/deepmodeling/colombo-academy-tutorials.git;fi;
```

```
Cloning into 'colombo-academy-tutorials'...
remote: Enumerating objects: 7164, done.
remote: Counting objects: 100% (174/174), done.
remote: Compressing objects: 100% (138/138), done.
remote: Total 7164 (delta 78), reused 71 (delta 32), pack-reused 6990
Receiving objects: 100% (7164/7164), 45.31 MiB | 3.85 MiB/s, done.
Resolving deltas: 100% (3378/3378), done.
Updating files: 100% (185/185), done.
```

1.2.4 General Introduction

This tutorial will introduce you to the basic usage of the DeePMD-kit, taking a gas phase methane molecule as an example. [DeePMD-kit's documentation](#) is recommended as the complete reference.

The DP model is generated using the DeePMD-kit package (v2.1.5). The training data is converted into the format of DeePMD-kit using a tool named dpdata (v0.2.14).

Details of dpdata can be found in [the dpdata documentation](#).

We've prepared initial data for CH_4 for you, and put them in the folder `colombo-academy-tutorials/DeePMD-kit/00.data`

```
import os

prefix_path = os.getcwd()
```

Folder `abacus_md` is obtained by performing ab-initio molecular dynamics with ABACUS. Detailed instructions on ABACUS can be found in its [document](#).

```
os.chdir(
    os.path.join(prefix_path, "colombo-academy-tutorials", "DeePMD-kit", "00.data")
)
os.listdir("abacus_md")
```

```
[ 'C_ONCV_PBE-1.2.upf',
  'C_gga_6au_100Ry_2s2p1d.orb',
  'H_ONCV_PBE-1.2.upf',
  'H_gga_6au_100Ry_2s1p.orb',
  'INPUT',
  'KPT',
  'OUT.ABACUS',
  'STRU']
```

1.2.5 Data preparation

The training data utilized by DeePMD-kit comprises essential information such as atom type, simulation box, atom coordinate, atom force, system energy, and virial. A snapshot of a molecular system that includes this data is called a **frame**. Multiple frames with the same number of atoms and atom types make up a **system** of data. For instance, a molecular dynamics trajectory can be converted into a system of data, with each time step corresponding to a frame in the system.

To simplify the process of converting data generated by popular simulation software like CP2K, Gaussian, Quantum-Espresso, ABACUS, and LAMMPS into the compressed format of DeePMD-kit, we offer a convenient tool called `dpdata`.

Next, the data from AIMD is splited randomly as training and validation data.

```
import dpdata
import numpy as np

# load data of abacus/md format
data = dpdata.LabeledSystem("abacus_md", fmt="abacus/md")
print("# the data contains %d frames" % len(data))

# random choose 40 index for validation_data
index_validation = np.random.choice(201, size=40, replace=False)

# other indexes are training_data
index_training = list(set(range(201)) - set(index_validation))
data_training = data.sub_system(index_training)
data_validation = data.sub_system(index_validation)

# all training data put into directory:"training_data"
data_training.to_deepmd_npy("training_data")

# all validation data put into directory:"validation_data"
data_validation.to_deepmd_npy("validation_data")

print("# the training data contains %d frames" % len(data_training))
print("# the validation data contains %d frames" % len(data_validation))
```

```
# the data contains 201 frames
# the training data contains 161 frames
# the validation data contains 40 frames
```

As you can see, 161 frames are picked as training data, and the other 40 frames are validation data.

The DeePMD-kit adopts a compressed data format. All training data should first be converted into this format and can then be used by DeePMD-kit. The data format is explained in detail in the DeePMD-kit manual that can be found in [the DeePMD-kit Data Introduction](#).

```
! tree training_data
```

```
training_data
  set.000
    box.npy
    coord.npy
    energy.npy
    force.npy
    virial.npy
  type.raw
  type_map.raw

1 directory, 7 files
```

Let's have a look at `type.raw`:

```
! cat training_data/type.raw
```

```
0
0
0
0
1
```

This tells us there are 5 atoms in this example, 4 atoms represented by type “0”, and 1 atom represented by type “1”. Sometimes one needs to map the integer types to atom name. The mapping can be given by the file `type_map.raw`

```
! cat training_data/type_map.raw
```

```
H
C
```

This tells us the type “0” is named by “H”, and the type “1” is named by “C”.

More detailed doc about Data conversion can be found [here](#).

1.2.6 Prepare input script

Once the data preparation is done, we can go on with training. Now go to the training directory

```
os.chdir(
    os.path.join(prefix_path, "colombo-academy-tutorials", "DeePMD-kit", "01.train")
)
```

DeePMD-kit requires a `json` format file to specify parameters for training.

In the `model` section, the parameters of embedding and fitting networks are specified.

```
"model":{
  "type_map":    ["H", "C"],
  "descriptor":{
    "type":      "se_e2_a",
    "rcut":      6.00,
    "rcut_smth": 0.50,
```

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```

    "sel":          "auto",
    "neuron":       [25, 50, 100],
    "resnet_dt":    false,
    "axis_neuron":  16,
    "seed":         1,
    "_comment":     "that's all"
  },
  "fitting_net":{
    "neuron":       [240, 240, 240],
    "resnet_dt":    true,
    "seed":         1,
    "_comment":     "that's all"
  },
  "_comment":      "that's all"
},

```

The explanation for some of the parameters is as follows:

| Parameter | Expiation |
|--------------------------|--|
| type_map | the name of each type of atom |
| descriptor > type | the type of descriptor |
| descriptor > rcut | cut-off radius |
| descriptor > rcut_smth | where the smoothing starts |
| descriptor > sel | the maximum number of type i atoms in the cut-off radius |
| descriptor > neuron | size of the embedding neural network |
| descriptor > axis_neuron | the size of the submatrix of G (embedding matrix) |
| fitting_net > neuron | size of the fitting neural network |

The `se_e2_a` descriptor is used to train the DP model. The item neurons set the size of the descriptors and fitting network to [25, 50, 100] and [240, 240, 240], respectively. The components in local environment to smoothly go to zero from 0.5 to 6 Å.

The following are the parameters that specify the learning rate and loss function.

```

"learning_rate" :{
  "type":          "exp",
  "decay_steps":   50,
  "start_lr":      0.001,
  "stop_lr":       3.51e-8,
  "_comment":     "that's all"
},
"loss" :{
  "type":          "ener",
  "start_pref_e":  0.02,
  "limit_pref_e":  1,
  "start_pref_f":  1000,
  "limit_pref_f":  1,
  "start_pref_v":  0,
  "limit_pref_v":  0,
  "_comment":     "that's all"
},

```

In the loss function, `pref_e` increases from 0.02 to 1, and `pref_f` decreases from 1000 to 1 progressively, which means that the force term dominates at the beginning, while energy and virial terms become important at the end. This strategy is very effective and reduces the total training time. `pref_v` is set to 0, indicating that

no virial data are included in the training process. The starting learning rate, stop learning rate, and decay steps are set to 0.001, $3.51\text{e-}8$, and 50, respectively. The model is trained for 10000 steps.

The training parameters are given in the following

```
"training" : {
  "training_data": {
    "systems":      ["../00.data/training_data"],
    "batch_size":   "auto",
    "_comment":     "that's all"
  },
  "validation_data":{
    "systems":      ["../00.data/validation_data/"],
    "batch_size":   "auto",
    "numb_btch":    1,
    "_comment":     "that's all"
  },
  "numb_steps":    10000,
  "seed":          10,
  "disp_file":     "lcurve.out",
  "disp_freq":     200,
  "save_freq":     10000,
}
```

More detailed docs about Data conversion can be found [here](#).

1.2.7 Train a model

After the training script is prepared, we can start the training with DeePMD-kit by simply running

```
! dp train input.json
```

```
WARNING:tensorflow:From /opt/deepmd-kit-2.2.1/lib/python3.10/site-packages/tensorflow/python/
↳ compat/v2_compat.py:107: disable_resource_variables (from tensorflow.python.ops.variable_scope)
↳ is deprecated and will be removed in a future version.
Instructions for updating:
non-resource variables are not supported in the long term
WARNING:root:To get the best performance, it is recommended to adjust the number of threads by
↳ setting the environment variables OMP_NUM_THREADS, TF_INTRA_OP_PARALLELISM_THREADS, and TF_INTER_
↳ OP_PARALLELISM_THREADS. See https://deepmd.rtfd.io/parallelism/ for more information.
WARNING:root:Environment variable KMP_BLOCKTIME is empty. Use the default value 0
WARNING:root:Environment variable KMP_AFFINITY is empty. Use the default value granularity=fine,
↳ verbose,compact,1,0
/opt/deepmd-kit-2.2.1/lib/python3.10/importlib/__init__.py:169: UserWarning: The NumPy module was
↳ reloaded (imported a second time). This can in some cases result in small but subtle issues and
↳ is discouraged.
  _bootstrap._exec(spec, module)
DEEPMO INFO    Calculate neighbor statistics... (add --skip-neighbor-stat to skip this step)
2023-04-20 23:35:59.335932: W tensorflow/stream_executor/platform/default/dso_loader.cc:64] Could
↳ not load dynamic library 'libcudart.so.1'; dlopen: libcudart.so.1: cannot open shared object file:
↳ No such file or directory; LD_LIBRARY_PATH: /usr/local/nvidia/lib:/usr/local/nvidia/lib64
2023-04-20 23:35:59.335979: W tensorflow/stream_executor/cuda/cuda_driver.cc:269] failed call to
↳ cuInit: UNKNOWN ERROR (303)
OMP: Info #155: KMP_AFFINITY: Initial OS proc set respected: 0-7
OMP: Info #216: KMP_AFFINITY: decoding x2APIC ids.
OMP: Info #216: KMP_AFFINITY: cpuid leaf 11 not supported.
```

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```

OMP: Info #216: KMP_AFFINITY: decoding legacy APIC ids.
OMP: Info #157: KMP_AFFINITY: 8 available OS procs
OMP: Info #158: KMP_AFFINITY: Uniform topology
OMP: Info #287: KMP_AFFINITY: topology layer "LL cache" is equivalent to "socket".
OMP: Info #192: KMP_AFFINITY: 1 socket x 4 cores/socket x 2 threads/core (4 total cores)
OMP: Info #218: KMP_AFFINITY: OS proc to physical thread map:
OMP: Info #172: KMP_AFFINITY: OS proc 0 maps to socket 0 core 0 thread 0
OMP: Info #172: KMP_AFFINITY: OS proc 1 maps to socket 0 core 0 thread 1
OMP: Info #172: KMP_AFFINITY: OS proc 2 maps to socket 0 core 1 thread 0
OMP: Info #172: KMP_AFFINITY: OS proc 3 maps to socket 0 core 1 thread 1
OMP: Info #172: KMP_AFFINITY: OS proc 4 maps to socket 0 core 2 thread 0
OMP: Info #172: KMP_AFFINITY: OS proc 5 maps to socket 0 core 2 thread 1
OMP: Info #172: KMP_AFFINITY: OS proc 6 maps to socket 0 core 3 thread 0
OMP: Info #172: KMP_AFFINITY: OS proc 7 maps to socket 0 core 3 thread 1
OMP: Info #254: KMP_AFFINITY: pid 118 tid 140 thread 1 bound to OS proc set 2
OMP: Info #254: KMP_AFFINITY: pid 118 tid 142 thread 2 bound to OS proc set 4
OMP: Info #254: KMP_AFFINITY: pid 118 tid 144 thread 4 bound to OS proc set 1
OMP: Info #254: KMP_AFFINITY: pid 118 tid 143 thread 3 bound to OS proc set 6
OMP: Info #254: KMP_AFFINITY: pid 118 tid 145 thread 5 bound to OS proc set 3
OMP: Info #254: KMP_AFFINITY: pid 118 tid 146 thread 6 bound to OS proc set 5
OMP: Info #254: KMP_AFFINITY: pid 118 tid 147 thread 7 bound to OS proc set 7
OMP: Info #254: KMP_AFFINITY: pid 118 tid 148 thread 8 bound to OS proc set 0
OMP: Info #254: KMP_AFFINITY: pid 118 tid 139 thread 9 bound to OS proc set 2
OMP: Info #254: KMP_AFFINITY: pid 118 tid 149 thread 10 bound to OS proc set 4
OMP: Info #254: KMP_AFFINITY: pid 118 tid 150 thread 11 bound to OS proc set 6
OMP: Info #254: KMP_AFFINITY: pid 118 tid 151 thread 12 bound to OS proc set 1
OMP: Info #254: KMP_AFFINITY: pid 118 tid 152 thread 13 bound to OS proc set 3
OMP: Info #254: KMP_AFFINITY: pid 118 tid 153 thread 14 bound to OS proc set 5
OMP: Info #254: KMP_AFFINITY: pid 118 tid 154 thread 15 bound to OS proc set 7
OMP: Info #254: KMP_AFFINITY: pid 118 tid 155 thread 16 bound to OS proc set 0
DEEPMO INFO      training data with min nbor dist: 1.045920568611028
DEEPMO INFO      training data with max nbor size: [4 1]
DEEPMO INFO
DEEPMO INFO      |  _ _ _ _ \      |  _ _ _ _ \  _ _ _ _ \      |  _ _ _ _ \  _ _ _ _ \
DEEPMO INFO      | | | | |  _ _ _ _ _ | | | | |  _ _ _ _ _ | | | | |  _ _ _ _ _ | | | | |  _ _ _ _ _
DEEPMO INFO      | | | | | / _ _ \ / _ _ \ | | | | | / _ _ \ | | | | | / _ _ \ | | | | | / _ _ \
DEEPMO INFO      | | _ _ | | _ _ / | _ _ / | | | | | | _ _ | | | | | | _ _ | | | | | | _ _
DEEPMO INFO      | _ _ _ _ /  \ _ _ \ \ _ _ \ | | | | | _ _ _ /  \ _ _ \ \ _ _ \ | | | | | _ _ _
DEEPMO INFO      Please read and cite:
DEEPMO INFO      Wang, Zhang, Han and E, Comput.Phys.Comm. 228, 178-184 (2018)
DEEPMO INFO      installed to:          /home/conda/feedstock_root/build_artifacts/deepmd-kit_
DEEPMO INFO      ↪1678943793317/work/_skbuild/linux-x86_64-3.10/cmake-install
DEEPMO INFO      source :                  v2.2.1
DEEPMO INFO      source brach:             HEAD
DEEPMO INFO      source commit:           3ac8c4c7
DEEPMO INFO      source commit at:       2023-03-16 12:33:24 +0800
DEEPMO INFO      build float prec:        double
DEEPMO INFO      build variant:           cuda
DEEPMO INFO      build with tf inc:         /opt/deepmd-kit-2.2.1/lib/python3.10/site-packages/tensorflow/
DEEPMO INFO      ↪include;/opt/deepmd-kit-2.2.1/lib/python3.10/site-packages/tensorflow/../../../../include
DEEPMO INFO      build with tf lib:
DEEPMO INFO      ---Summary of the training-----
DEEPMO INFO      running on:                   bohrium-14076-1013950
DEEPMO INFO      computing device:              cpu:0
DEEPMO INFO      CUDA_VISIBLE_DEVICES:          unset
DEEPMO INFO      Count of visible GPU: 0

```

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```

DEEPMD INFO    num_intra_threads:    0
DEEPMD INFO    num_inter_threads:    0
DEEPMD INFO    -----
DEEPMD INFO    ---Summary of DataSystem: training  -----
↪ --
DEEPMD INFO    found 1 system(s):
DEEPMD INFO
DEEPMD INFO              system  natoms  bch_sz  n_bch  prob  pbc
DEEPMD INFO              ../00.data/training_data      5      7     23  1.000  T
DEEPMD INFO    -----
↪ --
DEEPMD INFO    ---Summary of DataSystem: validation  -----
↪ --
DEEPMD INFO    found 1 system(s):
DEEPMD INFO
DEEPMD INFO              system  natoms  bch_sz  n_bch  prob  pbc
DEEPMD INFO              ../00.data/validation_data      5      7      5  1.000  T
DEEPMD INFO    -----
↪ --
DEEPMD INFO    training without frame parameter
DEEPMD INFO    data stating... (this step may take long time)
OMP: Info #254: KMP_AFFINITY: pid 118 tid 118 thread 0 bound to OS proc set 0
DEEPMD INFO    built lr
DEEPMD INFO    built network
DEEPMD INFO    built training
WARNING:root:To get the best performance, it is recommended to adjust the number of threads by
↪ setting the environment variables OMP_NUM_THREADS, TF_INTRA_OP_PARALLELISM_THREADS, and TF_INTER_
↪ OP_PARALLELISM_THREADS. See https://deepmd.rtd.io/parallelism/ for more information.
DEEPMD INFO    initialize model from scratch
DEEPMD INFO    start training at lr 1.00e-03 (== 1.00e-03), decay_step 50, decay_rate 0.950006,
↪ final lr will be 3.51e-08
DEEPMD INFO    batch      200 training time 6.10 s, testing time 0.02 s
DEEPMD INFO    batch      400 training time 4.83 s, testing time 0.02 s
DEEPMD INFO    batch      600 training time 4.84 s, testing time 0.02 s
DEEPMD INFO    batch      800 training time 4.85 s, testing time 0.02 s
DEEPMD INFO    batch     1000 training time 4.85 s, testing time 0.02 s
DEEPMD INFO    saved checkpoint model.ckpt
DEEPMD INFO    batch     1200 training time 4.86 s, testing time 0.02 s
DEEPMD INFO    batch     1400 training time 5.39 s, testing time 0.02 s
DEEPMD INFO    batch     1600 training time 4.84 s, testing time 0.02 s
DEEPMD INFO    batch     1800 training time 4.86 s, testing time 0.02 s
DEEPMD INFO    batch     2000 training time 4.84 s, testing time 0.02 s
DEEPMD INFO    saved checkpoint model.ckpt
DEEPMD INFO    batch     2200 training time 4.86 s, testing time 0.02 s
DEEPMD INFO    batch     2400 training time 4.90 s, testing time 0.02 s
DEEPMD INFO    batch     2600 training time 4.87 s, testing time 0.02 s
DEEPMD INFO    batch     2800 training time 4.84 s, testing time 0.02 s
DEEPMD INFO    batch     3000 training time 4.86 s, testing time 0.02 s
DEEPMD INFO    saved checkpoint model.ckpt
DEEPMD INFO    batch     3200 training time 4.86 s, testing time 0.02 s
DEEPMD INFO    batch     3400 training time 4.99 s, testing time 0.02 s
DEEPMD INFO    batch     3600 training time 4.88 s, testing time 0.02 s
DEEPMD INFO    batch     3800 training time 4.85 s, testing time 0.02 s
DEEPMD INFO    batch     4000 training time 4.88 s, testing time 0.02 s
DEEPMD INFO    saved checkpoint model.ckpt
DEEPMD INFO    batch     4200 training time 4.88 s, testing time 0.02 s
DEEPMD INFO    batch     4400 training time 4.86 s, testing time 0.02 s
DEEPMD INFO    batch     4600 training time 4.92 s, testing time 0.02 s

```

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```

DEEPMd INFO    batch    4800 training time 4.86 s, testing time 0.02 s
DEEPMd INFO    batch    5000 training time 4.86 s, testing time 0.02 s
DEEPMd INFO    saved checkpoint model.ckpt
DEEPMd INFO    batch    5200 training time 4.87 s, testing time 0.02 s
DEEPMd INFO    batch    5400 training time 4.88 s, testing time 0.02 s
DEEPMd INFO    batch    5600 training time 4.87 s, testing time 0.02 s
DEEPMd INFO    batch    5800 training time 4.87 s, testing time 0.02 s
DEEPMd INFO    batch    6000 training time 4.90 s, testing time 0.02 s
WARNING:tensorflow:From /opt/deepmd-kit-2.2.1/lib/python3.10/site-packages/tensorflow/python/
↳training/saver.py:1066: remove_checkpoint (from tensorflow.python.training.checkpoint_
↳management) is deprecated and will be removed in a future version.
Instructions for updating:
Use standard file APIs to delete files with this prefix.
WARNING:tensorflow:From /opt/deepmd-kit-2.2.1/lib/python3.10/site-packages/tensorflow/python/
↳training/saver.py:1066: remove_checkpoint (from tensorflow.python.training.checkpoint_
↳management) is deprecated and will be removed in a future version.
Instructions for updating:
Use standard file APIs to delete files with this prefix.
DEEPMd INFO    saved checkpoint model.ckpt
DEEPMd INFO    batch    6200 training time 4.86 s, testing time 0.02 s
DEEPMd INFO    batch    6400 training time 4.87 s, testing time 0.02 s
DEEPMd INFO    batch    6600 training time 4.86 s, testing time 0.02 s
DEEPMd INFO    batch    6800 training time 4.84 s, testing time 0.02 s
DEEPMd INFO    batch    7000 training time 4.93 s, testing time 0.02 s
DEEPMd INFO    saved checkpoint model.ckpt
DEEPMd INFO    batch    7200 training time 4.89 s, testing time 0.02 s
DEEPMd INFO    batch    7400 training time 4.88 s, testing time 0.02 s
DEEPMd INFO    batch    7600 training time 4.88 s, testing time 0.02 s
DEEPMd INFO    batch    7800 training time 4.87 s, testing time 0.02 s
DEEPMd INFO    batch    8000 training time 4.86 s, testing time 0.02 s
DEEPMd INFO    saved checkpoint model.ckpt
DEEPMd INFO    batch    8200 training time 4.87 s, testing time 0.02 s
DEEPMd INFO    batch    8400 training time 4.85 s, testing time 0.02 s
DEEPMd INFO    batch    8600 training time 4.86 s, testing time 0.02 s
DEEPMd INFO    batch    8800 training time 4.87 s, testing time 0.02 s
DEEPMd INFO    batch    9000 training time 4.83 s, testing time 0.02 s
DEEPMd INFO    saved checkpoint model.ckpt
DEEPMd INFO    batch    9200 training time 4.87 s, testing time 0.02 s
DEEPMd INFO    batch    9400 training time 4.95 s, testing time 0.02 s
DEEPMd INFO    batch    9600 training time 4.89 s, testing time 0.02 s
DEEPMd INFO    batch    9800 training time 4.87 s, testing time 0.02 s
DEEPMd INFO    batch    10000 training time 4.88 s, testing time 0.02 s
DEEPMd INFO    saved checkpoint model.ckpt
DEEPMd INFO    average training time: 0.0244 s/batch (exclude first 200 batches)
DEEPMd INFO    finished training
DEEPMd INFO    wall time: 256.669 s

```

On the screen, you will see the information of the data system(s)

```

DEEPMd INFO    -----
DEEPMd INFO    ---Summary of DataSystem: training -----
DEEPMd INFO    found 1 system(s):
DEEPMd INFO                system  natoms  bch_sz  n_bch  prob  pbc
DEEPMd INFO    ../00.data/training_data      5      7     23  1.000  T
DEEPMd INFO    -----
DEEPMd INFO    ---Summary of DataSystem: validation -----

```

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```

DEEPMD INFO      found 1 system(s):
DEEPMD INFO                               system  natoms  bch_sz  n_bch  prob  pbc
DEEPMD INFO      ../00.data/validation_data      5      7      5  1.000  T
DEEPMD INFO      -----

```

and the starting and final learning rate of this training

```

DEEPMD INFO      start training at lr 1.00e-03 (== 1.00e-03), decay_step 50, decay_rate 0.950006,
↪ final lr will be 3.51e-08

```

If everything works fine, you will see, on the screen, information printed every 1000 steps, like

```

DEEPMD INFO      batch      200 training time 6.04 s, testing time 0.02 s
DEEPMD INFO      batch      400 training time 4.80 s, testing time 0.02 s
DEEPMD INFO      batch      600 training time 4.80 s, testing time 0.02 s
DEEPMD INFO      batch      800 training time 4.78 s, testing time 0.02 s
DEEPMD INFO      batch     1000 training time 4.77 s, testing time 0.02 s
DEEPMD INFO      saved checkpoint model.ckpt
DEEPMD INFO      batch     1200 training time 4.47 s, testing time 0.02 s
DEEPMD INFO      batch     1400 training time 4.49 s, testing time 0.02 s
DEEPMD INFO      batch     1600 training time 4.45 s, testing time 0.02 s
DEEPMD INFO      batch     1800 training time 4.44 s, testing time 0.02 s
DEEPMD INFO      batch     2000 training time 4.46 s, testing time 0.02 s
DEEPMD INFO      saved checkpoint model.ckpt

```

They present the training and testing time counts. At the end of the 1000th batch, the model is saved in Tensorflow's checkpoint file `model.ckpt`. At the same time, the training and testing errors are presented in file `lcurve.out`.

The file contains 8 columns, from left to right, are the training step, the validation loss, training loss, root mean square (RMS) validation error of energy, RMS training error of energy, RMS validation error of force, RMS training error of force and the learning rate. The RMS error (RMSE) of the energy is normalized by number of atoms in the system.

```

head -n 2 lcurve.out
#  step      rmse_val  rmse_trn  rmse_e_val  rmse_e_trn  rmse_f_val  rmse_f_trn      lr
   0      2.02e+01  1.51e+01  1.37e-01  1.41e-01  6.40e-01  4.79e-01  1.0e-03

```

and

```

$ tail -n 2 lcurve.out
 9800      2.45e-02  4.02e-02  3.20e-04  3.88e-04  2.40e-02  3.94e-02  4.3e-08
10000      4.60e-02  3.76e-02  8.65e-04  5.35e-04  4.52e-02  3.69e-02  3.5e-08

```

Volumes 4, 5 and 6, 7 present energy and force training and testing errors, respectively.

```

! head -n 2 lcurve.out && tail -n 2 lcurve.out

```

```

#  step      rmse_val  rmse_trn  rmse_e_val  rmse_e_trn  rmse_f_val  rmse_f_trn      lr
   0      2.06e+01  1.94e+01  1.34e-01  1.35e-01  6.51e-01  6.14e-01  1.0e-03
 9800      5.49e-02  4.00e-02  7.55e-04  7.28e-04  5.37e-02  3.91e-02  4.3e-08
10000      6.56e-02  6.37e-02  1.13e-03  1.54e-03  6.44e-02  6.25e-02  3.5e-08

```

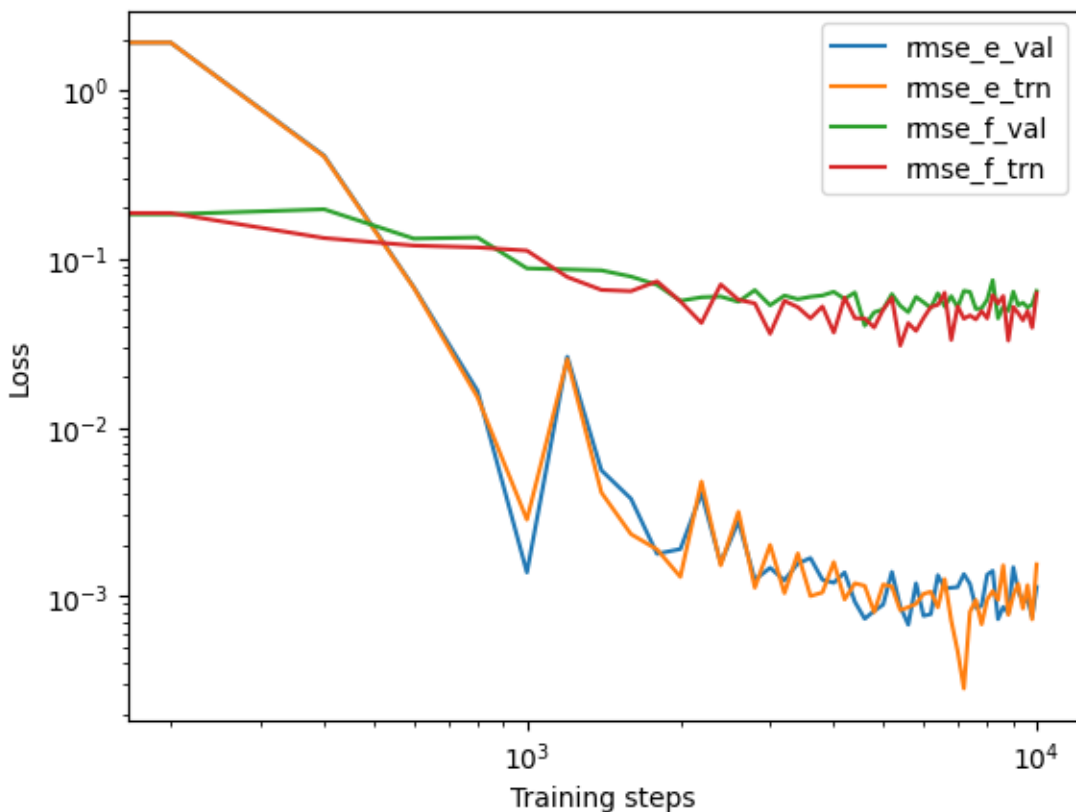
The loss function can be visualized to monitor the training process.

```

import numpy as np
import matplotlib.pyplot as plt
import pandas as pd

with open("lcurve.out") as f:
    headers = f.readline().split()[1:]
lcurve = pd.DataFrame(np.loadtxt("lcurve.out"), columns=headers)
legends = ["rmse_e_val", "rmse_e_trn", "rmse_f_val", "rmse_f_trn"]
for legend in legends:
    plt.loglog(lcurve["step"], lcurve[legend], label=legend)
plt.legend()
plt.xlabel("Training steps")
plt.ylabel("Loss")
plt.show()

```



1.2.8 Freeze a model

At the end of the training, the model parameters saved in TensorFlow's checkpoint file should be frozen as a model file that is usually ended with extension `.pb`. Simply execute

```
! dp freeze -o graph.pb
```

```

WARNING:tensorflow:From /opt/deepmd-kit-2.2.1/lib/python3.10/site-packages/tensorflow/python/
compat/v2_compat.py:107: disable_resource_variables (from tensorflow.python.ops.variable_scope)
is deprecated and will be removed in a future version.
Instructions for updating:

```

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```

non-resource variables are not supported in the long term
WARNING:root:To get the best performance, it is recommended to adjust the number of threads by
↳setting the environment variables OMP_NUM_THREADS, TF_INTRA_OP_PARALLELISM_THREADS, and TF_INTER_
↳OP_PARALLELISM_THREADS. See https://deepmd.rtd.io/parallelism/ for more information.
WARNING:root:Environment variable KMP_BLOCKTIME is empty. Use the default value 0
WARNING:root:Environment variable KMP_AFFINITY is empty. Use the default value granularity=fine,
↳verbose,compact,1,0
/opt/deepmd-kit-2.2.1/lib/python3.10/importlib/__init__.py:169: UserWarning: The NumPy module was
↳reloaded (imported a second time). This can in some cases result in small but subtle issues and
↳is discouraged.
_bootstrap._exec(spec, module)
2023-04-20 23:40:25.666203: W tensorflow/stream_executor/platform/default/dso_loader.cc:64] Could
↳not load dynamic library 'libcudart.so.1'; dLError: libcudart.so.1: cannot open shared object file:
↳No such file or directory; LD_LIBRARY_PATH: /usr/local/nvidia/lib:/usr/local/nvidia/lib64
2023-04-20 23:40:25.666257: W tensorflow/stream_executor/cuda/cuda_driver.cc:269] failed call to
↳cuInit: UNKNOWN ERROR (303)
DEEPMd INFO The following nodes will be frozen: ['model_type', 'descript_attr/rcut', 'descript_
↳attr/ntypes', 'model_attr/tmap', 'model_attr/model_type', 'model_attr/model_version', 'train_
↳attr/min_nbor_dist', 'train_attr/training_script', 'o_energy', 'o_force', 'o_virial', 'o_atom_
↳energy', 'o_atom_virial', 'fitting_attr/dparam', 'fitting_attr/daparam']
WARNING:tensorflow:From /opt/deepmd-kit-2.2.1/lib/python3.10/site-packages/deepmd/entrypoints/
↳freeze.py:354: convert_variables_to_constants (from tensorflow.python.framework.graph_util_impl)
↳is deprecated and will be removed in a future version.
Instructions for updating:
Use `tf.compat.v1.graph_util.convert_variables_to_constants`
WARNING:tensorflow:From /opt/deepmd-kit-2.2.1/lib/python3.10/site-packages/deepmd/entrypoints/
↳freeze.py:354: convert_variables_to_constants (from tensorflow.python.framework.graph_util_impl)
↳is deprecated and will be removed in a future version.
Instructions for updating:
Use `tf.compat.v1.graph_util.convert_variables_to_constants`
WARNING:tensorflow:From /opt/deepmd-kit-2.2.1/lib/python3.10/site-packages/tensorflow/python/
↳framework/convert_to_constants.py:925: extract_sub_graph (from tensorflow.python.framework.graph_
↳util_impl) is deprecated and will be removed in a future version.
Instructions for updating:
Use `tf.compat.v1.graph_util.extract_sub_graph`
WARNING:tensorflow:From /opt/deepmd-kit-2.2.1/lib/python3.10/site-packages/tensorflow/python/
↳framework/convert_to_constants.py:925: extract_sub_graph (from tensorflow.python.framework.graph_
↳util_impl) is deprecated and will be removed in a future version.
Instructions for updating:
Use `tf.compat.v1.graph_util.extract_sub_graph`
DEEPMd INFO 1211 ops in the final graph.

```

and it will output a model file named `graph.pb` in the current directory.

1.2.9 Test a model

We can check the quality of the trained model by running

```
! dp test -m graph.pb -s ../00.data/validation_data
```

```

WARNING:tensorflow:From /opt/deepmd-kit-2.2.1/lib/python3.10/site-packages/tensorflow/python/
↳compat/v2_compat.py:107: disable_resource_variables (from tensorflow.python.ops.variable_scope)
↳is deprecated and will be removed in a future version.
Instructions for updating:
non-resource variables are not supported in the long term

```

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```

WARNING:root:To get the best performance, it is recommended to adjust the number of threads by
↳setting the environment variables OMP_NUM_THREADS, TF_INTRA_OP_PARALLELISM_THREADS, and TF_INTER_
↳OP_PARALLELISM_THREADS. See https://deepmd.rtd.io/parallelism/ for more information.
WARNING:root:Environment variable KMP_BLOCKTIME is empty. Use the default value 0
WARNING:root:Environment variable KMP_AFFINITY is empty. Use the default value granularity=fine,
↳verbose,compact,1,0
/opt/deepmd-kit-2.2.1/lib/python3.10/importlib/__init__.py:169: UserWarning: The NumPy module was
↳reloaded (imported a second time). This can in some cases result in small but subtle issues and
↳is discouraged.
  _bootstrap._exec(spec, module)
2023-04-20 23:40:30.102300: W tensorflow/stream_executor/platform/default/dso_loader.cc:64] Could
↳not load dynamic library 'libcuda.so.1'; dLError: libcuda.so.1: cannot open shared object file:
↳No such file or directory; LD_LIBRARY_PATH: /usr/local/nvidia/lib:/usr/local/nvidia/lib64
2023-04-20 23:40:30.102346: W tensorflow/stream_executor/cuda/cuda_driver.cc:269] failed call to
↳cuInit: UNKNOWN ERROR (303)
WARNING:tensorflow:From /opt/deepmd-kit-2.2.1/lib/python3.10/site-packages/deepmd/utils/batch_size.
↳py:61: is_gpu_available (from tensorflow.python.framework.test_util) is deprecated and will be
↳removed in a future version.
Instructions for updating:
Use `tf.config.list_physical_devices('GPU')` instead.
WARNING:tensorflow:From /opt/deepmd-kit-2.2.1/lib/python3.10/site-packages/deepmd/utils/batch_size.
↳py:61: is_gpu_available (from tensorflow.python.framework.test_util) is deprecated and will be
↳removed in a future version.
Instructions for updating:
Use `tf.config.list_physical_devices('GPU')` instead.
DEEPMD WARNING You can use the environment variable DP_INFER_BATCH_SIZE to control the inference
↳batch size (nframes * natoms). The default value is 1024.
DEEPMD INFO      # -----output of dp test-----
DEEPMD INFO      # testing system : ../00.data/validation_data
OMP: Info #155: KMP_AFFINITY: Initial OS proc set respected: 0-7
OMP: Info #216: KMP_AFFINITY: decoding x2APIC ids.
OMP: Info #216: KMP_AFFINITY: cpuid leaf 11 not supported.
OMP: Info #216: KMP_AFFINITY: decoding legacy APIC ids.
OMP: Info #157: KMP_AFFINITY: 8 available OS procs
OMP: Info #158: KMP_AFFINITY: Uniform topology
OMP: Info #287: KMP_AFFINITY: topology layer "LL cache" is equivalent to "socket".
OMP: Info #192: KMP_AFFINITY: 1 socket x 4 cores/socket x 2 threads/core (4 total cores)
OMP: Info #218: KMP_AFFINITY: OS proc to physical thread map:
OMP: Info #172: KMP_AFFINITY: OS proc 0 maps to socket 0 core 0 thread 0
OMP: Info #172: KMP_AFFINITY: OS proc 1 maps to socket 0 core 0 thread 1
OMP: Info #172: KMP_AFFINITY: OS proc 2 maps to socket 0 core 1 thread 0
OMP: Info #172: KMP_AFFINITY: OS proc 3 maps to socket 0 core 1 thread 1
OMP: Info #172: KMP_AFFINITY: OS proc 4 maps to socket 0 core 2 thread 0
OMP: Info #172: KMP_AFFINITY: OS proc 5 maps to socket 0 core 2 thread 1
OMP: Info #172: KMP_AFFINITY: OS proc 6 maps to socket 0 core 3 thread 0
OMP: Info #172: KMP_AFFINITY: OS proc 7 maps to socket 0 core 3 thread 1
OMP: Info #254: KMP_AFFINITY: pid 254 tid 265 thread 1 bound to OS proc set 2
OMP: Info #254: KMP_AFFINITY: pid 254 tid 267 thread 2 bound to OS proc set 4
OMP: Info #254: KMP_AFFINITY: pid 254 tid 268 thread 3 bound to OS proc set 6
OMP: Info #254: KMP_AFFINITY: pid 254 tid 269 thread 4 bound to OS proc set 1
OMP: Info #254: KMP_AFFINITY: pid 254 tid 270 thread 5 bound to OS proc set 3
OMP: Info #254: KMP_AFFINITY: pid 254 tid 271 thread 6 bound to OS proc set 5
OMP: Info #254: KMP_AFFINITY: pid 254 tid 272 thread 7 bound to OS proc set 7
OMP: Info #254: KMP_AFFINITY: pid 254 tid 273 thread 8 bound to OS proc set 0
DEEPMD INFO      # number of test data : 40
DEEPMD INFO      Energy MAE           : 4.400922e-03 eV

```

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```

DEEPMD INFO   Energy RMSE       : 5.258026e-03 eV
DEEPMD INFO   Energy MAE/Natoms : 8.801843e-04 eV
DEEPMD INFO   Energy RMSE/Natoms : 1.051605e-03 eV
DEEPMD INFO   Force  MAE       : 4.277741e-02 eV/A
DEEPMD INFO   Force  RMSE      : 5.514855e-02 eV/A
DEEPMD INFO   Virial MAE      : 6.080471e-02 eV
DEEPMD INFO   Virial RMSE     : 7.882116e-02 eV
DEEPMD INFO   Virial MAE/Natoms : 1.216094e-02 eV
DEEPMD INFO   Virial RMSE/Natoms : 1.576423e-02 eV
DEEPMD INFO   # -----

```

The correlation between predicted data and original data can also be calculated.

```

import dpdata

training_systems = dpdata.LabeledSystem("../00.data/training_data", fmt="deepmd/npz")

predict = training_systems.predict("graph.pb")

```

```

2023-04-20 23:40:32.104716: I tensorflow/core/platform/cpu_feature_guard.cc:193] This TensorFlow
↳binary is optimized with oneAPI Deep Neural Network Library (oneDNN) to use the following CPU
↳instructions in performance-critical operations: AVX2 AVX512F FMA
To enable them in other operations, rebuild TensorFlow with the appropriate compiler flags.
2023-04-20 23:40:34.426193: W tensorflow/compiler/xla/stream_executor/platform/default/dso_loader.
↳cc:64] Could not load dynamic library 'libnvinfer.so.7'; dlerror: libnvinfer.so.7: cannot open
↳shared object file: No such file or directory; LD_LIBRARY_PATH: /usr/local/nvidia/lib:/usr/local/
↳nvidia/lib64
2023-04-20 23:40:34.427318: W tensorflow/compiler/xla/stream_executor/platform/default/dso_loader.
↳cc:64] Could not load dynamic library 'libnvinfer_plugin.so.7'; dlerror: libnvinfer_plugin.so.7:
↳cannot open shared object file: No such file or directory; LD_LIBRARY_PATH: /usr/local/nvidia/
↳lib:/usr/local/nvidia/lib64
2023-04-20 23:40:34.427332: W tensorflow/compiler/tf2tensorrt/utils/py_utils.cc:38] TF-TRT
↳Warning: Cannot dlopen some TensorRT libraries. If you would like to use Nvidia GPU with
↳TensorRT, please make sure the missing libraries mentioned above are installed properly.

```

```

WARNING:tensorflow:From /opt/mamba/lib/python3.10/site-packages/tensorflow/python/compat/v2_compat.
↳py:107: disable_resource_variables (from tensorflow.python.ops.variable_scope) is deprecated and
↳will be removed in a future version.
Instructions for updating:
non-resource variables are not supported in the long term

```

```

WARNING:root:To get the best performance, it is recommended to adjust the number of threads by
↳setting the environment variables OMP_NUM_THREADS, TF_INTRA_OP_PARALLELISM_THREADS, and TF_INTER_
↳OP_PARALLELISM_THREADS. See https://deepmd.rtfd.io/parallelism/ for more information.

```

```

WARNING:tensorflow:From /opt/mamba/lib/python3.10/site-packages/deepmd/utils/batch_size.py:61: is_
↳gpu_available (from tensorflow.python.framework.test_util) is deprecated and will be removed in
↳a future version.
Instructions for updating:
Use `tf.config.list_physical_devices('GPU')` instead.

```

```

2023-04-20 23:40:36.161142: I tensorflow/core/platform/cpu_feature_guard.cc:193] This TensorFlow
↳binary is optimized with oneAPI Deep Neural Network Library (oneDNN) to use the following CPU
↳instructions in performance-critical operations: AVX2 AVX512F FMA

```

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```

To enable them in other operations, rebuild TensorFlow with the appropriate compiler flags.
2023-04-20 23:40:36.165078: W tensorflow/compiler/xla/stream_executor/platform/default/dso_loader.
↳cc:64] Could not load dynamic library 'libcuda.so.1'; dLError: libcuda.so.1: cannot open shared
↳object file: No such file or directory; LD_LIBRARY_PATH: /usr/local/nvidia/lib:/usr/local/nvidia/
↳lib64
2023-04-20 23:40:36.165119: W tensorflow/compiler/xla/stream_executor/cuda/cuda_driver.cc:265]
↳failed call to cuInit: UNKNOWN ERROR (303)
2023-04-20 23:40:36.165142: I tensorflow/compiler/xla/stream_executor/cuda/cuda_diagnostics.
↳cc:156] kernel driver does not appear to be running on this host (bohrium-14076-1013950): /proc/
↳driver/nvidia/version does not exist
2023-04-20 23:40:36.181810: I tensorflow/compiler/mlir/mlir_graph_optimization_pass.cc:357] MLIR
↳V1 optimization pass is not enabled
WARNING:tensorflow:From /opt/mamba/lib/python3.10/site-packages/deepmd/utils/batch_size.py:61: is_
↳gpu_available (from tensorflow.python.framework.test_util) is deprecated and will be removed in
↳a future version.
Instructions for updating:
Use `tf.config.list_physical_devices('GPU')` instead.
WARNING:deepmd.utils.batch_size:You can use the environment variable DP_INFER_BATCH_SIZE to control
↳the inference batch size (nframes * natoms). The default value is 1024.

```

```

import matplotlib.pyplot as plt
import numpy as np

plt.scatter(training_systems["energies"], predict["energies"])

x_range = np.linspace(plt.xlim()[0], plt.xlim()[1])

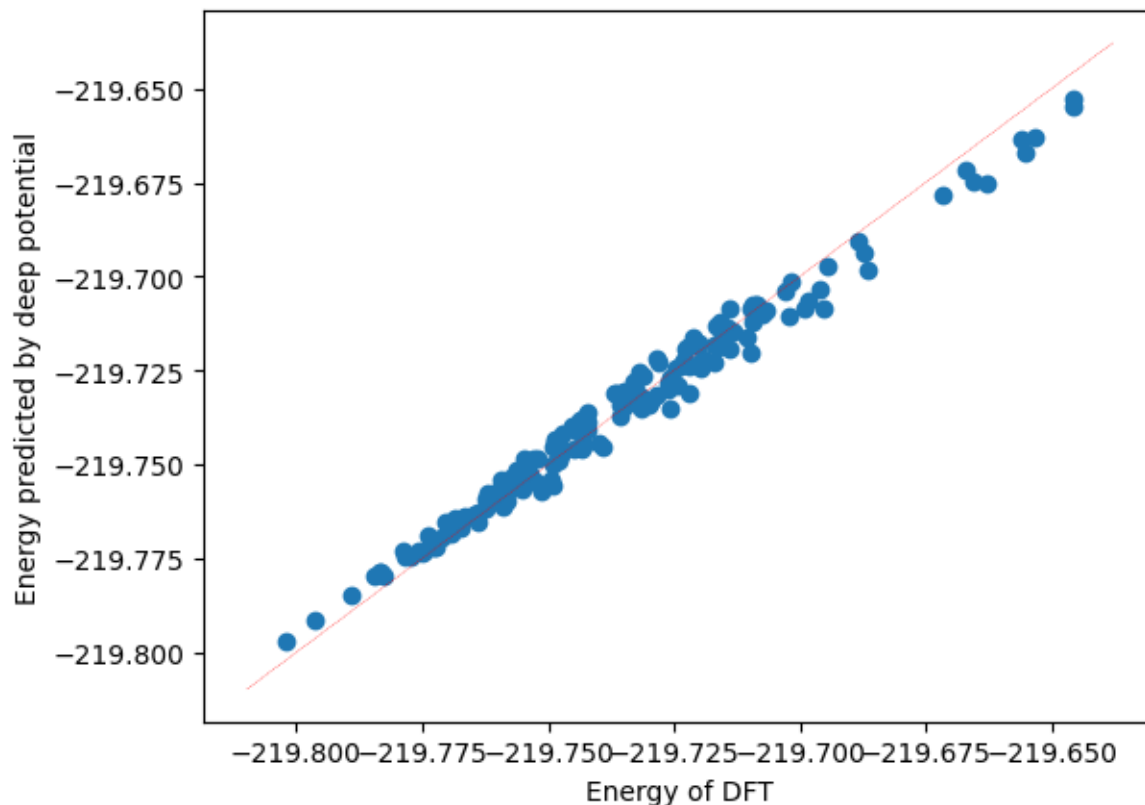
plt.plot(x_range, x_range, "r--", linewidth=0.25)
plt.xlabel("Energy of DFT")
plt.ylabel("Energy predicted by deep potential")
plt.plot()

```

```

[]

```



1.2.10 Run MD with LAMMPS

The model can drive molecular dynamics in LAMMPS.

```
! cd ../02.lmp && cp ../01.train/graph.pb ./ && ls
```

```
conf.lmp graph.pb in.lammps
```

Here `conf.lmp` gives the initial configuration of a gas phase methane MD simulation, and the file `in.lammps` is the LAMMPS input script. One may check `in.lammps` and finds that it is a rather standard LAMMPS input file for a MD simulation, with only two exception lines:

```
pair_style deepmd graph.pb
pair_coeff * *
```

where the pair style `deepmd` is invoked and the model file `graph.pb` is provided, which means the atomic interaction will be computed by the DP model that is stored in the file `graph.pb`.

In an environment with a compatible version of LAMMPS, the deep potential molecular dynamics can be performed via

```
lmp -i input.lammps
```

```
! cd ../02.lmp && cp ../01.train/graph.pb ./ && lmp -i in.lammps
```

```

Warning:
This LAMMPS executable is in a conda environment, but the environment has
not been activated. Libraries may fail to load. To activate this environment
please see https://conda.io/activation.
LAMMPS (23 Jun 2022 - Update 1)
OMP_NUM_THREADS environment is not set. Defaulting to 1 thread. (src/comm.cpp:98)
  using 1 OpenMP thread(s) per MPI task
Loaded 1 plugins from /opt/deepmd-kit-2.2.1/lib/deepmd_lmp
Reading data file ...
  triclinic box = (0 0 0) to (10.114259 10.263124 10.216793) with tilt (0.036749877 0.13833062 -0.
  ↪056322169)
  1 by 1 by 1 MPI processor grid
  reading atoms ...
  5 atoms
  read_data CPU = 0.004 seconds
DeePMD-kit WARNING: Environmental variable OMP_NUM_THREADS is not set. Tune OMP_NUM_THREADS for
  ↪the best performance. See https://deepmd.rtfd.io/parallelism/ for more information.
Summary of lammps deepmd module ...
>>> Info of deepmd-kit:
  installed to:      /opt/deepmd-kit-2.2.1
  source:            v2.2.1
  source branch:     HEAD
  source commit:     3ac8c4c7
  source commit at:  2023-03-16 12:33:24 +0800
  support model ver.: 1.1
  build variant:     cuda
  build with tf inc:  /opt/deepmd-kit-2.2.1/include;/opt/deepmd-kit-2.2.1/include
  build with tf lib:  /opt/deepmd-kit-2.2.1/lib/libtensorflow_cc.so
  set tf intra_op_parallelism_threads: 0
  set tf inter_op_parallelism_threads: 0
>>> Info of lammps module:
  use deepmd-kit at:  /opt/deepmd-kit-2.2.1
DeePMD-kit WARNING: Environmental variable OMP_NUM_
  ↪THREADS is not set. Tune OMP_NUM_THREADS for the best performance. See https://deepmd.rtfd.io/
  ↪parallelism/ for more information.
DeePMD-kit: Successfully load libcudart.so
2023-04-20 23:40:39.637091: I tensorflow/core/platform/cpu_feature_guard.cc:193] This TensorFlow
  ↪binary is optimized with oneAPI Deep Neural Network Library (oneDNN) to use the following CPU
  ↪instructions in performance-critical operations: SSE4.1 SSE4.2 AVX AVX2 AVX512F FMA
To enable them in other operations, rebuild TensorFlow with the appropriate compiler flags.
2023-04-20 23:40:39.643206: W tensorflow/stream_executor/platform/default/dso_loader.cc:64] Could
  ↪not load dynamic library 'libcuda.so.1'; dLError: libcuda.so.1: cannot open shared object file:
  ↪No such file or directory; LD_LIBRARY_PATH: /usr/local/nvidia/lib:/usr/local/nvidia/lib64
2023-04-20 23:40:39.643234: W tensorflow/stream_executor/cuda/cuda_driver.cc:269] failed call to
  ↪cuInit: UNKNOWN ERROR (303)
2023-04-20 23:40:39.643257: I tensorflow/stream_executor/cuda/cuda_diagnostics.cc:156] kernel
  ↪driver does not appear to be running on this host (bohrium-14076-1013950): /proc/driver/nvidia/
  ↪version does not exist
2023-04-20 23:40:39.645305: I tensorflow/core/common_runtime/process_util.cc:146] Creating new
  ↪thread pool with default inter op setting: 2. Tune using inter_op_parallelism_threads for best
  ↪performance.
2023-04-20 23:40:39.700559: I tensorflow/compiler/mlir/mlir_graph_optimization_pass.cc:354] MLIR
  ↪V1 optimization pass is not enabled
>>> Info of model(s):
  using 1 model(s): graph.pb
  rcut in model:    6
  ntypes in model:  2

```

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CITE-CITE-CITE-CITE-CITE-CITE-CITE-CITE-CITE-CITE-CITE-CITE

Your simulation uses code contributions which should be cited:

- USER-DEEPMO package:

The log file lists these citations in BibTeX format.

CITE-CITE-CITE-CITE-CITE-CITE-CITE-CITE-CITE-CITE-CITE-CITE

Generated 0 of 1 mixed pair_coeff terms from geometric mixing rule

Neighbor list info ...

update every 10 steps, delay 0 steps, check no

max neighbors/atom: 2000, page size: 100000

master list distance cutoff = 7

ghost atom cutoff = 7

binsize = 3.5, bins = 3 3 3

1 neighbor lists, perpetual/occasional/extra = 1 0 0

(1) pair deepmd, perpetual

attributes: full, newton on

pair build: full/bin/atomonly

stencil: full/bin/3d

bin: standard

Setting up Verlet run ...

Unit style : metal

Current step : 0

Time step : 0.001

Per MPI rank memory allocation (min/avg/max) = 3.809 | 3.809 | 3.809 Mbytes

| Step | PotEng | KinEng | TotEng | Temp | Press | Volume |
|------|------------|--------------|------------|-----------|------------|-----------|
| 0 | -219.77011 | 0.025852029 | -219.74426 | 50 | -810.10259 | 1060.5429 |
| 100 | -219.76784 | 0.023303362 | -219.74454 | 45.070664 | -605.50113 | 1060.5429 |
| 200 | -219.77863 | 0.032400378 | -219.74622 | 62.665059 | -53.929107 | 1060.5429 |
| 300 | -219.77403 | 0.027115352 | -219.74692 | 52.443373 | 642.24342 | 1060.5429 |
| 400 | -219.77126 | 0.023079501 | -219.74818 | 44.637697 | 861.365 | 1060.5429 |
| 500 | -219.786 | 0.034433001 | -219.75156 | 66.596322 | 256.47994 | 1060.5429 |
| 600 | -219.78295 | 0.029039598 | -219.75391 | 56.165027 | -527.21506 | 1060.5429 |
| 700 | -219.777 | 0.020227709 | -219.75677 | 39.122091 | -696.11258 | 1060.5429 |
| 800 | -219.78394 | 0.022893217 | -219.76105 | 44.277408 | -77.227892 | 1060.5429 |
| 900 | -219.77998 | 0.015506508 | -219.76447 | 29.990893 | 663.84491 | 1060.5429 |
| 1000 | -219.78328 | 0.015178419 | -219.7681 | 29.356341 | 482.8228 | 1060.5429 |
| 1100 | -219.7903 | 0.018763273 | -219.77154 | 36.28975 | -273.19351 | 1060.5429 |
| 1200 | -219.78639 | 0.012922048 | -219.77347 | 24.992328 | -577.90459 | 1060.5429 |
| 1300 | -219.79131 | 0.015848131 | -219.77546 | 30.65162 | -129.85247 | 1060.5429 |
| 1400 | -219.78829 | 0.011969602 | -219.77632 | 23.150218 | 545.58517 | 1060.5429 |
| 1500 | -219.78735 | 0.010610097 | -219.77674 | 20.520821 | 356.36805 | 1060.5429 |
| 1600 | -219.78834 | 0.011547453 | -219.77679 | 22.333746 | -386.08305 | 1060.5429 |
| 1700 | -219.78549 | 0.0095297364 | -219.77596 | 18.431312 | -522.29867 | 1060.5429 |
| 1800 | -219.78787 | 0.01302987 | -219.77484 | 25.200865 | 120.83085 | 1060.5429 |
| 1900 | -219.7845 | 0.012341623 | -219.77216 | 23.869737 | 643.66442 | 1060.5429 |
| 2000 | -219.7857 | 0.017597987 | -219.76811 | 34.035987 | 255.57892 | 1060.5429 |
| 2100 | -219.7853 | 0.023253088 | -219.76205 | 44.973429 | -465.61243 | 1060.5429 |
| 2200 | -219.77987 | 0.024650089 | -219.75522 | 47.675348 | -708.62743 | 1060.5429 |
| 2300 | -219.78134 | 0.030690759 | -219.75065 | 59.358512 | -221.82549 | 1060.5429 |
| 2400 | -219.77737 | 0.029446857 | -219.74792 | 56.952699 | 635.02431 | 1060.5429 |
| 2500 | -219.768 | 0.022122766 | -219.74587 | 42.787292 | 826.89652 | 1060.5429 |
| 2600 | -219.77246 | 0.02691536 | -219.74554 | 52.056572 | 168.88834 | 1060.5429 |
| 2700 | -219.77746 | 0.031963987 | -219.7455 | 61.821042 | -497.33107 | 1060.5429 |
| 2800 | -219.7733 | 0.02814671 | -219.74515 | 54.438107 | -792.71093 | 1060.5429 |

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| | | | | | | |
|------|------------|-------------|------------|-----------|------------|-----------|
| 2900 | -219.77498 | 0.029131114 | -219.74585 | 56.342026 | -685.23164 | 1060.5429 |
| 3000 | -219.78212 | 0.034326288 | -219.74779 | 66.38993 | -20.441816 | 1060.5429 |
| 3100 | -219.77222 | 0.02366469 | -219.74856 | 45.769502 | 708.42782 | 1060.5429 |
| 3200 | -219.77252 | 0.022334468 | -219.75019 | 43.196742 | 753.3138 | 1060.5429 |
| 3300 | -219.78538 | 0.032458098 | -219.75292 | 62.776693 | 36.172647 | 1060.5429 |
| 3400 | -219.78047 | 0.026131264 | -219.75434 | 50.540064 | -661.25487 | 1060.5429 |
| 3500 | -219.77926 | 0.022926821 | -219.75633 | 44.342401 | -623.5037 | 1060.5429 |
| 3600 | -219.78369 | 0.024854728 | -219.75884 | 48.071137 | 74.821258 | 1060.5429 |
| 3700 | -219.7768 | 0.016731114 | -219.76006 | 32.359382 | 709.57785 | 1060.5429 |
| 3800 | -219.77927 | 0.017595175 | -219.76168 | 34.03055 | 543.56168 | 1060.5429 |
| 3900 | -219.7864 | 0.023003584 | -219.7634 | 44.490867 | -230.55364 | 1060.5429 |
| 4000 | -219.78098 | 0.017102387 | -219.76388 | 33.077456 | -677.85161 | 1060.5429 |
| 4100 | -219.78581 | 0.020907229 | -219.7649 | 40.436341 | -343.9622 | 1060.5429 |
| 4200 | -219.78717 | 0.021708329 | -219.76546 | 41.985736 | 491.95578 | 1060.5429 |
| 4300 | -219.78328 | 0.018229256 | -219.76505 | 35.256916 | 680.5279 | 1060.5429 |
| 4400 | -219.79007 | 0.024931071 | -219.76514 | 48.21879 | -26.785455 | 1060.5429 |
| 4500 | -219.78331 | 0.019795452 | -219.76352 | 38.286071 | -624.98799 | 1060.5429 |
| 4600 | -219.78094 | 0.0196038 | -219.76134 | 37.915399 | -584.8297 | 1060.5429 |
| 4700 | -219.78608 | 0.027516802 | -219.75857 | 53.219812 | 74.218844 | 1060.5429 |
| 4800 | -219.77656 | 0.023488867 | -219.75307 | 45.429446 | 827.4406 | 1060.5429 |
| 4900 | -219.78039 | 0.032832529 | -219.74755 | 63.500874 | 634.64896 | 1060.5429 |
| 5000 | -219.78237 | 0.040761952 | -219.7416 | 78.837046 | -224.81626 | 1060.5429 |

Loop time of 12.1251 on 1 procs for 5000 steps with 5 atoms

Performance: 35.629 ns/day, 0.674 hours/ns, 412.369 timesteps/s
242.0% CPU use with 1 MPI tasks x 1 OpenMP threads

MPI task timing breakdown:

| Section | min time | avg time | max time | %varavg | %total |
|---------|-----------|-----------|-----------|---------|--------|
| Pair | 12.072 | 12.072 | 12.072 | 0.0 | 99.56 |
| Neigh | 0.0066181 | 0.0066181 | 0.0066181 | 0.0 | 0.05 |
| Comm | 0.012792 | 0.012792 | 0.012792 | 0.0 | 0.11 |
| Output | 0.0044695 | 0.0044695 | 0.0044695 | 0.0 | 0.04 |
| Modify | 0.022737 | 0.022737 | 0.022737 | 0.0 | 0.19 |
| Other | | 0.006263 | | | 0.05 |

| | | | | | | |
|-------------|-----|-----|-----|-----|-----|-----|
| Nlocal: | 5 | ave | 5 | max | 5 | min |
| Histogram: | 1 | 0 | 0 | 0 | 0 | 0 |
| Nghost: | 130 | ave | 130 | max | 130 | min |
| Histogram: | 1 | 0 | 0 | 0 | 0 | 0 |
| Neighs: | 0 | ave | 0 | max | 0 | min |
| Histogram: | 1 | 0 | 0 | 0 | 0 | 0 |
| FullNeighs: | 20 | ave | 20 | max | 20 | min |
| Histogram: | 1 | 0 | 0 | 0 | 0 | 0 |

Total # of neighbors = 20
Ave neighs/atom = 4
Neighbor list builds = 500
Dangerous builds not checked
Total wall time: 0:00:13

INSTALLATION

2.1 Easy install

There are various easy methods to install DeePMD-kit. Choose one that you prefer. If you want to build by yourself, jump to the next two sections.

After your easy installation, DeePMD-kit (`dp`) and LAMMPS (`lmp`) will be available to execute. You can try `dp -h` and `lmp -h` to see the help. `mpirun` is also available considering you may want to train models or run LAMMPS in parallel.

Note: Note: The off-line packages and conda packages require the [GNU C Library 2.17](#) or above. The GPU version requires [compatible NVIDIA driver](#) to be installed in advance. It is possible to force conda to [override detection](#) when installation, but these requirements are still necessary during runtime.

- [Install off-line packages](#)
- [Install with conda](#)
- [Install with docker](#)
- [Install Python interface with pip](#)

2.1.1 Install off-line packages

Both CPU and GPU version offline packages are available in [the Releases page](#).

Some packages are splited into two files due to size limit of GitHub. One may merge them into one after downloading:

```
cat deepmd-kit-2.1.1-cuda11.6_gpu-Linux-x86_64.sh.0 deepmd-kit-2.1.1-cuda11.6_gpu-Linux-x86_64.sh.  
↵1 > deepmd-kit-2.1.1-cuda11.6_gpu-Linux-x86_64.sh
```

One may enable the environment using

```
conda activate /path/to/deepmd-kit
```

2.1.2 Install with conda

DeePMD-kit is available with [conda](#). Install [Anaconda](#) or [Miniconda](#) first.

Official channel

One may create an environment that contains the CPU version of DeePMD-kit and LAMMPS:

```
conda create -n deepmd deepmd-kit==*cpu libdeepmd==*cpu lammps -c https://conda.deepmodeling.com
↪ -c defaults
```

Or one may want to create a GPU environment containing [CUDA Toolkit](#):

```
conda create -n deepmd deepmd-kit==*gpu libdeepmd==*gpu lammps cudatoolkit=11.6 horovod -c
↪ https://conda.deepmodeling.com -c defaults
```

One could change the CUDA Toolkit version from 10.2 or 11.6.

One may specify the DeePMD-kit version such as 2.1.1 using

```
conda create -n deepmd deepmd-kit=2.1.1=*cpu libdeepmd=2.1.1=*cpu lammps horovod -c https://conda.
↪ deepmodeling.com -c defaults
```

One may enable the environment using

```
conda activate deepmd
```

conda-forge channel

DeePMD-kit is also available on the [conda-forge](#) channel:

```
conda create -n deepmd deepmd-kit lammps -c conda-forge
```

The supported platform includes Linux x86-64, macOS x86-64, and macOS arm64. Read [conda-forge FAQ](#) to learn how to install CUDA-enabled packages.

2.1.3 Install with docker

A docker for installing the DeePMD-kit is available [here](#).

To pull the CPU version:

```
docker pull ghcr.io/deepmodeling/deepmd-kit:2.1.1_cpu
```

To pull the GPU version:

```
docker pull ghcr.io/deepmodeling/deepmd-kit:2.1.1_cuda11.6_gpu
```

To pull the ROCm version:

```
docker pull deepmodeling/dpmdkit-rocm:dp2.0.3-rocm4.5.2-tf2.6-lmp29Sep2021
```

2.1.4 Install Python interface with pip

If you have no existing TensorFlow installed, you can use `pip` to install the pre-built package of the Python interface with CUDA 11 supported:

```
pip install deepmd-kit[gpu,cu11]
```

`cu11` is required only when CUDA Toolkit and cuDNN were not installed.

Or install the CPU version without CUDA supported:

```
pip install deepmd-kit[cpu]
```

The LAMMPS module and the i-Pi driver are only provided on Linux and macOS. To install LAMMPS and/or i-Pi, add `lmp` and/or `ipi` to extras:

```
pip install deepmd-kit[gpu,cu11,lmp,ipi]
```

MPICH is required for parallel running. (The macOS arm64 package doesn't support MPI yet.)

It is suggested to install the package into an isolated environment. The supported platform includes Linux x86-64 and aarch64 with GNU C Library 2.28 or above, macOS x86-64 and arm64, and Windows x86-64. A specific version of TensorFlow which is compatible with DeePMD-kit will be also installed.

Warning: If your platform is not supported, or want to build against the installed TensorFlow, or want to enable ROCm support, please [build from source](#).

2.2 Install from source code

Please follow our [GitHub](#) webpage to download the [latest released version](#) and [development version](#).

Or get the DeePMD-kit source code by `git clone`

```
cd /some/workspace
git clone --recursive https://github.com/deepmodeling/deepmd-kit.git deepmd-kit
```

The `--recursive` option clones all [submodules](#) needed by DeePMD-kit.

For convenience, you may want to record the location of the source to a variable, saying `deepmd_source_dir` by

```
cd deepmd-kit
deepmd_source_dir=`pwd`
```

2.2.1 Install the python interface

Install Tensorflow's python interface

First, check the python version on your machine

```
python --version
```

We follow the virtual environment approach to install TensorFlow's Python interface. The full instruction can be found on the official [TensorFlow website](#). TensorFlow 1.8 or later is supported. Now we assume that the Python interface will be installed to the virtual environment directory `$tensorflow_venv`

```
virtualenv -p python3 $tensorflow_venv
source $tensorflow_venv/bin/activate
pip install --upgrade pip
pip install --upgrade tensorflow
```

It is important that every time a new shell is started and one wants to use DeePMD-kit, the virtual environment should be activated by

```
source $tensorflow_venv/bin/activate
```

if one wants to skip out of the virtual environment, he/she can do

```
deactivate
```

If one has multiple python interpreters named something like python3.x, it can be specified by, for example

```
virtualenv -p python3.8 $tensorflow_venv
```

If one does not need the GPU support of DeePMD-kit and is concerned about package size, the CPU-only version of TensorFlow should be installed by

```
pip install --upgrade tensorflow-cpu
```

To verify the installation, run

```
python -c "import tensorflow as tf;print(tf.reduce_sum(tf.random.normal([1000, 1000])))"
```

One should remember to activate the virtual environment every time he/she uses DeePMD-kit.

One can also [build the TensorFlow Python interface from source](#) for custom hardware optimization, such as CUDA, ROCM, or OneDNN support.

Install the DeePMD-kit's python interface

Check the compiler version on your machine

```
gcc --version
```

The compiler GCC 4.8 or later is supported in the DeePMD-kit. Note that TensorFlow may have specific requirements for the compiler version to support the C++ standard version and `_GLIBCXX_USE_CXX11_ABI` used by TensorFlow. It is recommended to use [the same compiler version as TensorFlow](#), which can be printed by `python -c "import tensorflow;print(tensorflow.version.COMPILER_VERSION)"`.

Execute

```
cd $deepmd_source_dir
pip install .
```

One may set the following environment variables before executing pip:

| Environment variables | Allowed value | Default value | Usage |
|-------------------------------|-----------------|------------------------|--|
| DP_VARIANT | cpu, cuda, rocm | cpu | Build CPU variant or GPU variant with CUDA or ROCM support. |
| CUDA-Toolkit_ROOT | Path | Detected automatically | The path to the CUDA toolkit directory. CUDA 7.0 or later is supported. NVCC is required. |
| ROCM_ROOT | Path | Detected automatically | The path to the ROCM toolkit directory. |
| TENSORFLOW_ROOT | Path | Detected automatically | The path to TensorFlow Python library. By default the installer only finds TensorFlow under user site-package directory (<code>site.getusersitepackages()</code>) or system site-package directory (<code>sysconfig.get_path("purelib")</code>) due to limitation of PEP-517 . If not found, the latest TensorFlow (or the environment variable <code>TENSORFLOW_VERSION</code> if given) from PyPI will be built against. |
| DP_ENABLE_NATIVE_OPTIMIZATION | ACTIVE | ACTIVE | OpenMP optimization for the native machine's CPU type. Do not enable it if generated code will run on different CPUs. |

To test the installation, one should first jump out of the source directory

```
cd /some/other/workspace
```

then execute

```
dp -h
```

It will print the help information like

```
usage: dp [-h] {train,freeze,test} ...

DeePMD-kit: A deep learning package for many-body potential energy
representation and molecular dynamics

optional arguments:
  -h, --help            show this help message and exit

Valid subcommands:
```

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```
{train,freeze,test}
  train      train a model
  freeze     freeze the model
  test       test the model
```

Install horovod and mpi4py

Horovod and mpi4py are used for parallel training. For better performance on GPU, please follow the tuning steps in [Horovod on GPU](#).

```
# With GPU, prefer NCCL as a communicator.
HOROVOD_WITHOUT_GLOO=1 HOROVOD_WITH_TENSORFLOW=1 HOROVOD_GPU_OPERATIONS=NCCL HOROVOD_NCCL_HOME=/
↪path/to/nccl pip install horovod mpi4py
```

If your work in a CPU environment, please prepare runtime as below:

```
# By default, MPI is used as communicator.
HOROVOD_WITHOUT_GLOO=1 HOROVOD_WITH_TENSORFLOW=1 pip install horovod mpi4py
```

To ensure Horovod has been built with proper framework support enabled, one can invoke the `horovodrun --check-build` command, e.g.,

```
$ horovodrun --check-build

Horovod v0.22.1:

Available Frameworks:
  [X] TensorFlow
  [X] PyTorch
  [ ] MXNet

Available Controllers:
  [X] MPI
  [X] Gloo

Available Tensor Operations:
  [X] NCCL
  [ ] DDL
  [ ] CCL
  [X] MPI
  [X] Gloo
```

Since version 2.0.1, Horovod and mpi4py with MPICH support are shipped with the installer.

If you don't install Horovod, DeePMD-kit will fall back to serial mode.

2.2.2 Install the C++ interface

If one does not need to use DeePMD-kit with Lammmps or I-Pi, then the python interface installed in the previous section does everything and he/she can safely skip this section.

Install Tensorflow's C++ interface (optional)

Since TensorFlow 2.12, TensorFlow C++ library (`libtensorflow_cc`) is packaged inside the Python library. Thus, you can skip building TensorFlow C++ library manually. If that does not work for you, you can still build it manually.

The C++ interface of DeePMD-kit was tested with compiler GCC ≥ 4.8 . It is noticed that the I-Pi support is only compiled with GCC ≥ 4.8 . Note that TensorFlow may have specific requirements for the compiler version.

First, the C++ interface of Tensorflow should be installed. It is noted that the version of Tensorflow should be consistent with the python interface. You may follow the instruction or run the script `$deepmd_source_dir/source/install/build_tf.py` to install the corresponding C++ interface.

Install DeePMD-kit's C++ interface

Now go to the source code directory of DeePMD-kit and make a building place.

```
cd $deepmd_source_dir/source
mkdir build
cd build
```

I assume you have activated the TensorFlow Python environment and want to install DeePMD-kit into path `$deepmd_root`, then execute CMake

```
cmake -DUSE_TF_PYTHON_LIBS=TRUE -DCMAKE_INSTALL_PREFIX=$deepmd_root ..
```

If you specify `-DUSE_TF_PYTHON_LIBS=FALSE`, you need to give the location where TensorFlow's C++ interface is installed to `-DTENSORFLOW_ROOT=${tensorflow_root}`.

One may add the following arguments to `cmake`:

| CMake Arguments | Allowed value | Default value | Usage |
|---|---------------|------------------------|--|
| - DTENSORFLOW_ROOT=<value> | Path | - | The Path to TensorFlow's C++ interface. |
| - DCMAKE_INSTALL_PREFIX=<value> | Path | - | The Path where DeePMD-kit will be installed. |
| - DUSE_CUDA_TOOLKIT=<value> | TRUE FALSE | FALSE | If TRUE, Build GPU support with CUDA toolkit. |
| - DCUDAToolkit_ROOT=<value> | Path | Detected automatically | The path to the CUDA toolkit directory. CUDA 7.0 or later is supported. NVCC is required. |
| - DUSE_ROCM_TOOLKIT=<value> | TRUE FALSE | FALSE | If TRUE, Build GPU support with ROCM toolkit. |
| - DCMAKE_HIP_COMPILER_ROCM_ROOT=<value> | Path | Detected automatically | The path to the ROCM toolkit directory. |
| - DLAMMPS_SOURCE_ROOT=<value> | Path | - | Only necessary for LAMMPS plugin mode. The path to the LAMMPS source code . LAMMPS 8Apr2021 or later is supported. If not assigned, the plugin mode will not be enabled. |
| - DUSE_TF_PYTHON_LIBS=<value> | TRUE FALSE | FALSE | If TRUE, Build C++ interface with TensorFlow's Python libraries(TensorFlow's Python Interface is required). And there's no need for building TensorFlow's C++ interface. |
| - DENABLE_NATIVE_OPTIMIZATION | TRUE FALSE | FALSE | Enable compilation optimization for the native machine's CPU type. Do not enable it if generated code will run on different CPUs. |

If the CMake has been executed successfully, then run the following make commands to build the package:

```
make -j4
make install
```

Option -j4 means using 4 processes in parallel. You may want to use a different number according to your hardware.

If everything works fine, you will have the executable and libraries installed in \$deepmd_root/bin and \$deepmd_root/lib

```
$ ls $deepmd_root/bin
$ ls $deepmd_root/lib
```


2.3 Install from pre-compiled C library

DeePMD-kit provides pre-compiled C library package (`libdeepmd_c.tar.gz`) in each [release](#). It can be used to build the [LAMMPS plugin](#) and [GROMACS patch](#), as well as many [third-party software packages](#), without building TensorFlow and DeePMD-kit on one's own.

The library is built in Linux (GLIBC 2.17) with CUDA 11.8. It's noted that this package does not contain CUDA Toolkit and cuDNN, so one needs to download them from the NVIDIA website.

2.3.1 Use Pre-compiled C Library to build the LAMMPS plugin and GROMACS patch

When one [installs DeePMD-kit's C++ interface](#), one can use the CMake argument `DEEPMDC_ROOT` to the path `libdeepmd_c`.

```
cd $deepmd_source_dir/source
mkdir build
cd build
cmake -DDEEPMDC_ROOT=/path/to/libdeepmd_c -DCMAKE_INSTALL_PREFIX=$deepmd_root ..
make -j8
make install
```

Then one can follow the manual [Install LAMMPS](#) and/or [Install GROMACS](#).

2.4 Install LAMMPS

There are two ways to install LAMMPS: the built-in mode and the plugin mode. The built-in mode builds LAMMPS along with the DeePMD-kit and DeePMD-kit will be loaded automatically when running LAMMPS. The plugin mode builds LAMMPS and a plugin separately, so one needs to use `plugin load` command to load the DeePMD-kit's LAMMPS plugin library.

2.4.1 Install LAMMPS's DeePMD-kit module (built-in mode)

Before following this section, [DeePMD-kit C++ interface](#) should have been installed.

DeePMD-kit provides a module for running MD simulations with LAMMPS. Now make the DeePMD-kit module for LAMMPS.

```
cd $deepmd_source_dir/source/build
make lammps
```

DeePMD-kit will generate a module called `USER-DEEPMDC` in the build directory, which supports either double or single float precision interface. Now download the LAMMPS code, and uncompress it.

```
cd /some/workspace
wget https://github.com/lammps/lammps/archive/stable_2Aug2023.tar.gz
tar xf stable_2Aug2023.tar.gz
```

The source code of LAMMPS is stored in the directory `lammps-stable_2Aug2023`. Now go into the LAMMPS code and copy the DeePMD-kit module like this

```
cd lammps-stable_2Aug2023/src/
cp -r $deepmd_source_dir/source/build/USER-DEEPMO .
make yes-kpspace
make yes-extra-fix
make yes-user-deepmd
```

You can enable any other package you want. Now build LAMMPS

```
make mpi -j4
```

If everything works fine, you will end up with an executable `lmp_mpi`.

```
./lmp_mpi -h
```

The DeePMD-kit module can be removed from the LAMMPS source code by

```
make no-user-deepmd
```

2.4.2 Install LAMMPS (plugin mode)

Starting from 8Apr2021, LAMMPS also provides a plugin mode, allowing one to build LAMMPS and a plugin separately.

Now download the LAMMPS code (8Apr2021 or later), and uncompress it:

```
cd /some/workspace
wget https://github.com/lammps/lammps/archive/stable_2Aug2023.tar.gz
tar xf stable_2Aug2023.tar.gz
```

The source code of LAMMPS is stored in the directory `lammps-stable_2Aug2023`. The directory of the source code should be specified as the CMAKE argument `LAMMPS_SOURCE_ROOT` during installation of the DeePMD-kit C++ interface. Now go into the LAMMPS directory and create a directory called `build`

```
mkdir -p lammps-stable_2Aug2023/build/
cd lammps-stable_2Aug2023/build/
```

Now build LAMMPS. Note that `PLUGIN` and `KSPACE` packages must be enabled, and `BUILD_SHARED_LIBS` must be set to `yes`. You can install any other package you want.

```
cmake -D PKG_PLUGIN=ON -D PKG_KSPACE=ON -D LAMMPS_INSTALL_RPATH=ON -D BUILD_SHARED_LIBS=yes -D
CMAKE_INSTALL_PREFIX=${deepmd_root} -D CMAKE_INSTALL_LIBDIR=lib -D CMAKE_INSTALL_FULL_LIBDIR=
${deepmd_root}/lib ../cmake
make -j4
make install
```

If everything works fine, you will end up with an executable `${deepmd_root}/bin/lmp`.

```
${deepmd_root}/bin/lmp -h
```

Note: If `${tensorflow_root}`, `${deepmd_root}`, or the path to TensorFlow Python package if applicable is different from the prefix of LAMMPS, you need to append the library path to `RUNPATH` of `liblammps.so`. For example, use `patchelf >= 0.13`

```
patchelf --add-rpath "${tensorflow_root}/lib" liblammps.so
```

2.5 Install i-PI

The i-PI works in a client-server model. The i-PI provides the server for integrating the replica positions of atoms, while the DeePMD-kit provides a client named `dp_ipi` that computes the interactions (including energy, forces and virials). The server and client communicate via the Unix domain socket or the Internet socket. Full documentation for i-PI can be found [here](#). The source code and a complete installation guide for i-PI can be found [here](#). To use i-PI with already existing drivers, install and update using Pip:

```
pip install -U i-PI
```

Test with Pytest:

```
pip install pytest
pytest --pyargs ipi.tests
```

2.6 Install GROMACS with DeepMD

Before following this section, DeePMD-kit C++ interface should have been installed.

2.6.1 Patch source code of GROMACS

Download the source code of a supported GROMACS version (2020.2) from <https://manual.gromacs.org/2020.2/download.html>. Run the following command:

```
export PATH=$PATH:$deepmd_kit_root/bin
dp_gmx_patch -d $gromacs_root -v $version -p
```

where `deepmd_kit_root` is the directory where the latest version of DeePMD-kit is installed, and `gromacs_root` refers to the source code directory of GROMACS. And `version` represents the version of GROMACS, where only 2020.2 is supported now. If attempting to patch another version of GROMACS you will still need to set `version` to 2020.2 as this is the only supported version, we cannot guarantee that patching other versions of GROMACS will work.

2.6.2 Compile GROMACS with deepmd-kit

The C++ interface of Deepmd-kit 2.x and TensorFlow 2.x are required. And be aware that only DeePMD-kit with high precision is supported now since we cannot ensure single precision is enough for a GROMACS simulation. Here is a sample compile script:

```
#!/bin/bash
export CC=/usr/bin/gcc
export CXX=/usr/bin/g++
export CMAKE_PREFIX_PATH="/path/to/fftw-3.3.9" # fftw libraries
mkdir build
cd build
```

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```
cmake3 .. -DCMAKE_CXX_STANDARD=14 \ # not required, but c++14 seems to be more compatible with ↵
↪ higher version of tensorflow
      -DGMX_MPI=ON \
      -DGMX_GPU=CUDA \ # Gromacs on ROCm has not been fully developed yet
      -DCUDAToolkit_ROOT=/path/to/cuda \
      -DCMAKE_INSTALL_PREFIX=/path/to/gromacs-2020.2-deepmd
make -j
make install
```

2.7 Building conda packages

One may want to keep both convenience and personalization of the DeePMD-kit. To achieve this goal, one can consider building conda packages. We provide building scripts in [deepmd-kit-recipes organization](#). These building tools are driven by [conda-build](#) and [conda-smithy](#).

For example, if one wants to turn on MPIIO package in LAMMPS, go to [lammps-feedstock](#) repository and modify `recipe/build.sh`. `-D PKG_MPIIO=OFF` should be changed to `-D PKG_MPIIO=ON`. Then go to the main directory and execute

```
./build-locally.py
```

This requires that Docker has been installed. After the building, the packages will be generated in `build_artifacts/linux-64` and `build_artifacts/noarch`, and then one can install then executing

```
conda create -n deepmd lammps -c file:///path/to/build_artifacts -c https://conda.deepmodeling.com ↵
↪ -c nvidia
```

One may also upload packages to one's Anaconda channel, so they can be installed on other machines:

```
anaconda upload /path/to/build_artifacts/linux-64/*.tar.bz2 /path/to/build_artifacts/noarch/*.tar ↵
↪ .bz2
```

2.8 Install Node.js interface

DeePMD-kit has an inference interface for Node.js, the most common programming language in the world, via a wrapper of the header-only C++ interface created by SWIG.

2.8.1 Install from npm

```
npm i deepmd-kit
# Or if you want to install globally
npm i -g deepmd-kit
```

2.8.2 Build from source

Before building DeePMD-kit, install [Node.js](#), [SWIG](#) (v4.1.0 for Node.js v12-v18 support), and [node-gyp](#) globally.

When using CMake to build DeePMD-kit from source, set argument `BUILD_NODEJS_IF=ON` and `NODEJS_INCLUDE_DIRS=/path/to/nodejs/include` (the path to the include directory of Node.js):

```
cmake -D BUILD_NODEJS_IF=ON \  
      -D NODEJS_INCLUDE_DIRS=/path/to/nodejs/include \  
      .. # and other arguments  
make  
make install
```

After installing DeePMD-kit, two files, `bind.gyp` and `deepmdJAVASCRIPT_wrap.cxx` will be generated in `$deepmd_source_dir/source/nodejs`.

Go to this directory, and install the Node.js package globally:

```
cd $deepmd_source_dir/source/nodejs  
npm i  
npm link
```

The `deepmd-kit` package should be globally available in Node.js environments:

```
const deepmd = require("deepmd-kit");
```


DATA

In this section, we will introduce how to convert the DFT-labeled data into the data format used by DeePMD-kit.

The DeePMD-kit organizes data in **systems**. Each **system** is composed of a number of **frames**. One may roughly view a **frame** as a snapshot of an MD trajectory, but it does not necessarily come from an MD simulation. A **frame** records the coordinates and types of atoms, cell vectors if the periodic boundary condition is assumed, energy, atomic forces and virials. It is noted that the **frames** in one **system** share the same number of atoms with the same type.

3.1 System

DeePMD-kit takes a system as the data structure. A snapshot of a system is called a frame. A system may contain multiple frames with the same atom types and numbers, i.e. the same formula (like H₂O). To contains data with different formulas, one usually needs to divide data into multiple systems, which may sometimes result in sparse-frame systems. See a [new system format](#) to further combine different systems with the same atom numbers, when training with descriptor `se_atten`.

A system should contain system properties, input frame properties, and labeled frame properties. The system property contains the following property:

| ID | Property | Raw file | Required/Optional | Shape | Description |
|----------|---------------------|--------------|-------------------|--------|--|
| type | Atom type indexes | type.raw | Required | Natoms | Integers that start with 0. If both the training parameter <code>type_map</code> is set and <code>type_map.raw</code> is provided, the system atom type should be mapped to <code>type_map.raw</code> in <code>type.raw</code> and will be mapped to the model atom type when training; otherwise, the system atom type will be always mapped to the model atom type (whether <code>type_map</code> is set or not) |
| type_map | Atom type names | type_map.raw | Optional | Ntypes | Atom names that map to atom type, which is unnecessary to be contained in the periodic table. Only works when the training parameter <code>type_map</code> is set |
| nopbc | Non-periodic system | nopbc | Optional | 1 | If True, this system is non-periodic; otherwise it's periodic |

The input frame properties contain the following property, the first axis of which is the number of frames:

| ID | Property | Raw file | Unit | Re-quired/Optional | Shape | Description |
|-----------|---|------------|------|----------------------|------------------------|---|
| coord | Atomic coordinates | co-ord.raw | Å | Required | Nframes * Natoms * 3 | |
| box | Boxes | box.raw | Å | Required if periodic | Nframes * 3 * 3 | in the order XX XY XZ YX YY YZ ZX ZY ZZ |
| fparam | Extra frame parameters | fparam.raw | Any | Optional | Nframes * Any | |
| aparam | Extra atomic parameters | aparam.raw | Any | Optional | Nframes * aparam * Any | |
| numb_copy | Each frame is copied by the numb_copy (int) times | prob.raw | 1 | Optional | Nframes | Integer; Default is 1 for all frames |

The labeled frame properties are listed as follows, all of which will be used for training if and only if the loss function contains such property:

| ID | Property | Raw file | Unit | Shape | Description |
|-----------------------|--|---------------------------|------|------------------------------------|---|
| energy | Frame energies | en-ergy.raw | eV | Nframes | |
| force | Atomic forces | force.raw | eV/Å | Nframes * Natoms * 3 | |
| virial | Frame virial | virial.raw | eV | Nframes * 9 | in the order XX XY XZ YX YY YZ ZX ZY ZZ |
| atom_ener | Atomic energies | atom_ener.raw | eV | Nframes * Natoms | |
| atom_pref | Weights of atomic forces | atom_pref.raw | 1 | Nframes * Natoms | |
| dipole | Frame dipole | dipole.raw | Any | Nframes * 3 | |
| atomic_dipole | Atomic dipole | atomic_dipole.raw | Any | Nframes * Natoms * 3 | |
| polarizability | Frame polarizability | polar-izabil-ity.raw | Any | Nframes * 9 | in the order XX XY XZ YX YY YZ ZX ZY ZZ |
| atomic_polarizability | Atomic polarizability | atomic_polarizability.raw | Any | Nframes * Natoms * 9 | in the order XX XY XZ YX YY YZ ZX ZY ZZ |
| drdq | Partial derivative of atomic coordinates with respect to generalized coordinates | drdq.raw | 1 | Nframes * Natoms * 3 * Ngen_coords | |

In general, we always use the following convention of units:

| Property | Unit |
|----------|------|
| Time | ps |
| Length | Å |
| Energy | eV |
| Force | eV/Å |
| Virial | eV |
| Pressure | Bar |

3.2 Formats of a system

Two binary formats, NumPy and HDF5, are supported for training. The raw format is not directly supported, but a tool is provided to convert data from the raw format to the NumPy format.

3.2.1 NumPy format

In a system with the Numpy format, the system properties are stored as text files ending with `.raw`, such as `type.raw` and `type_map.raw`, under the system directory. If one needs to train a non-periodic system, an empty `nopbc` file should be put under the system directory. Both input and labeled frame properties are saved as the [NumPy binary data \(NPY\) files](#) ending with `.numpy` in each of the `set.*` directories. Take an example, a system may contain the following files:

```
type.raw
type_map.raw
nopbc
set.000/coord.npy
set.000/energy.npy
set.000/force.npy
set.001/coord.npy
set.001/energy.npy
set.001/force.npy
```

We assume that the atom types do not change in all frames. It is provided by `type.raw`, which has one line with the types of atoms written one by one. The atom types should be integers. For example the `type.raw` of a system that has 2 atoms with 0 and 1:

```
$ cat type.raw
0 1
```

Sometimes one needs to map the integer types to atom names. The mapping can be given by the file `type_map.raw`. For example

```
$ cat type_map.raw
0 H
```

The type 0 is named by "0" and the type 1 is named by "H".

For training models with descriptor `se_atten`, a [new system format](#) is supported to put together the frame-sparse systems with the same atom number.

3.2.2 HDF5 format

A system with the HDF5 format has the same structure as the Numpy format, but in an HDF5 file, a system is organized as an [HDF5 group](#). The file name of a Numpy file is the key in an HDF5 file, and the data is the value of the key. One needs to use `#` in a DP path to divide the path to the HDF5 file and the HDF5 path:

```
/path/to/data.hdf5#/H20
```

Here, `/path/to/data.hdf5` is the file path and `/H20` is the HDF5 path. All HDF5 paths should start with `/`. There should be some data in the H20 group, such as `/H20/type.raw` and `/H20/set.000/force.npy`.

An HDF5 file with a large number of systems has better performance than multiple NumPy files in a large cluster.

3.2.3 Raw format and data conversion

A raw file is a plain text file with each information item written in one file and one frame written on one line. It's not directly supported, but we provide a tool to convert them.

In the raw format, the property of one frame is provided per line, ending with `.raw`. Take an example, the default files that provide box, coordinate, force, energy and virial are `box.raw`, `coord.raw`, `force.raw`, `energy.raw` and `virial.raw`, respectively. Here is an example of `force.raw`:

```
$ cat force.raw
-0.724  2.039 -0.951  0.841 -0.464  0.363
 6.737  1.554 -5.587 -2.803  0.062  2.222
-1.968 -0.163  1.020 -0.225 -0.789  0.343
```

This `force.raw` contains 3 frames with each frame having the forces of 2 atoms, thus it has 3 lines and 6 columns. Each line provides all the 3 force components of 2 atoms in 1 frame. The first three numbers are the 3 force components of the first atom, while the second three numbers are the 3 force components of the second atom. Other files are organized similarly. The number of lines of all raw files should be identical.

One can use the script `$deepmd_source_dir/data/raw/raw_to_set.sh` to convert the prepared raw files to the NumPy format. For example, if we have a raw file that contains 6000 frames,

```
$ ls
box.raw coord.raw energy.raw force.raw type.raw virial.raw
$ $deepmd_source_dir/data/raw/raw_to_set.sh 2000
nframe is 6000
nline per set is 2000
will make 3 sets
making set 0 ...
making set 1 ...
making set 2 ...
$ ls
box.raw coord.raw energy.raw force.raw set.000 set.001 set.002 type.raw virial.raw
```

It generates three sets `set.000`, `set.001` and `set.002`, with each set containing 2000 frames in the Numpy format.

3.3 Prepare data with dpdata

One can use a convenient tool `dpdata` to convert data directly from the output of first principle packages to the DeePMD-kit format.

To install one can execute

```
pip install dpdata
```

An example of converting data [VASP](#) data in OUTCAR format to DeePMD-kit data can be found at

```
$deepmd_source_dir/examples/data_conv
```

Switch to that directory, then one can convert data by using the following python script

```
import dpdata

dsys = dpdata.LabeledSystem("OUTCAR")
dsys.to("deepmd/npz", "deepmd_data", set_size=dsys.get_nframes())
```

`get_nframes()` method gets the number of frames in the OUTCAR, and the argument `set_size` enforces that the set size is equal to the number of frames in the system, viz. only one `set` is created in the `system`.

The data in DeePMD-kit format is stored in the folder `deepmd_data`.

A list of all [supported data format](#) and more nice features of `dpdata` can be found on the [official website](#).

4.1 Overall

A model has two parts, a descriptor that maps atomic configuration to a set of symmetry invariant features, and a fitting net that takes descriptor as input and predicts the atomic contribution to the target physical property. It's defined in the `model` section of the `input.json`, for example,

```
"model": {
  "type_map":      ["O", "H"],
  "descriptor" :{
    "...": "..."
  },
  "fitting_net" : {
    "...": "..."
  }
}
```

The two subsections, `descriptor` and `fitting_net`, define the descriptor and the fitting net, respectively.

The `type_map` is optional, which provides the element names (but not necessarily same as the actual name of the element) of the corresponding atom types. A water model, as in this example, has two kinds of atoms. The atom types are internally recorded as integers, e.g., 0 for oxygen and 1 for hydrogen here. A mapping from the atom type to their names is provided by `type_map`.

DeePMD-kit implements the following descriptors:

1. `se_e2_a`: DeepPot-SE constructed from all information (both angular and radial) of atomic configurations. The embedding takes the distance between atoms as input.
2. `se_e2_r`: DeepPot-SE constructed from radial information of atomic configurations. The embedding takes the distance between atoms as input.
3. `se_e3`: DeepPot-SE constructed from all information (both angular and radial) of atomic configurations. The embedding takes angles between two neighboring atoms as input.
4. `se_a_mask`: DeepPot-SE constructed from all information (both angular and radial) of atomic configurations. The input frames in one system can have a varied number of atoms. Input particles are padded with virtual particles of the same length.
5. `loc_frame`: Defines a local frame at each atom and compute the descriptor as local coordinates under this frame.
6. `hybrid`: Concatenate a list of descriptors to form a new descriptor.

The fitting of the following physical properties is supported

1. *ener*: Fit the energy of the system. The force (derivative with atom positions) and the virial (derivative with the box tensor) can also be trained.
2. *dipole*: The dipole moment.
3. *polar*: The polarizability.

4.2 Descriptor "se_e2_a"

The notation of `se_e2_a` is short for the Deep Potential Smooth Edition (DeepPot-SE) constructed from all information (both angular and radial) of atomic configurations. The `e2` stands for the embedding with two-atoms information. This descriptor was described in detail in [the DeepPot-SE paper](#).

Note that it is sometimes called a “two-atom embedding descriptor” which means the input of the embedding net is atomic distances. The descriptor does encode multi-body information (both angular and radial information of neighboring atoms).

In this example, we will train a DeepPot-SE model for a water system. A complete training input script of this example can be found in the directory.

```
$deepmd_source_dir/examples/water/se_e2_a/input.json
```

With the training input script, data are also provided in the example directory. One may train the model with the DeePMD-kit from the directory.

The construction of the descriptor is given by section descriptor. An example of the descriptor is provided as follows

```
"descriptor" :{
  "type":          "se_e2_a",
  "rcut_smth":     0.50,
  "rcut":          6.00,
  "sel":           [46, 92],
  "neuron":        [25, 50, 100],
  "type_one_side": true,
  "axis_neuron":   16,
  "resnet_dt":     false,
  "seed":          1
}
```

- The type of the descriptor is set to `"se_e2_a"`.
- `rcut` is the cut-off radius for neighbor searching, and the `rcut_smth` gives where the smoothing starts.
- `sel` gives the maximum possible number of neighbors in the cut-off radius. It is a list, the length of which is the same as the number of atom types in the system, and `sel[i]` denotes the maximum possible number of neighbors with type `i`.
- The neuron specifies the size of the embedding net. From left to right the members denote the sizes of each hidden layer from the input end to the output end, respectively. If the outer layer is twice the size of the inner layer, then the inner layer is copied and concatenated, then a [ResNet architecture](#) is built between them.
- If the option `type_one_side` is set to `true`, the embedding network parameters vary by types of neighbor atoms only, so there will be N_{types} sets of embedding network parameters. Otherwise, the embedding network parameters vary by types of centric atoms and types of neighbor atoms, so there will be N_{types}^2 sets of embedding network parameters.

- The `axis_neuron` specifies the size of the submatrix of the embedding matrix, the axis matrix as explained in the [DeepPot-SE paper](#)
- If the option `resnet_dt` is set to `true`, then a timestep is used in the ResNet.
- `seed` gives the random seed that is used to generate random numbers when initializing the model parameters.

4.3 Descriptor "se_e2_r"

The notation of `se_e2_r` is short for the Deep Potential Smooth Edition (DeepPot-SE) constructed from the radial information of atomic configurations. The `e2` stands for the embedding with two-atom information.

A complete training input script of this example can be found in the directory

```
$deepmd_source_dir/examples/water/se_e2_r/input.json
```

The training input script is very similar to that of `se_e2_a`. The only difference lies in the descriptor section

```
"descriptor": {
  "type":          "se_e2_r",
  "sel":           [46, 92],
  "rcut_smth":     0.50,
  "rcut":          6.00,
  "neuron":        [5, 10, 20],
  "resnet_dt":     false,
  "seed":          1,
  "_comment":     " that's all"
},
```

The type of the descriptor is set by the key type.

4.4 Descriptor "se_e3"

The notation of `se_e3` is short for the Deep Potential Smooth Edition (DeepPot-SE) constructed from all information (both angular and radial) of atomic configurations. The embedding takes angles between two neighboring atoms as input (denoted by `e3`).

A complete training input script of this example can be found in the directory

```
$deepmd_source_dir/examples/water/se_e3/input.json
```

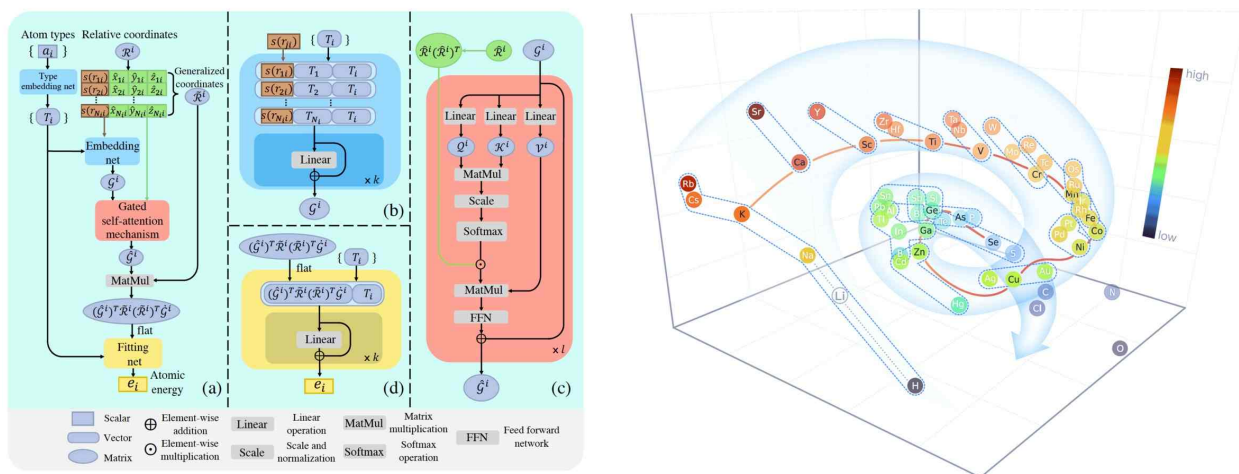
The training input script is very similar to that of `se_e2_a`. The only difference lies in the `descriptor` <model/descriptor> section

```
"descriptor": {
  "type":          "se_e3",
  "sel":           [40, 80],
  "rcut_smth":     0.50,
  "rcut":          6.00,
  "neuron":        [2, 4, 8],
  "resnet_dt":     false,
  "seed":          1,
  "_comment":     " that's all"
},
```

The type of the descriptor is set by the key type.

4.5 Descriptor "se_atten"

4.5.1 DPA-1: Pretraining of Attention-based Deep Potential Model for Molecular Simulation



Here we propose DPA-1, a Deep Potential model with a novel attention mechanism, which is highly effective for representing the conformation and chemical spaces of atomic systems and learning the PES.

See [this paper](#) for more information. DPA-1 is implemented as a new descriptor "se_atten" for model training, which can be used after simply editing the input.json.

4.5.2 Installation

Follow the [standard installation](#) of Python interface in the DeePMD-kit. After that, you can smoothly use the DPA-1 model with the following instructions.

4.5.3 Introduction to new features of DPA-1

Next, we will list the detailed settings in input.json and the data format, especially for large systems with dozens of elements. An example of DPA-1 input can be found [here](#).

Descriptor "se_atten"

The notation of `se_atten` is short for the smooth edition of Deep Potential with an attention mechanism. This descriptor was described in detail in [the DPA-1 paper](#) and the images above.

In this example, we will train a DPA-1 model for a water system. A complete training input script of this example can be found in the directory:

```
$deepmd_source_dir/examples/water/se_atten/input.json
```


With the training input script, data are also provided in the example directory. One may train the model with the DeePMD-kit from the directory.

An example of the DPA-1 descriptor is provided as follows

```
"descriptor" :{
  "type":          "se_atten",
  "rcut_smth":     0.50,
  "rcut":          6.00,
  "sel":           120,
  "neuron":        [25, 50, 100],
  "axis_neuron":   16,
  "resnet_dt":     false,
  "attn":          128,
  "attn_layer":    2,
  "attn_mask":     false,
  "attn_dotr":     true,
  "seed":         1
}
```

- The type of the descriptor is set to "se_atten", which will use DPA-1 structures.
- rcut is the cut-off radius for neighbor searching, and the rcut_smth gives where the smoothing starts.
- sel gives the maximum possible number of neighbors in the cut-off radius. It is an int. Note that this number highly affects the efficiency of training, which we usually use less than 200. (We use 120 for training 56 elements in [OC2M dataset](#))
- The neuron specifies the size of the embedding net. From left to right the members denote the sizes of each hidden layer from the input end to the output end, respectively. If the outer layer is twice the size of the inner layer, then the inner layer is copied and concatenated, then a [ResNet architecture](#) is built between them.
- The axis_neuron specifies the size of the submatrix of the embedding matrix, the axis matrix as explained in the [DeepPot-SE paper](#)
- If the option resnet_dt is set to true, then a timestep is used in the ResNet.
- seed gives the random seed that is used to generate random numbers when initializing the model parameters.
- attn sets the length of a hidden vector during scale-dot attention computation.
- attn_layer sets the number of layers in attention mechanism.
- attn_mask determines whether to mask the diagonal in the attention weights and False is recommended.
- attn_dotr determines whether to dot the relative coordinates on the attention weights as a gated scheme, True is recommended.

Descriptor "se_atten_v2"

We highly recommend using the version 2.0 of the attention-based descriptor "se_atten_v2", which is inherited from "se_atten" but with the following parameter modifications:

```
"stripped_type_embedding": true,  
"smooth_type_embdding": true,  
"set_davg_zero": false
```

Practical evidence demonstrates that "se_atten_v2" offers better and more stable performance compared to "se_atten".

Fitting "ener"

DPA-1 only supports "ener" fitting type, and you can refer [here](#) for detailed information.

Type embedding

DPA-1 only supports models with type embeddings. And the default setting is as follows:

```
"type_embedding":{  
    "neuron":      [8],  
    "resnet_dt":    false,  
    "seed":         1  
}
```

You can add these settings in input.json if you want to change the default ones, see [here](#) for detailed information.

Type map

For training large systems, especially those with dozens of elements, the `type` determines the element index of training data:

```
"type_map": [  
    "Mg",  
    "Al",  
    "Cu"  
]
```

which should include all the elements in the dataset you want to train on.

4.5.4 Data format

DPA-1 supports the standard data format, which is detailed in [data-conv.md](#) and [system.md](#). Note that in this format, only those frames with the same fingerprint (i.e. the number of atoms of different elements) can be put together as a unified system. This may lead to sparse frame numbers in those rare systems.

An ideal way is to put systems with the same total number of atoms together, which is the way we trained DPA-1 on [OC2M](#). This system format, which is called `mixed_type`, is proper to put frame-sparse systems together and is slightly different from the standard one. Take an example, a `mixed_type` may contain the following files:

```

type.raw
type_map.raw
set.*/box.npy
set.*/coord.npy
set.*/energy.npy
set.*/force.npy
set.*/real_atom_types.npy

```

This system contains `Nframes` frames with the same atom number `Natoms`, the total number of element types contained in all frames is `Ntypes`. Most files are the same as those in [standard formats](#), here we only list the distinct ones:

| ID | Property | File | Re- quired/Optional | Shape | Description |
|----------|----------------------------------|---------------------|------------------------|------------------|--|
| / | Atom type indexes (place holder) | type.raw | Re- quired | Natoms | All zeros to fake the type input |
| type_map | Atom type names | type_map.raw | Re- quired | Ntypes | Atom names that map to atom type contained in all the frames, which is unnecessary to be contained in the periodic table |
| type | Atom type indexes of each frame | real_atom_types.npy | Re- quired | Nframes * Natoms | Integers that describe atom types in each frame, corresponding to indexes in type_map. -1 means virtual atoms. |

With these edited files, one can put together frames with the same `Natoms`, instead of the same formula (like H2O). Note that this `mixed_type` format only supports `se_atten` descriptor.

To put frames with different `Natoms` into the same system, one can pad systems by adding virtual atoms whose type is -1. Virtual atoms do not contribute to any fitting property, so the atomic property of virtual atoms (e.g. forces) should be given zero.

The API to generate or transfer to `mixed_type` format is available on [dpdata](#) for a more convenient experience.

4.5.5 Training example

Here we upload the AlMgCu example shown in the paper, you can download it here: [Baidu disk](#); [Google disk](#).

4.6 Descriptor "hybrid"

This descriptor hybridizes multiple descriptors to form a new descriptor. For example, we have a list of descriptors denoted by $\mathcal{D}_1, \mathcal{D}_2, \dots, \mathcal{D}_N$, the hybrid descriptor is the concatenation of the list, i.e. $\mathcal{D} = (\mathcal{D}_1, \mathcal{D}_2, \dots, \mathcal{D}_N)$.

To use the descriptor in DeePMD-kit, one firstly set the type to hybrid, then provide the definitions of the descriptors by the items in the list,

```

"descriptor" :{
  "type": "hybrid",
  "list" : [
    {

```

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```

        "type" : "se_e2_a",
        ...
    },
    {
        "type" : "se_e2_r",
        ...
    }
]
},

```

A complete training input script of this example can be found in the directory

```
$deepmd_source_dir/examples/water/hybrid/input.json
```

4.7 Determine sel

All descriptors require to set `sel`, which means the expected maximum number of type-*i* neighbors of an atom. DeePMD-kit will allocate memory according to `sel`.

`sel` should not be too large or too small. If `sel` is too large, the computing will become much slower and cost more memory. If `sel` is not enough, the energy will be not conserved, making the accuracy of the model worse.

To determine a proper `sel`, one can calculate the neighbor stat of the training data before training:

```
dp neighbor-stat -s data -r 6.0 -t 0 H
```

where `data` is the directory of data, `6.0` is the cutoff radius, and `0` and `H` is the type map. The program will give the `max_nbor_size`. For example, `max_nbor_size` of the water example is `[38, 72]`, meaning an atom may have 38 O neighbors and 72 H neighbors in the training data.

The `sel` should be set to a higher value than that of the training data, considering there may be some extreme geometries during MD simulations. As a result, we set `sel` to `[46, 92]` in the water example.

4.8 Fit energy

In this section, we will take `$deepmd_source_dir/examples/water/se_e2_a/input.json` as an example of the input file.

4.8.1 The fitting network

The construction of the fitting net is given by section `fitting_net`

```

"fitting_net" : {
  "neuron":           [240, 240, 240],
  "resnet_dt":        true,
  "seed":             1
},

```

- `neuron` specifies the size of the fitting net. If two neighboring layers are of the same size, then a [ResNet architecture](#) is built between them.

- If the option `resnet_dt` is set to `true`, then a timestep is used in the ResNet.
- `seed` gives the random seed that is used to generate random numbers when initializing the model parameters.

4.8.2 Loss

The loss function L for training energy is given by

$$L = p_e L_e + p_f L_f + p_v L_v$$

where L_e , L_f , and L_v denote the loss in energy, forces and virials, respectively. p_e , p_f , and p_v give the prefactors of the energy, force and virial losses. The prefactors may not be a constant, rather it changes linearly with the learning rate. Taking the force prefactor for example, at training step t , it is given by

$$p_f(t) = p_f^0 \frac{\alpha(t)}{\alpha(0)} + p_f^\infty (1 - \frac{\alpha(t)}{\alpha(0)})$$

where $\alpha(t)$ denotes the learning rate at step t . p_f^0 and p_f^∞ specifies the p_f at the start of the training and the limit of $t \rightarrow \infty$ (set by `start_pref_f` and `limit_pref_f`, respectively), i.e.

$$\text{pref_f}(t) = \text{start_pref_f} * (\text{lr}(t) / \text{start_lr}) + \text{limit_pref_f} * (1 - \text{lr}(t) / \text{start_lr})$$

The `loss` section in the `input.json` is

```
"loss" : {
  "start_pref_e":      0.02,
  "limit_pref_e":      1,
  "start_pref_f":      1000,
  "limit_pref_f":      1,
  "start_pref_v":      0,
  "limit_pref_v":      0
}
```

The options `start_pref_e`, `limit_pref_e`, `start_pref_f`, `limit_pref_f`, `start_pref_v` and `limit_pref_v` determine the start and limit prefactors of energy, force and virial, respectively.

If one does not want to train with virial, then he/she may set the virial prefactors `start_pref_v` and `limit_pref_v` to 0.

4.9 Fit spin energy

In this section, we will take `$deepmd_source_dir/examples/NiO/se_e2_a/input.json` as an example of the input file.

4.9.1 Spin

The construction of the fitting net is give by section [spin](#)

```
"spin" : {
  "use_spin":      [true, false],
  "virtual_len":    [0.4],
  "spin_norm":     [1.2737],
},
```

- use_spin determines whether to turn on the magnetism of the atoms. The index of this option matches option type_map <model/type_map>.
- virtual_len specifies the distance between virtual atom and the belonging real atom.
- spin_norm gives the magnitude of the magnetic moment for each magnatic atom.

4.9.2 Spin Loss

The spin loss function L for training energy is given by

$$L = p_e L_e + p_{fr} L_{fr} + p_{fm} L_{fm} + p_v L_v$$

where L_e , L_{fr} , L_{fm} and L_v denote the loss in energy, atomic force, magnatic force and virial, respectively. p_e , p_{fr} , p_{fm} and p_v give the prefactors of the energy, atomic force, magnatic force and virial losses.

The prefactors may not be a constant, rather it changes linearly with the learning rate. Taking the atomic force prefactor for example, at training step t , it is given by

$$p_{fr}(t) = p_{fr}^0 \frac{\alpha(t)}{\alpha(0)} + p_{fr}^\infty (1 - \frac{\alpha(t)}{\alpha(0)})$$

where $\alpha(t)$ denotes the learning rate at step t . p_{fr}^0 and p_{fr}^∞ specifies the p_f at the start of the training and at the limit of $t \rightarrow \infty$ (set by [start_pref_fr](#) and [limit_pref_f](#), respectively), i.e.

```
pref_fr(t) = start_pref_fr * ( lr(t) / start_lr ) + limit_pref_fr * ( 1 - lr(t) / start_lr )
```

The [loss](#) section in the `input.json` is

```
"loss" :{
  "type":      "ener_spin",
  "start_pref_e":    0.02,
  "limit_pref_e":    1,
  "start_pref_fr":   1000,
  "limit_pref_fr":   1.0,
  "start_pref_fm":   10000,
  "limit_pref_fm":   10.0,
  "start_pref_v":    0,
  "limit_pref_v":    0,
},
```

The options [start_pref_e](#), [limit_pref_e](#), [start_pref_fr](#), [limit_pref_fm](#), [start_pref_v](#) and [limit_pref_v](#) determine the start and limit prefactors of energy, atomic force, magnatic force and virial, respectively.

If one does not want to train with virial, then he/she may set the virial prefactors [start_pref_v](#) and [limit_pref_v](#) to 0.

4.10 Fit tensor like Dipole and Polarizability

Unlike `energy`, which is a scalar, one may want to fit some high dimensional physical quantity, like `dipole` (vector) and `polarizability` (matrix, shorted as `polar`). Deep Potential has provided different APIs to do this. In this example, we will show you how to train a model to fit a water system. A complete training input script of the examples can be found in

```
$deepmd_source_dir/examples/water_tensor/dipole/dipole_input.json
$deepmd_source_dir/examples/water_tensor/polar/polar_input.json
```

The training and validation data are also provided our examples. But note that the data provided along with the examples are of limited amount, and should not be used to train a production model.

Similar to the `input.json` used in `ener` mode, training JSON is also divided into `model`, `learning_rate`, `loss` and `training`. Most keywords remain the same as `ener` mode, and their meaning can be found [here](#). To fit a tensor, one needs to modify `model/fitting_net` and `loss`.

4.10.1 The fitting Network

The `fitting_net` section tells DP which fitting net to use.

The JSON of `dipole` type should be provided like

```
"fitting_net" : {
    "type": "dipole",
    "sel_type": [0],
    "neuron": [100,100,100],
    "resnet_dt": true,
    "seed": 1,
},
```

The JSON of `polar` type should be provided like

```
"fitting_net" : {
    "type": "polar",
    "sel_type": [0],
    "neuron": [100,100,100],
    "resnet_dt": true,
    "seed": 1,
},
```

- `type` specifies which type of fitting net should be used. It should be either `dipole` or `polar`. Note that `global_polar` mode in version 1.x is already deprecated and is merged into `polar`. To specify whether a system is global or atomic, please see [here](#).
- `sel_type` is a list specifying which type of atoms have the quantity you want to fit. For example, in the water system, `sel_type` is `[0]` since 0 represents atom O. If left unset, all types of atoms will be fitted.
- The rest arguments have the same meaning as they do in `ener` mode.

4.10.2 Loss

DP supports a combinational training of the global system (only a global `tensor` label, i.e. dipole or polar, is provided in a frame) and atomic system (labels for each atom included in `sel_type` are provided). In a global system, each frame has just one `tensor` label. For example, when fitting `polar`, each frame will just provide a 1×9 vector which gives the elements of the polarizability tensor of that frame in order XX, XY, XZ, YX, YY, YZ, XZ, ZY, ZZ. By contrast, in an atomic system, each atom in `sel_type` has a `tensor` label. For example, when fitting a dipole, each frame will provide a `#sel_atom` \times 3 matrices, where `#sel_atom` is the number of atoms whose type are in `sel_type`.

The `loss` section tells DP the weight of these two kinds of loss, i.e.

```
loss = pref * global_loss + pref_atomic * atomic_loss
```

The loss section should be provided like

```
"loss" : {
    "type":          "tensor",
    "pref":          1.0,
    "pref_atomic":   1.0
},
```

- `type` should be written as `tensor` as a distinction from `ener` mode.
- `pref` and `pref_atomic` respectively specify the weight of global loss and atomic loss. It can not be left unset. If set to 0, the corresponding label will NOT be included in the training process.

4.10.3 Training Data Preparation

In tensor mode, the identification of the label's type (global or atomic) is derived from the file name. The global label should be named `dipole.npy/raw` or `polarizability.npy/raw`, while the atomic label should be named `atomic_dipole.npy/raw` or `atomic_polarizability.npy/raw`. If wrongly named, DP will report an error

```
ValueError: cannot reshape array of size xxx into shape (xx,xx). This error may occur when your
↳label mismatch it's name, i.e. you might store global tensor in `atomic_tensor.npy` or atomic
↳tensor in `tensor.npy`.
```

In this case, please check the file name of the label.

4.10.4 Train the Model

The training command is the same as `ener` mode, i.e.

```
dp train input.json
```

The detailed loss can be found in `lcurve.out`:

| # | step | rmse_val | rmse_trn | rmse_lc_val | rmse_lc_trn | rmse_gl_val | rmse_gl_trn | lr |
|---|------|----------|----------|-------------|-------------|-------------|-------------|---------|
| | 0 | 8.34e+00 | 8.26e+00 | 8.34e+00 | 8.26e+00 | 0.00e+00 | 0.00e+00 | 1.0e-02 |
| | 100 | 3.51e-02 | 8.55e-02 | 0.00e+00 | 8.55e-02 | 4.38e-03 | 0.00e+00 | 5.0e-03 |
| | 200 | 4.77e-02 | 5.61e-02 | 0.00e+00 | 5.61e-02 | 5.96e-03 | 0.00e+00 | 2.5e-03 |
| | 300 | 5.68e-02 | 1.47e-02 | 0.00e+00 | 0.00e+00 | 7.10e-03 | 1.84e-03 | 1.3e-03 |
| | 400 | 3.73e-02 | 3.48e-02 | 1.99e-02 | 0.00e+00 | 2.18e-03 | 4.35e-03 | 6.3e-04 |

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| | | | | | | | |
|------|----------|----------|----------|----------|----------|----------|---------|
| 500 | 2.77e-02 | 5.82e-02 | 1.08e-02 | 5.82e-02 | 2.11e-03 | 0.00e+00 | 3.2e-04 |
| 600 | 2.81e-02 | 5.43e-02 | 2.01e-02 | 0.00e+00 | 1.01e-03 | 6.79e-03 | 1.6e-04 |
| 700 | 2.97e-02 | 3.28e-02 | 2.03e-02 | 0.00e+00 | 1.17e-03 | 4.10e-03 | 7.9e-05 |
| 800 | 2.25e-02 | 6.19e-02 | 9.05e-03 | 0.00e+00 | 1.68e-03 | 7.74e-03 | 4.0e-05 |
| 900 | 3.18e-02 | 5.54e-02 | 9.93e-03 | 5.54e-02 | 2.74e-03 | 0.00e+00 | 2.0e-05 |
| 1000 | 2.63e-02 | 5.02e-02 | 1.02e-02 | 5.02e-02 | 2.01e-03 | 0.00e+00 | 1.0e-05 |
| 1100 | 3.27e-02 | 5.89e-02 | 2.13e-02 | 5.89e-02 | 1.43e-03 | 0.00e+00 | 5.0e-06 |
| 1200 | 2.85e-02 | 2.42e-02 | 2.85e-02 | 0.00e+00 | 0.00e+00 | 3.02e-03 | 2.5e-06 |
| 1300 | 3.47e-02 | 5.71e-02 | 1.07e-02 | 5.71e-02 | 3.00e-03 | 0.00e+00 | 1.3e-06 |
| 1400 | 3.13e-02 | 5.76e-02 | 3.13e-02 | 5.76e-02 | 0.00e+00 | 0.00e+00 | 6.3e-07 |
| 1500 | 3.34e-02 | 1.11e-02 | 2.09e-02 | 0.00e+00 | 1.57e-03 | 1.39e-03 | 3.2e-07 |
| 1600 | 3.11e-02 | 5.64e-02 | 3.11e-02 | 5.64e-02 | 0.00e+00 | 0.00e+00 | 1.6e-07 |
| 1700 | 2.97e-02 | 5.05e-02 | 2.97e-02 | 5.05e-02 | 0.00e+00 | 0.00e+00 | 7.9e-08 |
| 1800 | 2.64e-02 | 7.70e-02 | 1.09e-02 | 0.00e+00 | 1.94e-03 | 9.62e-03 | 4.0e-08 |
| 1900 | 3.28e-02 | 2.56e-02 | 3.28e-02 | 0.00e+00 | 0.00e+00 | 3.20e-03 | 2.0e-08 |
| 2000 | 2.59e-02 | 5.71e-02 | 1.03e-02 | 5.71e-02 | 1.94e-03 | 0.00e+00 | 1.0e-08 |

One may notice that in each step, some of the local loss and global loss will be 0.0. This is because our training data and validation data consist of the global system and atomic system, i.e.

```
--training_data
    >atomic_system
    >global_system
--validation_data
    >atomic_system
    >global_system
```

During training, at each step when the `lcurve.out` is printed, the system used for evaluating the training (validation) error may be either with only global or only atomic labels, thus the corresponding atomic or global errors are missing and are printed as zeros.

4.11 Fit electronic density of states (DOS)

Here we present an API to DeepDOS model, which can be used to fit electronic density of state (DOS) (which is a vector).

See the [PRB paper](#) for details.

In this example, we will show you how to train a model to fit a silicon system. A complete training input script of the examples can be found in

```
$deepmd_source_dir/examples/dos/input.json
```

The training and validation data are also provided our examples. But note that the data provided along with the examples are of limited amount, and should not be used to train a production model.

Similar to the `input.json` used in `ener` mode, training JSON is also divided into `model`, `learning_rate`, `loss` and `training`. Most keywords remain the same as `ener` mode, and their meaning can be found [here](#). To fit the `dos`, one needs to modify `model/fitting_net` and `loss`.

4.11.1 The fitting Network

The `fitting_net` section tells DP which fitting net to use.

The JSON of `dos` type should be provided like

```
"fitting_net" : {
  "type": "dos",
  "numb_dos": 250,
  "sel_type": [0],
  "neuron": [120,120,120],
  "resnet_dt": true,
  "fparam": 0,
  "seed": 1,
},
```

- `type` specifies which type of fitting net should be used. It should be `dos`.
- `numb_dos` specifies the length of output vector (density of states), which the same as the `NEDOS` set in VASP software, this argument defines the output length of the neural network. We note that the length of `dos` provided in training set should be the same.
- The rest arguments have the same meaning as they do in `ener` mode.

4.11.2 Loss

DeepDOS supports trainings of the global system (a global `dos` label is provided in a frame) or atomic system (atomic labels `atom_dos` is provided for each atom in a frame). In a global system, each frame has just one `dos` label. For example, when fitting `dos`, each frame will just provide a `1 x numb_dos` vector which gives the total electronic density of states. By contrast, in an atomic system, each atom in has a `atom_dos` label. For example, when fitting the site-projected electronic density of states, each frame will provide a `natom x numb_dos` matrices,

The `loss` section tells DP the weight of these two kinds of loss, i.e.

```
loss = pref * global_loss + pref_atomic * atomic_loss
```

The `loss` section should be provided like

```
"loss" : {
  "type": "dos",
  "start_pref_dos": 0.0,
  "limit_pref_dos": 0.0,
  "start_pref_cdf": 0.0,
  "limit_pref_cdf": 0.0,
  "start_pref_ados": 1.0,
  "limit_pref_ados": 1.0,
  "start_pref_acdf": 0.0,
  "limit_pref_acdf": 0.0
},
```

- `type` should be written as `dos` as a distinction from `ener` mode.
- `pref_dos` and `pref_ados`, respectively specify the weight of global and atomic loss. If set to 0, the corresponding label will not be included in the training process.
- We also provides a combination training of vector and its cumulative distribution function `cdf`, which can be defined as

$$D(\epsilon) = \int_{\epsilon_{min}}^{\epsilon} g(\epsilon') d\epsilon'$$

4.11.3 Training Data Preparation

The global label should be named `dos.npy/raw`, while the atomic label should be named `atomic_dos.npy/raw`. If wrongly named, DP will report an error.

To prepare the data, we recommend shifting the DOS data by the Fermi level.

4.11.4 Train the Model

The training command is the same as `ener` mode, i.e.

```
dp train input.json
```

The detailed loss can be found in `lcurve.out`:

| # | step | rmse_trn | rmse_ados_trn | rmse_ados_lr |
|---|------|----------|---------------|--------------|
| | 0 | 1.11e+00 | 1.11e+00 | 1.0e-03 |
| | 100 | 5.00e-02 | 5.00e-02 | 1.0e-03 |
| | 200 | 4.70e-02 | 4.70e-02 | 1.0e-03 |
| | 300 | 6.45e-02 | 6.45e-02 | 1.0e-03 |
| | 400 | 3.39e-02 | 3.39e-02 | 1.0e-03 |
| | 500 | 4.60e-02 | 4.60e-02 | 1.0e-03 |
| | 600 | 3.98e-02 | 3.98e-02 | 1.0e-03 |
| | 700 | 9.50e-02 | 9.50e-02 | 1.0e-03 |
| | 800 | 5.49e-02 | 5.49e-02 | 1.0e-03 |
| | 900 | 5.57e-02 | 5.57e-02 | 1.0e-03 |
| | 1000 | 3.73e-02 | 3.73e-02 | 1.0e-03 |
| | 1100 | 4.33e-02 | 4.33e-02 | 1.0e-03 |
| | 1200 | 3.27e-02 | 3.27e-02 | 1.0e-03 |
| | 1300 | 3.68e-02 | 3.68e-02 | 1.0e-03 |
| | 1400 | 3.09e-02 | 3.09e-02 | 1.0e-03 |
| | 1500 | 3.42e-02 | 3.42e-02 | 1.0e-03 |
| | 1600 | 5.62e-02 | 5.62e-02 | 1.0e-03 |
| | 1700 | 6.12e-02 | 6.12e-02 | 1.0e-03 |
| | 1800 | 4.10e-02 | 4.10e-02 | 1.0e-03 |
| | 1900 | 5.30e-02 | 5.30e-02 | 1.0e-03 |
| | 2000 | 3.85e-02 | 3.85e-02 | 1.0e-03 |

4.11.5 Test the Model

In this earlier version, we can use `dp test` to infer the electronic density of state for given frames.

```
$DP freeze -o frozen_model.pb
```

```
$DP test -m frozen_model.pb -s ../data/111/$k -d ${output_prefix} -a -n 100
```

if `dp test -d ${output_prefix} -a` is specified, the predicted DOS and atomic DOS for each frame is output in the working directory

```

${output_prefix}.ados.out.0  ${output_prefix}.ados.out.1  ${output_prefix}.ados.out.2  ${output_
↪prefix}.ados.out.3
${output_prefix}.dos.out.0  ${output_prefix}.dos.out.1  ${output_prefix}.dos.out.2  ${output_
↪prefix}.dos.out.3

```

for *.dos.out.*, it contains matrix with shape of (2, numb_dos), for *.ados.out.*, it contains matrix with shape of (2, natom x numb_dos),

```

# frame - 0: data_dos pred_dos
0.0000000000000000e+00  1.963193264917645342e-03
0.0000000000000000e+00  1.178440836781313727e-03
0.0000000000000000e+00  1.441258071790407769e-04
0.0000000000000000e+00  1.787297933314058174e-03
0.0000000000000000e+00  1.901603280243024940e-03
0.0000000000000000e+00  2.279848925571981155e-03
0.0000000000000000e+00  2.149355854688561607e-03
0.0000000000000000e+00  1.829848459515726056e-03
0.0000000000000000e+00  1.905156512419792225e-03

```

4.12 Type embedding approach

We generate specific a type embedding vector for each atom type so that we can share one descriptor embedding net and one fitting net in total, which decline training complexity largely.

The training input script is similar to that of `se_e2_a`, but different by adding the `type_embedding` section.

4.12.1 Type embedding net

The `model` defines how the model is constructed, adding a section of type embedding net:

```

"model": {
  "type_map":      ["O", "H"],
  "type_embedding":{
    ...
  },
  "descriptor" :{
    ...
  },
  "fitting_net" : {
    ...
  }
}

```

The model will automatically apply the type embedding approach and generate type embedding vectors. If the type embedding vector is detected, the descriptor and fitting net would take it as a part of the input.

The construction of type embedding net is given by `type_embedding`. An example of `type_embedding` is provided as follows

```

"type_embedding":{
  "neuron":      [2, 4, 8],
  "resnet_dt":   false,
  "seed":        1
}

```

- The `neuron` specifies the size of the type embedding net. From left to right the members denote the sizes of each hidden layer from the input end to the output end, respectively. It takes a one-hot vector as input and output dimension equals to the last dimension of the `neuron` list. If the outer layer is twice the size of the inner layer, then the inner layer is copied and concatenated, then a ResNet architecture is built between them.
- If the option `resnet_dt` is set to `true`, then a timestep is used in the ResNet.
- `seed` gives the random seed that is used to generate random numbers when initializing the model parameters.

A complete training input script of this example can be found in the directory.

```
$deepmd_source_dir/examples/water/se_e2_a_tebd/input.json
```

See [here](#) for further explanation of type embedding.

Note: You can't apply the compression method while using the atom type embedding.

4.13 Descriptor "se_a_mask"

Descriptor `se_a_mask` is a concise implementation of the descriptor `se_e2_a`, but functions slightly differently. `se_a_mask` is specially designed for DP/MM simulations where the number of atoms in DP regions is dynamically changed in simulations.

Therefore, the descriptor `se_a_mask` is not supported for training with PBC systems for simplicity. Besides, to make the output shape of the descriptor matrix consistent, the input coordinates are padded with virtual particle coordinates to the maximum number of atoms (specified with `sel` in the descriptor setting) in the system. The real/virtual sign of the atoms is specified with the `aparam.npy` (`[nframes * natoms]`) file in the input systems set directory. The `aparam.npy` can also be seen as the mask of the atoms in the system, which is also the origin of the name `se_a_mask`.

In this example, we will train a DP Mask model for zinc protein interactions. The input systems are the collection of zinc and its coordinates residues. A sample input system that contains 2 frames is included in the directory.

```
$deepmd_source_dir/examples/zinc_protein/data_dp_mask
```

A complete training input script of this example can be found in the directory.

```
$deepmd_source_dir/examples/zinc_protein/zinc_se_a_mask.json
```

The construction of the descriptor is given by section descriptor. An example of the descriptor is provided as follows

```
"descriptor" : {
  "type":      "se_a_mask",
  "sel":       [36, 16, 24, 64, 6, 1],
  "neuron":    [25, 50, 100],
  "axis_neuron": 16,
  "type_one_side": false,
  "resnet_dt":  false,
  "seed":      1
}
```

- The type of the descriptor is set to "se_a_mask".
- sel gives the maximum number of atoms in input coordinates. It is a list, the length of which is the same as the number of atom types in the system, and sel[i] denotes the maximum number of atoms with type i.
- The neuron specifies the size of the embedding net. From left to right the members denote the sizes of each hidden layer from the input end to the output end, respectively. If the outer layer is twice the size of the inner layer, then the inner layer is copied and concatenated, then a [ResNet architecture](#) is built between them.
- The axis_neuron specifies the size of the submatrix of the embedding matrix, the axis matrix as explained in the [DeepPot-SE paper](#)
- If the option type_one_side is set to true, the embedding network parameters vary by types of neighbor atoms only, so there will be N_{types} sets of embedding network parameters. Otherwise, the embedding network parameters vary by types of centric atoms and types of neighbor atoms, so there will be N_{types}^2 sets of embedding network parameters.
- If the option resnet_dt is set to true, then a timestep is used in the ResNet.
- seed gives the random seed that is used to generate random numbers when initializing the model parameters.

To make the aparam.npy used for descriptor se_a_mask, two variables in fitting_net section are needed.

```
"fitting_net" :{
  "neuron": [240, 240, 240],
  "resnet_dt": true,
  "seed": 1,
  "numb_aparam": 1,
  "use_aparam_as_mask": true
}
```

- neuron, resnet_dt and seed are the same as the fitting_net section for fitting energy.
- numb_aparam gives the dimension of the aparam.npy file. In this example, it is set to 1 and stores the real/virtual sign of the atoms. For real/virtual atoms, the corresponding sign in aparam.npy is set to 1/0.
- use_aparam_as_mask is set to true to use the aparam.npy as the mask of the atoms in the descriptor se_a_mask.

Finally, to make a reasonable fitting task with se_a_mask descriptor for DP/MM simulations, the loss function with se_a_mask is designed to include the atomic forces difference in specific atoms of the input particles only. More details about the selection of the specific atoms can be found in paper [DP/MM](left to be filled). Thus, atom_pref.npy ([nframes * natoms]) is required as the indicator of the specific atoms in the input particles. And the loss section in the training input script should be set as follows.

```
"loss": {
  "type": "ener",
  "start_pref_e": 0.0,
  "limit_pref_e": 0.0,
  "start_pref_f": 0.0,
  "limit_pref_f": 0.0,
  "start_pref_pf": 1.0,
  "limit_pref_pf": 1.0,
  "_comment": " that's all"
}
```

4.14 Deep potential long-range (DPLR)

Notice: The interfaces of DPLR are not stable and subject to change

The method of DPLR is described in [this paper](#). One is recommended to read the paper before using the DPLR.

In the following, we take the DPLR model for example to introduce the training and LAMMPS simulation with the DPLR model. The DPLR model is trained in two steps.

4.14.1 Train a deep Wannier model for Wannier centroids

We use the deep Wannier model (DW) to represent the relative position of the Wannier centroid (WC) with the atom with which it is associated. One may consult the introduction of the [dipole model](#) for a detailed introduction. An example input `wc.json` and a small dataset `data` for tutorial purposes can be found in

```
$deepmd_source_dir/examples/water/dplr/train/
```

It is noted that the tutorial dataset is not enough for training a productive model. Two settings make the training input script different from an energy training input:

```
"fitting_net": {
  "type":          "dipole",
  "dipole_type":   [0],
  "neuron":        [128, 128, 128],
  "seed":          1
},
```

The type of fitting is set to dipole. The dipole is associated with type 0 atoms (oxygen), by the setting `"dipole_type": [0]`. What we trained is the displacement of the WC from the corresponding oxygen atom. It shares the same training input as the atomic dipole because both are 3-dimensional vectors defined on atoms. The loss section is provided as follows

```
"loss": {
  "type":          "tensor",
  "pref":          0.0,
  "pref_atomic":   1.0
},
```

so that the atomic dipole is trained as labels. Note that the NumPy compressed file `atomic_dipole.npy` should be provided in each dataset.

The training and freezing can be started from the example directory by

```
dp train dw.json && dp freeze -o dw.pb
```

4.14.2 Train the DPLR model

The training of the DPLR model is very similar to the standard short-range DP models. An example input script can be found in the example directory. The following section is introduced to compute the long-range energy contribution of the DPLR model, and modify the short-range DP model by this part.

```
"modifier": {
  "type": "dipole_charge",
  "model_name": "dw.pb",
  "model_charge_map": [-8],
  "sys_charge_map": [6, 1],
  "ewald_h": 1.00,
  "ewald_beta": 0.40
},
```

The `model_name` specifies which DW model is used to predict the position of WCs. `model_charge_map` gives the amount of charge assigned to WCs. `sys_charge_map` provides the nuclear charge of oxygen (type 0) and hydrogen (type 1) atoms. `ewald_beta` (unit \AA^{-1}) gives the spread parameter controls the spread of Gaussian charges, and `ewald_h` (unit \AA) assigns the grid size of Fourier transformation. The DPLR model can be trained and frozen by (from the example directory)

```
dp train ener.json && dp freeze -o ener.pb
```

4.14.3 Molecular dynamics simulation with DPLR

In MD simulations, the long-range part of the DPLR is calculated by the LAMMPS `kspace` support. Then the long-range interaction is back-propagated to atoms by DeePMD-kit. This setup is commonly used in classical molecular dynamics simulations as the “virtual site”. Unfortunately, LAMMPS does not natively support virtual sites, so we have to hack the LAMMPS code, which makes the input configuration and script a little wired.

An example of an input configuration file and script can be found in

```
$deepmd_source_dir/examples/water/dplr/lmp/
```

We use `atom_style full` for DPLR simulations. the coordinates of the WCs are explicitly written in the configuration file. Moreover, a virtual bond is established between the oxygens and the WCs to indicate they are associated together. The configuration file containing 128 H2O molecules is thus written as

```
512 atoms
3 atom types
128 bonds
1 bond types

0 16.421037674 xlo xhi
0 16.421037674 ylo yhi
0 16.421037674 zlo zhi
0 0 0 xy xz yz

Masses
```

(continues on next page)

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```

1 16
2 2
3 16

Atoms

      1      1 1 6 8.4960699081e+00 7.5073699951e+00 9.6371297836e+00
      2      2 1 6 4.0597701073e+00 6.8156299591e+00 1.2051420212e+01
...

    385      1 3 -8 8.4960699081e+00 7.5073699951e+00 9.6371297836e+00
    386      2 3 -8 4.0597701073e+00 6.8156299591e+00 1.2051420212e+01
...

Bonds

1 1 1 385
2 1 2 386
...
```

The oxygens and hydrogens are assigned with atom types 1 and 2 (corresponding to training atom types 0 and 1), respectively. The WCs are assigned with atom type 3. We want to simulate heavy water so the mass of hydrogens is set to 2.

An example input script is provided in

```
$deepmd_source_dir/examples/water/dplr/lmp/in.lammps
```

Here are some explanations

```

# groups of real and virtual atoms
group          real_atom type 1 2
group          virtual_atom type 3

# bond between real and its corresponding virtual site should be given
# to setup a map between real and virtual atoms. However, no real
# bonded interaction is applied, thus bond_style "zero" is used.
pair_style     deepmd ener.pb
pair_coeff     * *
bond_style     zero
bond_coeff     *
special_bonds  lj/coul 1 1 1 angle no
```

Type 1 and 2 (O and H) are `real_atoms`, while type 3 (WCs) are `virtual_atoms`. The model file `ener.pb` stores both the DW and DPLR models, so the position of WCs and the energy can be inferred from it. A virtual bond type is specified by `bond_style zero`. The `special_bonds` command switches off the exclusion of intramolecular interactions.

```

# kspace_style "pppm/dplr" should be used. in addition the
# gewald(1/distance) should be set the same as that used in
# training. Currently only ik differentiation is supported.
kspace_style   pppm/dplr 1e-5
kspace_modify  gewald ${BETA} diff ik mesh ${KMESH} ${KMESH} ${KMESH}
```

The long-range part is calculated by the `kspace` support of LAMMPS. The `kspace_style pppm/dplr` is required. The spread parameter set by variable `BETA` should be set the same as that used in training. The `KMESH`

should be set dense enough so the long-range calculation is converged.

fix dplr command

Syntax

```
fix ID group-ID style_name keyword value ...
```

- ID, group-ID are documented in :doc:fix <fix> command
- style_name = dplr
- three or more keyword/value pairs may be appended

```
keyword = *model* or *type_associate* or *bond_type* or *efield*
*model* value = name
    name = name of DPLR model file (e.g. frozen_model.pb) (not DW model)
*type_associate* values = NR1 NW1 NR2 NW2 ...
    NRi = type of real atom in i-th (real atom, Wannier centroid) pair
    NWi = type of Wannier in i-th (real atom, Wannier centroid) pair
*bond_type* values = NB1 NB2 ...
    NBi = bond type of i-th (real atom, Wannier centroid) pair
*efield* (optional) values = Ex Ey Ez
    Ex/Ey/Ez = electric field along x/y/z direction
```

Examples

```
# "fix dplr" set the position of the virtual atom, and spread the
# electrostatic interaction asserting on the virtual atom to the real
# atoms. "type_associate" associates the real atom type its
# corresponding virtual atom type. "bond_type" gives the type of the
# bond between the real and virtual atoms.
fix          0 all dplr model ener.pb type_associate 1 3 bond_type 1
fix_modify   0 virial yes
```

The fix command dplr calculates the position of WCs by the DW model and back-propagates the long-range interaction on virtual atoms to real atoms. At this time, the training parameter `type_map` will be mapped to LAMMPS atom types.

To use a time-dependent electric field, LAMMPS's variable feature can be utilized:

```
variable EFIELD_Z equal 2*sin(2*PI*time/0.006)
fix 0 all dplr model ener.pb type_associate 1 3 bond_type 1 efield 0 0 v_EFIELD_Z
fix_modify 0 energy yes virial yes
```

The efield feature of fix dplr behaves similarly to LAMMPS's fix efield. Note that the atomic energy or potential in fix efield is not yet supported in fix dplr. For a detailed description on how a time-dependent variable can be defined, refer to LAMMPS's document of variable.

```
# compute the temperature of real atoms, excluding virtual atom contribution
compute      real_temp real_atom temp
compute      real_press all pressure real_temp
fix          1 real_atom nvt temp ${TEMP} ${TEMP} ${TAU_T}
fix_modify   1 temp real_temp
```

The temperature of the system should be computed from the real atoms. The kinetic contribution in the pressure tensor is also computed from the real atoms. The thermostat is applied to only real atoms. The computed temperature and pressure of real atoms can be accessed by, e.g.

```
fix                thermo_print all print ${THERMO_FREQ} "$(step) $(pe) $(ke) $(etotal) $(enthalpy)
↪$(c_real_temp) $(c_real_press) $(vol) $(c_real_press[1]) $(c_real_press[2]) $(c_real_press[3])"
↪append thermo.out screen no title "# step pe ke etotal enthalpy temp press vol pxx pyy pzz"
```

The LAMMPS simulation can be started from the example directory by

```
lmp -i in.lammps
```

If LAMMPS complains that no model file `ener.pb` exists, it can be copied from the training example directory.

The MD simulation lasts for only 20 steps. If one runs a longer simulation, it will blow up, because the model is trained with a very limited dataset for very short training steps, thus is of poor quality.

Another restriction that should be noted is that the energies printed at the zero steps are not correct. This is because at the zero steps the position of the WC has not been updated with the DW model. The energies printed in later steps are correct.

4.15 Deep Potential - Range Correction (DPRc)

Deep Potential - Range Correction (DPRc) is designed to combine with QM/MM method, and corrects energies from a low-level QM/MM method to a high-level QM/MM method:

$$E = E_{\text{QM}}(\text{R}; \text{P}) + E_{\text{QM/MM}}(\text{R}; \text{P}) + E_{\text{MM}}(\text{R}) + E_{\text{DPRc}}(\text{R})$$

See the [JCTC](#) paper for details.

4.15.1 Training data

Instead the normal ab initio data, one needs to provide the correction from a low-level QM/MM method to a high-level QM/MM method:

$$E = E_{\text{high-level QM/MM}} - E_{\text{low-level QM/MM}}$$

Two levels of data use the same MM method, so E_{MM} is eliminated.

4.15.2 Training the DPRc model

In a DPRc model, QM atoms and MM atoms have different atom types. Assuming we have 4 QM atom types (C, H, O, P) and 2 MM atom types (HW, OW):

```
"type_map": ["C", "H", "HW", "O", "OW", "P"]
```

As described in the paper, the DPRc model only corrects E_{QM} and $E_{\text{QM/MM}}$ within the cutoff, so we use a hybrid descriptor to describe them separately:

```
"descriptor" :{
  "type":      "hybrid",
  "list" : [
    {
      "type":    "se_e2_a",
      "sel":     [6, 11, 0, 6, 0, 1],
      "rcut_smth": 1.00,
```

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```

        "rcut":          9.00,
        "neuron":        [12, 25, 50],
        "exclude_types": [[2, 2], [2, 4], [4, 4], [0, 2], [0, 4], [1, 2], [1, 4], [3, 2],
↪ [3, 4], [5, 2], [5, 4]],
        "axis_neuron":    12,
        "set_davg_zero":  true,
        "_comment": " QM/QM interaction"
    },
    {
        "type":          "se_e2_a",
        "sel":            [6, 11, 100, 6, 50, 1],
        "rcut_smth":      0.50,
        "rcut":            6.00,
        "neuron":          [12, 25, 50],
        "exclude_types":  [[0, 0], [0, 1], [0, 3], [0, 5], [1, 1], [1, 3], [1, 5], [3, 3],
↪ [3, 5], [5, 5], [2, 2], [2, 4], [4, 4]],
        "axis_neuron":    12,
        "set_davg_zero":  true,
        "_comment": " QM/MM interaction"
    }
]
}

```

exclude_types can be generated by the following Python script:

```

from itertools import combinations_with_replacement, product

qm = (0, 1, 3, 5)
mm = (2, 4)
print(
    "QM/QM:",
    list(map(list, list(combinations_with_replacement(mm, 2)) + list(product(qm, mm)))),
)
print(
    "QM/MM:",
    list(
        map(
            list,
            list(combinations_with_replacement(qm, 2))
            + list(combinations_with_replacement(mm, 2)),
        )
    ),
)

```

Also, DPRc assumes MM atom energies (atom_ener) are zero:

```

"fitting_net": {
    "neuron": [240, 240, 240],
    "resnet_dt": true,
    "atom_ener": [null, null, 0.0, null, 0.0, null]
}

```

Note that atom_ener only works when descriptor/set_davg_zero is true.

4.15.3 Run MD simulations

The DPRc model has the best practices with the [AMBER](#) QM/MM module. An example is given by [GitLab RutgersLBSR/AmberDPRc](#). In theory, DPRc is able to be used with any QM/MM package, as long as the DeePMD-kit package accepts QM atoms and MM atoms within the cutoff range and returns energies and forces.

4.15.4 Pairwise DPRc

If one wants to correct from a low-level method into a full DFT level, and the system is too large to do full DFT calculation, one may try the experimental pairwise DPRc model. In a pairwise DPRc model, the total energy is divided into QM internal energy and the sum of QM/MM energy for each MM residue l :

$$E = E_{\text{QM}} + \sum_l E_{\text{QM/MM},l}$$

In this way, the interaction between the QM region and each MM fragmentation can be computed and trained separately. Thus, the pairwise DPRc model is divided into two sub-DPRc models. `qm_model` is for the QM internal interaction and `qmmm_model` is for the QM/MM interaction. The configuration for these two models is similar to the non-pairwise DPRc model. It is noted that the `se_attn` descriptor should be used, as it is the only descriptor to support the mixed type.

```
{
  "model": {
    "type": "pairwise_dprc",
    "type_map": [
      "C",
      "P",
      "O",
      "H",
      "OW",
      "HW"
    ],
    "type_embedding": {
      "neuron": [
        8
      ],
      "precision": "float32"
    },
    "qm_model": {
      "descriptor": {
        "type": "se_attn_v2",
        "sel": 24,
        "rcut_smth": 0.50,
        "rcut": 9.00,
        "attn_layer": 0,
        "neuron": [
          25,
          50,
          100
        ],
        "resnet_dt": false,
        "axis_neuron": 12,
        "precision": "float32",
        "seed": 1
      },
    },
  },
}
```

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```

    "fitting_net": {
        "type": "ener",
        "neuron": [
            240,
            240,
            240
        ],
        "resnet_dt": true,
        "precision": "float32",
        "atom_ener": [
            null,
            null,
            null,
            null,
            0.0,
            0.0
        ],
        "seed": 1
    }
},
"qmmm_model": {
    "descriptor": {
        "type": "se_atten_v2",
        "sel": 27,
        "rcut_smth": 0.50,
        "rcut": 6.00,
        "attn_layer": 0,
        "neuron": [
            25,
            50,
            100
        ],
        "resnet_dt": false,
        "axis_neuron": 12,
        "set_davg_zero": true,
        "exclude_types": [
            [
                0,
                0
            ],
            [
                0,
                1
            ],
            [
                0,
                2
            ],
            [
                0,
                3
            ],
            [
                1,
                1
            ]
        ]
    }
}

```

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```

        [
            1,
            2
        ],
        [
            1,
            3
        ],
        [
            2,
            2
        ],
        [
            2,
            3
        ],
        [
            3,
            3
        ],
        [
            4,
            4
        ],
        [
            4,
            5
        ],
        [
            5,
            5
        ]
    ],
    "precision": "float32",
    "seed": 1
},
"fitting_net": {
    "type": "ener",
    "neuron": [
        240,
        240,
        240
    ],
    "resnet_dt": true,
    "seed": 1,
    "precision": "float32",
    "atom_ener": [
        0.0,
        0.0,
        0.0,
        0.0,
        0.0,
        0.0
    ]
}
}

```

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```
}  
}
```

The pairwise model needs information for MM residues. The model uses *aparam* with the shape of `nframes` x `natoms` to get the residue index. The QM residue should always use 0 as the index. For example, 0 0 0 1 1 1 2 2 2 means these 9 atoms are grouped into one QM residue and two MM residues.

TRAINING

5.1 Train a model

Several examples of training can be found in the `examples` directory:

```
$ cd $deepmd_source_dir/examples/water/se_e2_a/
```

After switching to that directory, the training can be invoked by

```
$ dp train input.json
```

where `input.json` is the name of the input script.

By default, the verbosity level of the DeePMD-kit is `INFO`, one may see a lot of important information on the code and environment showing on the screen. Among them two pieces of information regarding data systems are worth special notice.

```
DEEPMD INFO    ---Summary of DataSystem: training  -----
↪--
DEEPMD INFO    found 3 system(s):
DEEPMD INFO
DEEPMD INFO          system  natoms  bch_sz  n_bch  prob  pbc
DEEPMD INFO    ../data_water/data_0/    192    1    80  0.250  T
DEEPMD INFO    ../data_water/data_1/    192    1   160  0.500  T
DEEPMD INFO    ../data_water/data_2/    192    1    80  0.250  T
DEEPMD INFO    -----
↪--
DEEPMD INFO    ---Summary of DataSystem: validation -----
↪--
DEEPMD INFO    found 1 system(s):
DEEPMD INFO
DEEPMD INFO          system  natoms  bch_sz  n_bch  prob  pbc
DEEPMD INFO    ../data_water/data_3    192    1    80  1.000  T
DEEPMD INFO    -----
↪--
```

The DeePMD-kit prints detailed information on the training and validation data sets. The data sets are defined by `training_data` and `validation_data` defined in the `training` section of the input script. The training data set is composed of three data systems, while the validation data set is composed by one data system. The number of atoms, batch size, the number of batches in the system and the probability of using the system are all shown on the screen. The last column presents if the periodic boundary condition is assumed for the system.

During the training, the error of the model is tested every `disp_freq` training steps with the batch used to train the model and with `numb_btch` batches from the validating data. The training error and validation error are printed correspondingly in the file `disp_file` (default is `lcurve.out`). The batch size can be set in the

input script by the key `batch_size` in the corresponding sections for the training and validation data set. An example of the output

| # | step | rmse_val | rmse_trn | rmse_e_val | rmse_e_trn | rmse_f_val | rmse_f_trn | lr |
|---|------|----------|----------|------------|------------|------------|------------|---------|
| | 0 | 3.33e+01 | 3.41e+01 | 1.03e+01 | 1.03e+01 | 8.39e-01 | 8.72e-01 | 1.0e-03 |
| | 100 | 2.57e+01 | 2.56e+01 | 1.87e+00 | 1.88e+00 | 8.03e-01 | 8.02e-01 | 1.0e-03 |
| | 200 | 2.45e+01 | 2.56e+01 | 2.26e-01 | 2.21e-01 | 7.73e-01 | 8.10e-01 | 1.0e-03 |
| | 300 | 1.62e+01 | 1.66e+01 | 5.01e-02 | 4.46e-02 | 5.11e-01 | 5.26e-01 | 1.0e-03 |
| | 400 | 1.36e+01 | 1.32e+01 | 1.07e-02 | 2.07e-03 | 4.29e-01 | 4.19e-01 | 1.0e-03 |
| | 500 | 1.07e+01 | 1.05e+01 | 2.45e-03 | 4.11e-03 | 3.38e-01 | 3.31e-01 | 1.0e-03 |

The file contains 8 columns, from left to right, which are the training step, the validation loss, training loss, root mean square (RMS) validation error of energy, RMS training error of energy, RMS validation error of force, RMS training error of force and the learning rate. The RMS error (RMSE) of the energy is normalized by the number of atoms in the system. One can visualize this file with a simple Python script:

```
import numpy as np
import matplotlib.pyplot as plt

data = np.genfromtxt("lcurve.out", names=True)
for name in data.dtype.names[1:-1]:
    plt.plot(data["step"], data[name], label=name)
plt.legend()
plt.xlabel("Step")
plt.ylabel("Loss")
plt.xscale("symlog")
plt.yscale("log")
plt.grid()
plt.show()
```

Checkpoints will be written to files with the prefix `save_ckpt` every `save_freq` training steps.

Warning: It is warned that the example water data (in folder `examples/water/data`) is of very limited amount, is provided only for testing purposes, and should not be used to train a production model.

5.2 Advanced options

In this section, we will take `$deepmd_source_dir/examples/water/se_e2_a/input.json` as an example of the input file.

5.2.1 Learning rate

The `learning_rate` section in `input.json` is given as follows

```
{
  "learning_rate" : {
    "type": "exp",
    "start_lr": 0.001,
    "stop_lr": 3.51e-8,
    "decay_steps": 5000,
    "_comment": "that's all"
  }
}
```

- `start_lr` gives the learning rate at the beginning of the training.

- `stop_lr` gives the learning rate at the end of the training. It should be small enough to ensure that the network parameters satisfactorily converge.
- During the training, the learning rate decays exponentially from `start_lr` to `stop_lr` following the formula:

$$\alpha(t) = \alpha_0 \lambda^{t/\tau}$$

where t is the training step, α is the learning rate, α_0 is the starting learning rate (set by `start_lr`), λ is the decay rate, and τ is the decay steps, i.e.

```
...
lr(t) = start_lr * decay_rate ^ ( t / decay_steps )
...
```

5.2.2 Training parameters

Other training parameters are given in the [training](#) section.

```
{
  "training": {
    "training_data": {
      "systems": ["../data_water/data_0/", "../data_water/data_1/", "../data_
↩water/data_2/"],
      "batch_size": "auto"
    },
    "validation_data": {
      "systems": ["../data_water/data_3/"],
      "batch_size": 1,
      "numb_btch": 3
    },
    "mixed_precision": {
      "output_prec": "float32",
      "compute_prec": "float16"
    },
    "numb_steps": 1000000,
    "seed": 1,
    "disp_file": "lcurve.out",
    "disp_freq": 100,
    "save_freq": 1000
  }
}
```

The sections `training_data` and `validation_data` give the training dataset and validation dataset, respectively. Taking the training dataset for example, the keys are explained below:

- `systems` provide paths of the training data systems. DeePMD-kit allows you to provide multiple systems with different numbers of atoms. This key can be a `list` or a `str`.
 - `list`: `systems` gives the training data systems.
 - `str`: `systems` should be a valid path. DeePMD-kit will recursively search all data systems in this path.
- At each training step, DeePMD-kit randomly picks `batch_size` frame(s) from one of the systems. The probability of using a system is by default in proportion to the number of batches in the system. More options are available for automatically determining the probability of using systems. One can set the key `auto_prob` to
 - `"prob_uniform"` all systems are used with the same probability.

- "prob_sys_size" the probability of using a system is proportional to its size (number of frames).
- "prob_sys_size; sidx_0:eidx_0:w_0; sidx_1:eidx_1:w_1;..." the list of systems is divided into blocks. Block *i* has systems ranging from *sidx_i* to *eidx_i*. The probability of using a system from block *i* is proportional to *w_i*. Within one block, the probability of using a system is proportional to its size.
- An example of using "auto_prob" is given below. The probability of using `systems[2]` is 0.4, and the sum of the probabilities of using `systems[0]` and `systems[1]` is 0.6. If the number of frames in `systems[1]` is twice of `system[0]`, then the probability of using `system[1]` is 0.4 and that of `system[0]` is 0.2.

```

    "training_data": {
        "systems":          ["../data_water/data_0/", "../data_water/data_1/", "../data_
↪water/data_2/"],
        "auto_prob":        "prob_sys_size; 0:2:0.6; 2:3:0.4",
        "batch_size":        "auto"
    }

```

- The probability of using systems can also be specified explicitly with key `sys_probs` which is a list having the length of the number of systems. For example

```

    "training_data": {
        "systems":          ["../data_water/data_0/", "../data_water/data_1/", "../data_
↪water/data_2/"],
        "sys_probs":        [0.5, 0.3, 0.2],
        "batch_size":        "auto:32"
    }

```

- The key `batch_size` specifies the number of frames used to train or validate the model in a training step. It can be set to
 - `list`: the length of which is the same as the systems. The batch size of each system is given by the elements of the list.
 - `int`: all systems use the same batch size.
 - `"auto"`: the same as `"auto:32"`, see `"auto:N"`
 - `"auto:N"`: automatically determines the batch size so that the `batch_size` times the number of atoms in the system is no less than *N*.
- The key `numb_batch` in `validate_data` gives the number of batches of model validation. Note that the batches may not be from the same system

The section `mixed_precision` specifies the mixed precision settings, which will enable the mixed precision training workflow for DeePMD-kit. The keys are explained below:

- `output_prec` precision used in the output tensors, only `float32` is supported currently.
- `compute_prec` precision used in the computing tensors, only `float16` is supported currently. Note there are several limitations about mixed precision training:
- Only `se_e2_a` type descriptor is supported by the mixed precision training workflow.
- The precision of the embedding net and the fitting net are forced to be set to `float32`.

Other keys in the `training` section are explained below:

- `numb_steps` The number of training steps.
- `seed` The random seed for getting frames from the training data set.

- `disp_file` The file for printing learning curve.
- `disp_freq` The frequency of printing learning curve. Set in the unit of training steps
- `save_freq` The frequency of saving checkpoint.

5.2.3 Options and environment variables

Several command line options can be passed to `dp train`, which can be checked with

```
$ dp train --help
```

An explanation will be provided

```
positional arguments:
  INPUT                the input json database

optional arguments:
  -h, --help            show this help message and exit

  --init-model INIT_MODEL
                        Initialize a model by the provided checkpoint

  --restart RESTART      Restart the training from the provided checkpoint

  --init-frz-model INIT_FRZ_MODEL
                        Initialize the training from the frozen model.

  --skip-neighbor-stat  Skip calculating neighbor statistics. Sel checking, automatic sel, and
  ↪model compression will be disabled. (default: False)
```

`--init-model model.ckpt`, initializes the model training with an existing model that is stored in the checkpoint `model.ckpt`, the network architectures should match.

`--restart model.ckpt`, continues the training from the checkpoint `model.ckpt`.

`--init-frz-model frozen_model.pb`, initializes the training with an existing model that is stored in `frozen_model.pb`.

`--skip-neighbor-stat` will skip calculating neighbor statistics if one is concerned about performance. Some features will be disabled.

To maximize the performance, one should follow [FAQ: How to control the parallelism of a job](#) to control the number of threads.

One can set other environmental variables:

| Environment variables | Allowed value | Default value | Usage |
|--------------------------------------|---------------|---------------|---|
| <code>DP_INTERFACE_PRECISION</code> | high, low | high | Control high (double) or low (float) precision of training. |
| <code>DP_AUTO_PARALLELIZATION</code> | 0, 1 | 0 | Enable auto parallelization for CPU operators. |
| <code>DP_JIT</code> | 0, 1 | 0 | Enable JIT. Note that this option may either improve or decrease the performance. Requires TensorFlow supports JIT. |

5.2.4 Adjust *sel* of a frozen model

One can use `--init-frz-model` features to adjust (increase or decrease) *sel* of a existing model. Firstly, one needs to adjust *sel* in `input.json`. For example, adjust from `[46, 92]` to `[23, 46]`.

```
"model": {
  "descriptor": {
    "sel": [23, 46]
  }
}
```

To obtain the new model at once, *numb_steps* should be set to zero:

```
"training": {
  "numb_steps": 0
}
```

Then, one can initialize the training from the frozen model and freeze the new model at once:

```
dp train input.json --init-frz-model frozen_model.pb
dp freeze -o frozen_model_adjusted_sel.pb
```

Two models should give the same result when the input satisfies both constraints.

Note: At this time, this feature is only supported by *se_e2_a* descriptor with *set_davg_true* enabled, or hybrid composed of the above descriptors.

5.3 Training Parameters

Note: One can load, modify, and export the input file by using our effective web-based tool [DP-GUI](#). All training parameters below can be set in DP-GUI. By clicking “SAVE JSON”, one can download the input file for further training.

model:

type: dict

argument path: model

type_map:

type: list, optional

argument path: model/type_map

A list of strings. Give the name to each type of atoms. It is noted that the number of atom type of training system must be less than 128 in a GPU environment. If not given, `type.raw` in each system should use the same type indexes, and `type_map.raw` will take no effect.

data_stat_nbatch:

type: int, optional, default: 10

argument path: model/data_stat_nbatch

The model determines the normalization from the statistics of the data. This key specifies the number of frames in each system used for statistics.

data_stat_protect:

type: float, optional, default: 0.01
 argument path: model/data_stat_protect

Protect parameter for atomic energy regression.

data_bias_nsample:

type: int, optional, default: 10
 argument path: model/data_bias_nsample

The number of training samples in a system to compute and change the energy bias.

use_srtab:

type: str, optional
 argument path: model/use_srtab

The table for the short-range pairwise interaction added on top of DP. The table is a text data file with $(N_t + 1) * N_t / 2 + 1$ columns. The first column is the distance between atoms. The second to the last columns are energies for pairs of certain types. For example we have two atom types, 0 and 1. The columns from 2nd to 4th are for 0-0, 0-1 and 1-1 correspondingly.

smin_alpha:

type: float, optional
 argument path: model/smin_alpha

The short-range tabulated interaction will be swithed according to the distance of the nearest neighbor. This distance is calculated by softmin. This parameter is the decaying parameter in the softmin. It is only required when use_srtab is provided.

sw_rmin:

type: float, optional
 argument path: model/sw_rmin

The lower boundary of the interpolation between short-range tabulated interaction and DP. It is only required when use_srtab is provided.

sw_rmax:

type: float, optional
 argument path: model/sw_rmax

The upper boundary of the interpolation between short-range tabulated interaction and DP. It is only required when use_srtab is provided.

srtab_add_bias:

type: bool, optional, default: True
 argument path: model/srtab_add_bias

Whether add energy bias from the statistics of the data to short-range tabulated atomic energy. It only takes effect when use_srtab is provided.

type_embedding:

type: dict, optional
 argument path: model/type_embedding

The type embedding.

neuron:

type: `list`, optional, default: `[8]`
argument path: `model/type_embedding/neuron`

Number of neurons in each hidden layers of the embedding net. When two layers are of the same size or one layer is twice as large as the previous layer, a skip connection is built.

activation_function:

type: `str`, optional, default: `tanh`
argument path: `model/type_embedding/activation_function`

The activation function in the embedding net. Supported activation functions are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”, “gelu_tf”, “None”, “none”. Note that “gelu” denotes the custom operator version, and “gelu_tf” denotes the TF standard version. If you set “None” or “none” here, no activation function will be used.

resnet_dt:

type: `bool`, optional, default: `False`
argument path: `model/type_embedding/resnet_dt`

Whether to use a “Timestep” in the skip connection

precision:

type: `str`, optional, default: `default`
argument path: `model/type_embedding/precision`

The precision of the embedding net parameters, supported options are “default”, “float16”, “float32”, “float64”, “bfloat16”. Default follows the interface precision.

trainable:

type: `bool`, optional, default: `True`
argument path: `model/type_embedding/trainable`

If the parameters in the embedding net are trainable

seed:

type: `NoneType` | `int`, optional, default: `None`
argument path: `model/type_embedding/seed`

Random seed for parameter initialization

modifier:

type: `dict`, optional
argument path: `model/modifier`

The modifier of model output.

Depending on the value of type, different sub args are accepted.

type:

type: `str` (flag key)
argument path: `model/modifier/type`
possible choices: *dipole_charge*

The type of modifier. See explanation below.

-dipole_charge: Use WFCC to model the electronic structure of the system. Correct the long-range interaction

When `type` is set to `dipole_charge`:

model_name:

type: str

argument path: model/modifier[dipole_charge]/model_name

The name of the frozen dipole model file.

model_charge_map:

type: list

argument path: model/modifier[dipole_charge]/model_charge_map

The charge of the WFCC. The list length should be the same as the `'sel_type <model/fitting_net[dipole]/sel_type_>'`.

sys_charge_map:

type: list

argument path: model/modifier[dipole_charge]/sys_charge_map

The charge of real atoms. The list length should be the same as the `type_map`

ewald_beta:

type: float, optional, default: 0.4

argument path: model/modifier[dipole_charge]/ewald_beta

The splitting parameter of Ewald sum. Unit is \AA^{-1}

ewald_h:

type: float, optional, default: 1.0

argument path: model/modifier[dipole_charge]/ewald_h

The grid spacing of the FFT grid. Unit is \AA

compress:

type: dict, optional

argument path: model/compress

Model compression configurations

spin:

type: dict, optional

argument path: model/spin

The settings for systems with spin.

use_spin:

type: list

argument path: model/spin/use_spin

Whether to use atomic spin model for each atom type

spin_norm:

type: list

argument path: model/spin/spin_norm

The magnitude of atomic spin for each atom type with spin

virtual_len:

type: list

argument path: model/spin/virtual_len

The distance between virtual atom representing spin and its corresponding real atom for each atom type with spin

Depending on the value of type, different sub args are accepted.

type:

type: str (flag key), default: standard

argument path: model/type

possible choices: *standard*, *multi*, *pairwise_dprc*

When *type* is set to *standard*:

Standard model, which contains a descriptor and a fitting.

descriptor:

type: dict

argument path: model[standard]/descriptor

The descriptor of atomic environment.

Depending on the value of type, different sub args are accepted.

type:

type: str (flag key)

argument path: model[standard]/descriptor/type

possible choices: *loc_frame*, *se_e2_a*, *se_e3*, *se_a_tpe*, *se_e2_r*, *hybrid*, *se_atten*, *se_atten_v2*, *se_a_mask*

The type of the descriptor. See explanation below.

- *loc_frame*: Defines a local frame at each atom, and the compute the descriptor as local coordinates under this frame.
- *se_e2_a*: Used by the smooth edition of Deep Potential. The full relative coordinates are used to construct the descriptor.
- *se_e2_r*: Used by the smooth edition of Deep Potential. Only the distance between atoms is used to construct the descriptor.
- *se_e3*: Used by the smooth edition of Deep Potential. The full relative coordinates are used to construct the descriptor. Three-body embedding will be used by this descriptor.
- *se_a_tpe*: Used by the smooth edition of Deep Potential. The full relative coordinates are used to construct the descriptor. Type embedding will be used by this descriptor.
- *se_atten*: Used by the smooth edition of Deep Potential. The full relative coordinates are used to construct the descriptor. Attention mechanism will be used by this descriptor.
- *se_atten_v2*: Used by the smooth edition of Deep Potential. The full relative coordinates are used to construct the descriptor. Attention mechanism with new modifications will be used by this descriptor.
- *se_a_mask*: Used by the smooth edition of Deep Potential. It can accept a variable number of atoms in a frame (Non-PBC system). aparam are required as an indicator matrix for the real/virtual sign of input atoms.
- *hybrid*: Concatenate of a list of descriptors as a new descriptor.

When *type* is set to *loc_frame*:

sel_a:
 type: list
 argument path: model[standard]/descriptor[loc_frame]/sel_a
 A list of integers. The length of the list should be the same as the number of atom types in the system. sel_a[i] gives the selected number of type-i neighbors. The full relative coordinates of the neighbors are used by the descriptor.

sel_r:
 type: list
 argument path: model[standard]/descriptor[loc_frame]/sel_r
 A list of integers. The length of the list should be the same as the number of atom types in the system. sel_r[i] gives the selected number of type-i neighbors. Only relative distance of the neighbors are used by the descriptor. sel_a[i] + sel_r[i] is recommended to be larger than the maximally possible number of type-i neighbors in the cut-off radius.

rcut:
 type: float, optional, default: 6.0
 argument path: model[standard]/descriptor[loc_frame]/rcut
 The cut-off radius. The default value is 6.0

axis_rule:
 type: list
 argument path:
 model[standard]/descriptor[loc_frame]/axis_rule
 A list of integers. The length should be 6 times of the number of types.

- axis_rule[i*6+0]: class of the atom defining the first axis of type-i atom. 0 for neighbors with full coordinates and 1 for neighbors only with relative distance.
- axis_rule[i*6+1]: type of the atom defining the first axis of type-i atom.
- axis_rule[i*6+2]: index of the axis atom defining the first axis. Note that the neighbors with the same class and type are sorted according to their relative distance.
- axis_rule[i*6+3]: class of the atom defining the second axis of type-i atom. 0 for neighbors with full coordinates and 1 for neighbors only with relative distance.
- axis_rule[i*6+4]: type of the atom defining the second axis of type-i atom.
- axis_rule[i*6+5]: index of the axis atom defining the second axis. Note that the neighbors with the same class and type are sorted according to their relative distance.

When `type` is set to `se_e2_a` (or its alias `se_a`):

sel:
 type: list | str, optional, default: auto
 argument path: model[standard]/descriptor[se_e2_a]/sel
 This parameter set the number of selected neighbors for each type of atom. It can be:

- List[int]. The length of the list should be the same as the number of atom types in the system. sel[i] gives the selected number of type-i

neighbors. `sel[i]` is recommended to be larger than the maximally possible number of type-*i* neighbors in the cut-off radius. It is noted that the total `sel` value must be less than 4096 in a GPU environment.

- `str`. Can be “auto:factor” or “auto”. “factor” is a float number larger than 1. This option will automatically determine the `sel`. In detail it counts the maximal number of neighbors with in the cutoff radius for each type of neighbor, then multiply the maximum by the “factor”. Finally the number is wrapped up to 4 divisible. The option “auto” is equivalent to “auto:1.1”.

rcut:

type: float, optional, default: 6.0

argument path: `model[standard]/descriptor[se_e2_a]/rcut`

The cut-off radius.

rcut_smth:

type: float, optional, default: 0.5

argument path: `model[standard]/descriptor[se_e2_a]/rcut_smth`

Where to start smoothing. For example the $1/r$ term is smoothed from `rcut` to `rcut_smth`

neuron:

type: list, optional, default: [10, 20, 40]

argument path: `model[standard]/descriptor[se_e2_a]/neuron`

Number of neurons in each hidden layers of the embedding net. When two layers are of the same size or one layer is twice as large as the previous layer, a skip connection is built.

axis_neuron:

type: int, optional, default: 4, alias: `n_axis_neuron`

argument path:

`model[standard]/descriptor[se_e2_a]/axis_neuron`

Size of the submatrix of *G* (embedding matrix).

activation_function:

type: str, optional, default: tanh

argument path:

`model[standard]/descriptor[se_e2_a]/activation_function`

The activation function in the embedding net. Supported activation functions are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”, “gelu_tf”, “None”, “none”. Note that “gelu” denotes the custom operator version, and “gelu_tf” denotes the TF standard version. If you set “None” or “none” here, no activation function will be used.

resnet_dt:

type: bool, optional, default: False

argument path: `model[standard]/descriptor[se_e2_a]/resnet_dt`

Whether to use a “Timestep” in the skip connection

type_one_side:

type: bool, optional, default: False

argument path:
`model[standard]/descriptor[se_e2_a]/type_one_side`

If true, the embedding network parameters vary by types of neighbor atoms only, so there will be N_{types} sets of embedding network parameters. Otherwise, the embedding network parameters vary by types of centric atoms and types of neighbor atoms, so there will be N_{types}^2 sets of embedding network parameters.

precision:

type: str, optional, default: default
 argument path: `model[standard]/descriptor[se_e2_a]/precision`

The precision of the embedding net parameters, supported options are “default”, “float16”, “float32”, “float64”, “bfloat16”. Default follows the interface precision.

trainable:

type: bool, optional, default: True
 argument path: `model[standard]/descriptor[se_e2_a]/trainable`

If the parameters in the embedding net is trainable

seed:

type: NoneType | int, optional
 argument path: `model[standard]/descriptor[se_e2_a]/seed`

Random seed for parameter initialization

exclude_types:

type: list, optional, default: []
 argument path:
`model[standard]/descriptor[se_e2_a]/exclude_types`

The excluded pairs of types which have no interaction with each other. For example, `[[0, 1]]` means no interaction between type 0 and type 1.

set_davg_zero:

type: bool, optional, default: False
 argument path:
`model[standard]/descriptor[se_e2_a]/set_davg_zero`

Set the normalization average to zero. This option should be set when `atom_ener` in the energy fitting is used

When `type` is set to `se_e3` (or its aliases `se_at`, `se_a_3be`, `se_t`):

sel:

type: list | str, optional, default: auto
 argument path: `model[standard]/descriptor[se_e3]/sel`

This parameter set the number of selected neighbors for each type of atom. It can be:

- List[int]. The length of the list should be the same as the number of atom types in the system. `sel[i]` gives the selected number of type-*i* neighbors. `sel[i]` is recommended to be larger than the maximally possible number of type-*i* neighbors in the cut-off radius. It is noted that the total `sel` value must be less than 4096 in a GPU environment.

- `str`. Can be “auto:factor” or “auto”. “factor” is a float number larger than 1. This option will automatically determine the sel. In detail it counts the maximal number of neighbors within the cutoff radius for each type of neighbor, then multiply the maximum by the “factor”. Finally the number is wrapped up to 4 divisible. The option “auto” is equivalent to “auto:1.1”.

rcut:

type: float, optional, default: 6.0

argument path: `model[standard]/descriptor[se_e3]/rcut`

The cut-off radius.

rcut_smth:

type: float, optional, default: 0.5

argument path: `model[standard]/descriptor[se_e3]/rcut_smth`

Where to start smoothing. For example the $1/r$ term is smoothed from `rcut` to `rcut_smth`

neuron:

type: list, optional, default: [10, 20, 40]

argument path: `model[standard]/descriptor[se_e3]/neuron`

Number of neurons in each hidden layers of the embedding net. When two layers are of the same size or one layer is twice as large as the previous layer, a skip connection is built.

activation_function:

type: str, optional, default: tanh

argument path:

`model[standard]/descriptor[se_e3]/activation_function`

The activation function in the embedding net. Supported activation functions are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”, “gelu_tf”, “None”, “none”. Note that “gelu” denotes the custom operator version, and “gelu_tf” denotes the TF standard version. If you set “None” or “none” here, no activation function will be used.

resnet_dt:

type: bool, optional, default: False

argument path: `model[standard]/descriptor[se_e3]/resnet_dt`

Whether to use a “Timestep” in the skip connection

precision:

type: str, optional, default: default

argument path: `model[standard]/descriptor[se_e3]/precision`

The precision of the embedding net parameters, supported options are “default”, “float16”, “float32”, “float64”, “bfloat16”. Default follows the interface precision.

trainable:

type: bool, optional, default: True

argument path: `model[standard]/descriptor[se_e3]/trainable`

If the parameters in the embedding net are trainable

seed:

type: `NoneType` | `int`, optional
 argument path: `model[standard]/descriptor[se_e3]/seed`
 Random seed for parameter initialization

set_davg_zero:

type: `bool`, optional, default: `False`
 argument path:
`model[standard]/descriptor[se_e3]/set_davg_zero`
 Set the normalization average to zero. This option should be set when `atom_ener` in the energy fitting is used

When `type` is set to `se_a_tpe` (or its alias `se_a_ebd`):

sel:

type: `list` | `str`, optional, default: `auto`
 argument path: `model[standard]/descriptor[se_a_tpe]/sel`
 This parameter set the number of selected neighbors for each type of atom. It can be:

- `List[int]`. The length of the list should be the same as the number of atom types in the system. `sel[i]` gives the selected number of type-*i* neighbors. `sel[i]` is recommended to be larger than the maximally possible number of type-*i* neighbors in the cut-off radius. It is noted that the total `sel` value must be less than 4096 in a GPU environment.
- `str`. Can be “auto:factor” or “auto”. “factor” is a float number larger than 1. This option will automatically determine the `sel`. In detail it counts the maximal number of neighbors with in the cutoff radius for each type of neighbor, then multiply the maximum by the “factor”. Finally the number is wrapped up to 4 divisible. The option “auto” is equivalent to “auto:1.1”.

rcut:

type: `float`, optional, default: 6.0
 argument path: `model[standard]/descriptor[se_a_tpe]/rcut`
 The cut-off radius.

rcut_smth:

type: `float`, optional, default: 0.5
 argument path: `model[standard]/descriptor[se_a_tpe]/rcut_smth`
 Where to start smoothing. For example the $1/r$ term is smoothed from `rcut` to `rcut_smth`

neuron:

type: `list`, optional, default: [10, 20, 40]
 argument path: `model[standard]/descriptor[se_a_tpe]/neuron`
 Number of neurons in each hidden layers of the embedding net. When two layers are of the same size or one layer is twice as large as the previous layer, a skip connection is built.

axis_neuron:

type: `int`, optional, default: 4, alias: `n_axis_neuron`

argument path:
`model[standard]/descriptor[se_a_tpe]/axis_neuron`
Size of the submatrix of G (embedding matrix).

activation_function:

type: `str`, optional, default: `tanh`
argument path:
`model[standard]/descriptor[se_a_tpe]/activation_function`

The activation function in the embedding net. Supported activation functions are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”, “gelu_tf”, “None”, “none”. Note that “gelu” denotes the custom operator version, and “gelu_tf” denotes the TF standard version. If you set “None” or “none” here, no activation function will be used.

resnet_dt:

type: `bool`, optional, default: `False`
argument path: `model[standard]/descriptor[se_a_tpe]/resnet_dt`
Whether to use a “Timestep” in the skip connection

type_one_side:

type: `bool`, optional, default: `False`
argument path:
`model[standard]/descriptor[se_a_tpe]/type_one_side`

If true, the embedding network parameters vary by types of neighbor atoms only, so there will be $N_{\text{text}}\{\text{types}\}$ sets of embedding network parameters. Otherwise, the embedding network parameters vary by types of centric atoms and types of neighbor atoms, so there will be $N_{\text{text}}\{\text{types}\}^2$ sets of embedding network parameters.

precision:

type: `str`, optional, default: `default`
argument path: `model[standard]/descriptor[se_a_tpe]/precision`

The precision of the embedding net parameters, supported options are “default”, “float16”, “float32”, “float64”, “bfloat16”. Default follows the interface precision.

trainable:

type: `bool`, optional, default: `True`
argument path: `model[standard]/descriptor[se_a_tpe]/trainable`
If the parameters in the embedding net is trainable

seed:

type: `NoneType` | `int`, optional
argument path: `model[standard]/descriptor[se_a_tpe]/seed`
Random seed for parameter initialization

exclude_types:

type: `list`, optional, default: `[]`
argument path:
`model[standard]/descriptor[se_a_tpe]/exclude_types`

The excluded pairs of types which have no interaction with each other. For example, `[[0, 1]]` means no interaction between type 0 and type 1.

set_davg_zero:

type: bool, optional, default: False

argument path:

`model[standard]/descriptor[se_a_tpe]/set_davg_zero`

Set the normalization average to zero. This option should be set when `atom_ener` in the energy fitting is used

type_nchanl:

type: int, optional, default: 4

argument path:

`model[standard]/descriptor[se_a_tpe]/type_nchanl`

number of channels for type embedding

type_nlayer:

type: int, optional, default: 2

argument path:

`model[standard]/descriptor[se_a_tpe]/type_nlayer`

number of hidden layers of type embedding net

numb_aparam:

type: int, optional, default: 0

argument path:

`model[standard]/descriptor[se_a_tpe]/numb_aparam`

dimension of atomic parameter. if set to a value > 0 , the atomic parameters are embedded.

When `type` is set to `se_e2_r` (or its alias `se_r`):

sel:

type: list | str, optional, default: auto

argument path: `model[standard]/descriptor[se_e2_r]/sel`

This parameter set the number of selected neighbors for each type of atom. It can be:

- List[int]. The length of the list should be the same as the number of atom types in the system. `sel[i]` gives the selected number of type-*i* neighbors. `sel[i]` is recommended to be larger than the maximally possible number of type-*i* neighbors in the cut-off radius. It is noted that the total sel value must be less than 4096 in a GPU environment.
- str. Can be “auto:factor” or “auto”. “factor” is a float number larger than 1. This option will automatically determine the sel. In detail it counts the maximal number of neighbors with in the cutoff radius for each type of neighbor, then multiply the maximum by the “factor”. Finally the number is wrapped up to 4 divisible. The option “auto” is equivalent to “auto:1.1”.

rcut:

type: float, optional, default: 6.0

argument path: `model[standard]/descriptor[se_e2_r]/rcut`

The cut-off radius.

rcut_smth:

type: float, optional, default: 0.5

argument path: model[standard]/descriptor[se_e2_r]/rcut_smth

Where to start smoothing. For example the $1/r$ term is smoothed from rcut to rcut_smth

neuron:

type: list, optional, default: [10, 20, 40]

argument path: model[standard]/descriptor[se_e2_r]/neuron

Number of neurons in each hidden layers of the embedding net. When two layers are of the same size or one layer is twice as large as the previous layer, a skip connection is built.

activation_function:

type: str, optional, default: tanh

argument path:

model[standard]/descriptor[se_e2_r]/activation_function

The activation function in the embedding net. Supported activation functions are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”, “gelu_tf”, “None”, “none”. Note that “gelu” denotes the custom operator version, and “gelu_tf” denotes the TF standard version. If you set “None” or “none” here, no activation function will be used.

resnet_dt:

type: bool, optional, default: False

argument path: model[standard]/descriptor[se_e2_r]/resnet_dt

Whether to use a “Timestep” in the skip connection

type_one_side:

type: bool, optional, default: False

argument path:

model[standard]/descriptor[se_e2_r]/type_one_side

If true, the embedding network parameters vary by types of neighbor atoms only, so there will be $N_{\text{text}}\{\text{types}\}$ sets of embedding network parameters. Otherwise, the embedding network parameters vary by types of centric atoms and types of neighbor atoms, so there will be $N_{\text{text}}\{\text{types}\}^2$ sets of embedding network parameters.

precision:

type: str, optional, default: default

argument path: model[standard]/descriptor[se_e2_r]/precision

The precision of the embedding net parameters, supported options are “default”, “float16”, “float32”, “float64”, “bfloat16”. Default follows the interface precision.

trainable:

type: bool, optional, default: True

argument path: model[standard]/descriptor[se_e2_r]/trainable

If the parameters in the embedding net are trainable

seed:

type: `NoneType` | `int`, optional
 argument path: `model[standard]/descriptor[se_e2_r]/seed`
 Random seed for parameter initialization

exclude_types:

type: `list`, optional, default: `[]`
 argument path:
`model[standard]/descriptor[se_e2_r]/exclude_types`
 The excluded pairs of types which have no interaction with each other.
 For example, `[[0, 1]]` means no interaction between type 0 and type 1.

set_davg_zero:

type: `bool`, optional, default: `False`
 argument path:
`model[standard]/descriptor[se_e2_r]/set_davg_zero`
 Set the normalization average to zero. This option should be set when
`atom_ener` in the energy fitting is used

When `type` is set to `hybrid`:

list:

type: `list`
 argument path: `model[standard]/descriptor[hybrid]/list`
 A list of descriptor definitions

When `type` is set to `se_atten`:

sel:

type: `list` | `str` | `int`, optional, default: `auto`
 argument path: `model[standard]/descriptor[se_atten]/sel`

This parameter set the number of selected neighbors. Note that this parameter is a little different from that in other descriptors. Instead of separating each type of atoms, only the summation matters. And this number is highly related with the efficiency, thus one should not make it too large. Usually 200 or less is enough, far away from the GPU limitation 4096. It can be:

- `int`. The maximum number of neighbor atoms to be considered. We recommend it to be less than 200.
- `List[int]`. The length of the list should be the same as the number of atom types in the system. `sel[i]` gives the selected number of type-`i` neighbors. Only the summation of `sel[i]` matters, and it is recommended to be less than 200. - `str`. Can be “auto:factor” or “auto”. “factor” is a float number larger than 1. This option will automatically determine the `sel`. In detail it counts the maximal number of neighbors with in the cutoff radius for each type of neighbor, then multiply the maximum by the “factor”. Finally the number is wrapped up to 4 divisible. The option “auto” is equivalent to “auto:1.1”.

rcut:

type: `float`, optional, default: 6.0
 argument path: `model[standard]/descriptor[se_atten]/rcut`

The cut-off radius.

rcut_smth:

type: float, optional, default: 0.5

argument path: model[standard]/descriptor[se_atten]/rcut_smth

Where to start smoothing. For example the $1/r$ term is smoothed from rcut to rcut_smth

neuron:

type: list, optional, default: [10, 20, 40]

argument path: model[standard]/descriptor[se_atten]/neuron

Number of neurons in each hidden layers of the embedding net. When two layers are of the same size or one layer is twice as large as the previous layer, a skip connection is built.

axis_neuron:

type: int, optional, default: 4, alias: n_axis_neuron

argument path:

model[standard]/descriptor[se_atten]/axis_neuron

Size of the submatrix of G (embedding matrix).

activation_function:

type: str, optional, default: tanh

argument path:

model[standard]/descriptor[se_atten]/activation_function

The activation function in the embedding net. Supported activation functions are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”, “gelu_tf”, “None”, “none”. Note that “gelu” denotes the custom operator version, and “gelu_tf” denotes the TF standard version. If you set “None” or “none” here, no activation function will be used.

resnet_dt:

type: bool, optional, default: False

argument path: model[standard]/descriptor[se_atten]/resnet_dt

Whether to use a “Timestep” in the skip connection

type_one_side:

type: bool, optional, default: False

argument path:

model[standard]/descriptor[se_atten]/type_one_side

If true, the embedding network parameters vary by types of neighbor atoms only, so there will be N_{types} sets of embedding network parameters. Otherwise, the embedding network parameters vary by types of centric atoms and types of neighbor atoms, so there will be N_{types}^2 sets of embedding network parameters.

precision:

type: str, optional, default: default

argument path: model[standard]/descriptor[se_atten]/precision

The precision of the embedding net parameters, supported options are “default”, “float16”, “float32”, “float64”, “bfloat16”. Default follows the interface precision.

trainable:
 type: bool, optional, default: True
 argument path: model[standard]/descriptor[se_atten]/trainable
 If the parameters in the embedding net is trainable

seed:
 type: NoneType | int, optional
 argument path: model[standard]/descriptor[se_atten]/seed
 Random seed for parameter initialization

exclude_types:
 type: list, optional, default: []
 argument path:
 model[standard]/descriptor[se_atten]/exclude_types
 The excluded pairs of types which have no interaction with each other.
 For example, [[0, 1]] means no interaction between type 0 and type 1.

attn:
 type: int, optional, default: 128
 argument path: model[standard]/descriptor[se_atten]/attn
 The length of hidden vectors in attention layers

attn_layer:
 type: int, optional, default: 2
 argument path:
 model[standard]/descriptor[se_atten]/attn_layer
 The number of attention layers. Note that model compression of se_atten is only enabled when attn_layer==0 and stripped_type_embedding is True

attn_dotr:
 type: bool, optional, default: True
 argument path: model[standard]/descriptor[se_atten]/attn_dotr
 Whether to do dot product with the normalized relative coordinates

attn_mask:
 type: bool, optional, default: False
 argument path: model[standard]/descriptor[se_atten]/attn_mask
 Whether to do mask on the diagonal in the attention matrix

stripped_type_embedding:
 type: bool, optional, default: False
 argument path:
 model[standard]/descriptor[se_atten]/stripped_type_embedding
 Whether to strip the type embedding into a separated embedding network. Setting it to False will fall back to the previous version of se_atten which is non-compressible.

smooth_type_embdding:
 type: bool, optional, default: False

argument path:
`model[standard]/descriptor[se_atten]/smooth_type_embdding`

When using stripped type embedding, whether to dot smooth factor on the network output of type embedding to keep the network smooth, instead of setting `set_davg_zero` to be `True`.

set_davg_zero:

type: `bool`, optional, default: `True`

argument path:

`model[standard]/descriptor[se_atten]/set_davg_zero`

Set the normalization average to zero. This option should be set when `se_atten` descriptor or `atom_ener` in the energy fitting is used

When `type` is set to `se_atten_v2`:

sel:

type: `list` | `str` | `int`, optional, default: `auto`

argument path: `model[standard]/descriptor[se_atten_v2]/sel`

This parameter set the number of selected neighbors. Note that this parameter is a little different from that in other descriptors. Instead of separating each type of atoms, only the summation matters. And this number is highly related with the efficiency, thus one should not make it too large. Usually 200 or less is enough, far away from the GPU limitation 4096. It can be:

- `int`. The maximum number of neighbor atoms to be considered. We recommend it to be less than 200.
- `List[int]`. The length of the list should be the same as the number of atom types in the system. `sel[i]` gives the selected number of type-*i* neighbors. Only the summation of `sel[i]` matters, and it is recommended to be less than 200. - `str`. Can be “auto:factor” or “auto”. “factor” is a float number larger than 1. This option will automatically determine the `sel`. In detail it counts the maximal number of neighbors with in the cutoff radius for each type of neighbor, then multiply the maximum by the “factor”. Finally the number is wrapped up to 4 divisible. The option “auto” is equivalent to “auto:1.1”.

rcut:

type: `float`, optional, default: 6.0

argument path: `model[standard]/descriptor[se_atten_v2]/rcut`

The cut-off radius.

rcut_smth:

type: `float`, optional, default: 0.5

argument path:

`model[standard]/descriptor[se_atten_v2]/rcut_smth`

Where to start smoothing. For example the $1/r$ term is smoothed from `rcut` to `rcut_smth`

neuron:

type: `list`, optional, default: [10, 20, 40]

argument path: `model[standard]/descriptor[se_atten_v2]/neuron`

Number of neurons in each hidden layers of the embedding net. When two layers are of the same size or one layer is twice as large as the previous layer, a skip connection is built.

axis_neuron:

type: int, optional, default: 4, alias: n_axis_neuron

argument path:

model[standard]/descriptor[se_attn_v2]/axis_neuron

Size of the submatrix of G (embedding matrix).

activation_function:

type: str, optional, default: tanh

argument path:

model[standard]/descriptor[se_attn_v2]/activation_function

The activation function in the embedding net. Supported activation functions are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”, “gelu_tf”, “None”, “none”. Note that “gelu” denotes the custom operator version, and “gelu_tf” denotes the TF standard version. If you set “None” or “none” here, no activation function will be used.

resnet_dt:

type: bool, optional, default: False

argument path:

model[standard]/descriptor[se_attn_v2]/resnet_dt

Whether to use a “Timestep” in the skip connection

type_one_side:

type: bool, optional, default: False

argument path:

model[standard]/descriptor[se_attn_v2]/type_one_side

If true, the embedding network parameters vary by types of neighbor atoms only, so there will be $N_{\text{text}}\{\text{types}\}$ sets of embedding network parameters. Otherwise, the embedding network parameters vary by types of centric atoms and types of neighbor atoms, so there will be $N_{\text{text}}\{\text{types}\}^2$ sets of embedding network parameters.

precision:

type: str, optional, default: default

argument path:

model[standard]/descriptor[se_attn_v2]/precision

The precision of the embedding net parameters, supported options are “default”, “float16”, “float32”, “float64”, “bfloat16”. Default follows the interface precision.

trainable:

type: bool, optional, default: True

argument path:

model[standard]/descriptor[se_attn_v2]/trainable

If the parameters in the embedding net is trainable

seed:

type: NoneType | int, optional

argument path: `model[standard]/descriptor[se_atten_v2]/seed`

Random seed for parameter initialization

exclude_types:

type: list, optional, default: []

argument path:

`model[standard]/descriptor[se_atten_v2]/exclude_types`

The excluded pairs of types which have no interaction with each other.

For example, `[[0, 1]]` means no interaction between type 0 and type 1.

attn:

type: int, optional, default: 128

argument path: `model[standard]/descriptor[se_atten_v2]/attn`

The length of hidden vectors in attention layers

attn_layer:

type: int, optional, default: 2

argument path:

`model[standard]/descriptor[se_atten_v2]/attn_layer`

The number of attention layers. Note that model compression of `se_atten` is only enabled when `attn_layer==0` and `stripped_type_embedding` is True

attn_dotr:

type: bool, optional, default: True

argument path:

`model[standard]/descriptor[se_atten_v2]/attn_dotr`

Whether to do dot product with the normalized relative coordinates

attn_mask:

type: bool, optional, default: False

argument path:

`model[standard]/descriptor[se_atten_v2]/attn_mask`

Whether to do mask on the diagonal in the attention matrix

set_davg_zero:

type: bool, optional, default: False

argument path:

`model[standard]/descriptor[se_atten_v2]/set_davg_zero`

Set the normalization average to zero. This option should be set when `se_atten` descriptor or `atom_ener` in the energy fitting is used

When `type` is set to `se_a_mask`:

sel:

type: list | str, optional, default: auto

argument path: `model[standard]/descriptor[se_a_mask]/sel`

This parameter sets the number of selected neighbors for each type of atom. It can be:

- List[int]. The length of the list should be the same as the number of atom types in the system. `sel[i]` gives the selected number of type-*i* neighbors. `sel[i]` is recommended to be larger than the maximally possible number of type-*i* neighbors in the cut-off radius. It is noted that the total `sel` value must be less than 4096 in a GPU environment.
- str. Can be “auto:factor” or “auto”. “factor” is a float number larger than 1. This option will automatically determine the `sel`. In detail it counts the maximal number of neighbors with in the cutoff radius for each type of neighbor, then multiply the maximum by the “factor”. Finally the number is wrapped up to 4 divisible. The option “auto” is equivalent to “auto:1.1”.

neuron:

type: list, optional, default: [10, 20, 40]
 argument path: `model[standard]/descriptor[se_a_mask]/neuron`

Number of neurons in each hidden layers of the embedding net. When two layers are of the same size or one layer is twice as large as the previous layer, a skip connection is built.

axis_neuron:

type: int, optional, default: 4, alias: `n_axis_neuron`
 argument path:
`model[standard]/descriptor[se_a_mask]/axis_neuron`

Size of the submatrix of *G* (embedding matrix).

activation_function:

type: str, optional, default: `tanh`
 argument path:
`model[standard]/descriptor[se_a_mask]/activation_function`

The activation function in the embedding net. Supported activation functions are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”, “gelu_tf”, “None”, “none”. Note that “gelu” denotes the custom operator version, and “gelu_tf” denotes the TF standard version. If you set “None” or “none” here, no activation function will be used.

resnet_dt:

type: bool, optional, default: `False`
 argument path:
`model[standard]/descriptor[se_a_mask]/resnet_dt`

Whether to use a “Timestep” in the skip connection

type_one_side:

type: bool, optional, default: `False`
 argument path:
`model[standard]/descriptor[se_a_mask]/type_one_side`

If true, the embedding network parameters vary by types of neighbor atoms only, so there will be $N_{\text{text}\{\text{types}\}}$ sets of embedding network parameters. Otherwise, the embedding network parameters vary by types of centric atoms and types of neighbor atoms, so there will be $N_{\text{text}\{\text{types}\}}^2$ sets of embedding network parameters.

exclude_types:

type: list, optional, default: []

argument path:

model[standard]/descriptor[se_a_mask]/exclude_types

The excluded pairs of types which have no interaction with each other.
For example, [[0, 1]] means no interaction between type 0 and type 1.

precision:

type: str, optional, default: default

argument path:

model[standard]/descriptor[se_a_mask]/precision

The precision of the embedding net parameters, supported options are “default”, “float16”, “float32”, “float64”, “bfloat16”. Default follows the interface precision.

trainable:

type: bool, optional, default: True

argument path:

model[standard]/descriptor[se_a_mask]/trainable

If the parameters in the embedding net is trainable

seed:

type: NoneType | int, optional

argument path: model[standard]/descriptor[se_a_mask]/seed

Random seed for parameter initialization

fitting_net:

type: dict

argument path: model[standard]/fitting_net

The fitting of physical properties.

Depending on the value of type, different sub args are accepted.

type:

type: str (flag key), default: ener

argument path: model[standard]/fitting_net/type

possible choices: *ener*, *dos*, *polar*, *dipole*

The type of the fitting. See explanation below.

- *ener*: Fit an energy model (potential energy surface).
- *dos*: Fit a density of states model. The total density of states / site-projected density of states labels should be provided by dos.npy or atom_dos.npy in each data system. The file has number of frames lines and number of energy grid columns (times number of atoms in atom_dos.npy). See loss parameter.
- *dipole*: Fit an atomic dipole model. Global dipole labels or atomic dipole labels for all the selected atoms (see sel_type) should be provided by dipole.npy in each data system. The file either has number of frames lines and 3 times of number of selected atoms columns, or has number of frames lines and 3 columns. See loss parameter.
- *polar*: Fit an atomic polarizability model. Global polarizability labels or atomic polarizability labels for all the selected atoms (see sel_type)

should be provided by `polarizability.npy` in each data system. The file either has number of frames lines and 9 times of number of selected atoms columns, or has number of frames lines and 9 columns. See `loss` parameter.

When `type` is set to `ener`:

numb_fparam:

type: `int`, optional, default: 0

argument path: `model[standard]/fitting_net[ener]/numb_fparam`

The dimension of the frame parameter. If set to `>0`, file `fparam.npy` should be included to provide the input fparams.

numb_aparam:

type: `int`, optional, default: 0

argument path: `model[standard]/fitting_net[ener]/numb_aparam`

The dimension of the atomic parameter. If set to `>0`, file `aparam.npy` should be included to provide the input aparams.

neuron:

type: `list`, optional, default: `[120, 120, 120]`, alias: `n_neuron`

argument path: `model[standard]/fitting_net[ener]/neuron`

The number of neurons in each hidden layers of the fitting net. When two hidden layers are of the same size, a skip connection is built.

activation_function:

type: `str`, optional, default: `tanh`

argument path:

`model[standard]/fitting_net[ener]/activation_function`

The activation function in the fitting net. Supported activation functions are “`relu`”, “`relu6`”, “`softplus`”, “`sigmoid`”, “`tanh`”, “`gelu`”, “`gelu_tf`”, “`None`”, “`none`”. Note that “`gelu`” denotes the custom operator version, and “`gelu_tf`” denotes the TF standard version. If you set “`None`” or “`none`” here, no activation function will be used.

precision:

type: `str`, optional, default: `default`

argument path: `model[standard]/fitting_net[ener]/precision`

The precision of the fitting net parameters, supported options are “`default`”, “`float16`”, “`float32`”, “`float64`”, “`bfloat16`”. Default follows the interface precision.

resnet_dt:

type: `bool`, optional, default: `True`

argument path: `model[standard]/fitting_net[ener]/resnet_dt`

Whether to use a “Timestep” in the skip connection

trainable:

type: `list` | `bool`, optional, default: `True`

argument path: `model[standard]/fitting_net[ener]/trainable`

Whether the parameters in the fitting net are trainable. This option can be

- `bool`: True if all parameters of the fitting net are trainable, False otherwise.
- `list of bool`: Specifies if each layer is trainable. Since the fitting net is composed by hidden layers followed by a output layer, the length of this list should be equal to `len(neuron)+1`.

rcond:

type: `float | NoneType`, optional, default: `None`

argument path: `model[standard]/fitting_net[ener]/rcond`

The condition number used to determine the initial energy shift for each type of atoms. See `rcond` in `numpy.linalg.lstsq()` for more details.

seed:

type: `NoneType | int`, optional

argument path: `model[standard]/fitting_net[ener]/seed`

Random seed for parameter initialization of the fitting net

atom_ener:

type: `list`, optional, default: `[]`

argument path: `model[standard]/fitting_net[ener]/atom_ener`

Specify the atomic energy in vacuum for each type

layer_name:

type: `list`, optional

argument path: `model[standard]/fitting_net[ener]/layer_name`

The name of the each layer. The length of this list should be equal to `n_neuron + 1`. If two layers, either in the same fitting or different fittings, have the same name, they will share the same neural network parameters. The shape of these layers should be the same. If null is given for a layer, parameters will not be shared.

use_aparam_as_mask:

type: `bool`, optional, default: `False`

argument path:

`model[standard]/fitting_net[ener]/use_aparam_as_mask`

Whether to use the `aparam` as a mask in input. If `True`, the `aparam` will not be used in fitting net for embedding. When `descrpt` is `se_a_mask`, the `aparam` will be used as a mask to indicate the input atom is real/virtual. And `use_aparam_as_mask` should be set to `True`.

When `type` is set to `dos`:

numb_fparam:

type: `int`, optional, default: `0`

argument path: `model[standard]/fitting_net[dos]/numb_fparam`

The dimension of the frame parameter. If set to `>0`, file `fparam.npy` should be included to provided the input `fparams`.

numb_aparam:

type: `int`, optional, default: `0`

argument path: `model[standard]/fitting_net[dos]/numb_aparam`

The dimension of the atomic parameter. If set to >0 , file `aparam.npy` should be included to provide the input `aparams`.

neuron:

type: `list`, optional, default: `[120, 120, 120]`

argument path: `model[standard]/fitting_net[dos]/neuron`

The number of neurons in each hidden layer of the fitting net. When two hidden layers are of the same size, a skip connection is built.

activation_function:

type: `str`, optional, default: `tanh`

argument path:

`model[standard]/fitting_net[dos]/activation_function`

The activation function in the fitting net. Supported activation functions are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”, “gelu_tf”, “None”, “none”. Note that “gelu” denotes the custom operator version, and “gelu_tf” denotes the TF standard version. If you set “None” or “none” here, no activation function will be used.

precision:

type: `str`, optional, default: `float64`

argument path: `model[standard]/fitting_net[dos]/precision`

The precision of the fitting net parameters, supported options are “default”, “float16”, “float32”, “float64”, “bfloat16”. Default follows the interface precision.

resnet_dt:

type: `bool`, optional, default: `True`

argument path: `model[standard]/fitting_net[dos]/resnet_dt`

Whether to use a “Timestep” in the skip connection

trainable:

type: `list | bool`, optional, default: `True`

argument path: `model[standard]/fitting_net[dos]/trainable`

Whether the parameters in the fitting net are trainable. This option can be

- `bool`: `True` if all parameters of the fitting net are trainable, `False` otherwise.
- `list of bool`: Specifies if each layer is trainable. Since the fitting net is composed by hidden layers followed by an output layer, the length of this list should be equal to `len(neuron)+1`.

rcond:

type: `float | NoneType`, optional, default: `None`

argument path: `model[standard]/fitting_net[dos]/rcond`

The condition number used to determine the initial energy shift for each type of atoms. See `rcond` in `numpy.linalg.lstsq()` for more details.

seed:

type: `NoneType | int`, optional

argument path: `model[standard]/fitting_net[dos]/seed`

Random seed for parameter initialization of the fitting net

numb_dos:

type: int, optional, default: 300

argument path: `model[standard]/fitting_net[dos]/numb_dos`

The number of gridpoints on which the DOS is evaluated (NEDOS in VASP)

When `type` is set to `polar`:

neuron:

type: list, optional, default: [120, 120, 120], alias: `n_neuron`

argument path: `model[standard]/fitting_net[polar]/neuron`

The number of neurons in each hidden layers of the fitting net. When two hidden layers are of the same size, a skip connection is built.

activation_function:

type: str, optional, default: `tanh`

argument path:

`model[standard]/fitting_net[polar]/activation_function`

The activation function in the fitting net. Supported activation functions are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”, “gelu_tf”, “None”, “none”. Note that “gelu” denotes the custom operator version, and “gelu_tf” denotes the TF standard version. If you set “None” or “none” here, no activation function will be used.

resnet_dt:

type: bool, optional, default: True

argument path: `model[standard]/fitting_net[polar]/resnet_dt`

Whether to use a “Timestep” in the skip connection

precision:

type: str, optional, default: `default`

argument path: `model[standard]/fitting_net[polar]/precision`

The precision of the fitting net parameters, supported options are “default”, “float16”, “float32”, “float64”, “bfloat16”. Default follows the interface precision.

fit_diag:

type: bool, optional, default: True

argument path: `model[standard]/fitting_net[polar]/fit_diag`

Fit the diagonal part of the rotational invariant polarizability matrix, which will be converted to normal polarizability matrix by contracting with the rotation matrix.

scale:

type: float | list, optional, default: 1.0

argument path: `model[standard]/fitting_net[polar]/scale`

The output of the fitting net (polarizability matrix) will be scaled by `scale`

shift_diag:

type: bool, optional, default: True

argument path: `model[standard]/fitting_net[polar]/shift_diag`

Whether to shift the diagonal of polar, which is beneficial to training. Default is true.

sel_type:

type: `list | NoneType | int`, optional, alias: `pol_type`

argument path: `model[standard]/fitting_net[polar]/sel_type`

The atom types for which the atomic polarizability will be provided. If not set, all types will be selected.

seed:

type: `NoneType | int`, optional

argument path: `model[standard]/fitting_net[polar]/seed`

Random seed for parameter initialization of the fitting net

When `type` is set to `dipole`:

neuron:

type: `list`, optional, default: `[120, 120, 120]`, alias: `n_neuron`

argument path: `model[standard]/fitting_net[dipole]/neuron`

The number of neurons in each hidden layers of the fitting net. When two hidden layers are of the same size, a skip connection is built.

activation_function:

type: `str`, optional, default: `tanh`

argument path:

`model[standard]/fitting_net[dipole]/activation_function`

The activation function in the fitting net. Supported activation functions are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”, “gelu_tf”, “None”, “none”. Note that “gelu” denotes the custom operator version, and “gelu_tf” denotes the TF standard version. If you set “None” or “none” here, no activation function will be used.

resnet_dt:

type: `bool`, optional, default: `True`

argument path: `model[standard]/fitting_net[dipole]/resnet_dt`

Whether to use a “Timestep” in the skip connection

precision:

type: `str`, optional, default: `default`

argument path: `model[standard]/fitting_net[dipole]/precision`

The precision of the fitting net parameters, supported options are “default”, “float16”, “float32”, “float64”, “bfloat16”. Default follows the interface precision.

sel_type:

type: `list | NoneType | int`, optional, alias: `dipole_type`

argument path: `model[standard]/fitting_net[dipole]/sel_type`

The atom types for which the atomic dipole will be provided. If not set, all types will be selected.

seed:

type: `NoneType` | `int`, optional
argument path: `model[standard]/fitting_net[dipole]/seed`
Random seed for parameter initialization of the fitting net

When `type` is set to `multi`:

Multiple-task model.

descriptor:

type: `dict`
argument path: `model[multi]/descriptor`
The descriptor of atomic environment. See `model[standard]/descriptor` for details.

fitting_net_dict:

type: `dict`
argument path: `model[multi]/fitting_net_dict`
The dictionary of multiple fitting nets in multi-task mode. Each `fitting_net_dict[fitting_key]` is the single definition of fitting of physical properties with user-defined name `fitting_key`.

When `type` is set to `pairwise_dprc`:

qm_model:

type: `dict`
argument path: `model[pairwise_dprc]/qm_model`

qmmm_model:

type: `dict`
argument path: `model[pairwise_dprc]/qmmm_model`

learning_rate:

type: `dict`, optional
argument path: `learning_rate`

The definitio of learning rate

scale_by_worker:

type: `str`, optional, default: `linear`
argument path: `learning_rate/scale_by_worker`
When parallel training or batch size scaled, how to alter learning rate. Valid values are `linear` (default), `'sqrt'` or `none`.

Depending on the value of `type`, different sub args are accepted.

type:

type: `str` (flag key), default: `exp`
argument path: `learning_rate/type`
possible choices: `exp`
The type of the learning rate.

When `type` is set to `exp`:

start_lr:

type: float, optional, default: 0.001

argument path: `learning_rate[exp]/start_lr`

The learning rate at the start of the training.

stop_lr:

type: float, optional, default: 1e-08

argument path: `learning_rate[exp]/stop_lr`

The desired learning rate at the end of the training.

decay_steps:

type: int, optional, default: 5000

argument path: `learning_rate[exp]/decay_steps`

The learning rate is decaying every this number of training steps.

learning_rate_dict:

type: dict, optional

argument path: `learning_rate_dict`

The dictionary of definitions of learning rates in multi-task mode. Each `learning_rate_dict[fitting_key]`, with user-defined name `fitting_key` in `model/fitting_net_dict`, is the single definition of learning rate.

loss:

type: dict, optional

argument path: `loss`

The definition of loss function. The loss type should be set to tensor, ener or left unset.

Depending on the value of type, different sub args are accepted.

type:

type: str (flag key), default: `ener`

argument path: `loss/type`

possible choices: `ener`, `ener_spin`, `dos`, `tensor`

The type of the loss. When the fitting type is `ener`, the loss type should be set to `ener` or left unset. When the fitting type is dipole or polar, the loss type should be set to `tensor`.

When `type` is set to `ener`:

start_pref_e:

type: float | int, optional, default: 0.02

argument path: `loss[ener]/start_pref_e`

The prefactor of energy loss at the start of the training. Should be larger than or equal to 0. If set to none-zero value, the energy label should be provided by file `energy.npy` in each data system. If both `start_pref_e` and `limit_pref_e` are set to 0, then the energy will be ignored.

limit_pref_e:

type: float | int, optional, default: 1.0

argument path: `loss[ener]/limit_pref_e`

The prefactor of energy loss at the limit of the training, Should be larger than or equal to 0. i.e. the training step goes to infinity.

start_pref_f:

type: `float | int`, optional, default: 1000

argument path: `loss[ener]/start_pref_f`

The prefactor of force loss at the start of the training. Should be larger than or equal to 0. If set to none-zero value, the force label should be provided by file `force.npy` in each data system. If both `start_pref_f` and `limit_pref_f` are set to 0, then the force will be ignored.

limit_pref_f:

type: `float | int`, optional, default: 1.0

argument path: `loss[ener]/limit_pref_f`

The prefactor of force loss at the limit of the training, Should be larger than or equal to 0. i.e. the training step goes to infinity.

start_pref_v:

type: `float | int`, optional, default: 0.0

argument path: `loss[ener]/start_pref_v`

The prefactor of virial loss at the start of the training. Should be larger than or equal to 0. If set to none-zero value, the virial label should be provided by file `virial.npy` in each data system. If both `start_pref_v` and `limit_pref_v` are set to 0, then the virial will be ignored.

limit_pref_v:

type: `float | int`, optional, default: 0.0

argument path: `loss[ener]/limit_pref_v`

The prefactor of virial loss at the limit of the training, Should be larger than or equal to 0. i.e. the training step goes to infinity.

start_pref_ae:

type: `float | int`, optional, default: 0.0

argument path: `loss[ener]/start_pref_ae`

The prefactor of atomic energy loss at the start of the training. Should be larger than or equal to 0. If set to none-zero value, the `atom_ener` label should be provided by file `atom_ener.npy` in each data system. If both `start_pref_ae` and `limit_pref_ae` are set to 0, then the atomic energy will be ignored.

limit_pref_ae:

type: `float | int`, optional, default: 0.0

argument path: `loss[ener]/limit_pref_ae`

The prefactor of atomic energy loss at the limit of the training, Should be larger than or equal to 0. i.e. the training step goes to infinity.

start_pref_pf:

type: `float | int`, optional, default: 0.0

argument path: `loss[ener]/start_pref_pf`

The prefactor of atomic prefactor force loss at the start of the training. Should be larger than or equal to 0. If set to none-zero value, the `atom_pref` label should

be provided by file `atom_pref.npy` in each data system. If both `start_pref_pf` and `limit_pref_pf` are set to 0, then the atomic prefactor force will be ignored.

limit_pref_pf:

type: float | int, optional, default: 0.0
argument path: `loss[ener]/limit_pref_pf`

The prefactor of atomic prefactor force loss at the limit of the training, Should be larger than or equal to 0. i.e. the training step goes to infinity.

relative_f:

type: float | NoneType, optional
argument path: `loss[ener]/relative_f`

If provided, relative force error will be used in the loss. The difference of force will be normalized by the magnitude of the force in the label with a shift given by `relative_f`, i.e. $DF_i / (\|F\| + \text{relative_f})$ with DF denoting the difference between prediction and label and $\|F\|$ denoting the L2 norm of the label.

enable_atom_ener_coeff:

type: bool, optional, default: False
argument path: `loss[ener]/enable_atom_ener_coeff`

If true, the energy will be computed as $\sum_i c_i E_i$. c_i should be provided by file `atom_ener_coeff.npy` in each data system, otherwise it's 1.

start_pref_gf:

type: float, optional, default: 0.0
argument path: `loss[ener]/start_pref_gf`

The prefactor of generalized force loss at the start of the training. Should be larger than or equal to 0. If set to none-zero value, the `drdq` label should be provided by file `drdq.npy` in each data system. If both `start_pref_gf` and `limit_pref_gf` are set to 0, then the generalized force will be ignored.

limit_pref_gf:

type: float, optional, default: 0.0
argument path: `loss[ener]/limit_pref_gf`

The prefactor of generalized force loss at the limit of the training, Should be larger than or equal to 0. i.e. the training step goes to infinity.

numb_generalized_coord:

type: int, optional, default: 0
argument path: `loss[ener]/numb_generalized_coord`

The dimension of generalized coordinates. Required when generalized force loss is used.

When `type` is set to `ener_spin`:

start_pref_e:

type: float | int, optional, default: 0.02
argument path: `loss[ener_spin]/start_pref_e`

The prefactor of energy loss at the start of the training. Should be larger than or equal to 0. If set to none-zero value, the energy label should be provided by file `energy.npy` in each data system. If both `start_pref_energy` and `limit_pref_energy` are set to 0, then the energy will be ignored.

limit_pref_e:

type: float | int, optional, default: 1.0

argument path: `loss[ener_spin]/limit_pref_e`

The prefactor of energy loss at the limit of the training, Should be larger than or equal to 0. i.e. the training step goes to infinity.

start_pref_fr:

type: float | int, optional, default: 1000

argument path: `loss[ener_spin]/start_pref_fr`

The prefactor of force_real_atom loss at the start of the training. Should be larger than or equal to 0. If set to none-zero value, the force_real_atom label should be provided by file `force_real_atom.npy` in each data system. If both `start_pref_force_real_atom` and `limit_pref_force_real_atom` are set to 0, then the force_real_atom will be ignored.

limit_pref_fr:

type: float | int, optional, default: 1.0

argument path: `loss[ener_spin]/limit_pref_fr`

The prefactor of force_real_atom loss at the limit of the training, Should be larger than or equal to 0. i.e. the training step goes to infinity.

start_pref_fm:

type: float | int, optional, default: 10000

argument path: `loss[ener_spin]/start_pref_fm`

The prefactor of force_magnetic loss at the start of the training. Should be larger than or equal to 0. If set to none-zero value, the force_magnetic label should be provided by file `force_magnetic.npy` in each data system. If both `start_pref_force_magnetic` and `limit_pref_force_magnetic` are set to 0, then the force_magnetic will be ignored.

limit_pref_fm:

type: float | int, optional, default: 10.0

argument path: `loss[ener_spin]/limit_pref_fm`

The prefactor of force_magnetic loss at the limit of the training, Should be larger than or equal to 0. i.e. the training step goes to infinity.

start_pref_v:

type: float | int, optional, default: 0.0

argument path: `loss[ener_spin]/start_pref_v`

The prefactor of virial loss at the start of the training. Should be larger than or equal to 0. If set to none-zero value, the virial label should be provided by file `virial.npy` in each data system. If both `start_pref_virial` and `limit_pref_virial` are set to 0, then the virial will be ignored.

limit_pref_v:

type: float | int, optional, default: 0.0

argument path: `loss[ener_spin]/limit_pref_v`

The prefactor of virial loss at the limit of the training, Should be larger than or equal to 0. i.e. the training step goes to infinity.

start_pref_ae:

type: float | int, optional, default: 0.0

argument path: `loss[ener_spin]/start_pref_ae`

The prefactor of atom_ener loss at the start of the training. Should be larger than or equal to 0. If set to none-zero value, the atom_ener label should be provided by file atom_ener.npy in each data system. If both start_pref_atom_ener and limit_pref_atom_ener are set to 0, then the atom_ener will be ignored.

limit_pref_ae:

type: float | int, optional, default: 0.0

argument path: `loss[ener_spin]/limit_pref_ae`

The prefactor of atom_ener loss at the limit of the training, Should be larger than or equal to 0. i.e. the training step goes to infinity.

start_pref_pf:

type: float | int, optional, default: 0.0

argument path: `loss[ener_spin]/start_pref_pf`

The prefactor of atom_pref loss at the start of the training. Should be larger than or equal to 0. If set to none-zero value, the atom_pref label should be provided by file atom_pref.npy in each data system. If both start_pref_atom_pref and limit_pref_atom_pref are set to 0, then the atom_pref will be ignored.

limit_pref_pf:

type: float | int, optional, default: 0.0

argument path: `loss[ener_spin]/limit_pref_pf`

The prefactor of atom_pref loss at the limit of the training, Should be larger than or equal to 0. i.e. the training step goes to infinity.

relative_f:

type: float | NoneType, optional

argument path: `loss[ener_spin]/relative_f`

If provided, relative force error will be used in the loss. The difference of force will be normalized by the magnitude of the force in the label with a shift given by relative_f, i.e. $DF_i / (\|F\| + \text{relative_f})$ with DF denoting the difference between prediction and label and $\|F\|$ denoting the L2 norm of the label.

enable_atom_ener_coeff:

type: bool, optional, default: False

argument path: `loss[ener_spin]/enable_atom_ener_coeff`

If true, the energy will be computed as $\sum_i c_i E_i$. c_i should be provided by file atom_ener_coeff.npy in each data system, otherwise it's 1.

When `type` is set to `dos`:

start_pref_dos:

type: float | int, optional, default: 0.0

argument path: `loss[dos]/start_pref_dos`

The prefactor of Density of State (DOS) loss at the start of the training. Should be larger than or equal to 0. If set to none-zero value, the Density of State (DOS) label should be provided by file Density of State (DOS).npy in each data system. If both start_pref_Density of State (DOS) and limit_pref_Density of State (DOS) are set to 0, then the Density of State (DOS) will be ignored.

limit_pref_dos:

type: float | int, optional, default: 0.0
argument path: `loss[dos]/limit_pref_dos`

The prefactor of Density of State (DOS) loss at the limit of the training, Should be larger than or equal to 0. i.e. the training step goes to infinity.

start_pref_cdf:

type: float | int, optional, default: 0.0
argument path: `loss[dos]/start_pref_cdf`

The prefactor of Cumulative Distribution Function (cumulative intergral of DOS) loss at the start of the training. Should be larger than or equal to 0. If set to none-zero value, the Cumulative Distribution Function (cumulative intergral of DOS) label should be provided by file Cumulative Distribution Function (cumulative intergral of DOS).npz in each data system. If both start_pref_Cumulative Distribution Function (cumulative intergral of DOS) and limit_pref_Cumulative Distribution Function (cumulative intergral of DOS) are set to 0, then the Cumulative Distribution Function (cumulative intergral of DOS) will be ignored.

limit_pref_cdf:

type: float | int, optional, default: 0.0
argument path: `loss[dos]/limit_pref_cdf`

The prefactor of Cumulative Distribution Function (cumulative intergral of DOS) loss at the limit of the training, Should be larger than or equal to 0. i.e. the training step goes to infinity.

start_pref_ados:

type: float | int, optional, default: 1.0
argument path: `loss[dos]/start_pref_ados`

The prefactor of atomic DOS (site-projected DOS) loss at the start of the training. Should be larger than or equal to 0. If set to none-zero value, the atomic DOS (site-projected DOS) label should be provided by file atomic DOS (site-projected DOS).npz in each data system. If both start_pref_atomic DOS (site-projected DOS) and limit_pref_atomic DOS (site-projected DOS) are set to 0, then the atomic DOS (site-projected DOS) will be ignored.

limit_pref_ados:

type: float | int, optional, default: 1.0
argument path: `loss[dos]/limit_pref_ados`

The prefactor of atomic DOS (site-projected DOS) loss at the limit of the training, Should be larger than or equal to 0. i.e. the training step goes to infinity.

start_pref_acdf:

type: float | int, optional, default: 0.0
argument path: `loss[dos]/start_pref_acdf`

The prefactor of Cumulative integral of atomic DOS loss at the start of the training. Should be larger than or equal to 0. If set to none-zero value, the Cumulative integral of atomic DOS label should be provided by file Cumulative integral of atomic DOS.npz in each data system. If both start_pref_Cumulative integral of atomic DOS and limit_pref_Cumulative integral of atomic DOS are set to 0, then the Cumulative integral of atomic DOS will be ignored.

limit_pref_acdf:

type: float | int, optional, default: 0.0
 argument path: `loss[dos]/limit_pref_acdf`

The prefactor of Cumulative integral of atomic DOS loss at the limit of the training, Should be larger than or equal to 0. i.e. the training step goes to infinity.

When `type` is set to `tensor`:

pref:

type: float | int
 argument path: `loss[tensor]/pref`

The prefactor of the weight of global loss. It should be larger than or equal to 0. It controls the weight of loss corresponding to global label, i.e. 'polarizability.npy' or dipole.npy, whose shape should be #frames x [9 or 3]. If it's larger than 0.0, this npy should be included.

pref_atomic:

type: float | int
 argument path: `loss[tensor]/pref_atomic`

The prefactor of the weight of atomic loss. It should be larger than or equal to 0. It controls the weight of loss corresponding to atomic label, i.e. atomic_polarizability.npy or atomic_dipole.npy, whose shape should be #frames x ([9 or 3] x #selected atoms). If it's larger than 0.0, this npy should be included. Both pref and pref_atomic should be provided, and either can be set to 0.0.

loss_dict:

type: dict, optional
 argument path: `loss_dict`

The dictionary of definitions of multiple loss functions in multi-task mode. Each `loss_dict[fitting_key]`, with user-defined name `fitting_key` in `model/fitting_net_dict`, is the single definition of loss function, whose type should be set to `tensor`, `ener` or left unset.

training:

type: dict
 argument path: `training`

The training options.

training_data:

type: dict, optional
 argument path: `training/training_data`

Configurations of training data.

systems:

type: list | str
 argument path: `training/training_data/systems`

The data systems for training. This key can be provided with a list that specifies the systems, or be provided with a string by which the prefix of all systems are given and the list of the systems is automatically generated.

set_prefix:

type: `str`, optional, default: `set`
argument path: `training/training_data/set_prefix`

The prefix of the sets in the [systems](#).

batch_size:

type: `list` | `str` | `int`, optional, default: `auto`
argument path: `training/training_data/batch_size`

This key can be

- `list`: the length of which is the same as the [systems](#). The batch size of each system is given by the elements of the list.
- `int`: all [systems](#) use the same batch size.
- string `"auto"`: automatically determines the batch size so that the `batch_size` times the number of atoms in the system is no less than 32.
- string `"auto:N"`: automatically determines the batch size so that the `batch_size` times the number of atoms in the system is no less than N.
- string `"mixed:N"`: the batch data will be sampled from all systems and merged into a mixed system with the batch size N. Only support the `se_atten` descriptor.

If MPI is used, the value should be considered as the batch size per task.

auto_prob:

type: `str`, optional, default: `prob_sys_size`, alias: `auto_prob_style`
argument path: `training/training_data/auto_prob`

Determine the probability of systems automatically. The method is assigned by this key and can be

- `"prob_uniform"` : the probability all the systems are equal, namely `1.0/self.get_nsystems()`
- `"prob_sys_size"` : the probability of a system is proportional to the number of batches in the system
- `"prob_sys_size;stt_idx:end_idx:weight;stt_idx:end_idx:weight;..."` : the list of systems is divided into blocks. A block is specified by `stt_idx:end_idx:weight`, where `stt_idx` is the starting index of the system, `end_idx` is then ending (not including) index of the system, the probabilities of the systems in this block sums up to `weight`, and the relatively probabilities within this block is proportional to the number of batches in the system.

sys_probs:

type: `list` | `NoneType`, optional, default: `None`, alias: `sys_weights`
argument path: `training/training_data/sys_probs`

A list of float if specified. Should be of the same length as [systems](#), specifying the probability of each system.

validation_data:

type: `dict` | `NoneType`, optional, default: `None`
argument path: `training/validation_data`

Configurations of validation data. Similar to that of training data, except that a `numb_btch` argument may be configured

systems:

type: `list` | `str`

argument path: `training/validation_data/systems`

The data systems for validation. This key can be provided with a list that specifies the systems, or be provided with a string by which the prefix of all systems are given and the list of the systems is automatically generated.

set_prefix:

type: `str`, optional, default: `set`

argument path: `training/validation_data/set_prefix`

The prefix of the sets in the `systems`.

batch_size:

type: `list` | `str` | `int`, optional, default: `auto`

argument path: `training/validation_data/batch_size`

This key can be

- `list`: the length of which is the same as the `systems`. The batch size of each system is given by the elements of the list.
- `int`: all `systems` use the same batch size.
- string `"auto"`: automatically determines the batch size so that the `batch_size` times the number of atoms in the system is no less than 32.
- string `"auto:N"`: automatically determines the batch size so that the `batch_size` times the number of atoms in the system is no less than N.

auto_prob:

type: `str`, optional, default: `prob_sys_size`, alias: `auto_prob_style`

argument path: `training/validation_data/auto_prob`

Determine the probability of systems automatically. The method is assigned by this key and can be

- `"prob_uniform"` : the probability all the systems are equal, namely `1.0/self.get_nsystems()`
- `"prob_sys_size"` : the probability of a system is proportional to the number of batches in the system
- `"prob_sys_size;stt_idx:end_idx:weight;stt_idx:end_idx:weight;..."` : the list of systems is divided into blocks. A block is specified by `stt_idx:end_idx:weight`, where `stt_idx` is the starting index of the system, `end_idx` is then ending (not including) index of the system, the probabilities of the systems in this block sums up to `weight`, and the relatively probabilities within this block is proportional to the number of batches in the system.

sys_probs:

type: `list` | `NoneType`, optional, default: `None`, alias: `sys_weights`

argument path: `training/validation_data/sys_probs`

A list of float if specified. Should be of the same length as `systems`, specifying the probability of each system.

numb_btch:

type: `int`, optional, default: `1`, alias: `numb_batch`

argument path: `training/validation_data/numb_btch`

An integer that specifies the number of batches to be sampled for each validation period.

mixed_precision:
type: dict, optional
argument path: `training/mixed_precision`
Configurations of mixed precision.

output_prec:
type: str, optional, default: float32
argument path: `training/mixed_precision/output_prec`
The precision for mixed precision params. " "The trainable variables precision during the mixed precision training process, " "supported options are float32 only currently.

compute_prec:
type: str
argument path: `training/mixed_precision/compute_prec`
The precision for mixed precision compute. " "The compute precision during the mixed precision training process, "" "supported options are float16 and bfloat16 currently.

numb_steps:
type: int, alias: stop_batch
argument path: `training/numb_steps`
Number of training batch. Each training uses one batch of data.

seed:
type: NoneType | int, optional
argument path: `training/seed`
The random seed for getting frames from the training data set.

disp_file:
type: str, optional, default: `lcurve.out`
argument path: `training/disp_file`
The file for printing learning curve.

disp_freq:
type: int, optional, default: 1000
argument path: `training/disp_freq`
The frequency of printing learning curve.

save_freq:
type: int, optional, default: 1000
argument path: `training/save_freq`
The frequency of saving check point.

save_ckpt:
type: str, optional, default: `model.ckpt`
argument path: `training/save_ckpt`
The file name of saving check point.

disp_training:
 type: bool, optional, default: True
 argument path: `training/disp_training`
 Displaying verbose information during training.

time_training:
 type: bool, optional, default: True
 argument path: `training/time_training`
 Timing during training.

profiling:
 type: bool, optional, default: False
 argument path: `training/profiling`
 Profiling during training.

profiling_file:
 type: str, optional, default: `timeline.json`
 argument path: `training/profiling_file`
 Output file for profiling.

enable_profiler:
 type: bool, optional, default: False
 argument path: `training/enable_profiler`
 Enable TensorFlow Profiler (available in TensorFlow 2.3) to analyze performance. The log will be saved to `tensorboard_log_dir`.

tensorboard:
 type: bool, optional, default: False
 argument path: `training/tensorboard`
 Enable tensorboard

tensorboard_log_dir:
 type: str, optional, default: `log`
 argument path: `training/tensorboard_log_dir`
 The log directory of tensorboard outputs

tensorboard_freq:
 type: int, optional, default: 1
 argument path: `training/tensorboard_freq`
 The frequency of writing tensorboard events.

data_dict:
 type: dict, optional
 argument path: `training/data_dict`
 The dictionary of multi DataSystems in multi-task mode. Each `data_dict[fitting_key]`, with user-defined name `fitting_key` in `model/fitting_net_dict`, contains training data and optional validation data definitions.

fitting_weight:

type: dict, optional

argument path: training/fitting_weight

Each fitting_weight[fitting_key], with user-defined name fitting_key in model/fitting_net_dict, is the training weight of fitting net fitting_key. Fitting nets with higher weights will be selected with higher probabilities to be trained in one step. Weights will be normalized and minus ones will be ignored. If not set, each fitting net will be equally selected when training.

nvnmmd:

type: dict, optional

argument path: nvnmmd

The nvnmmd options.

version:

type: int

argument path: nvnmmd/version

configuration the nvnmmd version (0 | 1), 0 for 4 types, 1 for 32 types

net_size:

type: int

argument path: nvnmmd/net_size

configuration the number of nodes of fitting_net, just can be set as 128

map_file:

type: str

argument path: nvnmmd/map_file

A file containing the mapping tables to replace the calculation of embedding nets

config_file:

type: str

argument path: nvnmmd/config_file

A file containing the parameters about how to implement the model in certain hardware

weight_file:

type: str

argument path: nvnmmd/weight_file

a *.npy file containing the weights of the model

enable:

type: bool

argument path: nvnmmd/enable

enable the nvnmmd training

restore_descriptor:

type: bool

argument path: nvnmmd/restore_descriptor

enable to restore the parameter of embedding_net from weight.npy

```

restore_fitting_net:
    type: bool
    argument path: nvnmmd/restore_fitting_net
    enable to restore the parameter of fitting_net from weight.npy

quantize_descriptor:
    type: bool
    argument path: nvnmmd/quantize_descriptor
    enable the quantization of descriptor

quantize_fitting_net:
    type: bool
    argument path: nvnmmd/quantize_fitting_net
    enable the quantization of fitting_net

```

5.4 Parallel training

Currently, parallel training is enabled in a synchronized way with help of [Horovod](#). Depending on the number of training processes (according to MPI context) and the number of GPU cards available, DeePMD-kit will decide whether to launch the training in parallel (distributed) mode or in serial mode. Therefore, no additional options are specified in your JSON/YAML input file.

5.4.1 Tuning learning rate

Horovod works in the data-parallel mode, resulting in a larger global batch size. For example, the real batch size is 8 when `batch_size` is set to 2 in the input file and you launch 4 workers. Thus, `learning_rate` is automatically scaled by the number of workers for better convergence. Technical details of such heuristic rule are discussed at [Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour](#).

The number of decay steps required to achieve the same accuracy can decrease by the number of cards (e.g., 1/2 of steps in the above case), but needs to be scaled manually in the input file.

In some cases, it won't work well when scaling the learning rate by worker count in a linear way. Then you can try `sqrt` or `none` by setting argument `scale_by_worker` like below.

```

"learning_rate" :{
  "scale_by_worker": "none",
  "type": "exp"
}

```

5.4.2 Scaling test

Testing `examples/water/se_e2_a` on an 8-GPU host, linear acceleration can be observed with the increasing number of cards.

| Num of GPU cards | Seconds every 100 samples | Samples per second | Speed up |
|------------------|---------------------------|--------------------|----------|
| 1 | 1.4515 | 68.89 | 1.00 |
| 2 | 1.5962 | 62.65*2 | 1.82 |
| 4 | 1.7635 | 56.71*4 | 3.29 |
| 8 | 1.7267 | 57.91*8 | 6.72 |

5.4.3 How to use

Training workers can be launched with `horovodrun`. The following command launches 4 processes on the same host:

```
CUDA_VISIBLE_DEVICES=4,5,6,7 horovodrun -np 4 \
dp train --mpi-log=workers input.json
```

Need to mention, the environment variable `CUDA_VISIBLE_DEVICES` must be set to control parallelism on the occupied host where one process is bound to one GPU card.

To maximize the performance, one should follow [FAQ: How to control the parallelism of a job](#) to control the number of threads.

When using MPI with Horovod, `horovodrun` is a simple wrapper around `mpirun`. In the case where fine-grained control over options is passed to `mpirun`, `mpirun` can be invoked directly, and it will be detected automatically by Horovod, e.g.,

```
CUDA_VISIBLE_DEVICES=4,5,6,7 mpirun -l -launcher=fork -hosts=localhost -np 4 \
dp train --mpi-log=workers input.json
```

this is sometimes necessary for an HPC environment.

Whether distributed workers are initiated can be observed in the “Summary of the training” section in the log (world size > 1, and distributed).

```
[0] DEEPMO INFO    ---Summary of the training-----
[0] DEEPMO INFO    distributed
[0] DEEPMO INFO    world size:           4
[0] DEEPMO INFO    my rank:              0
[0] DEEPMO INFO    node list:           ['exp-13-57']
[0] DEEPMO INFO    running on:         exp-13-57
[0] DEEPMO INFO    computing device:    gpu:0
[0] DEEPMO INFO    CUDA_VISIBLE_DEVICES: 0,1,2,3
[0] DEEPMO INFO    Count of visible GPU: 4
[0] DEEPMO INFO    num_intra_threads:   0
[0] DEEPMO INFO    num_inter_threads:   0
[0] DEEPMO INFO    -----
```

5.4.4 Logging

What’s more, 2 command-line arguments are defined to control the logging behavior when performing parallel training with MPI.

```
optional arguments:
  -l LOG_PATH, --log-path LOG_PATH
                        set log file to log messages to disk, if not
                        specified, the logs will only be output to console
                        (default: None)
  -m {master,collect,workers}, --mpi-log {master,collect,workers}
                        Set the manner of logging when running with MPI.
                        'master' logs only on main process, 'collect'
                        broadcasts logs from workers to master and 'workers'
                        means each process will output its own log (default:
                        master)
```

5.5 Multi-task training

5.5.1 Perform the multi-task training

Training on multiple data sets (each data set contains several data systems) can be performed in multi-task mode, with one common descriptor and multiple specific fitting nets for each data set. One can simply switch the following parameters in training input script to perform multi-task mode:

- `fitting_net` -> `fitting_net_dict`, each key of which can be one individual fitting net.
- `training_data`, `validation_data` -> `data_dict`, each key of which can be one individual data set contains several data systems for corresponding fitting net, the keys must be consistent with those in `fitting_net_dict`.
- `loss` -> `loss_dict`, each key of which can be one individual loss setting for corresponding fitting net, the keys must be consistent with those in `fitting_net_dict`, if not set, the corresponding fitting net will use the default loss.
- (Optional) `fitting_weight`, each key of which can be a non-negative integer or float, deciding the chosen probability for corresponding fitting net in training, if not set or invalid, the corresponding fitting net will not be used.

The training procedure will automatically choose single-task or multi-task mode, based on the above parameters. Note that parameters of single-task mode and multi-task mode can not be mixed.

An example input for training energy and dipole in water system can be found here: [multi-task input on water](#).

The supported descriptors for multi-task mode are listed:

- `se_a` (`se_e2_a`)
- `se_r` (`se_e2_r`)
- `se_at` (`se_e3`)
- `se_atten`
- `se_atten_v2`
- `hybrid`

The supported fitting nets for multi-task mode are listed:

- `ener`
- `dipole`
- `polar`

The output of `dp freeze` command in multi-task mode can be seen in [freeze command](#).

5.5.2 Initialization from pretrained multi-task model

For advance training in multi-task mode, one can first train the descriptor on several upstream datasets and then transfer it on new downstream ones with newly added fitting nets. At the second step, you can also inherit some fitting nets trained on upstream datasets, by merely adding fitting net keys in `fitting_net_dict` and optional fitting net weights in `fitting_weight`.

Take multi-task input on water again for example. You can first train a multi-task model using input script with the following `model` part:

```
"model": {
  "type_map": ["O", "H"],
  "descriptor": {
    "type": "se_e2_a",
    "sel": [46, 92],
    "rcut_smth": 0.5,
    "rcut": 6.0,
    "neuron": [25, 50, 100],
  },
  "fitting_net_dict": {
    "water_dipole": {
      "type": "dipole",
      "neuron": [100, 100, 100],
    },
    "water_ener": {
      "neuron": [240, 240, 240],
      "resnet_dt": true,
    }
  }
}
```

After training, you can freeze this multi-task model into one unit graph:

```
$ dp freeze -o graph.pb --united-model
```

Then if you want to transfer the trained descriptor and some fitting nets (take `water_ener` for example) to newly added datasets with new fitting net `water_ener_2`, you can modify the `model` part of the new input script in a more simplified way:

```
"model": {
  "type_map": ["O", "H"],
  "descriptor": {},
  "fitting_net_dict": {
    "water_ener": {},
    "water_ener_2": {
      "neuron": [240, 240, 240],
      "resnet_dt": true,
    }
  }
}
```

It will autocomplete the configurations according to the frozen graph.

Note that for newly added fitting net keys, other parts in the input script, including `data_dict` and `loss_dict` (optionally `fitting_weight`), should be set explicitly. While for old fitting net keys, it will inherit the old configurations if not set.

Finally, you can perform the modified multi-task training from the frozen model with command:


```
$ dp train input.json --init_frz_model graph.pb
```

5.5.3 Share layers among energy fitting networks

The multi-task training can be used to train multiple levels of energies (e.g. DFT and CCSD(T)) at the same time. In this situation, one can set `model/fitting_net[ener]/layer_name>` to share some of layers among fitting networks. The architecture of the layers with the same name should be the same.

For example, if one want to share the first and the third layers for two three-hidden-layer fitting networks, the following parameters should be set.

```
"fitting_net_dict": {
  "ccsd": {
    "neuron": [
      240,
      240,
      240
    ],
    "layer_name": ["l0", null, "l2", null]
  },
  "wb97m": {
    "neuron": [
      240,
      240,
      240
    ],
    "layer_name": ["l0", null, "l2", null]
  }
}
```

5.6 TensorBoard Usage

TensorBoard provides the visualization and tooling needed for machine learning experimentation. Full instructions for TensorBoard can be found [here](#).

5.6.1 Highlighted features

DeePMD-kit can now use most of the interesting features enabled by TensorBoard!

- Tracking and visualizing metrics, such as `l2_loss`, `l2_energy_loss` and `l2_force_loss`
- Visualizing the model graph (ops and layers)
- Viewing histograms of weights, biases, or other tensors as they change over time.
- Viewing summaries of trainable variables

5.6.2 How to use Tensorboard with DeePMD-kit

Before running TensorBoard, make sure you have generated summary data in a log directory by modifying the input script, setting `tensorboard` to true in the training subsection will enable the TensorBoard data analysis. eg. `water_se_a.json`.

```
"training" : {
  "systems":      ["../data/"],
  "set_prefix":    "set",
  "stop_batch":    1000000,
  "batch_size":    1,

  "seed":          1,

  "_comment": " display and restart",
  "_comment": " frequencies counted in batch",
  "disp_file":     "lcurve.out",
  "disp_freq":     100,
  "numb_test":     10,
  "save_freq":     1000,
  "save_ckpt":     "model.ckpt",

  "disp_training": true,
  "time_training": true,
  "tensorboard":   true,
  "tensorboard_log_dir": "log",
  "tensorboard_freq": 1000,
  "profiling":     false,
  "profiling_file": "timeline.json",
  "_comment":     "that's all"
}
```

Once you have event files, run TensorBoard and provide the log directory. This should print that TensorBoard has started. Next, connect to `http://tensorboard_server_ip:6006`.

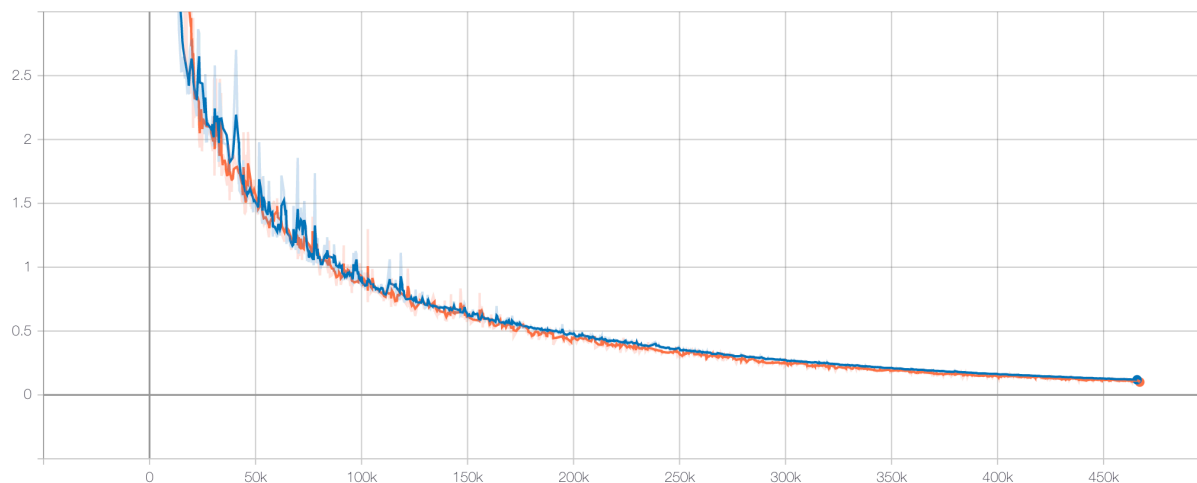
TensorBoard requires a logdir to read logs from. For info on configuring TensorBoard, run `TensorBoard -help`. One can easily change the log name with “`tensorboard_log_dir`” and the sampling frequency with “`tensorboard_freq`”.

```
tensorboard --logdir path/to/logs
```

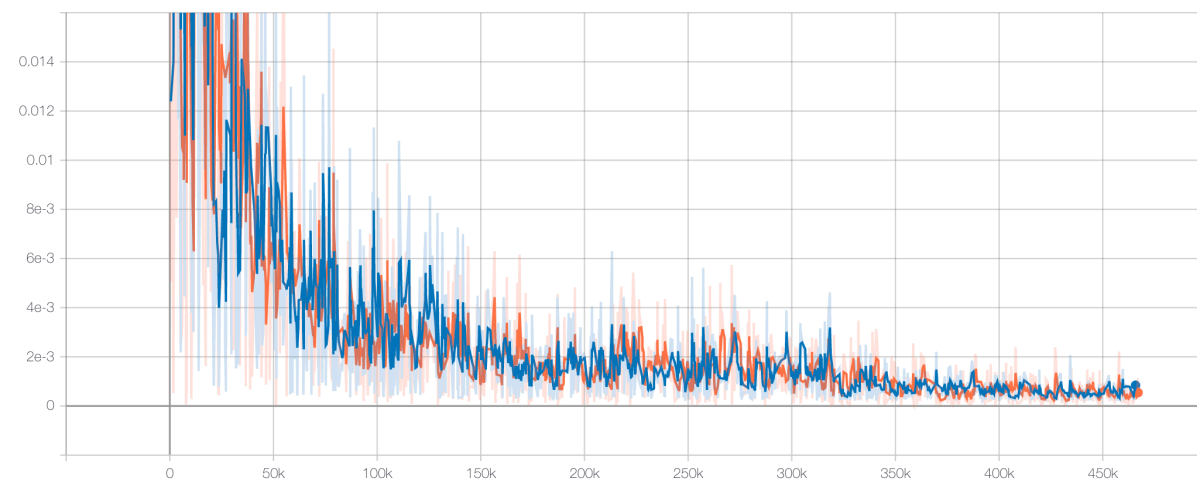
5.6.3 Examples

Tracking and visualizing loss metrics(red:train, blue:test)

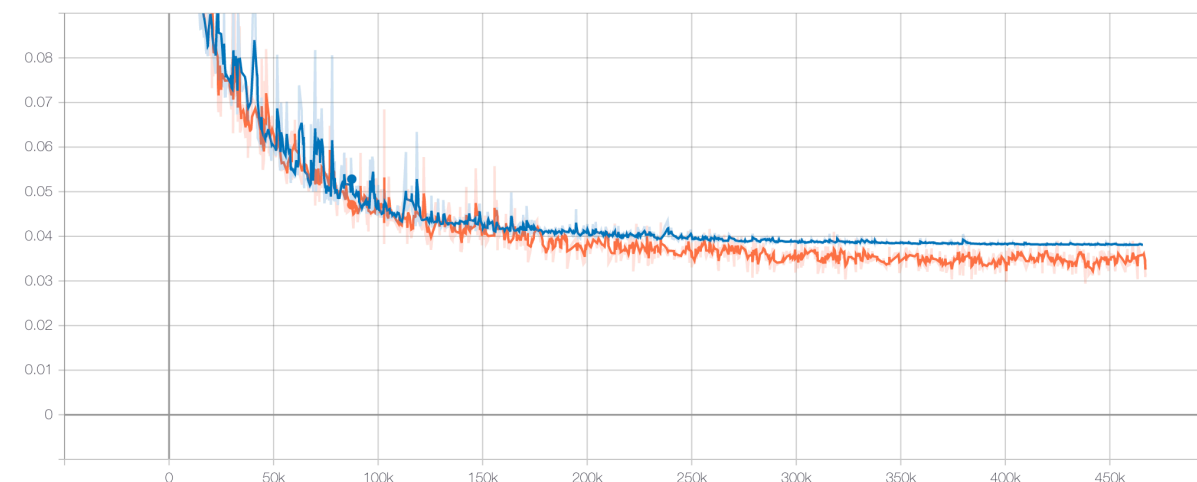
l2_loss



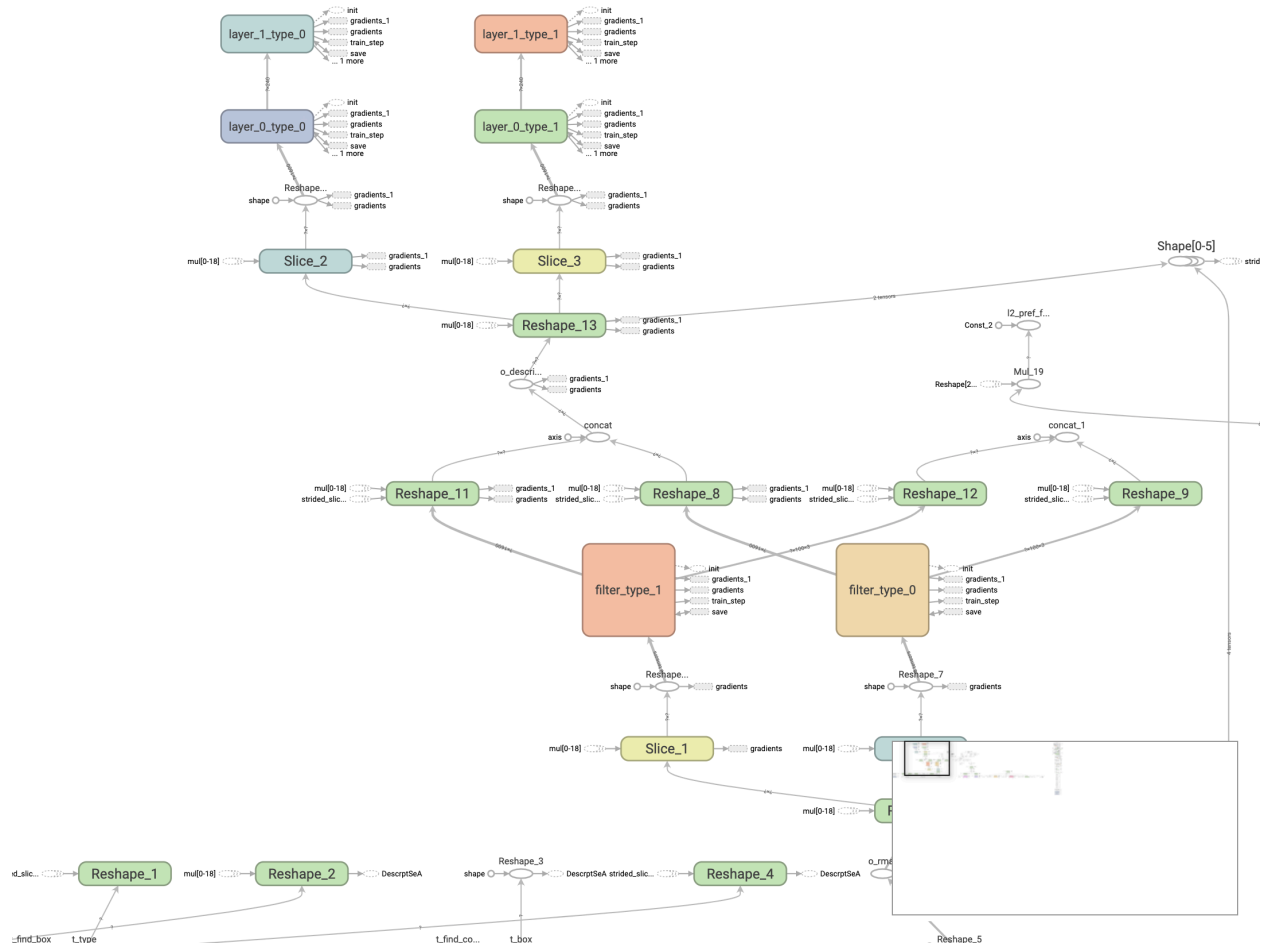
l2_ener_loss



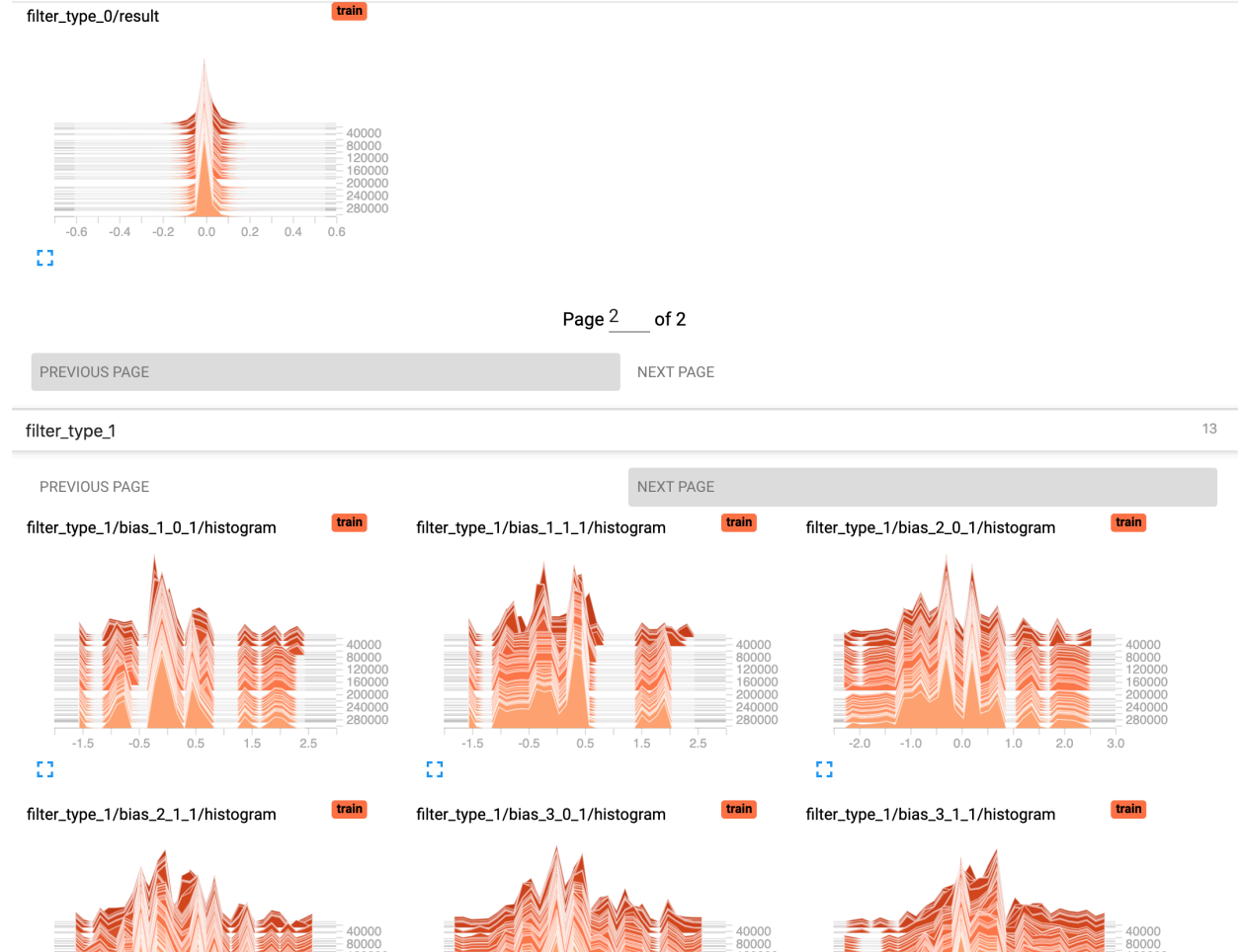
l2_force_loss



Visualizing DeePMD-kit model graph



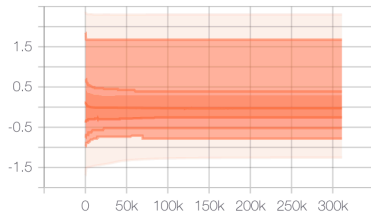
Viewing histograms of weights, biases, or other tensors as they change over time



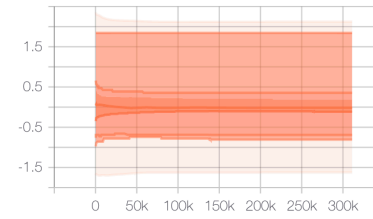
filter_type_0

[PREVIOUS PAGE](#)[NEXT PAGE](#)

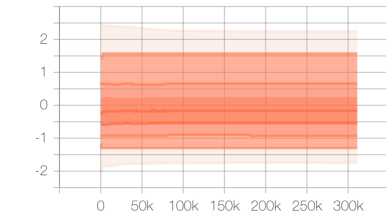
filter_type_0/bias_1_0_1/histogram



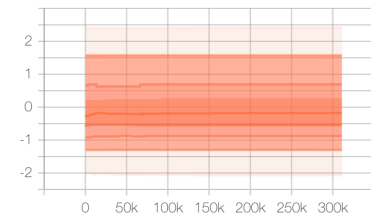
filter_type_0/bias_1_1_1/histogram



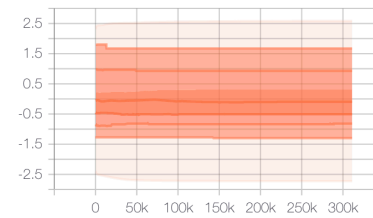
filter_type_0/bias_2_0_1/histogram



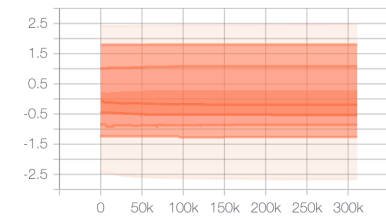
filter_type_0/bias_2_1_1/histogram



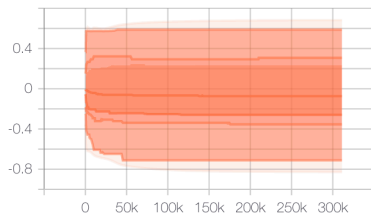
filter_type_0/bias_3_0_1/histogram



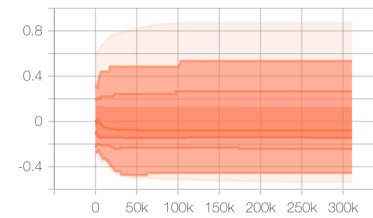
filter_type_0/bias_3_1_1/histogram



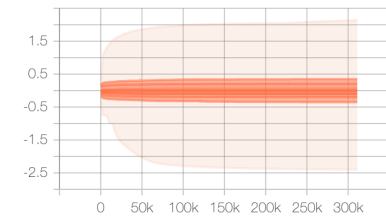
filter_type_0/matrix_1_0_1/histogram



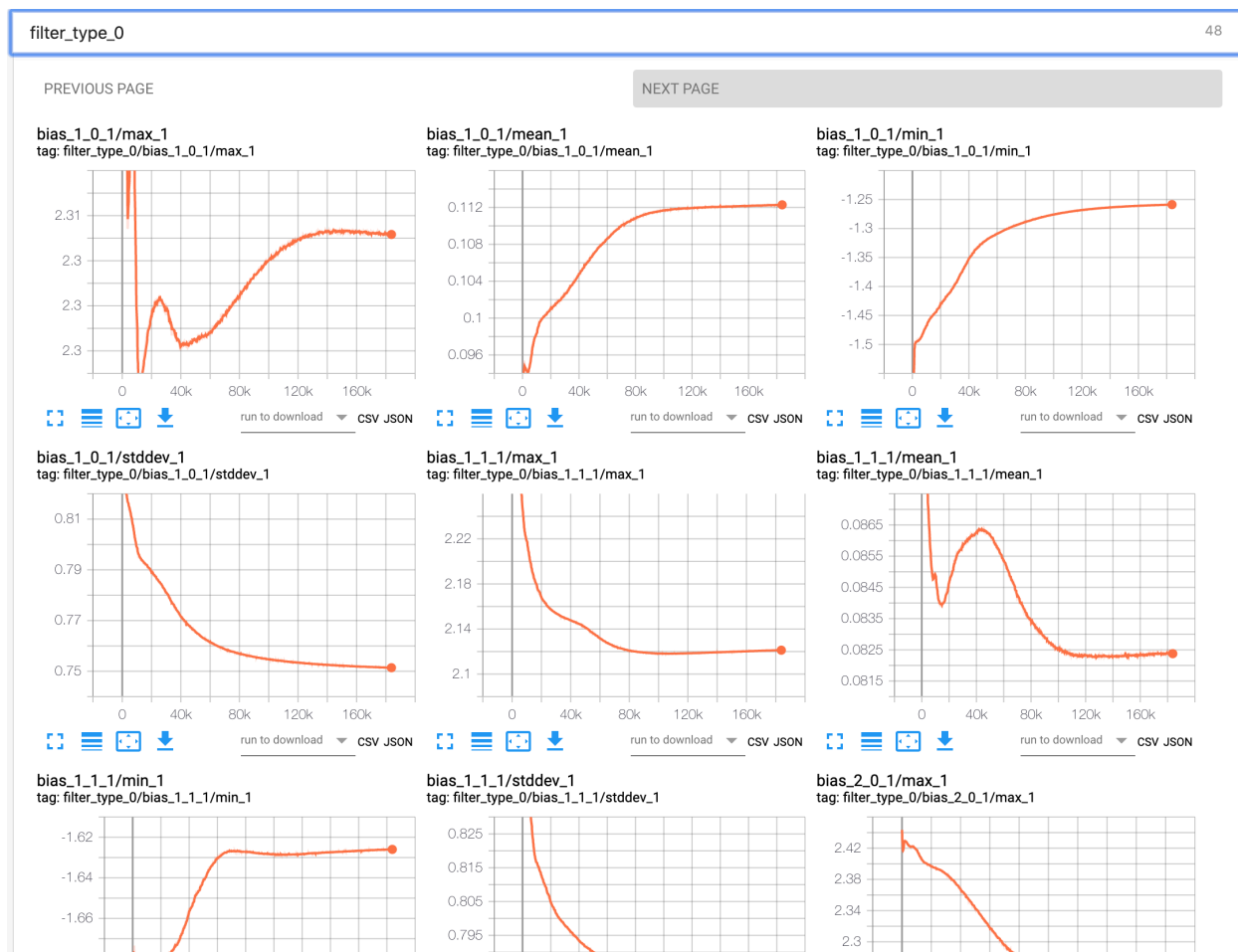
filter_type_0/matrix_1_1_1/histogram



filter_type_0/matrix_2_0_1/histogram



Viewing summaries of trainable variables



5.6.4 Attention

Allowing the tensorboard analysis will takes extra execution time.(eg, 15% increasing @Nvidia GTX 1080Ti double precision with default water sample)

TensorBoard can be used in Google Chrome or Firefox. Other browsers might work, but there may be bugs or performance issues.

5.7 Known limitations of using GPUs

If you use DeePMD-kit in a GPU environment, the acceptable value range of some variables is additionally restricted compared to the CPU environment due to the software's GPU implementations:

1. The number of atom types of a given system must be less than 128.
2. The maximum distance between an atom and its neighbors must be less than 128. It can be controlled by setting the rcut value of training parameters.

3. Theoretically, the maximum number of atoms that a single GPU can accept is about 10,000,000. However, this value is limited by the GPU memory size currently, usually within 1000,000 atoms even in the model compression mode.
4. The total sel value of training parameters(in `model/descriptor` section) must be less than 4096.
5. The size of the last layer of the embedding net must be less than 1024 during the model compression process.

5.8 Finetune the pretrained model

Pretraining-and-finetuning is a widely used approach in other fields such as Computer Vision (CV) or Natural Language Processing (NLP) to vastly reduce the training cost, while it's not trivial in potential models. Compositions and configurations of data samples or even computational parameters in upstream software (such as VASP) may be different between the pretrained and target datasets, leading to energy shifts or other diversities of training data.

Recently the emerging of methods such as [DPA-1](#) has brought us to a new stage where we can perform similar pretraining-finetuning approaches. DPA-1 can hopefully learn the common knowledge in the pretrained dataset (especially the `force` information) and thus reduce the computational cost in downstream training tasks. If you have a pretrained model `pretrained.pb` (here we support models using `se_atten` descriptor and `ener` fitting net) on a large dataset (for example, [OC2M](#) in [DPA-1 paper](#)), a finetuning strategy can be performed by simply running:

```
$ dp train input.json --finetune pretrained.pb
```

The command above will change the energy bias in the last layer of the fitting net in `pretrained.pb`, according to the training dataset in `input.json`.

Warning: Note that the elements in the training dataset must be contained in the pretrained dataset.

The finetune procedure will inherit the model structures in `pretrained.pb`, and thus it will ignore the model parameters in `input.json`, such as `descriptor`, `fitting_net`, `type_embedding` and `type_map`. However, you can still set the `trainable` parameters in each part of `input.json` to control the training procedure.

To obtain a more simplified script, for example, you can change the `model` part in `input.json` to perform finetuning:

```
"model": {
  "type_map":      ["O", "H"],
  "type_embedding": {"trainable": true},
  "descriptor" : {},
  "fitting_net" : {}
}
```


FREEZE AND COMPRESS

6.1 Freeze a model

The trained neural network is extracted from a checkpoint and dumped into a protobuf(.pb) file. This process is called “freezing” a model. The idea and part of our code are from [Morgan](#). To freeze a model, typically one does

```
$ dp freeze -o graph.pb
```

in the folder where the model is trained. The output model is called `graph.pb`.

In [multi-task mode](#):

- This process will in default output several models, each of which contains the common descriptor and one of the user-defined fitting nets in `fitting_net_dict`, let's name it `fitting_key`, together frozen in `graph_{fitting_key}.pb`. Those frozen models are exactly the same as single-task output with fitting net `fitting_key`.
- If you add `--united-model` option in this situation, the total multi-task model will be frozen into one unit `graph.pb`, which is mainly for multi-task initialization and can not be used directly for inference.

6.2 Compress a model

Once the frozen model is obtained from DeePMD-kit, we can get the neural network structure and its parameters (weights, biases, etc.) from the trained model, and compress it in the following way:

```
dp compress -i graph.pb -o graph-compress.pb
```

where `-i` gives the original frozen model, `-o` gives the compressed model. Several other command line options can be passed to `dp compress`, which can be checked with

```
$ dp compress --help
```

An explanation will be provided

```
usage: dp compress [-h] [-v {DEBUG,3,INFO,2,WARNING,1,ERROR,0}] [-l LOG_PATH]
                  [-m {master,collect,workers}] [-i INPUT] [-o OUTPUT]
                  [-s STEP] [-e EXTRAPOLATE] [-f FREQUENCY]
                  [-c CHECKPOINT_FOLDER]
```

optional arguments:

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```

-h, --help          show this help message and exit
-v {DEBUG,3,INFO,2,WARNING,1,ERROR,0}, --log-level {DEBUG,3,INFO,2,WARNING,1,ERROR,0}
                    set verbosity level by string or number, 0=ERROR,
                    1=WARNING, 2=INFO and 3=DEBUG (default: INFO)
-l LOG_PATH, --log-path LOG_PATH
                    set log file to log messages to disk, if not
                    specified, the logs will only be output to console
                    (default: None)
-m {master,collect,workers}, --mpi-log {master,collect,workers}
                    Set the manner of logging when running with MPI.
                    'master' logs only on main process, 'collect'
                    broadcasts logs from workers to master and 'workers'
                    means each process will output its own log (default:
                    master)
-i INPUT, --input INPUT
                    The original frozen model, which will be compressed by
                    the code (default: frozen_model.pb)
-o OUTPUT, --output OUTPUT
                    The compressed model (default:
                    frozen_model_compressed.pb)
-s STEP, --step STEP Model compression uses fifth-order polynomials to
                    interpolate the embedding-net. It introduces two
                    tables with different step size to store the
                    parameters of the polynomials. The first table covers
                    the range of the training data, while the second table
                    is an extrapolation of the training data. The domain
                    of each table is uniformly divided by a given step
                    size. And the step(parameter) denotes the step size of
                    the first table and the second table will use 10 *
                    step as it's step size to save the memory. Usually the
                    value ranges from 0.1 to 0.001. Smaller step means
                    higher accuracy and bigger model size (default: 0.01)
-e EXTRAPOLATE, --extrapolate EXTRAPOLATE
                    The domain range of the first table is automatically
                    detected by the code: [d_low, d_up]. While the second
                    table ranges from the first table's upper
                    boundary(d_up) to the extrapolate(parameter) * d_up:
                    [d_up, extrapolate * d_up] (default: 5)
-f FREQUENCY, --frequency FREQUENCY
                    The frequency of tabulation overflow check(Whether the
                    input environment matrix overflow the first or second
                    table range). By default do not check the overflow
                    (default: -1)
-c CHECKPOINT_FOLDER, --checkpoint-folder CHECKPOINT_FOLDER
                    path to checkpoint folder (default: .)
-t TRAINING_SCRIPT, --training-script TRAINING_SCRIPT
                    The training script of the input frozen model
                    (default: None)

```

Parameter explanation

Model compression, which includes tabulating the embedding net. The table is composed of fifth-order polynomial coefficients and is assembled from two sub-tables. For model descriptor with `se_e2_a` type, the first sub-table takes the `stride(parameter)` as its uniform stride, while the second sub-table takes `10 * stride` as its uniform stride; For model descriptor with `se_e3` type, the first sub-table takes `10 * stride` as its uniform stride, while the second sub-table takes `100 * stride` as its uniform stride. The range of the first table is automatically detected by DeePMD-kit, while the second table ranges from the first table's upper boundary(upper) to

the `extrapolate(parameter) * upper`. Finally, we added a check frequency parameter. It indicates how often the program checks for overflow(if the input environment matrix overflows the first or second table range) during the MD inference.

Justification of model compression

Model compression, with little loss of accuracy, can greatly speed up MD inference time. According to different simulation systems and training parameters, the speedup can reach more than 10 times at both CPU and GPU devices. At the same time, model compression can greatly change memory usage, reducing as much as 20 times under the same hardware conditions.

Acceptable original model version

The model compression interface requires the version of DeePMD-kit used in the original model generation should be `2.0.0-alpha.0` or above. If one has a frozen 1.2 or 1.3 model, one can upgrade it through the `dp convert-from` interface. (eg: `dp convert-from 1.2/1.3 -i old_frozen_model.pb -o new_frozen_model.pb`)

Acceptable descriptor type

Descriptors with `se_e2_a`, `se_e3`, `se_e2_r` and `se_atten_v2` types are supported by the model compression feature. `Hybrid` mixed with the above descriptors is also supported.

Available activation functions for descriptor:

- `tanh`
- `gelu`
- `relu`
- `relu6`
- `softplus`
- `sigmoid`

TEST

7.1 Test a model

The frozen model can be used in many ways. The most straightforward test can be performed using `dp test`. A typical usage of `dp test` is

```
dp test -m graph.pb -s /path/to/system -n 30
```

where `-m` gives the tested model, `-s` the path to the tested system and `-n` the number of tested frames. Several other command line options can be passed to `dp test`, which can be checked with

```
$ dp test --help
```

An explanation will be provided

```
usage: dp test [-h] [-m MODEL] [-s SYSTEM] [-S SET_PREFIX] [-n NUMB_TEST]
              [-r RAND_SEED] [--shuffle-test] [-d DETAIL_FILE]

optional arguments:
  -h, --help            show this help message and exit
  -m MODEL, --model MODEL
                        Frozen model file to import
  -s SYSTEM, --system SYSTEM
                        The system dir
  -S SET_PREFIX, --set-prefix SET_PREFIX
                        The set prefix
  -n NUMB_TEST, --numb-test NUMB_TEST
                        The number of data for test
  -r RAND_SEED, --rand-seed RAND_SEED
                        The random seed
  --shuffle-test         Shuffle test data
  -d DETAIL_FILE, --detail-file DETAIL_FILE
                        The prefix to files where details of energy, force and virial accuracy/
                        accuracy per atom will be written
  -a, --atomic           Test the accuracy of atomic label, i.e. energy / tensor (dipole, polar)
```

7.2 Calculate Model Deviation

One can also use a subcommand to calculate the deviation of predicted forces or virials for a bunch of models in the following way:

```
dp model-devi -m graph.000.pb graph.001.pb graph.002.pb graph.003.pb -s ./data -o model_devi.out
```

where `-m` specifies graph files to be calculated, `-s` gives the data to be evaluated, `-o` the file to which model deviation results is dumped. Here is more information on this sub-command:

```
usage: dp model-devi [-h] [-v {DEBUG,3,INFO,2,WARNING,1,ERROR,0}]
                    [-l LOG_PATH] [-m MODELS [MODELS ...]] [-s SYSTEM]
                    [-S SET_PREFIX] [-o OUTPUT] [-f FREQUENCY] [-i ITEMS]

optional arguments:
  -h, --help            show this help message and exit
  -v {DEBUG,3,INFO,2,WARNING,1,ERROR,0}, --log-level {DEBUG,3,INFO,2,WARNING,1,ERROR,0}
                        set verbosity level by string or number, 0=ERROR,
                        1=WARNING, 2=INFO and 3=DEBUG (default: INFO)
  -l LOG_PATH, --log-path LOG_PATH
                        set log file to log messages to disk, if not
                        specified, the logs will only be output to console
                        (default: None)
  -m MODELS [MODELS ...], --models MODELS [MODELS ...]
                        Frozen models file to import (default:
                        ['graph.000.pb', 'graph.001.pb', 'graph.002.pb',
                        'graph.003.pb'])
  -s SYSTEM, --system SYSTEM
                        The system directory, not support recursive detection.
                        (default: .)
  -S SET_PREFIX, --set-prefix SET_PREFIX
                        The set prefix (default: set)
  -o OUTPUT, --output OUTPUT
                        The output file for results of model deviation
                        (default: model_devi.out)
  -f FREQUENCY, --frequency FREQUENCY
                        The trajectory frequency of the system (default: 1)
```

For more details concerning the definition of model deviation and its application, please refer to Yuzhi Zhang, Haidi Wang, Weijie Chen, Jinzhe Zeng, Linfeng Zhang, Han Wang, and Weinan E, DP-GEN: A concurrent learning platform for the generation of reliable deep learning based potential energy models, Computer Physics Communications, 2020, 253, 107206.

INFERENCE

Note that the model for inference is required to be compatible with the DeePMD-kit package. See [Model compatibility](#) for details.

8.1 Python interface

One may use the python interface of DeePMD-kit for model inference, an example is given as follows

```
from deepmd.infer import DeepPot
import numpy as np

dp = DeepPot("graph.pb")
coord = np.array([[1, 0, 0], [0, 0, 1.5], [1, 0, 3]]).reshape([1, -1])
cell = np.diag(10 * np.ones(3)).reshape([1, -1])
atype = [1, 0, 1]
e, f, v = dp.eval(coord, cell, atype)
```

where *e*, *f* and *v* are predicted energy, force and virial of the system, respectively.

Furthermore, one can use the python interface to calculate model deviation.

```
from deepmd.infer import calc_model_devi
from deepmd.infer import DeepPot as DP
import numpy as np

coord = np.array([[1, 0, 0], [0, 0, 1.5], [1, 0, 3]]).reshape([1, -1])
cell = np.diag(10 * np.ones(3)).reshape([1, -1])
atype = [1, 0, 1]
graphs = [DP("graph.000.pb"), DP("graph.001.pb")]
model_devi = calc_model_devi(coord, cell, atype, graphs)
```

Note that if the model inference or model deviation is performed cyclically, one should avoid calling the same model multiple times. Otherwise, tensorflow will never release the memory and this may lead to an out-of-memory (OOM) error.

8.2 C/C++ interface

8.2.1 C++ interface

The C++ interface of DeePMD-kit is also available for the model interface, which is considered faster than the Python interface. An example `infer_water.cpp` is given below:

```
#include "deepmd/DeepPot.h"

int main(){
    deepmd::DeepPot dp ("graph.pb");
    std::vector<double> coord = {1., 0., 0., 0., 0., 1.5, 1., 0., 3.};
    std::vector<double> cell = {10., 0., 0., 0., 10., 0., 0., 0., 10.};
    std::vector<int> atype = {1, 0, 1};
    double e;
    std::vector<double> f, v;
    dp.compute (e, f, v, coord, atype, cell);
}
```

where `e`, `f` and `v` are predicted energy, force and virial of the system, respectively. See `deepmd::DeepPot` for details.

You can compile `infer_water.cpp` using `gcc`:

```
gcc infer_water.cpp -L $deepmd_root/lib -L $tensorflow_root/lib -I $deepmd_root/include -Wl,--no-
as-needed -ldeepmd_cc -lstdc++ -ltensorflow_cc -Wl,-rpath=$deepmd_root/lib -Wl,-rpath=
$tensorflow_root/lib -o infer_water
```

and then run the program:

```
./infer_water
```

8.2.2 C interface

Although C is harder to write, the C library will not be affected by different versions of C++ compilers.

An example `infer_water.c` is given below:

```
#include <stdio.h>
#include <stdlib.h>
#include "deepmd/c_api.h"

int main(){
    const char* model = "graph.pb";
    double coord[] = {1., 0., 0., 0., 0., 1.5, 1., 0., 3.};
    double cell[] = {10., 0., 0., 0., 10., 0., 0., 0., 10.};
    int atype[] = {1, 0, 1};
    // init C pointers with given memory
    double* e = malloc(sizeof(*e));
    double* f = malloc(sizeof(*f) * 9); // natoms * 3
    double* v = malloc(sizeof(*v) * 9);
    double* ae = malloc(sizeof(*ae) * 9); // natoms
    double* av = malloc(sizeof(*av) * 27); // natoms * 9
    // DP model
    DP_DeepPot* dp = DP_NewDeepPot(model);
```

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```

DP_DeepPotCompute (dp, 3, coord, atype, cell, e, f, v, ae, av);
// print results
printf("energy: %f\n", *e);
for (int ii = 0; ii < 9; ++ii)
    printf("force[%d]: %f\n", ii, f[ii]);
for (int ii = 0; ii < 9; ++ii)
    printf("force[%d]: %f\n", ii, v[ii]);
// free memory
free(e);
free(f);
free(v);
free(ae);
free(av);
free(dp);
}

```

where `e`, `f` and `v` are predicted energy, force and virial of the system, respectively. `ae` and `av` are atomic energy and atomic virials, respectively. See `DP_DeepPotCompute()` for details.

You can compile `infer_water.c` using `gcc`:

```

gcc infer_water.c -L $deepmd_root/lib -L $tensorflow_root/lib -I $deepmd_root/include -Wl,--no-as-
-needed -ldeepmd_c -Wl,-rpath=$deepmd_root/lib -Wl,-rpath=$tensorflow_root/lib -o infer_water

```

and then run the program:

```
./infer_water
```

8.2.3 Header-only C++ library interface (recommended)

The header-only C++ library is built based on the C library. Thus, it has the same ABI compatibility as the C library but provides a powerful C++ interface. To use it, include `deepmd/deepmd.hpp`.

```

#include "deepmd/deepmd.hpp"

int main(){
    deepmd::hpp::DeepPot dp ("graph.pb");
    std::vector<double> coord = {1., 0., 0., 0., 0., 1.5, 1., 0., 3.};
    std::vector<double> cell = {10., 0., 0., 0., 10., 0., 0., 0., 10.};
    std::vector<int> atype = {1, 0, 1};
    double e;
    std::vector<double> f, v;
    dp.compute (e, f, v, coord, atype, cell);
}

```

Note that the feature of the header-only C++ library is still limited compared to the original C++ library. See `deepmd::hpp::DeepPot` for details.

You can compile `infer_water_hpp.cpp` using `gcc`:

```

gcc infer_water_hpp.cpp -L $deepmd_root/lib -L $tensorflow_root/lib -I $deepmd_root/include -Wl,--
no-as-needed -ldeepmd_c -Wl,-rpath=$deepmd_root/lib -Wl,-rpath=$tensorflow_root/lib -o infer_
water_hpp

```

and then run the program:

```
./infer_water_hpp
```

In some cases, one may want to pass the custom neighbor list instead of the native neighbor list. The above code can be revised as follows:

```
// neighbor list
std::vector<std::vector<int>> nlist_vec = {
    {1, 2},
    {0, 2},
    {0, 1}
};
std::vector<int>  ilist(3), numneigh(3);
std::vector<int*> firstneigh(3);
InputNlist nlist(3, &ilist[0], &numneigh[0], &firstneigh[0]);
convert_nlist(nlist, nlist_vec);
dp.compute(e, f, v, coord, atype, cell, 0, nlist, 0);
```

Here, `nlist_vec` means the neighbors of atom 0 are atom 1 and atom 2, the neighbors of atom 1 are atom 0 and atom 2, and the neighbors of atom 2 are atom 0 and atom 1.

8.3 Node.js interface

If `Node.js interface` is installed, one can use the Node.js interface for model inference, which is a wrapper of the header-only C++ API.

A simple example is shown below.

```
const deepmd = require("deepmd-kit");

const dp = new deepmd.DeepPot("graph.pb");

const coord = [1., 0., 0., 0., 0., 1.5, 1., 0., 3.];
const atype = [1, 0, 1];
const cell = [10., 0., 0., 0., 10., 0., 0., 0., 10.];

const v_coord = new deepmd.vectord(coord.length);
const v_atype = new deepmd.vectori(atype.length);
const v_cell = new deepmd.vectord(cell.length);
for (var i = 0; i < coord.length; i++) v_coord.set(i, coord[i]);
for (var i = 0; i < atype.length; i++) v_atype.set(i, atype[i]);
for (var i = 0; i < cell.length; i++) v_cell.set(i, cell[i]);

var energy = 0.0
var v_forces = new deepmd.vectord();
var v_virials = new deepmd.vectord();

energy = dp.compute(energy, v_forces, v_virials, v_coord, v_atype, v_cell);

console.log("energy:", energy);
console.log("forces:", [...Array(v_forces.size()).keys()].map(i => v_forces.get(i)));
console.log("virials:", [...Array(v_virials.size()).keys()].map(i => v_virials.get(i)));
```

Energy, forces, and virials will be printed to the screen.

COMMAND LINE INTERFACE

DeePMD-kit: A deep learning package for many-body potential energy representation and molecular dynamics

```
usage: dp [-h] [--version]
          {transfer,train,freeze,test,compress,doc-train-input,model-devi,convert-from,neighbor-
↪stat,train-nvnmd}
          ...
```

9.1 Named Arguments

| | |
|------------------------|--|
| <code>--version</code> | show program's version number and exit |
|------------------------|--|

9.2 Valid subcommands

| | |
|----------------------|--|
| <code>command</code> | Possible choices: transfer, train, freeze, test, compress, doc-train-input, model-devi, convert-from, neighbor-stat, train-nvnmd |
|----------------------|--|

9.3 Sub-commands

9.3.1 transfer

pass parameters to another model

```
dp transfer [-h] [-v {DEBUG,3,INFO,2,WARNING,1,ERROR,0}] [-l LOG_PATH]
            [-r RAW_MODEL] [-O OLD_MODEL] [-o OUTPUT]
```

Named Arguments

| | |
|------------------------------|--|
| <code>-v, --log-level</code> | <p>Possible choices: DEBUG, 3, INFO, 2, WARNING, 1, ERROR, 0</p> <p>set verbosity level by string or number, 0=ERROR, 1=WARNING, 2=INFO and 3=DEBUG</p> <p>Default: “INFO”</p> |
| <code>-l, --log-path</code> | <p>set log file to log messages to disk, if not specified, the logs will only be output to console</p> |
| <code>-r, --raw-model</code> | <p>the model receiving parameters</p> <p>Default: “raw_frozen_model.pb”</p> |
| <code>-O, --old-model</code> | <p>the model providing parameters</p> <p>Default: “old_frozen_model.pb”</p> |
| <code>-o, --output</code> | <p>the model after passing parameters</p> <p>Default: “frozen_model.pb”</p> |

9.3.2 train

train a model

```
dp train [-h] [-v {DEBUG,3,INFO,2,WARNING,1,ERROR,0}] [-l LOG_PATH]
        [-m {master,collect,workers}]
        [-i INIT_MODEL | -r RESTART | -f INIT_FRZ_MODEL | -t FINETUNE]
        [-o OUTPUT] [--skip-neighbor-stat]
        INPUT
```

Positional Arguments

| | |
|-------|---|
| INPUT | the input parameter file in json or yaml format |
|-------|---|

Named Arguments

| | |
|-------------------------------|--|
| <code>-v, --log-level</code> | <p>Possible choices: DEBUG, 3, INFO, 2, WARNING, 1, ERROR, 0</p> <p>set verbosity level by string or number, 0=ERROR, 1=WARNING, 2=INFO and 3=DEBUG</p> <p>Default: “INFO”</p> |
| <code>-l, --log-path</code> | <p>set log file to log messages to disk, if not specified, the logs will only be output to console</p> |
| <code>-m, --mpi-log</code> | <p>Possible choices: master, collect, workers</p> <p>Set the manner of logging when running with MPI. ‘master’ logs only on main process, ‘collect’ broadcasts logs from workers to master and ‘workers’ means each process will output its own log</p> <p>Default: “master”</p> |
| <code>-i, --init-model</code> | <p>Initialize the model by the provided checkpoint.</p> |

- r, --restart Restart the training from the provided checkpoint.
- f, --init-frz-model Initialize the training from the frozen model.
- t, --finetune Finetune the frozen pretrained model.
- o, --output The output file of the parameters used in training.
Default: “out.json”
- skip-neighbor-stat Skip calculating neighbor statistics. Sel checking, automatic sel, and
model compression will be disabled.
Default: False

examples:

```
dp train input.json dp train input.json -restart model.ckpt dp train input.json -init-model model.ckpt
```

9.3.3 freeze

freeze the model

```
dp freeze [-h] [-v {DEBUG,3,INFO,2,WARNING,1,ERROR,0}] [-l LOG_PATH]
          [-c CHECKPOINT_FOLDER] [-o OUTPUT] [-n NODE_NAMES] [-w NVNMD_WEIGHT]
          [--united-model]
```

Named Arguments

- v, --log-level Possible choices: DEBUG, 3, INFO, 2, WARNING, 1, ERROR, 0
set verbosity level by string or number, 0=ERROR, 1=WARNING,
2=INFO and 3=DEBUG
Default: “INFO”
- l, --log-path set log file to log messages to disk, if not specified, the logs will only be
output to console
- c, --checkpoint-folder path to checkpoint folder
Default: “.”
- o, --output name of graph, will output to the checkpoint folder
Default: “frozen_model.pb”
- n, --node-names the frozen nodes, if not set, determined from the model type
- w, --nvnmd-weight the name of weight file (.npy), if set, save the model’s weight into the file
- united-model When in multi-task mode, freeze all nodes into one united model
Default: False

examples:

```
dp freeze dp freeze -o graph.pb
```

9.3.4 test

test the model

```
dp test [-h] [-v {DEBUG,3,INFO,2,WARNING,1,ERROR,0}] [-l LOG_PATH] [-m MODEL]
        [-s SYSTEM | -f DATAFILE] [-S SET_PREFIX] [-n NUMB_TEST]
        [-r RAND_SEED] [--shuffle-test] [-d DETAIL_FILE] [-a]
```

Named Arguments

| | |
|-------------------|---|
| -v, --log-level | Possible choices: DEBUG, 3, INFO, 2, WARNING, 1, ERROR, 0 set verbosity level by string or number, 0=ERROR, 1=WARNING, 2=INFO and 3=DEBUG Default: "INFO" |
| -l, --log-path | set log file to log messages to disk, if not specified, the logs will only be output to console |
| -m, --model | Frozen model file to import Default: "frozen_model.pb" |
| -s, --system | The system dir. Recursively detect systems in this directory Default: "." |
| -f, --datafile | The path to file of test list. |
| -S, --set-prefix | The set prefix Default: "set" |
| -n, --numb-test | The number of data for test. 0 means all data. Default: 0 |
| -r, --rand-seed | The random seed |
| --shuffle-test | Shuffle test data Default: False |
| -d, --detail-file | The prefix to files where details of energy, force and virial accuracy/accuracy per atom will be written |
| -a, --atomic | Test the accuracy of atomic label, i.e. energy / tensor (dipole, polar) Default: False |

examples:

```
dp test -m graph.pb -s /path/to/system -n 30
```

9.3.5 compress

compress a model

```
dp compress [-h] [-v {DEBUG,3,INFO,2,WARNING,1,ERROR,0}] [-l LOG_PATH]
            [-m {master,collect,workers}] [-i INPUT] [-o OUTPUT] [-s STEP]
            [-e EXTRAPOLATE] [-f FREQUENCY] [-c CHECKPOINT_FOLDER]
            [-t TRAINING_SCRIPT]
```

Named Arguments

| | |
|-------------------|--|
| -v, --log-level | <p>Possible choices: DEBUG, 3, INFO, 2, WARNING, 1, ERROR, 0</p> <p>set verbosity level by string or number, 0=ERROR, 1=WARNING, 2=INFO and 3=DEBUG</p> <p>Default: "INFO"</p> |
| -l, --log-path | <p>set log file to log messages to disk, if not specified, the logs will only be output to console</p> |
| -m, --mpi-log | <p>Possible choices: master, collect, workers</p> <p>Set the manner of logging when running with MPI. 'master' logs only on main process, 'collect' broadcasts logs from workers to master and 'workers' means each process will output its own log</p> <p>Default: "master"</p> |
| -i, --input | <p>The original frozen model, which will be compressed by the code</p> <p>Default: "frozen_model.pb"</p> |
| -o, --output | <p>The compressed model</p> <p>Default: "frozen_model_compressed.pb"</p> |
| -s, --step | <p>Model compression uses fifth-order polynomials to interpolate the embedding-net. It introduces two tables with different step size to store the parameters of the polynomials. The first table covers the range of the training data, while the second table is an extrapolation of the training data. The domain of each table is uniformly divided by a given step size. And the step(parameter) denotes the step size of the first table and the second table will use 10 * step as it's step size to save the memory. Usually the value ranges from 0.1 to 0.001. Smaller step means higher accuracy and bigger model size</p> <p>Default: 0.01</p> |
| -e, --extrapolate | <p>The domain range of the first table is automatically detected by the code: [d_low, d_up]. While the second table ranges from the first table's upper boundary(d_up) to the extrapolate(parameter) * d_up: [d_up, extrapolate * d_up]</p> <p>Default: 5</p> |
| -f, --frequency | <p>The frequency of tabulation overflow check(Whether the input environment matrix overflow the first or second table range). By default do not check the overflow</p> <p>Default: -1</p> |

- c, --checkpoint-folder path to checkpoint folder
Default: “model-compression”
- t, --training-script The training script of the input frozen model

examples:

```
dp compress dp compress -i graph.pb -o compressed.pb
```

9.3.6 doc-train-input

print the documentation (in rst format) of input training parameters.

```
dp doc-train-input [-h] [-v {DEBUG,3,INFO,2,WARNING,1,ERROR,0}] [-l LOG_PATH]
                  [--out-type {rst,json}]
```

Named Arguments

- v, --log-level Possible choices: DEBUG, 3, INFO, 2, WARNING, 1, ERROR, 0
set verbosity level by string or number, 0=ERROR, 1=WARNING, 2=INFO and 3=DEBUG
Default: “INFO”
- l, --log-path set log file to log messages to disk, if not specified, the logs will only be output to console
- out-type Possible choices: rst, json
The output type
Default: “rst”

9.3.7 model-devi

calculate model deviation

```
dp model-devi [-h] [-v {DEBUG,3,INFO,2,WARNING,1,ERROR,0}] [-l LOG_PATH]
               [-m MODELS [MODELS ...]] [-s SYSTEM] [-S SET_PREFIX] [-o OUTPUT]
               [-f FREQUENCY] [--real_error]
```

Named Arguments

- v, --log-level Possible choices: DEBUG, 3, INFO, 2, WARNING, 1, ERROR, 0
set verbosity level by string or number, 0=ERROR, 1=WARNING, 2=INFO and 3=DEBUG
Default: “INFO”
- l, --log-path set log file to log messages to disk, if not specified, the logs will only be output to console
- m, --models Frozen models file to import
Default: ['graph.000.pb', 'graph.001.pb', 'graph.002.pb', 'graph.003.pb']

| | |
|------------------|--|
| -s, --system | The system directory. Recursively detect systems in this directory. Default: “.” |
| -S, --set-prefix | The set prefix Default: “set” |
| -o, --output | The output file for results of model deviation Default: “model_devi.out” |
| -f, --frequency | The trajectory frequency of the system Default: 1 |
| --real_error | Calculate the RMS real error of the model. The real data should be given in the systems. Default: False |

examples:

```
dp model-devi -m graph.000.pb graph.001.pb graph.002.pb graph.003.pb -s ./data -o model_devi.out
```

9.3.8 convert-from

convert lower model version to supported version

```
dp convert-from [-h] [-v {DEBUG,3,INFO,2,WARNING,1,ERROR,0}] [-l LOG_PATH]
                [-i INPUT_MODEL] [-o OUTPUT_MODEL]
                [{auto,0.12,1.0,1.1,1.2,1.3,2.0,pbtxt}]
```

Positional Arguments

| | |
|------|---|
| FROM | Possible choices: auto, 0.12, 1.0, 1.1, 1.2, 1.3, 2.0, pbtxt The original model compatibility Default: “auto” |
|------|---|

Named Arguments

| | |
|--------------------|---|
| -v, --log-level | Possible choices: DEBUG, 3, INFO, 2, WARNING, 1, ERROR, 0 set verbosity level by string or number, 0=ERROR, 1=WARNING, 2=INFO and 3=DEBUG Default: “INFO” |
| -l, --log-path | set log file to log messages to disk, if not specified, the logs will only be output to console |
| -i, --input-model | the input model Default: “frozen_model.pb” |
| -o, --output-model | the output model Default: “convert_out.pb” |

examples:

```
dp convert-from -i graph.pb -o graph_new.pb dp convert-from auto -i graph.pb -o graph_new.pb dp
convert-from 1.0 -i graph.pb -o graph_new.pb
```

9.3.9 neighbor-stat

Calculate neighbor statistics

```
dp neighbor-stat [-h] [-v {DEBUG,3,INFO,2,WARNING,1,ERROR,0}] [-l LOG_PATH]
                 [-s SYSTEM] -r RCUT -t TYPE_MAP [TYPE_MAP ...] [--one-type]
```

Named Arguments

| | |
|------------------------------|---|
| <code>-v, --log-level</code> | Possible choices: DEBUG, 3, INFO, 2, WARNING, 1, ERROR, 0 set verbosity level by string or number, 0=ERROR, 1=WARNING, 2=INFO and 3=DEBUG Default: "INFO" |
| <code>-l, --log-path</code> | set log file to log messages to disk, if not specified, the logs will only be output to console |
| <code>-s, --system</code> | The system dir. Recursively detect systems in this directory Default: "." |
| <code>-r, --rcut</code> | cutoff radius |
| <code>-t, --type-map</code> | type map |
| <code>--one-type</code> | treat all types as a single type. Used with se_atten descriptor. Default: False |

examples:

```
dp neighbor-stat -s data -r 6.0 -t O H
```

9.3.10 train-nvnmd

train nvnmd model

```
dp train-nvnmd [-h] [-v {DEBUG,3,INFO,2,WARNING,1,ERROR,0}] [-l LOG_PATH]
                [-r RESTART] [-s {s1,s2}] [--skip-neighbor-stat]
                INPUT
```

Positional Arguments

INPUT the input parameter file in json format

Named Arguments

-v, --log-level Possible choices: DEBUG, 3, INFO, 2, WARNING, 1, ERROR, 0
 set verbosity level by string or number, 0=ERROR, 1=WARNING,
 2=INFO and 3=DEBUG
 Default: "INFO"

-l, --log-path set log file to log messages to disk, if not specified, the logs will only be
 output to console

-r, --restart Restart the training from the provided checkpoint.

-s, --step Possible choices: s1, s2
 steps to train model of NVNMD: s1 (train CNN), s2 (train QNN)
 Default: "s1"

--skip-neighbor-stat Skip calculating neighbor statistics. Sel checking, automatic sel, and
 model compression will be disabled.
 Default: False

INTEGRATE WITH THIRD-PARTY PACKAGES

Note that the model for inference is required to be compatible with the DeePMD-kit package. See [Model compatibility](#) for details.

10.1 Use deep potential with ASE

Deep potential can be set up as a calculator with ASE to obtain potential energies and forces.

```
from ase import Atoms
from deepmd.calculator import DP

water = Atoms(
    "H2O",
    positions=[(0.7601, 1.9270, 1), (1.9575, 1, 1), (1.0, 1.0, 1.0)],
    cell=[100, 100, 100],
    calculator=DP(model="frozen_model.pb"),
)
print(water.get_potential_energy())
print(water.get_forces())
```

Optimization is also available:

```
from ase.optimize import BFGS

dyn = BFGS(water)
dyn.run(fmax=1e-6)
print(water.get_positions())
```

10.2 Run MD with LAMMPS

Running an MD simulation with LAMMPS is simpler. In the LAMMPS input file, one needs to specify the pair style as follows

```
pair_style      deepmd graph.pb
pair_coeff      * * O H
```

where `graph.pb` is the file name of the frozen model. `pair_coeff` maps atom names (O H) with LAMMPS atom types (integers from 1 to Ntypes, i.e. 1 2).

10.3 LAMMPS commands

10.3.1 Enable DeePMD-kit plugin (plugin mode)

If you are using the plugin mode, enable DeePMD-kit package in LAMMPS with `plugin` command:

```
plugin load libdeepmd_lmp.so
```

After LAMMPS version `patch_24Mar2022`, another way to load plugins is to set the environmental variable `LAMMPS_PLUGIN_PATH`:

```
LAMMPS_PLUGIN_PATH=$deepmd_root/lib/deepmd_lmp
```

where `$deepmd_root` is the directory to [install C++ interface](#).

The built-in mode doesn't need this step.

10.3.2 `pair_style deepmd`

The DeePMD-kit package provides the `pair_style deepmd`

```
pair_style deepmd models ... keyword value ...
```

- `deepmd` = style of this `pair_style`
- `models` = frozen model(s) to compute the interaction. If multiple models are provided, then only the first model serves to provide energy and force prediction for each timestep of molecular dynamics, and the model deviation will be computed among all models every `out_freq` timesteps.
- `keyword` = `out_file` or `out_freq` or `fparam` or `fparam_from_compute` or `atomic` or `relative` or `relative_v` or `aparam` or `ttm`

Examples

```
pair_style deepmd graph.pb
pair_style deepmd graph.pb fparam 1.2
pair_style deepmd graph_0.pb graph_1.pb graph_2.pb out_file md.out out_freq 10 atomic relative 1.0
pair_coeff * * O H

pair_style deepmd cp.pb fparam_from_compute TEMP
compute TEMP all temp
```

Description

Evaluate the interaction of the system by using [Deep Potential](#) or [Deep Potential Smooth Edition](#). It is noticed that deep potential is not a “pairwise” interaction, but a multi-body interaction.

This pair style takes the deep potential defined in a model file that usually has the `.pb` extension. The model can be trained and frozen by package [DeePMD-kit](#), which can have either double or single float precision interface.

The model deviation evaluates the consistency of the force predictions from multiple models. By default, only the maximal, minimal and average model deviations are output. If the key `atomic` is set, then the model deviation of force prediction of each atom will be output.

By default, the model deviation is output in absolute value. If the keyword `relative` is set, then the relative model deviation of the force will be output, including values output by the keyword `atomic`. The relative model deviation of the force on atom i is defined by

$$E_{f_i} = \frac{|D_{f_i}|}{|f_i| + l}$$

where D_{f_i} is the absolute model deviation of the force on atom i , f_i is the norm of the force and l is provided as the parameter of the keyword `relative`. If the keyword `relative_v` is set, then the relative model deviation of the virial will be output instead of the absolute value, with the same definition of that of the force:

$$E_{v_i} = \frac{|D_{v_i}|}{|v_i| + l}$$

If the keyword `fparam` is set, the given frame parameter(s) will be fed to the model. If the keyword `fparam_from_compute` is set, the global parameter(s) from compute command (e.g., temperature from `compute temp command`) will be fed to the model as the frame parameter(s). If the keyword `aparam` is set, the given atomic parameter(s) will be fed to the model, where each atom is assumed to have the same atomic parameter(s). If the keyword `ttm` is set, electronic temperatures from `fix ttm command` will be fed to the model as the atomic parameters.

Only a single `pair_coeff` command is used with the deepmd style which specifies atom names. These are mapped to LAMMPS atom types (integers from 1 to Ntypes) by specifying Ntypes additional arguments after `*` in the `pair_coeff` command. If atom names are not set in the `pair_coeff` command, the training parameter `type_map` will be used by default. If a mapping value is specified as `NULL`, the mapping is not performed. This can be used when a deepmd potential is used as part of the hybrid pair style. The `NULL` values are placeholders for atom types that will be used with other potentials. If the training parameter `type_map` is not set, atom names in the `pair_coeff` command cannot be set. In this case, atom type indexes in `type.raw` (integers from 0 to Ntypes-1) will map to LAMMPS atom types.

Spin is specified by keywords `virtual_len` and `spin_norm`. If the keyword `virtual_len` is set, the distance between virtual atom and its corresponding real atom for each type of magnetic atoms will be fed to the model as the spin parameters. If the keyword `spin_norm` is set, the magnitude of the magnetic moment for each type of magnetic atoms will be fed to the model as the spin parameters.

Restrictions

- The deepmd pair style is provided in the USER-DEEPMK package, which is compiled from the DeePMD-kit, visit the [DeePMD-kit website](#) for more information.

10.3.3 Compute tensorial properties

The DeePMD-kit package provides the compute `deeptensor/atom` for computing atomic tensorial properties.

```
compute ID group-ID deeptensor/atom model_file
```

- ID: user-assigned name of the computation
- group-ID: ID of the group of atoms to compute
- deeptensor/atom: the style of this compute
- model_file: the name of the binary model file.

At this time, the training parameter `type_map` will be mapped to LAMMPS atom types.

Examples

```
compute          dipole all deeptensor/atom dipole.pb
```

The result of the compute can be dumped to trajectory file by

```
dump            1 all custom 100 water.dump id type c_dipole[1] c_dipole[2] c_dipole[3]
```

Restrictions

- The `deeptensor/atom` compute is provided in the USER-DEEPMO package, which is compiled from the DeePMD-kit, visit the [DeePMD-kit website](#) for more information.

10.3.4 Long-range interaction

The reciprocal space part of the long-range interaction can be calculated by LAMMPS command `kpspace_style`. To use it with DeePMD-kit, one writes

```
pair_style      deepmd graph.pb
pair_coeff      * *
kpspace_style    pppm 1.0e-5
kpspace_modify   gewald 0.45
```

Please notice that the DeePMD does nothing to the direct space part of the electrostatic interaction, because this part is assumed to be fitted in the DeePMD model (the direct space cut-off is thus the cut-off of the DeePMD model). The splitting parameter `gewald` is modified by the `kpspace_modify` command.

10.3.5 Use of the centroid/stress/atom to get the full 3x3 “atomic-virial”

The DeePMD-kit also allows the computation of per-atom stress tensor defined as:

$$d_{\text{vatom}} = - \sum_m (r_n - r_m) \frac{de_m}{dr_n}$$

Where r_n is the atomic position of n th atom, v_n velocity of the atom and $\frac{de_m}{dr_n}$ the derivative of the atomic energy.

In LAMMPS one can get the per-atom stress using the command `centroid/stress/atom`:

```
compute ID group-ID centroid/stress/atom NULL virial
```

see [LAMMPS doc page](#) for more details on the meaning of the keywords.

Changed in version v2.2.3: v2.2.2 or previous versions passed per-atom stress (`cvatom`) with the per-atom pressure tensor, which is inconsistent with LAMMPS's definition. LAMMPS defines per-atom stress as the negative of the per-atom pressure tensor. Such behavior is corrected in v2.2.3.

Examples

In order of computing the 9-component per-atom stress

```
compute stress all centroid/stress/atom NULL virial
```

Thus `c_stress` is an array with 9 components in the order `xx,yy,zz,xy,xz,yz,yx,zx,zy`.

If you use this feature please cite D. Tisi, L. Zhang, R. Bertossa, H. Wang, R. Car, S. Baroni - arXiv preprint arXiv:2108.10850, 2021

10.3.6 Computation of heat flux

Using a per-atom stress tensor one can, for example, compute the heat flux defined as:

$$J = \sum_n e_n v_n + \sum_{n,m} (r_m - r_n) \frac{de_m}{dr_n} v_n$$

to compute the heat flux with LAMMPS:

```
compute ke_ID all ke/atom
compute pe_ID all pe/atom
compute stress_ID group-ID centroid/stress/atom NULL virial
compute flux_ID all heat/flux ke_ID pe_ID stress_ID
```

Examples

```
compute ke all ke/atom
compute pe all pe/atom
compute stress all centroid/stress/atom NULL virial
compute flux all heat/flux ke pe stress
```

`c_flux` is a global vector of length 6. The first three components are the x , y and z components of the full heat flux vector. The others are the components of the so-called convective portion, see [LAMMPS doc page](#) for more details.

If you use these features please cite D. Tisi, L. Zhang, R. Bertossa, H. Wang, R. Car, S. Baroni - arXiv preprint arXiv:2108.10850, 2021

10.4 Run path-integral MD with i-PI

The i-PI works in a client-server model. The i-PI provides the server for integrating the replica positions of atoms, while the DeePMD-kit provides a client named `dp_ipi` that computes the interactions (including energy, forces and virials). The server and client communicate via the Unix domain socket or the Internet socket. Installation instructions for i-PI can be found [here](#). The client can be started by

```
i-pi input.xml &
dp_ipi water.json
```

It is noted that multiple instances of the client allow for computing, in parallel, the interactions of multiple replicas of the path-integral MD.

`water.json` is the parameter file for the client `dp_ipi`, and an example is provided:

```
{
  "verbose":          false,
  "use_unix":         true,
  "port":             31415,
  "host":             "localhost",
  "graph_file":       "graph.pb",
  "coord_file":       "conf.xyz",
  "atom_type" : {
    "OW":             0,
    "HW1":            1,
    "HW2":            1
  }
}
```

The option `use_unix` is set to `true` to activate the Unix domain socket, otherwise, the Internet socket is used.

The option `port` should be the same as that in `input.xml`:

```
<port>31415</port>
```

The option `graph_file` provides the file name of the frozen model. The model can have either double or single float precision interface.

The `dp_ipi` gets the atom names from an `XYZ` file provided by `coord_file` (meanwhile ignores all coordinates in it) and translates the names to atom types by rules provided by `atom_type`.

10.5 Running MD with GROMACS

10.5.1 DP/MM Simulation

This part gives a simple tutorial on how to run a DP/MM simulation for methane in water, which means using DP for methane and TIP3P for water. All relevant files can be found in `examples/methane`.

Topology Preparation

Similar to QM/MM simulation, the internal interactions (including bond, angle, dihedrals, LJ, Columb) of the region described by a neural network potential (NNP) have to be turned off. In GROMACS, bonded interactions can be turned off by modifying [`bonds`], [`angles`], [`dihedrals`] and [`pairs`] sections. And LJ and Columb interactions must be turned off by [`exclusions`] section.

For example, if one wants to simulate ethane in water, using DeepPotential for methane and TIP3P for water, the topology of methane should be like the following (as presented in `examples/methane/methane.itp`):

```
[ atomtypes ]
;name btype  mass  charge ptype    sigma  epsilon
c3    c3    0.0    0.0    A  0.339771 0.451035
hc    hc    0.0    0.0    A  0.260018 0.087027

[ moleculetype ]
;name          nrexcl
methane        3

[ atoms ]
; nr  type  resnr residue atom  cgnr  charge  mass
```

(continues on next page)

(continued from previous page)

```

1  c3      1  MOL  C1   1 -0.1068 12.010
2  hc      1  MOL  H1   2  0.0267  1.008
3  hc      1  MOL  H2   3  0.0267  1.008
4  hc      1  MOL  H3   4  0.0267  1.008
5  hc      1  MOL  H4   5  0.0267  1.008

```

```
[ bonds ]
```

```
; i j func b0 kb
```

```

1  2      5
1  3      5
1  4      5
1  5      5

```

```
[ exclusions ]
```

```
; ai aj1 aj2 aj3 aj4
```

```

1  2  3  4  5
2  1  3  4  5
3  1  2  4  5
4  1  2  3  5
5  1  2  3  4

```

For comparison, the original topology file generated by acpype will be:

```
; methane_GMX.itp created by acpype (v: 2021-02-05T22:15:50CET) on Wed Sep  8 01:21:53 2021
```

```
[ atomtypes ]
```

```

;name  bond_type      mass      charge  ptype  sigma      epsilon      Amb
c3      c3            0.00000  0.00000  A      3.39771e-01  4.51035e-01 ; 1.91  0.1078
hc      hc            0.00000  0.00000  A      2.60018e-01  8.70272e-02 ; 1.46  0.0208

```

```
[ moleculetype ]
```

```

;name      nrexcl
methane      3

```

```
[ atoms ]
```

```

;  nr  type  resi  res  atom  cgnr      charge      mass      ; qtot  bond_type
   1  c3     1  MOL  C1    1   -0.106800   12.01000 ; qtot -0.107
   2  hc     1  MOL  H1    2    0.026700    1.00800 ; qtot -0.080
   3  hc     1  MOL  H2    3    0.026700    1.00800 ; qtot -0.053
   4  hc     1  MOL  H3    4    0.026700    1.00800 ; qtot -0.027
   5  hc     1  MOL  H4    5    0.026700    1.00800 ; qtot  0.000

```

```
[ bonds ]
```

```

;  ai  aj  funct  r      k
   1  2  1      1.0970e-01  3.1455e+05 ; C1 - H1
   1  3  1      1.0970e-01  3.1455e+05 ; C1 - H2
   1  4  1      1.0970e-01  3.1455e+05 ; C1 - H3
   1  5  1      1.0970e-01  3.1455e+05 ; C1 - H4

```

```
[ angles ]
```

```

;  ai  aj  ak  funct  theta      cth
   2  1  3    1      1.0758e+02  3.2635e+02 ; H1 - C1 - H2
   2  1  4    1      1.0758e+02  3.2635e+02 ; H1 - C1 - H3
   2  1  5    1      1.0758e+02  3.2635e+02 ; H1 - C1 - H4
   3  1  4    1      1.0758e+02  3.2635e+02 ; H2 - C1 - H3
   3  1  5    1      1.0758e+02  3.2635e+02 ; H2 - C1 - H4
   4  1  5    1      1.0758e+02  3.2635e+02 ; H3 - C1 - H4

```

DeepMD Settings

Before running simulations, we need to tell GROMACS to use DeepPotential by setting the environment variable `GMX_DEEPMD_INPUT_JSON`:

```
export GMX_DEEPMD_INPUT_JSON=input.json
```

Then, in your working directories, we have to write `input.json` file:

```
{
  "graph_file": "/path/to/graph.pb",
  "type_file": "type.raw",
  "index_file": "index.raw",
  "lambda": 1.0,
  "pbc": false
}
```

Here is an explanation for these settings:

- `graph_file`: The graph file (with suffix `.pb`) generated by `dp freeze` command
- `type_file`: File to specify DP atom types (in space-separated format). Here, `type.raw` looks like

```
1 0 0 0 0
```

- `index_file`: File containing indices of DP atoms (in space-separated format), which should be consistent with the indices' order in `.gro` file but starting from zero. Here, `index.raw` looks like

```
0 1 2 3 4
```

- `lambda`: Optional, default 1.0. Used in alchemical calculations.
- `pbc`: Optional, default true. If true, the GROMACS periodic condition is passed to DeepMD.

Run Simulation

Finally, you can run GROMACS using `gmx mdrun` as usual.

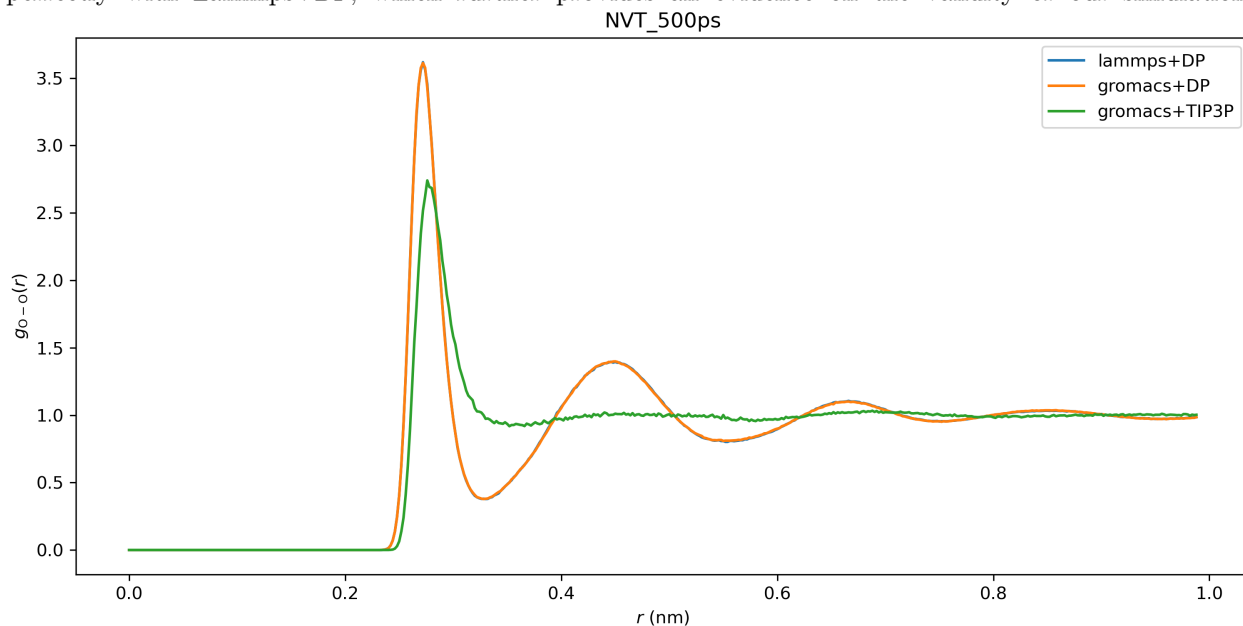
10.5.2 All-atom DP Simulation

This part gives an example of how to simulate all atoms described by a DeepPotential with Gromacs, taking water as an example. Instead of using `[exclusions]` to turn off the non-bonded energies, we can simply do this by setting LJ parameters (i.e. `epsilon` and `sigma`) and partial charges to 0, as shown in `examples/water/gmx/water.top`:

```
[ atomtypes ]
; name      at.num  mass      charge ptype  sigma      epsilon
HW          1       1.008    0.0000  A    0.00000e+00  0.00000e+00
OW          8       16.00    0.0000  A    0.00000e+00  0.00000e+00
```

As mentioned in the above section, `input.json` and relevant files (`index.raw`, `type.raw`) should also be created. Then, we can start the simulation under the NVT ensemble and plot the radial distribution function (RDF) by `gmx rdf` command. We can see that the RDF given by Gromacs+DP matches

perfectly with Lammmps+DP, which further provides an evidence on the validity of our simulation.



However, we still recommend you run an all-atom DP simulation using LAMMPS since it is more stable and efficient.

10.6 Interfaces out of DeePMD-kit

The codes of the following interfaces are not a part of the DeePMD-kit package and maintained by other repositories. We list these interfaces here for user convenience.

10.6.1 dpdata

`dpdata` provides the `predict` method for `System` class:

```
import dpdata

dsys = dpdata.LabeledSystem("OUTCAR")
dp_sys = dsys.predict("frozen_model_compressed.pb")
```

By inferring with the DP model `frozen_model_compressed.pb`, `dpdata` will generate a new labeled system `dp_sys` with inferred energies, forces, and virials.

10.6.2 OpenMM plugin for DeePMD-kit

An [OpenMM](#) plugin is provided from [JingHuangLab/openmm_deepmd_plugin](#), written by the [Huang Lab](#) at Westlake University.

10.6.3 AMBER interface to DeePMD-kit

An [AMBER](#) interface to DeePMD-kit is written by the [\[York Lab\]](#) from Rutgers University. It is open-source at [GitLab RutgersLBSR/AmberDPRc](#). Details can be found in [this paper](#).

10.6.4 DP-GEN

[DP-GEN](#) provides a workflow to generate accurate DP models by calling DeePMD-kit's command line interface (CLI) in the local or remote server. Details can be found in [this paper](#).

10.6.5 MLatom

[MLatom](#) provides an interface to the DeePMD-kit within MLatom's workflow by calling DeePMD-kit's CLI. Details can be found in [this paper](#).

10.6.6 ABACUS

[ABACUS](#) can run molecular dynamics with a DP model. User is required to [build ABACUS with DeePMD-kit](#).

USE NVNMD

11.1 Introduction

NVNMD stands for non-von Neumann molecular dynamics.

This is the training code we used to generate the results in our paper entitled “Accurate and Efficient Molecular Dynamics based on Machine Learning and non von Neumann Architecture”, which has been accepted by npj Computational Materials (DOI: [10.1038/s41524-022-00773-z](https://doi.org/10.1038/s41524-022-00773-z)).

Any user can follow two consecutive steps to run molecular dynamics (MD) on the proposed NVNMD computer, which has been released online: (i) to train a machine learning (ML) model that can decently reproduce the potential energy surface (PES); and (ii) to deploy the trained ML model on the proposed NVNMD computer, then run MD there to obtain the atomistic trajectories.

11.2 Training

Our training procedure consists of not only continuous neural network (CNN) training but also quantized neural network (QNN) training which uses the results of CNN as inputs. It is performed on CPU or GPU by using the training codes we open-sourced online.

To train an ML model that can decently reproduce the PES, a training and testing data set should be prepared first. This can be done by using either the state-of-the-art active learning tools or the outdated (i.e., less efficient) brute-force density functional theory (DFT)-based ab-initio molecular dynamics (AIMD) sampling.

If you just want to simply test the training function, you can use the example in the `$deepmd_source_dir/examples/nvnmd` directory. If you want to fully experience training and running MD functions, you can download the complete example from the [website](#).

Then, copy the data set to the working directory

```
mkdir -p $workspace
cd $workspace
mkdir -p data
cp -r $dataset data
```

where `$dataset` is the path to the data set and `$workspace` is the path to the working directory.

11.2.1 Input script

Create and go to the training directory.

```
mkdir train
cd train
```

Then copy the input script `train_cnn.json` and `train_qnn.json` to the directory `train`

```
cp -r $deepmd_source_dir/examples/nvnmd/train/train_cnn.json train_cnn.json
cp -r $deepmd_source_dir/examples/nvnmd/train/train_qnn.json train_qnn.json
```

The structure of the input script is as follows

```
{
  "nvnmd" : {},
  "learning_rate" : {},
  "loss" : {},
  "training": {}
}
```

nvnmd

The “nvnmd” section is defined as

```
{
  "version": 0,
  "net_size": 128,
  "sel": [60, 60],
  "rcut": 6.0,
  "rcut_smth": 0.5,
  "type_map": ["Ge", "Te"]
}
```

where items are defined as:

| Item | Mean | Optional Value |
|-----------|--|---|
| version | the version of network structure | 0 or 1 |
| net_size | the size of nueral network | 128 |
| sel | the number of neighbors | version 0: integer list of lengths 1 to 4 are acceptable; version 1: integer |
| rcut | the cutoff radial | (0, 8.0] |
| rcut_smth | the smooth cutoff parameter | (0, 8.0] |
| type_map | mapping atom type to the name (str) of the type | string list, optional |

Multiple versions of the nvnmd model correspond to different network structures. `nvnmd-v0` and `nvnmd-v1` differ in the following ways:

1. `nvnmd-v0` and `nvnmd-v1` use the `se_a` descriptor and `se_atten` descriptor, respectively
2. `nvnmd-v0` has 1 set of parameters for each element and supports up to 4 element types. `nvnmd-v1` shares 1 set of parameters for each element and supports up to 31 types.
3. `nvnmd-v0` distinguishes between neighboring atoms, so `sel` is a list of integers. `nvnmd-v1` does not distinguish between neighboring atoms, so `sel` is an integer.

learning_rate

The “learning_rate” section is defined as

```
{
  "type": "exp",
  "start_lr": 1e-3,
  "stop_lr": 3e-8,
  "decay_steps": 5000
}
```

where items are defined as:

| Item | Mean | Optional Value |
|-------------|--|------------------------|
| type | learning rate variant type | exp |
| start_lr | the learning rate at the beginning of the training | a positive real number |
| stop_lr | the desired learning rate at the end of the training | a positive real number |
| decay_stops | the learning rate is decaying every {decay_stops} training steps | a positive integer |

loss

The “loss” section is defined as

```
{
  "start_pref_e": 0.02,
  "limit_pref_e": 2,
  "start_pref_f": 1000,
  "limit_pref_f": 1,
  "start_pref_v": 0,
  "limit_pref_v": 0
}
```

where items are defined as:

| Item | Mean | Optional Value |
|--------------|--|------------------------------|
| start_pref_e | the loss factor of energy at the beginning of the training | zero or positive real number |
| limit_pref_e | the loss factor of energy at the end of the training | zero or positive real number |
| start_pref_f | the loss factor of force at the beginning of the training | zero or positive real number |
| limit_pref_f | the loss factor of force at the end of the training | zero or positive real number |
| start_pref_v | the loss factor of virial at the beginning of the training | zero or positive real number |
| limit_pref_v | the loss factor of virial at the end of the training | zero or positive real number |

training

The “training” section is defined as

```
{
  "seed": 1,
  "stop_batch": 1000000,
  "numb_test": 1,
  "disp_file": "lcurve.out",
  "disp_freq": 1000,

```

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```

"save_ckpt": "model.ckpt",
"save_freq": 10000,
"training_data":{
  "systems":["system1_path", "system2_path", "..."],
  "set_prefix": "set",
  "batch_size": ["batch_size_of_system1", "batch_size_of_system2", "..."]
}
}

```

where items are defined as:

| Item | Mean | Optional Value |
|------------|---|--------------------|
| seed | the random seed | a integer |
| stop_batch | the total training steps | a positive integer |
| numb_test | the accuracy is test by using {numb_test} sample | a positive integer |
| disp_file | the log file where the training message display | a string |
| disp_freq | display frequency | a positive integer |
| save_ckpt | check point file | a string |
| save_freq | save frequency | a positive integer |
| systems | a list of data directory which contains the dataset | string list |
| set_prefix | the prefix of dataset | a string |
| batch_size | a list of batch size of corresponding dataset | a integer list |

11.2.2 Training

Training can be invoked by

```

# step1: train CNN
dp train-nvnmd train_cnn.json -s s1
# step2: train QNN
dp train-nvnmd train_qnn.json -s s2

```

After the training process, you will get two folders: `nvnmdd_cnn` and `nvnmdd_qnn`. The `nvnmdd_cnn` contains the model after continuous neural network (CNN) training. The `nvnmdd_qnn` contains the model after quantized neural network (QNN) training. The binary file `nvnmdd_qnn/model.pb` is the model file that is used to perform NVNMD in the server [<http://nvnmdd.picp.vip>].

You can also restart the CNN training from the checkpoint (`nvnmdd_cnn/model.ckpt`) by

```
dp train-nvnmd train_cnn.json -r nvnmdd_cnn/model.ckpt -s s1
```

11.3 Testing

The frozen model can be used in many ways. The most straightforward testing can be invoked by

```

mkdir test
dp test -m ./nvnmdd_qnn/frozen_model.pb -s path/to/system -d ./test/detail -n 99999 -l test/output.
log

```

where the frozen model file to import is given via the `-m` command line flag, the path to the testing data set is given via the `-s` command line flag, and the file containing details of energy, forces and virials accuracy is given via the `-d` command line flag, the amount of data for testing is given via the `-n` command line flag.

11.4 Running MD in Bohrium

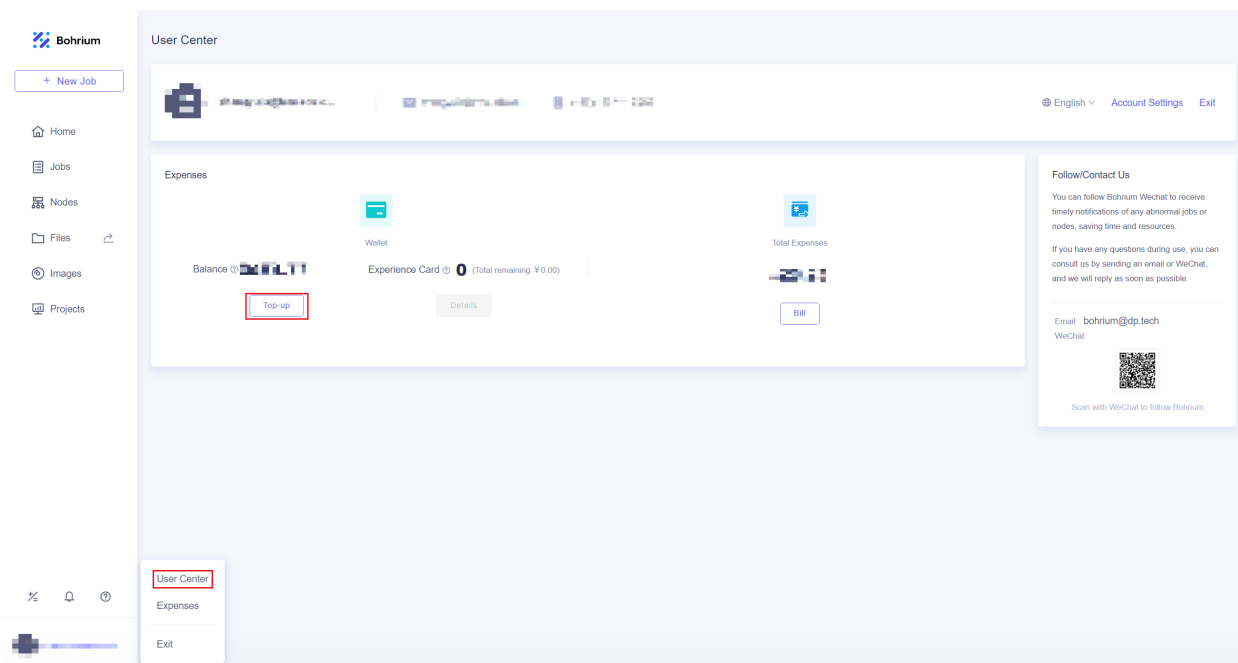
After CNN and QNN training, you can upload the ML model to our online NVNMD system and run MD there through Bohrium (<https://bohrium.dp.tech>). Bohrium is a research platform designed for AI for Science Era. For more information, please refer to [Bohrium Introduction](#).

11.4.1 Registration

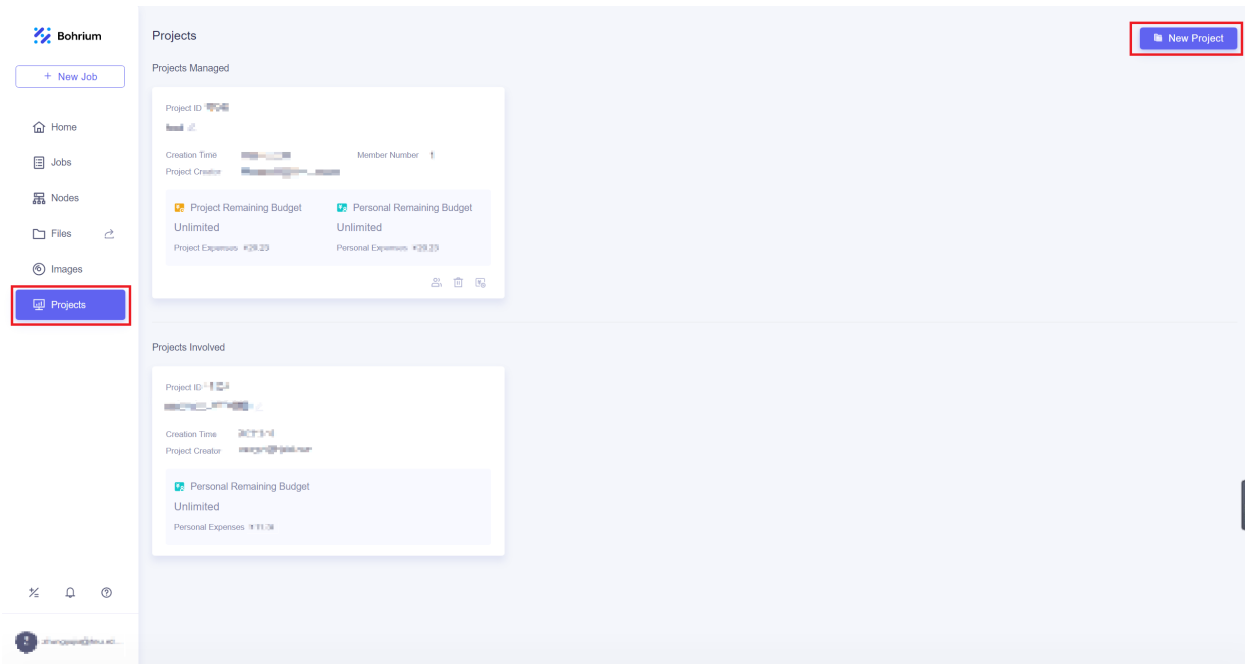
Click [here](#) to register a Bohrium account. If you already have an account for other DP products, you can skip this step and log in directly.

11.4.2 Top-up and create a project

After entering the homepage, you can click on the **User Center** in the lower left corner to top-up by yourself.



After completing the top-up, click on the **Projects**, and then click **New Project** in the upper right corner of the page. Give the project a name that is easy for you to recognize and click OK. If the project has other collaborators, you can refer to [Project Collaboration](#) for more information.



11.4.3 Run job

We will use Utility to submit jobs, you can install it with the following command

```
pip install lbg
```

When using the Lebesgue Utility for the first time, you need to configure your account by

```
lbg config account
```

Enter your Bohrium account and the corresponding password.

Then you need prepare the configuration file `job.json`, the configuration file is as follows

```
{
  "job_name": "test",
  "command": "/usr/bin/lmp_mpi < in.lmp;",
  "log_file": "OUTCAR",
  "machine_type": "c8_m32_cpu",
  "job_type": "container",
  "image_name": "lammps_dp:29Sep2021",
  "platform": "hnu",
  "region": "default",
  "project_id": 0000
}
```

where items are defined as:

| Item | Mean | Optional Value |
|---------------|--|-----------------------|
| job_name | the name of computing job, which can be named freely | a string |
| com-mand | the command to be executed on the computing node | a string |
| log_file | the log file that can be viewed at any time during the calculation process, which can be viewed on the Bohrium “Jobs” page | a string |
| ma-chine_type | the machine type used for the job | “c8_m32_cpu” |
| job_type | the job type | “container” |
| im-age_name | the image name used for the job | “lammps_dp:29Sep2021” |
| plat-form | resource provider | “hnu” |
| project_id | the project ID to which the job belongs, which can be viewed on the “Projects” page | a integer |

Notice: The task will use 8 CPU cores for computation, so do not repeatedly use the `mpirun` command, otherwise an error will be reported. All 0000 after “project_id” need to be replaced with your own project ID, which can be viewed on the “Projects” page. Also, the JSON file format requires that no commas be added after the last field within the {}, otherwise, there will be a syntax error.

In addition, it is necessary to prepare input script of the MD simulation, the ML model named `model.pb` obtained by QNN training and data files containing information required for running an MD simulation (e.g., `coord.lmp` containing initial atom coordinates).

In the input script, one needs to specify the pair style as follows

```
pair_style nvnmmd model.pb 6 2
pair_coeff * *
```

where `model.pb` is the path to model, 6 is the cutoff radius, 2 is the number of FPGA cards used with the maximum of 2.

After preparing the configuration file and the required files for calculation, using Lebesgue Utility to submit the job

```
lbg job submit -i job.json -p ./
```

where the configuration file for the job is given via the `-i` command line flag, the directory where the input files are located is given via the `-p` command line flag. Bohrium will package and upload the specified directory, and after decompressing it on the computing node, it will switch the working directory to that directory.

After the job is submitted successfully, the JOB ID and JOB GROUP ID will be output.

11.4.4 Check job status

After successfully submitting the job, you can view the progress and related logs of the submitted jobs on the Jobs page.

The screenshot shows the 'Jobs' page in the DeePMD-kit interface. On the left, a sidebar contains navigation links: Home, Jobs (highlighted), Nodes, Files, Images, and Projects. The main area displays a table of jobs. The job with ID 7742231, named 'test', is shown with a 'Completed' status. Below the table, the 'Job Details' section provides information about the job's configuration: Image (lanmps_dp29Sep2021), Directory (/home/sy/test), Command (/usr/bin/imp_mpi < in.imp), Max run time (-min), Platform (hnu), Machine Type (c8_m32_cpu), Region (default), and Automatic Download? (No). The 'Log' section shows the output of the job, including performance metrics and MPI task timing breakdown. The 'Result Files' section lists the output file 'out.zip' with its update time, size, and download options. The 'Computing Node' section shows the node configuration: Machine Type (c8_m32_cpu), Cores (8 Cores), Memory (32 GB), GPU (-), and Status (Completed).

11.4.5 Terminate and delete jobs

You can choose between `terminate` and `delete` operations.

- **Terminate:** To end running jobs/job groups in advance, save the generated result files, and the status of the terminated jobs will be changed to “completed”.
- **Delete:** To end running jobs/job groups, the status of the jobs will be changed to “failed”. Job result files will be deleted, and the jobs/job groups disappear from the list. The delete operation cannot be undone.

The Jobs page provides buttons to end jobs and job groups

The screenshot shows the 'Jobs' page in the DeePMD-kit interface. The main area displays a table of jobs. The job with ID 10913979, named 'test', is shown with a 'Completed' status. Below the table, the 'Job Details' section provides information about the job's configuration: Image (lanmps_dp29Sep2021), Directory (/home/sy/test), Command (/usr/bin/imp_mpi < in.imp), Max run time (-min), Platform (hnu), Machine Type (c8_m32_cpu), Region (default), and Automatic Download? (No). The 'Log' section shows the output of the job, including performance metrics and MPI task timing breakdown. The 'Result Files' section lists the output file 'out.zip' with its update time, size, and download options. The 'Computing Node' section shows the node configuration: Machine Type (c8_m32_cpu), Cores (8 Cores), Memory (32 GB), GPU (-), and Status (Completed).

You can also use the Lebesgue Utility tool to end jobs

```
lbg jobgroup terminate <JOB GROUP ID>
```

```
lbg job terminate <JOB ID>
```

```
lbg jobgroup rm <JOB GROUP ID>
```

```
lbg job rm <JOB ID>
```

11.4.6 Download Results

After the calculation is completed, you can download the results on the Jobs page, or save them to the data disk.

The screenshot displays the DeePMD-kit web interface. On the left, a sidebar contains navigation links: Home, Jobs (highlighted with a red box), Nodes, Files, Images, and Projects. The main area shows a table of jobs with columns for Job ID, Job Name, and Job Status. Job ID 7742231 is highlighted with a red box, and its status is 'Completed'. Below the table, there are buttons for 'Select All', '0 Jobs Selected', 'Details', and 'Terminate'. To the right, the 'Job Details' section for job 7742231 is shown, including fields for Image, Directory, Command, Machine type, Platform, Region, and Automatic Download?. Below this is a 'Log' section with a table of performance metrics. At the bottom, the 'Result Files' section is highlighted with a red box, showing a table with columns for File Name, Update Time, Size, and Operation. The file 'out.zip' is listed with a size of 1.46MB and options to 'Download' or 'Save to Data Disk'. Below the result files is a 'Computing Node' section with a table showing machine type, cores, memory, GPU, status, and operation.

Job Details

| | | | | | |
|-----------|----------------------------|----------------|------|---------------------|------------|
| Image | lammps_dp29Sep2021 | Max run time | -min | Machine type | c8_m32_cpu |
| Directory | /home/zyj/test | Platform | hnu | Region | default |
| Command | /usr/bin/imp_mpi < in.lmp; | backward files | - | Automatic Download? | No |

Automatic Download Directory

Log

| W | U | W | U | W | U | W | U |
|-----|-----------|-----------|-----------|-----------|------------|-----------|---|
| 100 | 6610.1871 | 612.75139 | 7222.9385 | 342.93938 | -13140.843 | 410636.35 | |

Loop time of 0.281256 on 8 procs for 100 steps with 13824 atoms
Performance: 30.719 ns/day, 0.781 hours/ns, 355.547 timesteps/s
82.7% CPU use with 8 MPI tasks x no OpenMP threads
MPI task timing breakdown:
Section | min time | avg time | max time | [Svaravg] | %total
-----|-----|-----|-----|-----|-----
Pair | 0.078213 | 0.15639 | 0.24332 | 14.5 | 55.60
Neigh | 0.026712 | 0.026975 | 0.027214 | 0.1 | 9.59
Comm | 0.000000 | 0.000000 | 0.000000 | 0.0 | 0.00

Result Files Input Files Log Files

| File Name | Update Time | Size | Operation |
|-----------|---------------------|--------|--|
| out.zip | 2023-07-04 20:59:33 | 1.46MB | Download Save to Data Disk ⓘ |

Computing Node

| Machine Type | Cores | Memory | GPU | Status | Operation |
|--------------|---------|--------|-----|-----------|-------------------------|
| c8_m32_cpu | 8 Cores | 32 GB | - | Completed | Details |

You can also download it using the commands of Lebesgue Utility

```
lbg job download <JOB ID>
```

or

```
lbg jobgroup download <JOB GROUP ID>
```

11.5 Running MD in Nvnmd website

After CNN and QNN training, you can upload the ML model to our online NVNMD system and run MD there.

11.5.1 Account application

The server website of NVNMD is available at <http://nvnmd.picp.vip>. You can visit the URL and enter the login interface.

NVNMD

[User guide](#)

[Switch to Chinese](#)

Username

Password

Login

To apply for an account, please email:
jie_liu@hnu.edu.cn, liujie@uw.edu

To obtain an account, please send your application to the email (jie_liu@hnu.edu.cn, liujie@uw.edu). The username and password will be sent to you by email.

11.5.2 Adding task

After successfully obtaining the account, enter the username and password in the login interface, and click “Login” to enter the homepage.

NVNMD

Current user: test1 [Logout](#)

Remaining calculation time: 6:22:29

[Add a new task](#)

[Operation records](#)

Calculation records [Refresh](#)
[Clear calculation records](#)

| Submission time | Task name | Input script | Calculation status | Cancel calculation | Calculation time | Download results | Delete record |
|-----------------|-----------|--------------|--------------------|--------------------|------------------|------------------|---------------|
|-----------------|-----------|--------------|--------------------|--------------------|------------------|------------------|---------------|

The homepage displays the remaining calculation time and all calculation records not deleted. Click **Add a new task** to enter the interface for adding a new task.

NVNMD

Current user:test1 [Return to home page](#)

Remaining calculation time:6:22:29

| | |
|---------------|--|
| Task name | <input type="text" value="test"/> |
| Upload mode ? | <input type="button" value="Manual upload"/> ▾ |
| Input script | <input type="button" value="Browse..."/> in.lmp |
| Model file | <input type="button" value="Browse..."/> model.pb |
| Data files | <input type="button" value="Browse..."/> coord.lmp |

- Task name: name of the task
- Upload mode: two modes of uploading results to online data storage, including **Manual upload** and **Automatic upload**. Results need to be uploaded manually to online data storage with **Manual upload** mode and will be uploaded automatically with **Automatic upload** mode.
- Input script: input file of the MD simulation.

In the input script, one needs to specify the pair style as follows

```
pair_style nvnmd model.pb
pair_coeff * *
```

- Model file: the ML model named `model.pb` obtained by QNN training.
- Data files: data files containing the information required for running an MD simulation (e.g., `coord.lmp` containing initial atom coordinates).

Next, you can click **Submit** to submit the task and then automatically return to the homepage.

NVNMD

Current user:test1 [Logout](#)

Remaining calculation time:6:22:29

[Add a new task](#)

[Operation records](#)

Calculation records [Refresh](#)

[Clear calculation records](#)

| Submission time | Task name | Input script | Calculation status | Cancel calculation | Calculation time | Download results | Delete record |
|---------------------|-----------|--------------|--------------------|------------------------|------------------|------------------|---------------|
| 2022-05-17 21:31:20 | test | in.lmp | Running | Cancel | | | |

Then, click **Refresh** to view the latest status of all calculation tasks.

11.5.3 Cancelling calculation

For the task whose calculation status is **Pending** and **Running**, you can click the corresponding **Cancel** on the homepage to stop the calculation.

NVNMD

Current user: test1 [Logout](#)
 Remaining calculation time: 6:21:09
[Add a new task](#)
[Operation records](#)

Calculation records [Refresh](#)
[Clear calculation records](#)

| Submission time | Task name | Input script | Calculation status | Cancel calculation | Calculation time | Download results | Delete record |
|---------------------|-----------|--------------|--------------------|--------------------|------------------|---|------------------------|
| 2022-05-17 21:31:20 | test | in.lmp | Cancelled | | 0:01:20 | Package Separate files | Delete |

11.5.4 Downloading results

For the task whose calculation status is **Completed**, **Failed** and **Cancelled**, you can click the corresponding **Package** or **Separate files** in the **Download results** bar on the homepage to download results.

Click **Package** to download a zipped package of all files including input files and output results.

NVNMD

Current user: test1 [Return to home page](#)
 Remaining calculation time: 6:21:09

Files

| Name | Size | Download directly | Download from online data storage | Upload to online data storage ^② |
|------------|--------|--------------------------|-----------------------------------|--|
| output.zip | 1.2 MB | Download | | Upload |

Click **Separate files** to download the required separate files.

NVNMD

Current user:test1 [Return to home page](#)

Remaining calculation time:6:21:09

Files

| Name | Size | Download directly | Download from online data storage | Upload to online data storage? |
|------------|---------|--------------------------|-----------------------------------|--------------------------------|
| coord.lmp | 15.4 KB | Download | | Upload |
| in.lmp | 3.1 KB | Download | | Upload |
| lammps.xyz | 2.1 MB | Download | | Upload |
| log.lammps | 14.0 KB | Download | | Upload |
| model.pb | 8.1 MB | Download | | Upload |
| result.out | 13.5 KB | Download | | Upload |

If **Manual upload** mode is selected or the file has expired, click **Upload** on the download interface to upload manually.

11.5.5 Deleting record

For the task no longer needed, you can click the corresponding **Delete** on the homepage to delete the record. Records cannot be retrieved after deletion.

11.5.6 Clearing records

Click **Clear calculation records** on the homepage to clear all records.

Records cannot be retrieved after clearing.

FAQS

As a consequence of differences in computers or systems, problems may occur. Some common circumstances are listed as follows. In addition, some frequently asked questions are listed as follows. If other unexpected problems occur, you're welcome to contact us for help.

12.1 How to tune Fitting/embedding-net size ?

Here are some test forms on fitting-net size tuning or embedding-net size tuning performed on several different systems.

12.1.1 Al2O3

Fitting net size tuning form on Al2O3: (embedding-net size: [25,50,100])

| Fitting-net size | Energy L2err(eV) | Energy L2err/Natoms(eV) | Force L2err(eV/Angstrom) |
|------------------|------------------|-------------------------|--------------------------|
| [240,240,240] | 1.742252e-02 | 7.259383e-05 | 4.014115e-02 |
| [80,80,80] | 1.799349e-02 | 7.497287e-05 | 4.042977e-02 |
| [40,40,40] | 1.799036e-02 | 7.495984e-05 | 4.068806e-02 |
| [20,20,20] | 1.834032e-02 | 7.641801e-05 | 4.094784e-02 |
| [10,10,10] | 1.913058e-02 | 7.971073e-05 | 4.154775e-02 |
| [5,5,5] | 1.932914e-02 | 8.053808e-05 | 4.188052e-02 |
| [4,4,4] | 1.944832e-02 | 8.103467e-05 | 4.217826e-02 |
| [3,3,3] | 2.068631e-02 | 8.619296e-05 | 4.300497e-02 |
| [2,2,2] | 2.267962e-02 | 9.449840e-05 | 4.413609e-02 |
| [1,1,1] | 2.813596e-02 | 1.172332e-04 | 4.781115e-02 |
| [] | 3.135002e-02 | 1.306251e-04 | 5.373120e-02 |

[] means no hidden layer, but there is still a linear output layer. This situation is equal to the linear regression.

Embedding net size tuning form on Al₂O₃: (Fitting-net size: [240,240,240])

| Embedding-net size | Energy L2err(eV) | Energy L2err/Natoms(eV) | Force L2err(eV/Angstrom) |
|--------------------|------------------|-------------------------|--------------------------|
| [25,50,100] | 1.742252e-02 | 7.259383e-05 | 4.014115e-02 |
| [10,20,40] | 2.909990e-02 | 1.212496e-04 | 4.734667e-02 |
| [5,10,20] | 3.357767e-02 | 1.399070e-04 | 5.706385e-02 |
| [4,8,16] | 6.060367e-02 | 2.525153e-04 | 7.333304e-02 |
| [3,6,12] | 5.656043e-02 | 2.356685e-04 | 7.793539e-02 |
| [2,4,8] | 5.277023e-02 | 2.198759e-04 | 7.459995e-02 |
| [1,2,4] | 1.302282e-01 | 5.426174e-04 | 9.672238e-02 |

12.1.2 Cu**Fitting net size tuning form on Cu: (embedding-net size: [25,50,100])**

| Fitting-net size | Energy L2err(eV) | Energy L2err/Natoms(eV) | Force L2err(eV/Angstrom) |
|------------------|------------------|-------------------------|--------------------------|
| [240,240,240] | 4.135548e-02 | 1.615449e-04 | 8.940946e-02 |
| [20,20,20] | 4.323858e-02 | 1.689007e-04 | 8.955762e-02 |
| [10,10,10] | 4.399364e-02 | 1.718502e-04 | 8.962891e-02 |
| [5,5,5] | 4.468404e-02 | 1.745470e-04 | 8.970111e-02 |
| [4,4,4] | 4.463580e-02 | 1.743586e-04 | 8.972011e-02 |
| [3,3,3] | 4.493758e-02 | 1.755374e-04 | 8.971303e-02 |
| [2,2,2] | 4.500736e-02 | 1.758100e-04 | 8.973878e-02 |
| [1,1,1] | 4.542073e-02 | 1.774247e-04 | 8.964761e-02 |
| [] | 4.545168e-02 | 1.775456e-04 | 8.983201e-02 |

Embedding net size tuning form on Cu: (Fitting-net size: [240,240,240])

| Embedding-net size | Energy L2err(eV) | Energy L2err/Natoms(eV) | Force L2err(eV/Angstrom) |
|---------------------|------------------|-------------------------|--------------------------|
| [25,50,100] | 4.135548e-02 | 1.615449e-04 | 8.940946e-02 |
| [20,40,80] | 4.203562e-02 | 1.642016e-04 | 8.925881e-02 |
| [15,30,60] | 4.146672e-02 | 1.619794e-04 | 8.936911e-02 |
| [10,20,40] | 4.263060e-02 | 1.665258e-04 | 8.955818e-02 |
| [5,10,20] | 4.994913e-02 | 1.951138e-04 | 9.007786e-02 |
| [4,8,16] | 1.022157e-01 | 3.992802e-04 | 9.532119e-02 |
| [3,6,12] | 1.362098e-01 | 5.320695e-04 | 1.073860e-01 |
| [2,4,8] | 7.061800e-02 | 2.758515e-04 | 9.126418e-02 |
| [1,2,4] && seed = 1 | 9.843161e-02 | 3.844985e-04 | 9.348505e-02 |
| [1,2,4] && seed = 2 | 9.404335e-02 | 3.673568e-04 | 9.304089e-02 |
| [1,2,4] && seed = 3 | 1.508016e-01 | 5.890688e-04 | 1.382356e-01 |
| [1,2,4] && seed = 4 | 9.686949e-02 | 3.783965e-04 | 9.294820e-02 |

12.1.3 Water

Fitting net size tuning form on water: (embedding-net size: [25,50,100])

| Fitting-net size | Energy L2err/Natoms(eV) | Force L2err(eV/Angstrom) |
|------------------|-------------------------|--------------------------|
| [240,240,240] | 9.1589E-04 | 5.1540E-02 |
| [200,200,200] | 9.3221E-04 | 5.2366E-02 |
| [160,160,160] | 9.4274E-04 | 5.3403E-02 |
| [120,120,120] | 9.5407E-04 | 5.3093E-02 |
| [80,80,80] | 9.4605E-04 | 5.3402E-02 |
| [40,40,40] | 9.8533E-04 | 5.5790E-02 |
| [20,20,20] | 1.0057E-03 | 5.8232E-02 |
| [10,10,10] | 1.0466E-03 | 6.2279E-02 |
| [5,5,5] | 1.1154E-03 | 6.7994E-02 |
| [4,4,4] | 1.1289E-03 | 6.9613E-02 |
| [3,3,3] | 1.2368E-03 | 7.9786E-02 |
| [2,2,2] | 1.3558E-03 | 9.7042E-02 |
| [1,1,1] | 1.4633E-03 | 1.1265E-01 |
| [] | 1.5193E-03 | 1.2136E-01 |

Embedding net size tuning form on water: (Fitting-net size: [240,240,240])

| Embedding-net size | Energy L2err/Natoms(eV) | Force L2err(eV/Angstrom) |
|--------------------|-------------------------|--------------------------|
| [25,50,100] | 9.1589E-04 | 5.1540E-02 |
| [20,40,80] | 9.5080E-04 | 5.3593E-02 |
| [15,30,60] | 9.7996E-04 | 5.6338E-02 |
| [10,20,40] | 1.0353E-03 | 6.2776E-02 |
| [5,10,20] | 1.1254E-03 | 7.3195E-02 |
| [4,8,16] | 1.2495E-03 | 8.0371E-02 |
| [3,6,12] | 1.3604E-03 | 9.9883E-02 |
| [2,4,8] | 1.4358E-03 | 9.7389E-02 |
| [1,2,4] | 2.1765E-03 | 1.7276E-01 |

12.1.4 Mg-Al

Fitting net size tuning form on Mg-Al: (embedding-net size: [25,50,100])

| Fitting-net size | Energy L2err/Natoms(eV) | Force L2err(eV/Angstrom) |
|------------------|-------------------------|--------------------------|
| [240,240,240] | 3.9606e-03 | 1.6289e-02 |
| [200,200,200] | 3.9449e-03 | 1.6471e-02 |
| [160,160,160] | 4.0947e-03 | 1.6413e-02 |
| [120,120,120] | 3.9234e-03 | 1.6283e-02 |
| [80,80,80] | 3.9758e-03 | 1.6506e-02 |
| [40,40,40] | 3.9142e-03 | 1.6348e-02 |
| [20,20,20] | 4.1302e-03 | 1.7006e-02 |
| [10,10,10] | 4.3433e-03 | 1.7524e-02 |
| [5,5,5] | 5.3154e-03 | 1.9716e-02 |
| [4,4,4] | 5.4210e-03 | 1.9710e-02 |
| [2,2,2] | 6.2667e-03 | 2.2568e-02 |
| [1,1,1] | 7.3676e-03 | 2.6375e-02 |
| [] | 7.3999e-03 | 2.6097e-02 |

Embedding net size tuning form on Mg-Al: (Fitting-net size: [240,240,240])

| Embedding-net size | Energy L2err/Natoms(eV) | Force L2err(eV/Angstrom) |
|--------------------|-------------------------|--------------------------|
| [25,50,100] | 3.9606e-03 | 1.6289e-02 |
| [20,40,80] | 4.0292e-03 | 1.6555e-02 |
| [15,30,60] | 4.1743e-03 | 1.7026e-02 |
| [10,20,40] | 4.8138e-03 | 1.8516e-02 |
| [5,10,20] | 5.6052e-03 | 2.0709e-02 |
| [4,8,16] | 6.1335e-03 | 2.1450e-02 |
| [3,6,12] | 6.6469e-03 | 2.3003e-02 |
| [2,4,8] | 6.8222e-03 | 2.6318e-02 |
| [1,2,4] | 1.0678e-02 | 3.9559e-02 |

12.2 How to control the parallelism of a job?

DeePMD-kit has three levels of parallelism. To get the best performance, one should control the number of threads used by DeePMD-kit. One should make sure the product of the parallel numbers is less than or equal to the number of cores available.

12.2.1 MPI (optional)

Parallelism for MPI is optional and used for multiple nodes, multiple GPU cards, or sometimes multiple CPU cores.

To enable MPI support for training, one should [install horovod](#) in advance. Note that the parallelism mode is data parallelism, so it is not expected to see the training time per batch decreases.

MPI support for inference is not directly supported by DeePMD-kit, but indirectly supported by the third-party software. For example, [LAMMPS enables running simulations in parallel](#) using the MPI parallel communication standard with distributed data. That software has to build against MPI.

Set the number of processes with:

```
mpirun -np $num_nodes dp
```

Note that `mpirun` here should be the same as the MPI used to build software. For example, one can use `mpirun -h` and `lmp -h` to see if `mpirun` and LAMMPS has the same MPI version.

Sometimes, `$num_nodes` and the nodes information can be directly given by the HPC scheduler system, if the MPI used here is the same as the MPI used to build the scheduler system. Otherwise, one have to manually assign these information.

12.2.2 Parallelism between independent operators

For CPU devices, TensorFlow use multiple streams to run independent operators (OP).

```
export TF_INTER_OP_PARALLELISM_THREADS=3
```

However, for GPU devices, TensorFlow uses only one compute stream and multiple copy streams. Note that some of DeePMD-kit OPs do not have GPU support, so it is still encouraged to set environmental variables even if one has a GPU.

12.2.3 Parallelism within an individual operators

For CPU devices, `TF_INTRA_OP_PARALLELISM_THREADS` controls parallelism within TensorFlow native OPs when TensorFlow is built against Eigen.

```
export TF_INTRA_OP_PARALLELISM_THREADS=2
```

`OMP_NUM_THREADS` is threads for OpenMP parallelism. It controls parallelism within TensorFlow native OPs when TensorFlow is built by Intel OneDNN and DeePMD-kit custom CPU OPs. It may also control parallelism for NumPy when NumPy is built against OpenMP, so one who uses GPUs for training should also care this environmental variable.

```
export OMP_NUM_THREADS=2
```

There are several other environmental variables for OpenMP, such as `KMP_BLOCKTIME`. See [Intel documentation](#) for detailed information.

12.2.4 Tune the performance

There is no one general parallel configuration that works for all situations, so you are encouraged to tune parallel configurations yourself after empirical testing.

Here are some empirical examples. If you wish to use 3 cores of 2 CPUs on one node, you may set the environmental variables and run DeePMD-kit as follows:

```
export OMP_NUM_THREADS=3
export TF_INTRA_OP_PARALLELISM_THREADS=3
export TF_INTER_OP_PARALLELISM_THREADS=2
dp train input.json
```

For a node with 128 cores, it is recommended to start with the following variables:

```
export OMP_NUM_THREADS=16
export TF_INTRA_OP_PARALLELISM_THREADS=16
export TF_INTER_OP_PARALLELISM_THREADS=8
```

Again, in general, one should make sure the product of the parallel numbers is less than or equal to the number of cores available. In the above case, $16 \times 8 = 128$, so threads will not compete with each other.

12.3 Do we need to set $rcut < \text{half boxsize}$?

When seeking the neighbors of atom i under periodic boundary conditions, DeePMD-kit considers all j atoms within cutoff $rcut$ from atom i in all mirror cells.

So, there is no limitation on the setting of $rcut$.

PS: The reason why some software requires $rcut < \text{half box size}$ is that they only consider the nearest mirrors from the center cell. DeePMD-kit is different from them.

12.4 How to set sel ?

sel is short for “selected number of atoms in $rcut$ ”.

$sel_a[i]$ is a list of integers. The length of the list should be the same as the number of atom types in the system.

$sel_a[i]$ gives the number of the selected number of type i neighbors within $rcut$. To ensure that the results are strictly accurate, $sel_a[i]$ should be larger than the largest number of type i neighbors in the $rcut$.

However, the computation overhead increases with $sel_a[i]$, therefore, $sel_a[i]$ should be as small as possible.

The setting of $sel_a[i]$ should balance the above two considerations.

12.5 Installation

12.5.1 Inadequate versions of gcc/g++

Sometimes you may use a gcc/g++ of version < 4.8. In this way, you can still compile all the parts of TensorFlow and most of the parts of DeePMD-kit, but i-Pi and GROMACS plugins will be disabled automatically. Or if you have a gcc/g++ of version > 4.8, say, 7.2.0, you may choose to use it by doing

```
export CC=/path/to/gcc-7.2.0/bin/gcc
export CXX=/path/to/gcc-7.2.0/bin/g++
```

12.5.2 Build files left in DeePMD-kit

When you try to build a second time when installing DeePMD-kit, files produced before may contribute to failure. Thus, you may clear them by

```
cd build
rm -r *
```

and redo the cmake process.

12.6 The temperature undulates violently during the early stages of MD

This is probably because your structure is too far from the equilibrium configuration.

To make sure the potential model is truly accurate, we recommend checking model deviation.

12.7 MD: cannot run LAMMPS after installing a new version of DeePMD-kit

This typically happens when you install a new version of DeePMD-kit and copy directly the generated USER-DEEPM to a LAMMPS source code folder and re-install LAMMPS.

To solve this problem, it suffices to first remove USER-DEEPM from the LAMMPS source code by

```
make no-user-deepmd
```

and then install the new USER-DEEPM.

If this does not solve your problem, try to decompress the LAMMPS source tarball and install LAMMPS from scratch again, which typically should be very fast.

12.8 Model compatibility

When the version of DeePMD-kit used to train the model is different from the that of DeePMD-kit running MDs, one has the problem of model compatibility.

DeePMD-kit guarantees that the codes with the same major and minor revisions are compatible. That is to say, v0.12.5 is compatible with v0.12.0, but is not compatible with v0.11.0 or v1.0.0.

One can execute `dp convert-from` to convert an old model to a new one.

| Model version | v0.12 | v1.0 | v1.1 | v1.2 | v1.3 | v2.0 | v2.1 | v2.2 |
|---------------|-------|------|------|------|------|------|------|------|
| Compatibility | 😊 | 😊 | 😊 | 😊 | 😊 | 😊 | 😊 | 😊 |

Legend:

- 😊: The model is compatible with the DeePMD-kit package.
- 😊: The model is incompatible with the DeePMD-kit package, but one can execute `dp convert-from` to convert an old model to v2.2.
- ☹️: The model is incompatible with the DeePMD-kit package, and there is no way to convert models.

12.9 Why does a model have low precision?

Many phenomena are caused by model accuracy. For example, during simulations, temperatures explode, structures fall apart, and atoms are lost. One can [test the model](#) to confirm whether the model has the enough accuracy.

There are many reasons for a low-quality model. Some common reasons are listed below.

12.9.1 Data

Data units and signs

The unit of training data should follow what is listed in [data section](#). Usually, the package to calculate the training data has different units from those of the DeePMD-kit. It is noted that some software label the energy gradient as forces, instead of the negative energy gradient. It is necessary to check them carefully to avoid inconsistent data.

SCF coverage and data accuracy

The accuracy of models will not exceed the accuracy of training data, so the training data should reach enough accuracy. Here is a checklist for the accuracy of data:

- SCF should converge to a suitable threshold for all points in the training data.
- The convergence of the energy, force and virial with respect to the energy cutoff and k-spacing sample is checked.
- Sometimes, QM software may generate unstable outliers, which should be removed.
- The data should be extracted with enough digits and stored with the proper precision. Large energies may have low precision when they are stored as the single-precision floating-point format (FP32).

Enough data

If the model performs good on the training data, but has bad accuracy on another data, this means some data space is not covered by the training data. It can be validated by evaluating the [model deviation](#) with multiple models. If the model deviation of these data is high for some data, try to collect more data using [DP-GEN](#).

Values of data

One should be aware that the errors of some data is also affected by the absolute values of this data. Stable structures tend to be more precise than unstable structures because unstable structures may have larger forces. Also, errors will be introduced in the Projector augmented wave (PAW) DFT calculations when the atoms are very close due to the overlap of pseudo-potentials. It is expected to see that data with large forces has larger errors and it is better to compare different models only with the same data.

12.9.2 Model

Enough sel

The `sel` of the descriptors must be enough for both training and test data. Otherwise, the model will be unreliable and give wrong results.

Cutoff radius

The model cannot fit the long-term interaction out of the cutoff radius. This is a designed approximation for performance, but one has to choose proper cutoff radius for the system.

Neural network size

The size of neural networks will affect the accuracy, but if one follows the parameters in the examples, this effect is insignificant. See [FAQ: How to tune Fitting/embedding-net size](#) for details.

Neural network precision

In some cases, one may want to use the FP32 precision to make the model faster. For some applications, FP32 is enough and thus is recommended, but one should still be aware that the precision of FP32 is not as high as that of FP64.

12.9.3 Training

Training steps

Generally speaking, the longer the number of training steps, the better the model. A balance between model accuracy and training time can be achieved. If one finds that model accuracy decreases with training time, there may be a problem with the data. See the [data section](#) for details.

Learning rate

Both too large and too small learning rate may affect the training. It is recommended to start with a large learning rate and end with a small learning rate. The learning rate from the examples is a good choice to start.

FIND DEEPMD-KIT C/C++ LIBRARY FROM CMAKE

After DeePMD-kit C/C++ library is installed, one can find DeePMD-kit from CMake:

```
find_package(DeePMD REQUIRED)
```

Note that you may need to add `${deepmd_root}` to the cached CMake variable `CMAKE_PREFIX_PATH`.

To link against the C interface library, using

```
target_link_libraries(some_library PRIVATE DeePMD::deepmd_c)
```

To link against the C++ interface library, using

```
target_link_libraries(some_library PRIVATE DeePMD::deepmd_cc)
```


CODING CONVENTIONS

14.1 Preface

The aim of these coding standards is to help create a codebase with a defined and consistent coding style that every contributor can get easily familiar with. This will enhance code readability as there will be no different coding styles from different contributors and everything will be documented. Also, PR diffs will be smaller because of the unified coding style. Finally, static typing will help in hunting down potential bugs before the code is even run.

Contributed code will not be refused merely because it does not strictly adhere to these conditions; as long as it's internally consistent, clean, and correct, it probably will be accepted. But don't be surprised if the "offending" code gets fiddled with overtime to conform to these conventions.

There are also GitHub actions CI checks for python code style which will annotate the PR diff for you to see the areas where your code is lacking compared to the set standard.

14.2 Rules

The code must be compatible with the oldest supported version of python which is 3.7

The project follows the generic coding conventions as specified in the [Style Guide for Python Code](#), [Docstring Conventions](#) and [Typing Conventions](#) PEPs, clarified and extended as follows:

- Do not use "*" imports such as `from module import *`. Instead, list imports explicitly.
- Use 4 spaces per indentation level. No tabs.
- No one-liner compound statements (i.e., no `if x: return:` use two lines).
- Maximum line length is 88 characters as recommended by [black](#) which is less strict than [Docstring Conventions](#) suggests.
- Use "StudlyCaps" for class names.
- Use "lowercase" or "lowercase_with_underscores" for function, method, variable names and module names. For short names, joined lowercase may be used (e.g. "tagname"). Choose what is most readable.
- No single-character variable names, except indices in loops that encompass a very small number of lines (`for i in range(5): ...`).
- Avoid lambda expressions. Use named functions instead.
- Avoid functional constructs (filter, map, etc.). Use list comprehensions instead.
- Use "double quotes" for string literals, and `"""triple double quotes"""` for docstring's. Single quotes are OK for something like

```
f"something {'this' if x else 'that'}"
```

- Use f-strings `s = f"{x:.2f}"` instead of old style formatting with `"%f" % x`. string format method `"{x:.2f}".format()` may be used sparsely where it is more convenient than f-strings.

14.3 Whitespace

Python is not C/C++ so whitespace should be used sparingly to maintain code readability

- Read the Whitespace in Expressions and Statements section of [PEP8](#).
- Avoid [trailing whitespaces](#).
- Do not use excessive whitespace in your expressions and statements.
- You should have blank spaces after commas, colons, and semi-colons if it isn't trailing next to the end of a bracket, brace, or parentheses.
- With any operators you should use space on both sides of the operator.
- Colons for slicing are considered a binary operator, and should not have any spaces between them.
- You should have parentheses with no space, directly next to the function when calling functions `function()`.
- When indexing or slicing the brackets should be directly next to the collection with no space `collection["index"]`.
- Whitespace used to line up variable values is not recommended.
- Make sure you are consistent with the formats you choose when optional choices are available.

14.4 General advice

- Get rid of as many `break` and `continue` statements as possible.
- Write short functions. All functions should fit within a standard screen.
- Use descriptive variable names.

14.5 Writing documentation in the code

Here is an example of how to write good docstrings:

<https://github.com/numpy/numpy/blob/master/doc/example.py>

The NumPy docstring documentation can be found [here](#)

It is a good practice to run [pydocstyle](#) check on your code or use a text editor that does it automatically):

```
$ pydocstyle filename.py
```

14.6 Run pycodestyle on your code

It's a good idea to run `pycodestyle` on your code (or use a text editor that does it automatically):

```
$ pycodestyle filename.py
```

14.7 Run mypy on your code

It's a good idea to run `mypy` on your code (or use a text editor that does it automatically):

```
$ mypy filename.py
```

14.8 Run pydocstyle on your code

It's a good idea to run `pycodestyle` on your code (or use a text editor that does it automatically):

```
$ pycodestyle filename.py --max-line-length=88
```

14.9 Run black on your code

Another method of enforcing `PEP8` is using a tool such as `black`. These tools tend to be very effective at cleaning up code but should be used carefully and code should be retested after cleaning it. Try:

```
$ black --help
```


CREATE A MODEL

If you'd like to create a new model that isn't covered by the existing DeePMD-kit library, but reuse DeePMD-kit's other efficient modules such as data processing, trainer, etc, you may want to read this section.

To incorporate your custom model you'll need to:

1. Register and implement new components (e.g. descriptor) in a Python file. You may also want to register new TensorFlow OPs if necessary.
2. Register new arguments for user inputs.
3. Package new codes into a Python package.
4. Test new models.

15.1 Design a new component

When creating a new component, take descriptor as the example, you should inherit `deepmd.descriptor.descriptor.Descriptor` class and override several methods. Abstract methods such as `deepmd.descriptor.descriptor.Descriptor.build` must be implemented and others are not. You should keep arguments of these methods unchanged.

After implementation, you need to register the component with a key:

```
from deepmd.descriptor import Descriptor

@Descriptor.register("some_descrpt")
class SomeDescriptor(Descriptor):
    def __init__(self, arg1: bool, arg2: float) -> None:
        pass
```

15.2 Register new arguments

To let someone uses your new component in their input file, you need to create a new method that returns some `Argument` of your new component, and then register new arguments. For example, the code below

```
from typing import List

from dargs import Argument
from deepmd.utils.argcheck import descrpt_args_plugin
```

(continues on next page)

(continued from previous page)

```
@descript_args_plugin.register("some_descript")
def descript_some_args() -> List[Argument]:
    return [
        Argument("arg1", bool, optional=False, doc="balabala"),
        Argument("arg2", float, optional=True, default=6.0, doc="haha"),
    ]
```

allows one to use your new descriptor as below:

```
"descriptor" :{
    "type": "some_descript",
    "arg1": true,
    "arg2": 6.0
}
```

The arguments here should be consistent with the class arguments of your new component.

15.3 Package new codes

You may use `setuptools` to package new codes into a new Python package. It's crucial to add your new component to `entry_points['deepmd']` in `setup.py`:

```
entry_points = (
    {
        "deepmd": [
            "some_descript=deepmd_some_descriptpt:SomeDescript",
        ],
    },
)
```

where `deepmd_some_descriptpt` is the module of your codes. It is equivalent to `from deepmd_some_descriptpt import SomeDescript`.

If you place `SomeDescript` and `descript_some_args` into different modules, you are also expected to add `descript_some_args` to `entry_points`.

After you install your new package, you can now use `dp train` to run your new model.

ATOM TYPE EMBEDDING

16.1 Overview

Here is an overview of the DeePMD-kit algorithm. Given a specific centric atom, we can obtain the matrix describing its local environment, named \mathcal{R} . It consists of the distance between the centric atom and its neighbors, as well as a direction vector. We can embed each distance into a vector of M_1 dimension by an **embedding net**, so the environment matrix \mathcal{R} can be embedded into matrix \mathcal{G} . We can thus extract a descriptor vector (of $M_1 \times M_2$ dim) of the centric atom from the \mathcal{G} by some matrix multiplication, and put the descriptor into **fitting net** to get predicted energy E . The vanilla version of DeePMD-kit builds **embedding net** and **fitting net** relying on the atom type, resulting in $O(N)$ memory usage. After applying atom type embedding, in DeePMD-kit v2.0, we can share one **embedding net** and one **fitting net** in total, which decline training complexity largely.

16.2 Preliminary

In the following chart, you can find the meaning of symbols used to clarify the atom-type embedding algorithm.

i : Type of centric atom

j : Type of neighbor atom

s_{ij} : Distance between centric atom and neighbor atom

$\mathcal{G}_{ij}(\cdot)$: Origin embedding net, take s_{ij} as input and output embedding vector of M_1 dim

$\mathcal{G}(\cdot)$: Shared embedding net

$\text{Multi}(\cdot)$: Matrix multiplication and flattening, output the descriptor vector of $M_1 \times M_2$ dim

$F_i(\cdot)$: Origin fitting net, take the descriptor vector as input and output energy

$F(\cdot)$: Shared fitting net

$A(\cdot)$: Atom type embedding net, input is atom type, the output is type embedding vector of dim `nchan1`

So, we can formulate the training process as follows. Vanilla DeePMD-kit algorithm:

$$E = F_i(\text{Multi}(\mathcal{G}_{ij}(s_{ij})))$$

DeePMD-kit applying atom type embedding:

$$E = F([\text{Multi}(\mathcal{G}([s_{ij}, A(i), A(j)])), A(j)])$$

or

$$E = F([\text{Multi}(\mathcal{G}([s_{ij}, A(j)])), A(j)])$$

The difference between the two variants above is whether using the information of centric atom when generating the descriptor. Users can choose by modifying the `type_one_side` hyper-parameter in the input JSON file.

16.3 How to use

A detailed introduction can be found at [se_e2_a_tebd](#). Looking for a fast start-up, you can simply add a `type_embedding` section in the input JSON file as displayed in the following, and the algorithm will adopt the atom type embedding algorithm automatically. An example of `type_embedding` is like

```
"type_embedding":{
  "neuron":      [2, 4, 8],
  "resnet_dt":   false,
  "seed":        1
}
```

16.4 Code Modification

Atom-type embedding can be applied to varied `embedding net` and `fitting net`, as a result, we build a class `TypeEmbedNet` to support this free combination. In the following, we will go through the execution process of the code to explain our code modification.

16.4.1 trainer (train/trainer.py)

In `trainer.py`, it will parse the parameter from the input JSON file. If a `type_embedding` section is detected, it will build a `TypeEmbedNet`, which will be later input in the `model`. `model` will be built in the function `_build_network`.

16.4.2 model (model/ener.py)

When building the operation graph of the `model` in `model.build`. If a `TypeEmbedNet` is detected, it will build the operation graph of `type embed net`, `embedding net` and `fitting net` by order. The building process of `type embed net` can be found in `TypeEmbedNet.build`, which output the type embedding vector of each atom type (of `[ntypes × nchan]` dimensions). We then save the type embedding vector into `input_dict`, so that they can be fetched later in `embedding net` and `fitting net`.

16.4.3 embedding net (descriptor/se*.py)

In `embedding net`, we shall take local environment \mathcal{R} as input and output matrix \mathcal{G} . Functions called in this process by the order is

```
build -> _pass_filter -> _filter -> _filter_lower
```

`_pass_filter`: It will first detect whether an atom type embedding exists, if so, it will apply atom type embedding algorithm and doesn't divide the input by type.

`_filter`: It will call `_filter_lower` function to obtain the result of matrix multiplication ($\mathcal{G}^T \cdot \mathcal{R}$), do further multiplication involved in `Multi()`, and finally output the result of descriptor vector of $M_1 \times M_2$ dim.

`_filter_lower`: The main function handling input modification. If type embedding exists, it will call `_concat_type_embedding` function to concat the first column of input \mathcal{R} (the column of s_{ij}) with the atom type embedding information. It will decide whether to use the atom type embedding vector of the centric atom according to the value of `type_one_side` (if set True, then we only use the vector of the neighbor atom). The modified input will be put into the `fitting net` to get \mathcal{G} for further matrix multiplication stage.

16.4.4 fitting net (fit/ener.py)

In `fitting net`, it takes the descriptor vector as input, whose dimension is $[\text{natoms}, M_1 \times M_2]$. Because we need to involve information on the centric atom in this step, we need to generate a matrix named `atype_embed` (of dim $[\text{natoms}, \text{nchanl}]$), in which each row is the type embedding vector of the specific centric atom. The input is sorted by type of centric atom, we also know the number of a particular atom type (stored in `natoms[2+i]`), thus we get the type vector of the centric atom. In the build phase of the fitting net, it will check whether type embedding exists in `input_dict` and fetch them. After that, call `embed_atom_type` function to look up the embedding vector for the type vector of the centric atom to obtain `atype_embed`, and concat input with it (`[input, atype_embed]`). The modified input goes through `fitting net` to get predicted energy.

Note: You can't apply the compression method while using atom-type embedding.

17.1 deepmd package

Root of the deepmd package, exposes all public classes and submodules.

```
class deepmd.DeepEval(model_file: Path, load_prefix: str = 'load', default_tf_graph: bool = False,
                      auto_batch_size: Union[bool, int, AutoBatchSize] = False)
```

Bases: `object`

Common methods for DeepPot, DeepWFC, DeepPolar, ...

Parameters

`model_file`

[`Path`] The name of the frozen model file.

`load_prefix`: `str`

The prefix in the load computational graph

`default_tf_graph`

[`bool`] If uses the default tf graph, otherwise build a new tf graph for evaluation

`auto_batch_size`

[`bool` or `int` or `AutomaticBatchSize`, default: `False`] If True, automatic batch size will be used. If int, it will be used as the initial batch size.

Attributes

`model_type`

Get type of model.

`model_version`

Get version of model.

`sess`

Get TF session.

Methods

| | |
|---|--|
| <code>eval_typeebd()</code> | Evaluate output of type embedding network by using this model. |
| <code>make_natoms_vec(atom_types[, mixed_type])</code> | Make the natom vector used by deepmd-kit. |
| <code>reverse_map(vec, imap)</code> | Reverse mapping of a vector according to the index map. |
| <code>sort_input(coord, atom_type[, sel_atoms, ...])</code> | Sort atoms in the system according their types. |

`eval_typeebd()` → `ndarray`

Evaluate output of type embedding network by using this model.

Returns

`np.ndarray`

The output of type embedding network. The shape is `[ntypes, o_size]`, where `ntypes` is the number of types, and `o_size` is the number of nodes in the output layer.

Raises

`KeyError`

If the model does not enable type embedding.

See also:

`deepmd.utils.type_embed.TypeEmbedNet`

The type embedding network.

Examples

Get the output of type embedding network of graph.pb:

```
>>> from deepmd.infer import DeepPotential
>>> dp = DeepPotential('graph.pb')
>>> dp.eval_typeebd()
```

`load_prefix:` `str`

`make_natoms_vec(atom_types: ndarray, mixed_type: bool = False)` → `ndarray`

Make the natom vector used by deepmd-kit.

Parameters

`atom_types`

The type of atoms

`mixed_type`

Whether to perform the mixed_type mode. If True, the input data has the mixed_type format (see doc/model/train_se_atten.md), in which frames in a system may have different natoms_vec(s), with the same nloc.

Returns

`natoms`

The number of atoms. This tensor has the length of `Ntypes + 2` `natoms[0]`: number of local atoms `natoms[1]`: total number of atoms held by this processor `natoms[i]`: $2 \leq i < Ntypes+2$, number of type `i` atoms

```

property model_type: str
    Get type of model.

    :type:str

property model_version: str
    Get version of model.

    Returns

    str
        version of model

static reverse_map(vec: ndarray, imap: List[int]) → ndarray
    Reverse mapping of a vector according to the index map.

    Parameters

    vec
        Input vector. Be of shape [nframes, natoms, -1]

    imap
        Index map. Be of shape [natoms]

    Returns

    vec_out
        Reverse mapped vector.

property sess: Session
    Get TF session.

static sort_input(coord: ndarray, atom_type: ndarray, sel_atoms: Optional[List[int]] = None,
    mixed_type: bool = False)

    Sort atoms in the system according their types.

    Parameters

    coord
        The coordinates of atoms. Should be of shape [nframes, natoms, 3]

    atom_type
        The type of atoms Should be of shape [natoms]

    sel_atoms
        The selected atoms by type

    mixed_type
        Whether to perform the mixed_type mode. If True, the input data has the
        mixed_type format (see doc/model/train_se_atten.md), in which frames in a sys-
        tem may have different natoms_vec(s), with the same nloc.

    Returns

    coord_out
        The coordinates after sorting

    atom_type_out
        The atom types after sorting

    idx_map
        The index mapping from the input to the output. For example coord_out = co-
        ord[:,idx_map,:]

```

sel_atom_type

Only output if sel_atoms is not None The sorted selected atom types

sel_idx_map

Only output if sel_atoms is not None The index mapping from the selected atoms to sorted selected atoms.

`deepmd.DeepPotential(model_file: Union[str, Path], load_prefix: str = 'load', default_tf_graph: bool = False) → Union[DeepDipole, DeepGlobalPolar, DeepPolar, DeepPot, DeepDOS, DeepWFC]`

Factory function that will initialize appropriate potential read from model_file.

Parameters

model_file

[str] The name of the frozen model file.

load_prefix

[str] The prefix in the load computational graph

default_tf_graph

[bool] If uses the default tf graph, otherwise build a new tf graph for evaluation

Returns

Union[DeepDipole, DeepGlobalPolar, DeepPolar, DeepPot, DeepWFC]

one of the available potentials

Raises

RuntimeError

if model file does not correspond to any implemented potential

`class deepmd.DipoleChargeModifier(model_name: str, model_charge_map: List[float], sys_charge_map: List[float], ewald_h: float = 1, ewald_beta: float = 1)`

Bases: *DeepDipole*

Parameters

model_name

The model file for the DeepDipole model

model_charge_map

Gives the amount of charge for the wfcc

sys_charge_map

Gives the amount of charge for the real atoms

ewald_h

Grid spacing of the reciprocal part of Ewald sum. Unit: Å

ewald_beta

Splitting parameter of the Ewald sum. Unit: Å⁻¹

Attributes

model_type

Get type of model.

model_version

Get version of model.

sess

Get TF session.

Methods

| | |
|--|---|
| <i>build_fv_graph()</i> | Build the computational graph for the force and virial inference. |
| <i>eval</i> (coord, box, atype[, eval_fv]) | Evaluate the modification. |
| <i>eval_full</i> (coords, cells, atom_types[, ...]) | Evaluate the model with interface similar to the energy model. |
| <i>eval_typeebd</i> () | Evaluate output of type embedding network by using this model. |
| <i>get_dim_apham</i> () | Unsupported in this model. |
| <i>get_dim_fparam</i> () | Unsupported in this model. |
| <i>get_ntypes</i> () | Get the number of atom types of this model. |
| <i>get_rcut</i> () | Get the cut-off radius of this model. |
| <i>get_sel_type</i> () | Get the selected atom types of this model. |
| <i>get_type_map</i> () | Get the type map (element name of the atom types) of this model. |
| <i>make_natoms_vec</i> (atom_types[, mixed_type]) | Make the natom vector used by deepmd-kit. |
| <i>modify_data</i> (data, data_sys) | Modify data. |
| <i>reverse_map</i> (vec, imap) | Reverse mapping of a vector according to the index map. |
| <i>sort_input</i> (coord, atom_type[, sel_atoms, ...]) | Sort atoms in the system according their types. |

build_fv_graph() → Tensor

Build the computational graph for the force and virial inference.

eval(coord: ndarray, box: ndarray, atype: ndarray, eval_fv: bool = True) → Tuple[ndarray, ndarray, ndarray]

Evaluate the modification.

Parameters

coord

The coordinates of atoms

box

The simulation region. PBC is assumed

atype

The atom types

eval_fv

Evaluate force and virial

Returns

tot_e

The energy modification

tot_f

The force modification

tot_v

The virial modification

`load_prefix: str`

`modify_data(data: dict, data_sys: DeepmdData) → None`

Modify data.

Parameters

`data`

Internal data of DeepmdData. Be a dict, has the following keys - coord coordinates - box simulation box - type atom types - find_energy tells if data has energy - find_force tells if data has force - find_virial tells if data has virial - energy energy - force force - virial virial

`data_sys`

[DeepmdData] The data system.

17.1.1 Subpackages

deepmd.cluster package

Module that reads node resources, auto detects if running local or on SLURM.

`deepmd.cluster.get_resource() → Tuple[str, List[str], Optional[List[int]]]`

Get local or slurm resources: nodename, nodelist, and gpus.

Returns

`Tuple[str, List[str], Optional[List[int]]]`
nodename, nodelist, and gpus

Submodules

deepmd.cluster.local module

Get local GPU resources.

`deepmd.cluster.local.get_gpus()`

Get available IDs of GPU cards at local. These IDs are valid when used as the TensorFlow device ID.

Returns

`Optional[List[int]]`
List of available GPU IDs. Otherwise, None.

`deepmd.cluster.local.get_resource() → Tuple[str, List[str], Optional[List[int]]]`

Get local resources: nodename, nodelist, and gpus.

Returns

`Tuple[str, List[str], Optional[List[int]]]`
nodename, nodelist, and gpus

deepmd.cluster.slurm module

Module to get resources on SLURM cluster.

References

https://github.com/deepsense-ai/tensorflow_on_slurm ####

`deepmd.cluster.slurm.get_resource()` → `Tuple[str, List[str], Optional[List[int]]]`

Get SLURM resources: nodename, nodelist, and gpus.

Returns

`Tuple[str, List[str], Optional[List[int]]]`
nodename, nodelist, and gpus

Raises

`RuntimeError`
if number of nodes could not be retrieved

`ValueError`
list of nodes is not of the same length as a number of nodes

`ValueError`
if current nodename is not found in node list

deepmd.descriptor package

`class deepmd.descriptor.Descriptor(*args, **kwargs)`

Bases: *PluginVariant*

The abstract class for descriptors. All specific descriptors should be based on this class.

The descriptor \mathcal{D} describes the environment of an atom, which should be a function of coordinates and types of its neighbour atoms.

Notes

Only methods and attributes defined in this class are generally public, that can be called by other classes.

Examples

```
>>> descript = Descriptor(type="se_e2_a", rcut=6., rcut_smth=0.5, sel=[50])
>>> type(descript)
<class 'deepmd.descriptor.se_a.DescriptSeA'>
```

Attributes

`explicit_ntypes`
Explicit ntypes with type embedding.

Methods

| | |
|--|---|
| <i>build</i> (coord_, atype_, natoms, box_, mesh, ...) | Build the computational graph for the descriptor. |
| <i>build_type_exclude_mask</i> (exclude_types, ...) | Build the type exclude mask for the descriptor. |
| <i>compute_input_stats</i> (data_coord, data_box, ...) | Compute the statistics (avg and std) of the training data. |
| <i>enable_compression</i> (min_nbor_dist, graph, ...) | Receive the statistics (distance, max_nbor_size and env_mat_range) of the training data. |
| <i>enable_mixed_precision</i> ([mixed_prec]) | Receive the mixed precision setting. |
| <i>get_dim_out</i> () | Returns the output dimension of this descriptor. |
| <i>get_dim_rot_mat_1</i> () | Returns the first dimension of the rotation matrix. |
| <i>get_nlist</i> () | Returns neighbor information. |
| <i>get_ntypes</i> () | Returns the number of atom types. |
| <i>get_rcut</i> () | Returns the cut-off radius. |
| <i>get_tensor_names</i> ([suffix]) | Get names of tensors. |
| <i>init_variables</i> (graph, graph_def[, suffix]) | Init the embedding net variables with the given dict. |
| <i>pass_tensors_from_frz_model</i> (*tensors) | Pass the descript_reshape tensor as well as descript_deriv tensor from the frz graph_def. |
| <i>prod_force_virial</i> (atom_ener, natoms) | Compute force and virial. |
| <i>register</i> (key) | Register a descriptor plugin. |

abstract *build*(coord_: Tensor, atype_: Tensor, natoms: Tensor, box_: Tensor, mesh: Tensor, input_dict: Dict[str, Any], reuse: Optional[bool] = None, suffix: str = '') → Tensor

Build the computational graph for the descriptor.

Parameters

coord_
[tf.Tensor] The coordinate of atoms

atype_
[tf.Tensor] The type of atoms

natoms
[tf.Tensor] The number of atoms. This tensor has the length of Ntypes + 2
natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor
natoms[i]: 2 ≤ i < Ntypes+2, number of type i atoms

box_
[tf.Tensor] The box of frames

mesh
[tf.Tensor] For historical reasons, only the length of the Tensor matters. if size of mesh == 6, pbc is assumed. if size of mesh == 0, no-pbc is assumed.

input_dict
[dict[str, Any]] Dictionary for additional inputs

reuse
[bool, optional] The weights in the networks should be reused when get the variable.

suffix
[str, optional] Name suffix to identify this descriptor

Returns

descriptor: `tf.Tensor`
The output descriptor

Notes

This method must be implemented, as it's called by other classes.

build_type_exclude_mask(exclude_types: List[Tuple[int, int]], ntypes: int, sel: List[int], ndescript: int, atype: Tensor, shape0: Tensor) → Tensor

Build the type exclude mask for the descriptor.

Parameters

exclude_types
[List[Tuple[int, int]]] The list of excluded types, e.g. [(0, 1), (1, 0)] means the interaction between type 0 and type 1 is excluded.

ntypes
[int] The number of types.

sel
[List[int]] The list of the number of selected neighbors for each type.

ndescript
[int] The number of descriptors for each atom.

atype
[tf.Tensor] The type of atoms, with the size of shape0.

shape0
[tf.Tensor] The shape of the first dimension of the inputs, which is equal to nsamples * natoms.

Returns

`tf.Tensor`
The type exclude mask, with the shape of (shape0, ndescript), and the precision of GLOBAL_TF_FLOAT_PRECISION. The mask has the value of 1 if the interaction between two types is not excluded, and 0 otherwise.

Notes

To exclude the interaction between two types, the derivative of energy with respect to distances (or angles) between two atoms should be zero [R08579741114c-1], i.e.

$$\forall i \in \text{type 1}, j \in \text{type 2}, \frac{\partial E}{\partial r_{ij}} = 0$$

When embedding networks between every two types are built, we can just remove that network. But when type_one_side is enabled, a network may be built for multiple pairs of types. In this case, we need to build a mask to exclude the interaction between two types.

The mask assumes the descriptors are sorted by neighbor type with the fixed number of given sel and each neighbor has the same number of descriptors (for example 4).

References

[1]

```
abstract compute_input_stats(data_coord: List[ndarray], data_box: List[ndarray], data_atype:
                             List[ndarray], natoms_vec: List[ndarray], mesh: List[ndarray],
                             input_dict: Dict[str, List[ndarray]], **kwargs) → None
```

Compute the statisitcs (avg and std) of the training data. The input will be normalized by the statistics.

Parameters

data_coord
`[list[np.ndarray]]` The coordinates. Can be generated by `deepmd.model.model_stat.make_stat_input()`

data_box
`[list[np.ndarray]]` The box. Can be generated by `deepmd.model.model_stat.make_stat_input()`

data_atype
`[list[np.ndarray]]` The atom types. Can be generated by `deepmd.model.model_stat.make_stat_input()`

natoms_vec
`[list[np.ndarray]]` The vector for the number of atoms of the system and different types of atoms. Can be generated by `deepmd.model.model_stat.make_stat_input()`

mesh
`[list[np.ndarray]]` The mesh for neighbor searching. Can be generated by `deepmd.model.model_stat.make_stat_input()`

input_dict
`[dict[str, list[np.ndarray]]]` Dictionary for additional input

****kwargs**
 Additional keyword arguments which may contain `mixed_type` and `real_natoms_vec`.

Notes

This method must be implemented, as it's called by other classes.

```
enable_compression(min_nbor_dist: float, graph: Graph, graph_def: GraphDef, table_extrapolate:
                    float = 5.0, table_stride_1: float = 0.01, table_stride_2: float = 0.1,
                    check_frequency: int = -1, suffix: str = "") → None
```

Reveive the statisitcs (distance, max_nbor_size and env_mat_range) of the training data.

Parameters

min_nbor_dist
`[float]` The nearest distance between atoms

graph
`[tf.Graph]` The graph of the model

graph_def
`[tf.GraphDef]` The graph definition of the model

`table_extrapolate`
 [`float`, default: 5.] The scale of model extrapolation
`table_stride_1`
 [`float`, default: 0.01] The uniform stride of the first table
`table_stride_2`
 [`float`, default: 0.1] The uniform stride of the second table
`check_frequency`
 [`int`, default: -1] The overflow check frequency
`suffix`
 [`str`, optional] The suffix of the scope

Notes

This method is called by others when the descriptor supported compression.

`enable_mixed_precision`(mixed_prec: `Optional[dict]` = None) → `None`

Reveive the mixed precision setting.

Parameters

`mixed_prec`
 The mixed precision setting used in the embedding net

Notes

This method is called by others when the descriptor supported compression.

property `explicit_ntypes`: `bool`

Explicit ntypes with type embedding.

abstract `get_dim_out`() → `int`

Returns the output dimension of this descriptor.

Returns

`int`
 the output dimension of this descriptor

Notes

This method must be implemented, as it's called by other classes.

`get_dim_rot_mat_1`() → `int`

Returns the first dimension of the rotation matrix. The rotation is of shape dim_1 x 3.

Returns

`int`
 the first dimension of the rotation matrix

`get_nlist`() → `Tuple[Tensor, Tensor, List[int], List[int]]`

Returns neighbor information.

Returns

`nlist`
[`tf.Tensor`] Neighbor list

`rij`
[`tf.Tensor`] The relative distance between the neighbor and the center atom.

`sel_a`
[`list[int]`] The number of neighbors with full information

`sel_r`
[`list[int]`] The number of neighbors with only radial information

abstract `get_ntypes()` → `int`
Returns the number of atom types.

Returns

`int`
the number of atom types

Notes

This method must be implemented, as it's called by other classes.

abstract `get_rcut()` → `float`
Returns the cut-off radius.

Returns

`float`
the cut-off radius

Notes

This method must be implemented, as it's called by other classes.

`get_tensor_names(suffix: str = '')` → `Tuple[str]`
Get names of tensors.

Parameters

`suffix`
[`str`] The suffix of the scope

Returns

`Tuple[str]`
Names of tensors

init_variables(`graph`: `Graph`, `graph_def`: `GraphDef`, `suffix`: `str` = '') → `None`
Init the embedding net variables with the given dict.

Parameters

`graph`
[`tf.Graph`] The input frozen model graph

`graph_def`
[`tf.GraphDef`] The input frozen model graph_def

suffix
 [str, optional] The suffix of the scope

Notes

This method is called by others when the descriptor supported initialization from the given variables.

pass_tensors_from_frz_model(*tensors: Tensor) → None

Pass the descrtpt_reshape tensor as well as descrtpt_deriv tensor from the frz graph_def.

Parameters

*tensors
 [tf.Tensor] passed tensors

Notes

The number of parameters in the method must be equal to the numbers of returns in *get_tensor_names()*.

abstract prod_force_virial(atom_ener: Tensor, natoms: Tensor) → Tuple[Tensor, Tensor, Tensor]

Compute force and virial.

Parameters

atom_ener
 [tf.Tensor] The atomic energy

natoms
 [tf.Tensor] The number of atoms. This tensor has the length of Ntypes + 2
 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this
 processor natoms[i]: 2 ≤ i < Ntypes+2, number of type i atoms

Returns

force
 [tf.Tensor] The force on atoms

virial
 [tf.Tensor] The total virial

atom_virial
 [tf.Tensor] The atomic virial

static register(key: str) → Callable

Register a descriptor plugin.

Parameters

key
 [str] the key of a descriptor

Returns

Descriptor
 the registered descriptor

Examples

```
>>> @Descriptor.register("some_descrpt")
class SomeDescript(Descriptor):
    pass
```

```
class deepmd.descriptor.DescriptHybrid(*args, **kwargs)
```

Bases: *Descriptor*

Concat a list of descriptors to form a new descriptor.

Parameters

list

[list] Build a descriptor from the concatenation of the list of descriptors.

Attributes

explicit_ntypes

Explicit ntypes with type embedding.

Methods

| | |
|--|--|
| <i>build</i> (coord_, atype_, natoms, box_, mesh, ...) | Build the computational graph for the descriptor. |
| <i>build_type_exclude_mask</i> (exclude_types, ...) | Build the type exclude mask for the descriptor. |
| <i>compute_input_stats</i> (data_coord, data_box, ...) | Compute the statisitcs (avg and std) of the training data. |
| <i>enable_compression</i> (min_nbor_dist, graph, ...) | Reveive the statisitcs (distance, max_nbor_size and env_mat_range) of the training data. |
| <i>enable_mixed_precision</i> ([mixed_prec]) | Reveive the mixed precision setting. |
| <i>get_dim_out</i> () | Returns the output dimension of this descriptor. |
| <i>get_dim_rot_mat_1</i> () | Returns the first dimension of the rotation matrix. |
| <i>get_nlist</i> () | Get the neighbor information of the descriptor, returns the nlist of the descriptor with the largest cut-off radius. |
| <i>get_nlist_i</i> (ii) | Get the neighbor information of the ii-th descriptor. |
| <i>get_ntypes</i> () | Returns the number of atom types. |
| <i>get_rcut</i> () | Returns the cut-off radius. |
| <i>get_tensor_names</i> ([suffix]) | Get names of tensors. |
| <i>init_variables</i> (graph, graph_def[, suffix]) | Init the embedding net variables with the given dict. |
| <i>merge_input_stats</i> (stat_dict) | Merge the statisitcs computed from compute_input_stats to obtain the self.davg and self.dstd. |
| <i>pass_tensors_from_frz_model</i> (*tensors) | Pass the descrpt_reshape tensor as well as descrpt_deriv tensor from the frz graph_def. |
| <i>prod_force_virial</i> (atom_ener, natoms) | Compute force and virial. |
| <i>register</i> (key) | Register a descriptor plugin. |

build(coord_: Tensor, atype_: Tensor, natoms: Tensor, box_: Tensor, mesh: Tensor, input_dict: dict, reuse: Optional[bool] = None, suffix: str = "") → Tensor

Build the computational graph for the descriptor.

Parameters

`coord_`
The coordinate of atoms

`atype_`
The type of atoms

`natoms`
The number of atoms. This tensor has the length of `Ntypes + 2` `natoms[0]`: number of local atoms `natoms[1]`: total number of atoms held by this processor `natoms[i]`: $2 \leq i < Ntypes+2$, number of type `i` atoms

`box_`
[`tf.Tensor`] The box of the system

`mesh`
For historical reasons, only the length of the Tensor matters. if size of mesh == 6, pbc is assumed. if size of mesh == 0, no-pbc is assumed.

`input_dict`
Dictionary for additional inputs

`reuse`
The weights in the networks should be reused when get the variable.

`suffix`
Name suffix to identify this descriptor

Returns

descriptor
The output descriptor

`compute_input_stats`(data_coord: list, data_box: list, data_atype: list, natoms_vec: list, mesh: list, input_dict: dict, mixed_type: bool = False, real_natoms_vec: Optional[list] = None, **kwargs) → None

Compute the statistics (avg and std) of the training data. The input will be normalized by the statistics.

Parameters

`data_coord`
The coordinates. Can be generated by `deepmd.model.make_stat_input`

`data_box`
The box. Can be generated by `deepmd.model.make_stat_input`

`data_atype`
The atom types. Can be generated by `deepmd.model.make_stat_input`

`natoms_vec`
The vector for the number of atoms of the system and different types of atoms. Can be generated by `deepmd.model.make_stat_input`

`mesh`
The mesh for neighbor searching. Can be generated by `deepmd.model.make_stat_input`

`input_dict`
Dictionary for additional input

`mixed_type`
Whether to perform the `mixed_type` mode. If `True`, the input data has the `mixed_type` format (see `doc/model/train_se_atten.md`), in which frames in a system may have different `natoms_vec(s)`, with the same `nloc`.

`real_natoms_vec`
If `mixed_type` is `True`, it takes in the `real_natoms_vec` for each frame.

`**kwargs`
Additional keyword arguments.

`enable_compression`(`min_nbor_dist`: `float`, `graph`: `Graph`, `graph_def`: `GraphDef`, `table_extrapolate`: `float` = 5.0, `table_stride_1`: `float` = 0.01, `table_stride_2`: `float` = 0.1, `check_frequency`: `int` = -1, `suffix`: `str` = "") \rightarrow `None`
Reveive the statisitcs (distance, `max_nbor_size` and `env_mat_range`) of the training data.

Parameters

`min_nbor_dist`
[`float`] The nearest distance between atoms

`graph`
[`tf.Graph`] The graph of the model

`graph_def`
[`tf.GraphDef`] The `graph_def` of the model

`table_extrapolate`
[`float`, default: 5.] The scale of model extrapolation

`table_stride_1`
[`float`, default: 0.01] The uniform stride of the first table

`table_stride_2`
[`float`, default: 0.1] The uniform stride of the second table

`check_frequency`
[`int`, default: -1] The overflow check frequency

`suffix`
[`str`, optional] The suffix of the scope

`enable_mixed_precision`(`mixed_prec`: `Optional[dict]` = `None`) \rightarrow `None`
Reveive the mixed precision setting.

Parameters

`mixed_prec`
The mixed precision setting used in the embedding net

`property explicit_ntypes`: `bool`
Explicit ntypes with type embedding.

`get_dim_out()` \rightarrow `int`
Returns the output dimension of this descriptor.

`get_nlist()` \rightarrow `Tuple`[`Tensor`, `Tensor`, `List[int]`, `List[int]`]
Get the neighbor information of the descriptor, returns the `nlist` of the descriptor with the largest cut-off radius.

Returns

nlist
Neighbor list

rij
The relative distance between the neighbor and the center atom.

sel_a
The number of neighbors with full information

sel_r
The number of neighbors with only radial information

get_nlist_i(ii: `int`) → `Tuple`[`Tensor`, `Tensor`, `List`[`int`], `List`[`int`]]

Get the neighbor information of the ii-th descriptor.

Parameters

ii
[`int`] The index of the descriptor

Returns

nlist
Neighbor list

rij
The relative distance between the neighbor and the center atom.

sel_a
The number of neighbors with full information

sel_r
The number of neighbors with only radial information

get_ntypes() → `int`

Returns the number of atom types.

get_rcut() → `float`

Returns the cut-off radius.

get_tensor_names(suffix: `str` = '') → `Tuple`[`str`]

Get names of tensors.

Parameters

suffix
[`str`] The suffix of the scope

Returns

`Tuple`[`str`]
Names of tensors

init_variables(graph: `Graph`, graph_def: `GraphDef`, suffix: `str` = '') → `None`

Init the embedding net variables with the given dict.

Parameters

graph
[`tf.Graph`] The input frozen model graph

`graph_def`
[`tf.GraphDef`] The input frozen model `graph_def`

`suffix`
[`str`, `optional`] The suffix of the scope

`merge_input_stats`(`stat_dict`)

Merge the statistics computed from `compute_input_stats` to obtain the `self.davg` and `self.dstd`.

Parameters

`stat_dict`
The dict of statistics computed from `compute_input_stats`, including:

`sumr`
The sum of radial statistics.

`suma`
The sum of relative coord statistics.

`sumn`
The sum of neighbor numbers.

`sumr2`
The sum of square of radial statistics.

`suma2`
The sum of square of relative coord statistics.

`pass_tensors_from_frz_model`(*`tensors`: `Tensor`) → `None`

Pass the `descript_reshape` tensor as well as `descript_deriv` tensor from the `frz_graph_def`.

Parameters

*`tensors`
[`tf.Tensor`] passed tensors

`prod_force_virial`(`atom_ener`: `Tensor`, `natoms`: `Tensor`) → `Tuple`[`Tensor`, `Tensor`, `Tensor`]

Compute force and virial.

Parameters

`atom_ener`
The atomic energy

`natoms`
The number of atoms. This tensor has the length of `Ntypes + 2` `natoms[0]`: number of local atoms `natoms[1]`: total number of atoms held by this processor `natoms[i]`: $2 \leq i < Ntypes + 2$, number of type `i` atoms

Returns

`force`
The force on atoms

`virial`
The total virial

`atom_virial`
The atomic virial

```
class deepmd.descriptor.DescriptLocFrame(*args, **kwargs)
```

Bases: *Descriptor*

Defines a local frame at each atom, and the compute the descriptor as local coordinates under this frame.

Parameters

`rcut`

The cut-off radius

`sel_a`

[`list[str]`] The length of the list should be the same as the number of atom types in the system. `sel_a[i]` gives the selected number of type-*i* neighbors. The full relative coordinates of the neighbors are used by the descriptor.

`sel_r`

[`list[str]`] The length of the list should be the same as the number of atom types in the system. `sel_r[i]` gives the selected number of type-*i* neighbors. Only relative distance of the neighbors are used by the descriptor. `sel_a[i] + sel_r[i]` is recommended to be larger than the maximally possible number of type-*i* neighbors in the cut-off radius.

`axis_rule`: `list[int]`

The length should be 6 times of the number of types. - `axis_rule[i*6+0]`: class of the atom defining the first axis of type-*i* atom. 0 for neighbors with full coordinates and 1 for neighbors only with relative distance. - `axis_rule[i*6+1]`: type of the atom defining the first axis of type-*i* atom. - `axis_rule[i*6+2]`: index of the axis atom defining the first axis. Note that the neighbors with the same class and type are sorted according to their relative distance. - `axis_rule[i*6+3]`: class of the atom defining the second axis of type-*i* atom. 0 for neighbors with full coordinates and 1 for neighbors only with relative distance. - `axis_rule[i*6+4]`: type of the atom defining the second axis of type-*i* atom. - `axis_rule[i*6+5]`: index of the axis atom defining the second axis. Note that the neighbors with the same class and type are sorted according to their relative distance.

Attributes

`explicit_ntypes`

Explicit ntypes with type embedding.

Methods

| | |
|---|---|
| <code>build(coord_, atype_, natoms, box_, mesh, ...)</code> | Build the computational graph for the descriptor. |
| <code>build_type_exclude_mask(exclude_types, ...)</code> | Build the type exclude mask for the descriptor. |
| <code>compute_input_stats(data_coord, data_box, ...)</code> | Compute the statistics (avg and std) of the training data. |
| <code>enable_compression(min_nbor_dist, graph, ...)</code> | Receive the statistics (distance, max_nbor_size and env_mat_range) of the training data. |
| <code>enable_mixed_precision([mixed_prec])</code> | Receive the mixed precision setting. |
| <code>get_dim_out()</code> | Returns the output dimension of this descriptor. |
| <code>get_dim_rot_mat_1()</code> | Returns the first dimension of the rotation matrix. |
| <code>get_nlist()</code> | Returns |
| <code>get_ntypes()</code> | Returns the number of atom types. |
| <code>get_rcut()</code> | Returns the cut-off radius. |
| <code>get_rot_mat()</code> | Get rotational matrix. |
| <code>get_tensor_names([suffix])</code> | Get names of tensors. |
| <code>init_variables(graph, graph_def[, suffix])</code> | Init the embedding net variables with the given dict. |
| <code>pass_tensors_from_frz_model(*tensors)</code> | Pass the <code>descript_reshape</code> tensor as well as <code>descript_deriv</code> tensor from the <code>frz_graph_def</code> . |
| <code>prod_force_virial(atom_ener, natoms)</code> | Compute force and virial. |
| <code>register(key)</code> | Register a descriptor plugin. |

build(coord_: Tensor, atype_: Tensor, natoms: Tensor, box_: Tensor, mesh: Tensor, input_dict: dict, reuse: Optional[bool] = None, suffix: str = '') → Tensor

Build the computational graph for the descriptor.

Parameters

coord_
The coordinate of atoms

atype_
The type of atoms

natoms
The number of atoms. This tensor has the length of Ntypes + 2. natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 ≤ i < Ntypes+2, number of type i atoms

box_
[tf.Tensor] The box of the system

mesh
For historical reasons, only the length of the Tensor matters. if size of mesh == 6, pbc is assumed. if size of mesh == 0, no-pbc is assumed.

input_dict
Dictionary for additional inputs

reuse
The weights in the networks should be reused when get the variable.

suffix
Name suffix to identify this descriptor

Returns

descriptor
The output descriptor

compute_input_stats(data_coord: list, data_box: list, data_atype: list, natoms_vec: list, mesh: list, input_dict: dict, **kwargs) → None

Compute the statistics (avg and std) of the training data. The input will be normalized by the statistics.

Parameters

data_coord
The coordinates. Can be generated by `deepmd.model.make_stat_input`

data_box
The box. Can be generated by `deepmd.model.make_stat_input`

data_atype
The atom types. Can be generated by `deepmd.model.make_stat_input`

natoms_vec
The vector for the number of atoms of the system and different types of atoms.
Can be generated by `deepmd.model.make_stat_input`

mesh
The mesh for neighbor searching. Can be generated by `deepmd.model.make_stat_input`

input_dict
Dictionary for additional input

****kwargs**
Additional keyword arguments.

get_dim_out() → int
Returns the output dimension of this descriptor.

get_nlist() → Tuple[Tensor, Tensor, List[int], List[int]]

Returns

nlist
Neighbor list

rij
The relative distance between the neighbor and the center atom.

sel_a
The number of neighbors with full information

sel_r
The number of neighbors with only radial information

get_ntypes() → int
Returns the number of atom types.

get_rcut() → float
Returns the cut-off radius.

`get_rot_mat()` \rightarrow Tensor

Get rotational matrix.

`init_variables(graph: Graph, graph_def: GraphDef, suffix: str = "")` \rightarrow None

Init the embedding net variables with the given dict.

Parameters

`graph`

[`tf.Graph`] The input frozen model graph

`graph_def`

[`tf.GraphDef`] The input frozen model graph_def

`suffix`

[`str`, optional] The suffix of the scope

`prod_force_virial(atom_ener: Tensor, natoms: Tensor)` \rightarrow Tuple[Tensor, Tensor, Tensor]

Compute force and virial.

Parameters

`atom_ener`

The atomic energy

`natoms`

The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 <= i < Ntypes+2, number of type i atoms

Returns

force

The force on atoms

virial

The total virial

atom_virial

The atomic virial

`class deepmd.descriptor.DescriptSeA(*args, **kwargs)`

Bases: *DescriptSe*

DeepPot-SE constructed from all information (both angular and radial) of atomic configurations. The embedding takes the distance between atoms as input.

The descriptor $\mathcal{D}^i \in \mathbb{R}^{M_1 \times M_2}$ is given by [1]

$$\mathcal{D}^i = (\mathcal{G}^i)^T \mathcal{R}^i (\mathcal{R}^i)^T \mathcal{G}_{<}^i$$

where $\mathcal{R}^i \in \mathbb{R}^{N \times 4}$ is the coordinate matrix, and each row of \mathcal{R}^i can be constructed as follows

$$(\mathcal{R}^i)_j = \begin{bmatrix} \frac{s(r_{ji})}{s(r_{ji})x_{ji}} \\ \frac{r_{ji}}{s(r_{ji})y_{ji}} \\ \frac{r_{ji}}{s(r_{ji})z_{ji}} \\ \frac{r_{ji}}{r_{ji}} \end{bmatrix}$$

where $\mathbf{R}_{ji} = \mathbf{R}_j - \mathbf{R}_i = (x_{ji}, y_{ji}, z_{ji})$ is the relative coordinate and $r_{ji} = \|\mathbf{R}_{ji}\|$ is its norm. The switching function $s(r)$ is defined as:

$$s(r) = \begin{cases} \frac{1}{r}, & r < r_s \\ \frac{1}{r} \left\{ \left(\frac{r-r_s}{r_c-r_s} \right)^3 \left(-6 \left(\frac{r-r_s}{r_c-r_s} \right)^2 + 15 \frac{r-r_s}{r_c-r_s} - 10 \right) + 1 \right\}, & r_s \leq r < r_c \\ 0, & r \geq r_c \end{cases}$$

Each row of the embedding matrix $\mathcal{G}^i \in \mathbb{R}^{N \times M_1}$ consists of outputs of a embedding network \mathcal{N} of $s(r_{ji})$:

$$(\mathcal{G}^i)_j = \mathcal{N}(s(r_{ji}))$$

$\mathcal{G}^i_{<} \in \mathbb{R}^{N \times M_2}$ takes first M_2 columns of \mathcal{G}^i . The equation of embedding network \mathcal{N} can be found at [deepmd.utils.network.embedding_net\(\)](#).

Parameters

- rcut
The cut-off radius r_c
- rcut_smth
From where the environment matrix should be smoothed r_s
- sel
[[list](#)[[str](#)]] sel[i] specifies the maximum number of type i atoms in the cut-off radius
- neuron
[[list](#)[[int](#)]] Number of neurons in each hidden layers of the embedding net \mathcal{N}
- axis_neuron
Number of the axis neuron M_2 (number of columns of the sub-matrix of the embedding matrix)
- resnet_dt
Time-step dt in the resnet construction: $y = x + dt * \phi(Wx + b)$
- trainable
If the weights of embedding net are trainable.
- seed
Random seed for initializing the network parameters.
- type_one_side
Try to build N_types embedding nets. Otherwise, building N_types^2 embedding nets
- exclude_types
[[List](#)[[List](#)[[int](#)]]] The excluded pairs of types which have no interaction with each other. For example, [\[\[0, 1\]\]](#) means no interaction between type 0 and type 1.
- set_davg_zero
Set the shift of embedding net input to zero.
- activation_function
The activation function in the embedding net. Supported options are "relu", "relu6", "softplus", "sigmoid", "tanh", "gelu", "gelu_tf", "None", "none".
- precision
The precision of the embedding net parameters. Supported options are "default", "float16", "float32", "float64", "bfloat16".

`uniform_seed`

Only for the purpose of backward compatibility, retrieves the old behavior of using the random seed

`multi_task`

If the model has multi fitting nets to train.

References

[1]

Attributes

`explicit_ntypes`

Explicit ntypes with type embedding.

`precision`

Precision of filter network.

Methods

| | |
|--|---|
| <code>build(coord_, atype_, natoms, box_, mesh, ...)</code> | Build the computational graph for the descriptor. |
| <code>build_type_exclude_mask(exclude_types, ...)</code> | Build the type exclude mask for the descriptor. |
| <code>compute_input_stats(data_coord, data_box, ...)</code> | Compute the statisitcs (avg and std) of the training data. |
| <code>enable_compression(min_nbor_dist, graph, ...)</code> | Reveive the statisitcs (distance, max_nbor_size and env_mat_range) of the training data. |
| <code>enable_mixed_precision([mixed_prec])</code> | Reveive the mixed precision setting. |
| <code>get_dim_out()</code> | Returns the output dimension of this descriptor. |
| <code>get_dim_rot_mat_1()</code> | Returns the first dimension of the rotation matrix. |
| <code>get_nlist()</code> | Returns neighbor information. |
| <code>get_ntypes()</code> | Returns the number of atom types. |
| <code>get_rcut()</code> | Returns the cut-off radius. |
| <code>get_rot_mat()</code> | Get rotational matrix. |
| <code>get_tensor_names([suffix])</code> | Get names of tensors. |
| <code>init_variables(graph, graph_def[, suffix])</code> | Init the embedding net variables with the given dict. |
| <code>merge_input_stats(stat_dict)</code> | Merge the statisitcs computed from <code>compute_input_stats</code> to obtain the <code>self.davg</code> and <code>self.dstd</code> . |
| <code>pass_tensors_from_frz_model(descrpt_reshape, ...)</code> | Pass the <code>descrpt_reshape</code> tensor as well as <code>descrpt_deriv</code> tensor from the <code>frz_graph_def</code> . |
| <code>prod_force_virial(atom_ener, natoms)</code> | Compute force and virial. |
| <code>register(key)</code> | Register a descriptor plugin. |

`build`(coord_: Tensor, atype_: Tensor, natoms: Tensor, box_: Tensor, mesh: Tensor, input_dict: dict, reuse: Optional[bool] = None, suffix: str = "") → Tensor

Build the computational graph for the descriptor.

Parameters

`coord_`
The coordinate of atoms

`atype_`
The type of atoms

`natoms`
The number of atoms. This tensor has the length of `Ntypes + 2` `natoms[0]`: number of local atoms `natoms[1]`: total number of atoms held by this processor `natoms[i]`: $2 \leq i < Ntypes+2$, number of type `i` atoms

`box_`
[`tf.Tensor`] The box of the system

`mesh`
For historical reasons, only the length of the Tensor matters. if size of mesh == 6, pbc is assumed. if size of mesh == 0, no-pbc is assumed.

`input_dict`
Dictionary for additional inputs

`reuse`
The weights in the networks should be reused when get the variable.

`suffix`
Name suffix to identify this descriptor

Returns

descriptor
The output descriptor

`compute_input_stats`(`data_coord`: list, `data_box`: list, `data_atype`: list, `natoms_vec`: list, `mesh`: list, `input_dict`: dict, `**kwargs`) → None

Compute the statistics (avg and std) of the training data. The input will be normalized by the statistics.

Parameters

`data_coord`
The coordinates. Can be generated by `deepmd.model.make_stat_input`

`data_box`
The box. Can be generated by `deepmd.model.make_stat_input`

`data_atype`
The atom types. Can be generated by `deepmd.model.make_stat_input`

`natoms_vec`
The vector for the number of atoms of the system and different types of atoms. Can be generated by `deepmd.model.make_stat_input`

`mesh`
The mesh for neighbor searching. Can be generated by `deepmd.model.make_stat_input`

`input_dict`
Dictionary for additional input

`**kwargs`
Additional keyword arguments.

```
enable_compression(min_nbor_dist: float, graph: Graph, graph_def: GraphDef, table_extrapolate:
    float = 5, table_stride_1: float = 0.01, table_stride_2: float = 0.1,
    check_frequency: int = -1, suffix: str = '') → None
```

Reveive the statisitcs (distance, max_nbor_size and env_mat_range) of the training data.

Parameters

min_nbor_dist
The nearest distance between atoms

graph
[[tf.Graph](#)] The graph of the model

graph_def
[[tf.GraphDef](#)] The graph_def of the model

table_extrapolate
The scale of model extrapolation

table_stride_1
The uniform stride of the first table

table_stride_2
The uniform stride of the second table

check_frequency
The overflow check frequency

suffix
[[str](#), optional] The suffix of the scope

```
enable_mixed_precision(mixed_prec: Optional[dict] = None) → None
```

Reveive the mixed precision setting.

Parameters

mixed_prec
The mixed precision setting used in the embedding net

```
get_dim_out() → int
```

Returns the output dimension of this descriptor.

```
get_dim_rot_mat_1() → int
```

Returns the first dimension of the rotation matrix. The rotation is of shape dim_1 x 3.

```
get_nlist() → Tuple[Tensor, Tensor, List[int], List[int]]
```

Returns neighbor information.

Returns

nlist
Neighbor list

rij
The relative distance between the neighbor and the center atom.

sel_a
The number of neighbors with full information

sel_r
The number of neighbors with only radial information

get_ntypes() → `int`

Returns the number of atom types.

get_rcut() → `float`

Returns the cut-off radius.

get_rot_mat() → `Tensor`

Get rotational matrix.

init_variables(graph: `Graph`, graph_def: `GraphDef`, suffix: `str` = "") → `None`

Init the embedding net variables with the given dict.

Parameters

graph

[`tf.Graph`] The input frozen model graph

graph_def

[`tf.GraphDef`] The input frozen model graph_def

suffix

[`str`, `optional`] The suffix of the scope

merge_input_stats(stat_dict)

Merge the statistics computed from compute_input_stats to obtain the self.davg and self.dstd.

Parameters

stat_dict

The dict of statistics computed from compute_input_stats, including:

sumr

The sum of radial statistics.

suma

The sum of relative coord statistics.

sumn

The sum of neighbor numbers.

sumr2

The sum of square of radial statistics.

suma2

The sum of square of relative coord statistics.

prod_force_virial(atom_ener: `Tensor`, natoms: `Tensor`) → `Tuple`[`Tensor`, `Tensor`, `Tensor`]

Compute force and virial.

Parameters

atom_ener

The atomic energy

natoms

The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 ≤ i < Ntypes+2, number of type i atoms

Returns

```
    force
        The force on atoms

    virial
        The total virial

    atom_virial
        The atomic virial

class deepmd.descriptor.DescriptSeAEbd(*args, **kwargs)
    Bases: DescriptSeA
    DeepPot-SE descriptor with type embedding approach.

    Parameters

    rcut
        The cut-off radius

    rcut_smth
        From where the environment matrix should be smoothed

    sel
        [list[str]] sel[i] specifies the maxmum number of type i atoms in the cut-off radius

    neuron
        [list[int]] Number of neurons in each hidden layers of the embedding net

    axis_neuron
        Number of the axis neuron (number of columns of the sub-matrix of the embedding
        matrix)

    resnet_dt
        Time-step dt in the resnet construction:  $y = x + dt * \phi(Wx + b)$ 

    trainable
        If the weights of embedding net are trainable.

    seed
        Random seed for initializing the network parameters.

    type_one_side
        Try to build  $N\_types$  embedding nets. Otherwise, building  $N\_types^2$  embedding
        nets

    type_nchanl
        Number of channels for type representation

    type_nlayer
        Number of hidden layers for the type embedding net (skip connected).

    numb_aparam
        Number of atomic parameters. If  $>0$  it will be embedded with atom types.

    set_davg_zero
        Set the shift of embedding net input to zero.

    activation_function
        The activation function in the embedding net. Supported options are {0}

    precision
        The precision of the embedding net parameters. Supported options are {1}
```

exclude_types
 [List[List[int]]] The excluded pairs of types which have no interaction with each other. For example, [[0, 1]] means no interaction between type 0 and type 1.

Attributes

explicit_ntypes
 Explicit ntypes with type embedding.

precision
 Precision of filter network.

Methods

| | |
|--|---|
| <i>build</i> (coord_, atype_, natoms, box_, mesh, ...) | Build the computational graph for the descriptor. |
| <i>build_type_exclude_mask</i> (exclude_types, ...) | Build the type exclude mask for the descriptor. |
| <i>compute_input_stats</i> (data_coord, data_box, ...) | Compute the statisitcs (avg and std) of the training data. |
| <i>enable_compression</i> (min_nbor_dist, graph, ...) | Reveive the statisitcs (distance, max_nbor_size and env_mat_range) of the training data. |
| <i>enable_mixed_precision</i> ([mixed_prec]) | Reveive the mixed precision setting. |
| <i>get_dim_out</i> () | Returns the output dimension of this descriptor. |
| <i>get_dim_rot_mat_1</i> () | Returns the first dimension of the rotation matrix. |
| <i>get_nlist</i> () | Returns neighbor information. |
| <i>get_ntypes</i> () | Returns the number of atom types. |
| <i>get_rcut</i> () | Returns the cut-off radius. |
| <i>get_rot_mat</i> () | Get rotational matrix. |
| <i>get_tensor_names</i> ([suffix]) | Get names of tensors. |
| <i>init_variables</i> (graph, graph_def[, suffix]) | Init the embedding net variables with the given dict. |
| <i>merge_input_stats</i> (stat_dict) | Merge the statisitcs computed from compute_input_stats to obtain the self.davg and self.dstd. |
| <i>pass_tensors_from_frz_model</i> (descript_reshape, ...) | Pass the descript_reshape tensor as well as descript_deriv tensor from the frz_graph_def. |
| <i>prod_force_virial</i> (atom_ener, natoms) | Compute force and virial. |
| <i>register</i> (key) | Register a descriptor plugin. |

build(coord_: Tensor, atype_: Tensor, natoms: Tensor, box_: Tensor, mesh: Tensor, input_dict: dict, reuse: Optional[bool] = None, suffix: str = '') → Tensor

Build the computational graph for the descriptor.

Parameters

coord_
 The coordinate of atoms

atype_
 The type of atoms

natoms
 The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number

of local atoms `natoms[1]`: total number of atoms held by this processor `natoms[i]`:
 $2 \leq i < N_{\text{types}} + 2$, number of type i atoms

`box_`
`[tf.Tensor]` The box of the system

`mesh`
 For historical reasons, only the length of the Tensor matters. if size of `mesh == 6`,
 pbc is assumed. if size of `mesh == 0`, no-pbc is assumed.

`input_dict`
 Dictionary for additional inputs

`reuse`
 The weights in the networks should be reused when get the variable.

`suffix`
 Name suffix to identify this descriptor

Returns

descriptor
 The output descriptor

class `deepmd.descriptor.DescriptSeAEf(*args, **kwargs)`
 Bases: *Descriptor*
 Smooth edition descriptor with Ef.

Parameters

`rcut`
 The cut-off radius

`rcut_smth`
 From where the environment matrix should be smoothed

`sel`
`[list[str]]` `sel[i]` specifies the maximum number of type i atoms in the cut-off radius

`neuron`
`[list[int]]` Number of neurons in each hidden layers of the embedding net

`axis_neuron`
 Number of the axis neuron (number of columns of the sub-matrix of the embedding
 matrix)

`resnet_dt`
 Time-step dt in the resnet construction: $y = x + dt * \phi(Wx + b)$

`trainable`
 If the weights of embedding net are trainable.

`seed`
 Random seed for initializing the network parameters.

`type_one_side`
 Try to build N_{types} embedding nets. Otherwise, building N_{types}^2 embedding
 nets

`exclude_types`
`[List[List[int]]]` The excluded pairs of types which have no interaction with each
 other. For example, `[[0, 1]]` means no interaction between type 0 and type 1.

`set_davg_zero`
Set the shift of embedding net input to zero.

`activation_function`
The activation function in the embedding net. Supported options are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”, “gelu_tf”, “None”, “none”.

`precision`
The precision of the embedding net parameters. Supported options are “default”, “float16”, “float32”, “float64”, “bfloat16”.

`uniform_seed`
Only for the purpose of backward compatibility, retrieves the old behavior of using the random seed

Attributes

`explicit_ntypes`
Explicit ntypes with type embedding.

Methods

| | |
|---|--|
| <code>build(coord_, atype_, natoms, box_, mesh, ...)</code> | Build the computational graph for the descriptor. |
| <code>build_type_exclude_mask(exclude_types, ...)</code> | Build the type exclude mask for the descriptor. |
| <code>compute_input_stats(data_coord, data_box, ...)</code> | Compute the statistics (avg and std) of the training data. |
| <code>enable_compression(min_nbor_dist, graph, ...)</code> | Reveive the statistics (distance, max_nbor_size and env_mat_range) of the training data. |
| <code>enable_mixed_precision([mixed_prec])</code> | Reveive the mixed precision setting. |
| <code>get_dim_out()</code> | Returns the output dimension of this descriptor. |
| <code>get_dim_rot_mat_1()</code> | Returns the first dimension of the rotation matrix. |
| <code>get_nlist()</code> | Returns neighbor information. |
| <code>get_ntypes()</code> | Returns the number of atom types. |
| <code>get_rcut()</code> | Returns the cut-off radius. |
| <code>get_rot_mat()</code> | Get rotational matrix. |
| <code>get_tensor_names([suffix])</code> | Get names of tensors. |
| <code>init_variables(graph, graph_def[, suffix])</code> | Init the embedding net variables with the given dict. |
| <code>pass_tensors_from_frz_model(*tensors)</code> | Pass the descrpt_reshape tensor as well as descrpt_deriv tensor from the frz graph_def. |
| <code>prod_force_virial(atom_ener, natoms)</code> | Compute force and virial. |
| <code>register(key)</code> | Register a descriptor plugin. |

`build(coord_: Tensor, atype_: Tensor, natoms: Tensor, box_: Tensor, mesh: Tensor, input_dict: dict, reuse: Optional[bool] = None, suffix: str = '') → Tensor`

Build the computational graph for the descriptor.

Parameters

`coord_`
The coordinate of atoms

`atype_`
The type of atoms

`natoms`
The number of atoms. This tensor has the length of `Ntypes + 2` `natoms[0]`: number of local atoms `natoms[1]`: total number of atoms held by this processor `natoms[i]`: $2 \leq i < Ntypes+2$, number of type `i` atoms

`box_`
[`tf.Tensor`] The box of the system

`mesh`
For historical reasons, only the length of the Tensor matters. if size of `mesh == 6`, pbc is assumed. if size of `mesh == 0`, no-pbc is assumed.

`input_dict`
Dictionary for additional inputs. Should have 'efield'.

`reuse`
The weights in the networks should be reused when get the variable.

`suffix`
Name suffix to identify this descriptor

Returns

descriptor
The output descriptor

`compute_input_stats`(`data_coord`: list, `data_box`: list, `data_atype`: list, `natoms_vec`: list, `mesh`: list, `input_dict`: dict, `**kwargs`) → None

Compute the statistics (avg and std) of the training data. The input will be normalized by the statistics.

Parameters

`data_coord`
The coordinates. Can be generated by `deepmd.model.make_stat_input`

`data_box`
The box. Can be generated by `deepmd.model.make_stat_input`

`data_atype`
The atom types. Can be generated by `deepmd.model.make_stat_input`

`natoms_vec`
The vector for the number of atoms of the system and different types of atoms. Can be generated by `deepmd.model.make_stat_input`

`mesh`
The mesh for neighbor searching. Can be generated by `deepmd.model.make_stat_input`

`input_dict`
Dictionary for additional input

`**kwargs`
Additional keyword arguments.

`get_dim_out()` → int
Returns the output dimension of this descriptor.

`get_dim_rot_mat_1()` → int
Returns the first dimension of the rotation matrix. The rotation is of shape `dim_1 x 3`.

`get_nlist()` → `Tuple[Tensor, Tensor, List[int], List[int]]`

Returns neighbor information.

Returns

nlist

Neighbor list

rij

The relative distance between the neighbor and the center atom.

sel_a

The number of neighbors with full information

sel_r

The number of neighbors with only radial information

`get_ntypes()` → `int`

Returns the number of atom types.

`get_rcut()` → `float`

Returns the cut-off radius.

`get_rot_mat()` → `Tensor`

Get rotational matrix.

`prod_force_virial(atom_ener: Tensor, natoms: Tensor)` → `Tuple[Tensor, Tensor, Tensor]`

Compute force and virial.

Parameters

atom_ener

The atomic energy

natoms

The number of atoms. This tensor has the length of `Ntypes + 2` `natoms[0]`: number of local atoms `natoms[1]`: total number of atoms held by this processor `natoms[i]`: $2 \leq i < Ntypes + 2$, number of type `i` atoms

Returns

force

The force on atoms

virial

The total virial

atom_virial

The atomic virial

`class deepmd.descriptor.DescriptSeAEfLower(*args, **kwargs)`

Bases: *DescriptSeA*

Helper class for implementing DescriptSeAEf.

Attributes

explicit_ntypes

Explicit ntypes with type embedding.

precision

Precision of filter network.

Methods

| | |
|--|---|
| <code>build(coord_, atype_, natoms, box_, mesh, ...)</code> | Build the computational graph for the descriptor. |
| <code>build_type_exclude_mask(exclude_types, ...)</code> | Build the type exclude mask for the descriptor. |
| <code>compute_input_stats(data_coord, data_box, ...)</code> | Compute the statistics (avg and std) of the training data. |
| <code>enable_compression(min_nbor_dist, graph, ...)</code> | Receive the statistics (distance, max_nbor_size and env_mat_range) of the training data. |
| <code>enable_mixed_precision([mixed_prec])</code> | Receive the mixed precision setting. |
| <code>get_dim_out()</code> | Returns the output dimension of this descriptor. |
| <code>get_dim_rot_mat_1()</code> | Returns the first dimension of the rotation matrix. |
| <code>get_nlist()</code> | Returns neighbor information. |
| <code>get_ntypes()</code> | Returns the number of atom types. |
| <code>get_rcut()</code> | Returns the cut-off radius. |
| <code>get_rot_mat()</code> | Get rotational matrix. |
| <code>get_tensor_names([suffix])</code> | Get names of tensors. |
| <code>init_variables(graph, graph_def[, suffix])</code> | Init the embedding net variables with the given dict. |
| <code>merge_input_stats(stat_dict)</code> | Merge the statistics computed from <code>compute_input_stats</code> to obtain the <code>self.davg</code> and <code>self.dstd</code> . |
| <code>pass_tensors_from_frz_model(descrpt_reshape, ...)</code> | Pass the <code>descrpt_reshape</code> tensor as well as <code>descrpt_deriv</code> tensor from the <code>frz_graph_def</code> . |
| <code>prod_force_virial(atom_ener, natoms)</code> | Compute force and virial. |
| <code>register(key)</code> | Register a descriptor plugin. |

build(coord_, atype_, natoms, box_, mesh, input_dict, suffix='', reuse=None)

Build the computational graph for the descriptor.

Parameters

coord_

The coordinate of atoms

atype_

The type of atoms

natoms

The number of atoms. This tensor has the length of `Ntypes + 2`: `natoms[0]`: number of local atoms `natoms[1]`: total number of atoms held by this processor `natoms[i]`: $2 \leq i < Ntypes + 2$, number of type `i` atoms

box_

[`tf.Tensor`] The box of the system

mesh

For historical reasons, only the length of the Tensor matters. if size of `mesh == 6`, pbc is assumed. if size of `mesh == 0`, no-pbc is assumed.

input_dict

Dictionary for additional inputs

reuse

The weights in the networks should be reused when get the variable.

suffix
Name suffix to identify this descriptor

Returns

descriptor
The output descriptor

compute_input_stats(data_coord, data_box, data_atype, natoms_vec, mesh, input_dict, **kwargs)
Compute the statisitcs (avg and std) of the training data. The input will be normalized by the statistics.

Parameters

data_coord
The coordinates. Can be generated by deepmd.model.make_stat_input

data_box
The box. Can be generated by deepmd.model.make_stat_input

data_atype
The atom types. Can be generated by deepmd.model.make_stat_input

natoms_vec
The vector for the number of atoms of the system and different types of atoms.
Can be generated by deepmd.model.make_stat_input

mesh
The mesh for neighbor searching. Can be generated by
deepmd.model.make_stat_input

input_dict
Dictionary for additional input

**kwargs
Additional keyword arguments.

class deepmd.descriptor.DescriptSeAMask(*args, **kwargs)

Bases: *DescriptSeA*

DeepPot-SE constructed from all information (both angular and radial) of atomic configurations. The embedding takes the distance between atoms as input.

The descriptor $\mathcal{D}^i \in \mathbb{R}^{M_1 \times M_2}$ is given by [1]

$$\mathcal{D}^i = (\mathcal{G}^i)^T \mathcal{R}^i (\mathcal{R}^i)^T \mathcal{G}_{<}^i$$

where $\mathcal{R}^i \in \mathbb{R}^{N \times 4}$ is the coordinate matrix, and each row of \mathcal{R}^i can be constructed as follows

$$(\mathcal{R}^i)_j = \begin{bmatrix} \frac{s(r_{ji})}{s(r_{ji})x_{ji}} \\ \frac{r_{ji}}{s(r_{ji})y_{ji}} \\ \frac{r_{ji}}{s(r_{ji})z_{ji}} \\ \frac{r_{ji}}{r_{ji}} \end{bmatrix}$$

where $\mathbf{R}_{ji} = \mathbf{R}_j - \mathbf{R}_i = (x_{ji}, y_{ji}, z_{ji})$ is the relative coordinate and $r_{ji} = \|\mathbf{R}_{ji}\|$ is its norm. The switching function $s(r)$ is defined as:

$$s(r) = \begin{cases} \frac{1}{r}, & r < r_s \\ \frac{1}{r} \left\{ \left(\frac{r-r_s}{r_c-r_s} \right)^3 \left(-6 \left(\frac{r-r_s}{r_c-r_s} \right)^2 + 15 \frac{r-r_s}{r_c-r_s} - 10 \right) + 1 \right\}, & r_s \leq r < r_c \\ 0, & r \geq r_c \end{cases}$$

Each row of the embedding matrix $\mathcal{G}^i \in \mathbb{R}^{N \times M_1}$ consists of outputs of a embedding network \mathcal{N} of $s(r_{ji})$:

$$(\mathcal{G}^i)_j = \mathcal{N}(s(r_{ji}))$$

$\mathcal{G}^i_{<} \in \mathbb{R}^{N \times M_2}$ takes first M_2 columns of \mathcal{G}^i . The equation of embedding network \mathcal{N} can be found at `deepmd.utils.network.embedding_net()`. Specially for descriptor `se_a_mask` is a concise implementation of `se_a`. The difference is that `se_a_mask` only considered a non-pbc system. And accept a mask matrix to indicate the atom i in frame j is a real atom or not. (1 means real atom, 0 means ghost atom) Thus `se_a_mask` can accept a variable number of atoms in a frame.

Parameters

`sel`
`[list[str]]` `sel[i]` specifies the maximum number of type i atoms in the neighbor list.

`neuron`
`[list[int]]` Number of neurons in each hidden layers of the embedding net \mathcal{N}

`axis_neuron`
 Number of the axis neuron M_2 (number of columns of the sub-matrix of the embedding matrix)

`resnet_dt`
 Time-step dt in the resnet construction: $y = x + dt * \phi(Wx + b)$

`trainable`
 If the weights of embedding net are trainable.

`seed`
 Random seed for initializing the network parameters.

`type_one_side`
 Try to build N_{types} embedding nets. Otherwise, building N_{types}^2 embedding nets

`exclude_types`
`[List[List[int]]]` The excluded pairs of types which have no interaction with each other. For example, `[[0, 1]]` means no interaction between type 0 and type 1.

`activation_function`
 The activation function in the embedding net. Supported options are {0}

`precision`
 The precision of the embedding net parameters. Supported options are {1}

`uniform_seed`
 Only for the purpose of backward compatibility, retrieves the old behavior of using the random seed

References

[1]

Attributes

`explicit_ntypes`
 Explicit ntypes with type embedding.

`precision`
 Precision of filter network.

Methods

| | |
|--|---|
| <code>build(coord_, atype_, natoms, box_, mesh, ...)</code> | Build the computational graph for the descriptor. |
| <code>build_type_exclude_mask(exclude_types, ...)</code> | Build the type exclude mask for the descriptor. |
| <code>compute_input_stats(data_coord, data_box, ...)</code> | Compute the statisitcs (avg and std) of the training data. |
| <code>enable_compression(min_nbor_dist, graph, ...)</code> | Reveive the statisitcs (distance, max_nbor_size and env_mat_range) of the training data. |
| <code>enable_mixed_precision([mixed_prec])</code> | Reveive the mixed precision setting. |
| <code>get_dim_out()</code> | Returns the output dimension of this descriptor. |
| <code>get_dim_rot_mat_1()</code> | Returns the first dimension of the rotation matrix. |
| <code>get_nlist()</code> | Returns neighbor information. |
| <code>get_ntypes()</code> | Returns the number of atom types. |
| <code>get_rcut()</code> | Returns the cutoff radius. |
| <code>get_rot_mat()</code> | Get rotational matrix. |
| <code>get_tensor_names([suffix])</code> | Get names of tensors. |
| <code>init_variables(graph, graph_def[, suffix])</code> | Init the embedding net variables with the given dict. |
| <code>merge_input_stats(stat_dict)</code> | Merge the statisitcs computed from compute_input_stats to obtain the self.davg and self.dstd. |
| <code>pass_tensors_from_frz_model(descrpt_reshape, ...)</code> | Pass the descrpt_reshape tensor as well as descrpt_deriv tensor from the frz graph_def. |
| <code>prod_force_virial(atom_ener, natoms)</code> | Compute force and virial. |
| <code>register(key)</code> | Register a descriptor plugin. |

build(coord_ : Tensor, atype_ : Tensor, natoms: Tensor, box_ : Tensor, mesh: Tensor, input_dict: Dict[str, Any], reuse: Optional[bool] = None, suffix: str = '') → Tensor

Build the computational graph for the descriptor.

Parameters

coord_
The coordinate of atoms

atype_
The type of atoms

natoms
The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 ≤ i < Ntypes+2, number of type i atoms

box_
[tf.Tensor] The box of the system

mesh
For historical reasons, only the length of the Tensor matters. if size of mesh == 6, pbc is assumed. if size of mesh == 0, no-pbc is assumed.

input_dict
Dictionary for additional inputs

reuse

The weights in the networks should be reused when get the variable.

suffix

Name suffix to identify this descriptor

Returns

descriptor

The output descriptor

compute_input_stats(data_coord: list, data_box: list, data_atype: list, natoms_vec: list, mesh: list, input_dict: dict, **kwargs) → None

Compute the statistics (avg and std) of the training data. The input will be normalized by the statistics.

Parameters

data_coord

The coordinates. Can be generated by `deepmd.model.make_stat_input`

data_box

The box. Can be generated by `deepmd.model.make_stat_input`

data_atype

The atom types. Can be generated by `deepmd.model.make_stat_input`

natoms_vec

The vector for the number of atoms of the system and different types of atoms.
Can be generated by `deepmd.model.make_stat_input`

mesh

The mesh for neighbor searching. Can be generated by
`deepmd.model.make_stat_input`

input_dict

Dictionary for additional input

**kwargs

Additional keyword arguments.

get_rcut() → float

Returns the cutoff radius.

prod_force_virial(atom_ener: Tensor, natoms: Tensor) → Tuple[Tensor, Tensor, Tensor]

Compute force and virial.

Parameters

atom_ener

The atomic energy

natoms

The number of atoms. This tensor has the length of `Ntypes + 2`
`natoms[0]`: number of local atoms
`natoms[1]`: total number of atoms held by this processor
`natoms[i]`: $2 \leq i < Ntypes + 2$, number of type *i* atoms

Returns

force

The force on atoms


```

    virial
        None for se_a_mask op
    atom_virial
        None for se_a_mask op
class deepmd.descriptor.DescriptSeAtten(*args, **kwargs)
    Bases: DescriptSeA
    Smooth version descriptor with attention.
    Parameters
        rcut
            The cut-off radius  $r_c$ 
        rcut_smth
            From where the environment matrix should be smoothed  $r_s$ 
        sel
            [list[str]] sel[i] specifies the maximum number of type i atoms in the cut-off radius
        neuron
            [list[int]] Number of neurons in each hidden layers of the embedding net  $\mathcal{N}$ 
        axis_neuron
            Number of the axis neuron  $M_2$  (number of columns of the sub-matrix of the embedding matrix)
        resnet_dt
            Time-step dt in the resnet construction:  $y = x + dt * \phi(Wx + b)$ 
        trainable
            If the weights of embedding net are trainable.
        seed
            Random seed for initializing the network parameters.
        type_one_side
            Try to build  $N_{\text{types}}$  embedding nets. Otherwise, building  $N_{\text{types}}^2$  embedding nets
        exclude_types
            [List[List[int]]] The excluded pairs of types which have no interaction with each other. For example,  $[[0, 1]]$  means no interaction between type 0 and type 1.
        set_davg_zero
            Set the shift of embedding net input to zero.
        activation_function
            The activation function in the embedding net. Supported options are "relu", "relu6", "softplus", "sigmoid", "tanh", "gelu", "gelu_tf", "None", "none".
        precision
            The precision of the embedding net parameters. Supported options are "default", "float16", "float32", "float64", "bfloat16".
        uniform_seed
            Only for the purpose of backward compatibility, retrieves the old behavior of using the random seed
        attn
            The length of hidden vector during scale-dot attention computation.

```

`attn_layer`

The number of layers in attention mechanism.

`attn_dotr`

Whether to dot the relative coordinates on the attention weights as a gated scheme.

`attn_mask`

Whether to mask the diagonal in the attention weights.

`multi_task`

If the model has multi fitting nets to train.

`stripped_type_embedding`

Whether to strip the type embedding into a separated embedding network. Default value will be True in `se_attn_v2` descriptor.

`smooth_type_embdding`

When using stripped type embedding, whether to dot smooth factor on the network output of type embedding to keep the network smooth, instead of setting `set_davg_zero` to be True. Default value will be True in `se_attn_v2` descriptor.

Attributes

`explicit_ntypes`

Explicit ntypes with type embedding.

`precision`

Precision of filter network.

Methods

| | |
|--|---|
| <code>build(coord_, atype_, natoms, box_, mesh, ...)</code> | Build the computational graph for the descriptor. |
| <code>build_type_exclude_mask(exclude_types, ...)</code> | Build the type exclude mask for the attention descriptor. |
| <code>compute_input_stats(data_coord, data_box, ...)</code> | Compute the statistics (avg and std) of the training data. |
| <code>enable_compression(min_nbor_dist, graph, ...)</code> | Reveive the statistics (distance, max_nbor_size and env_mat_range) of the training data. |
| <code>enable_mixed_precision([mixed_prec])</code> | Reveive the mixed precision setting. |
| <code>get_dim_out()</code> | Returns the output dimension of this descriptor. |
| <code>get_dim_rot_mat_1()</code> | Returns the first dimension of the rotation matrix. |
| <code>get_nlist()</code> | Returns neighbor information. |
| <code>get_ntypes()</code> | Returns the number of atom types. |
| <code>get_rcut()</code> | Returns the cut-off radius. |
| <code>get_rot_mat()</code> | Get rotational matrix. |
| <code>get_tensor_names([suffix])</code> | Get names of tensors. |
| <code>init_variables(graph, graph_def[, suffix])</code> | Init the embedding net variables with the given dict. |
| <code>merge_input_stats(stat_dict)</code> | Merge the statistics computed from compute_input_stats to obtain the self.davg and self.dstd. |
| <code>pass_tensors_from_frz_model(descrpt_reshape, ...)</code> | Pass the descrpt_reshape tensor as well as descrpt_deriv tensor from the frz graph_def. |
| <code>prod_force_virial(atom_ener, natoms)</code> | Compute force and virial. |
| <code>register(key)</code> | Register a descriptor plugin. |

`build(coord_ : Tensor, atype_ : Tensor, natoms: Tensor, box_ : Tensor, mesh: Tensor, input_dict: dict, reuse: Optional[bool] = None, suffix: str = "") → Tensor`

Build the computational graph for the descriptor.

Parameters

`coord_`
The coordinate of atoms

`atype_`
The type of atoms

`natoms`
The number of atoms. This tensor has the length of Ntypes + 2 `natoms[0]`: number of local atoms `natoms[1]`: total number of atoms held by this processor `natoms[i]`: $2 \leq i < \text{Ntypes} + 2$, number of type i atoms

`box_`
[`tf.Tensor`] The box of the system

`mesh`
For historical reasons, only the length of the Tensor matters. if size of mesh == 6, pbc is assumed. if size of mesh == 0, no-pbc is assumed.

`input_dict`
Dictionary for additional inputs

reuse

The weights in the networks should be reused when get the variable.

suffix

Name suffix to identify this descriptor

Returns

descriptor

The output descriptor

build_type_exclude_mask(exclude_types: List[Tuple[int, int]], ntypes: int, sel: List[int], ndescript: int, atype: Tensor, shape0: Tensor, nei_type_vec: Tensor) → Tensor

Build the type exclude mask for the attention descriptor.

Parameters

exclude_types

[List[Tuple[int, int]]] The list of excluded types, e.g. [(0, 1), (1, 0)] means the interaction between type 0 and type 1 is excluded.

ntypes

[int] The number of types.

sel

[List[int]] The list of the number of selected neighbors for each type.

ndescript

[int] The number of descriptors for each atom.

atype

[tf.Tensor] The type of atoms, with the size of shape0.

shape0

[tf.Tensor] The shape of the first dimension of the inputs, which is equal to nsamples * natoms.

nei_type_vec

[tf.Tensor] The type of neighbors, with the size of (shape0, nnei).

Returns

tf.Tensor

The type exclude mask, with the shape of (shape0, ndescript), and the precision of GLOBAL_TF_FLOAT_PRECISION. The mask has the value of 1 if the interaction between two types is not excluded, and 0 otherwise.

See also:

`deepmd.descriptor.descriptor.Descriptor.build_type_exclude_mask`

Notes

This method has the similar way to build the type exclude mask as `deepmd.descriptor.descriptor.Descriptor.build_type_exclude_mask()`. The mathematical expression has been explained in that method. The difference is that the attention descriptor has provided the type of the neighbors (`idx_j`) that is not in order, so we use it from an extra input.

```
compute_input_stats(data_coord: list, data_box: list, data_atype: list, natoms_vec: list, mesh: list,
                    input_dict: dict, mixed_type: bool = False, real_natoms_vec: Optional[list] =
                    None, **kwargs) → None
```

Compute the statistics (avg and std) of the training data. The input will be normalized by the statistics.

Parameters

`data_coord`

The coordinates. Can be generated by `deepmd.model.make_stat_input`

`data_box`

The box. Can be generated by `deepmd.model.make_stat_input`

`data_atype`

The atom types. Can be generated by `deepmd.model.make_stat_input`

`natoms_vec`

The vector for the number of atoms of the system and different types of atoms. If `mixed_type` is True, this para is blank. See `real_natoms_vec`.

`mesh`

The mesh for neighbor searching. Can be generated by `deepmd.model.make_stat_input`

`input_dict`

Dictionary for additional input

`mixed_type`

Whether to perform the `mixed_type` mode. If True, the input data has the `mixed_type` format (see `doc/model/train_se_atten.md`), in which frames in a system may have different `natoms_vec(s)`, with the same `nloc`.

`real_natoms_vec`

If `mixed_type` is True, it takes in the `real_natoms_vec` for each frame.

`**kwargs`

Additional keyword arguments.

```
enable_compression(min_nbor_dist: float, graph: Graph, graph_def: GraphDef, table_extrapolate:
                    float = 5, table_stride_1: float = 0.01, table_stride_2: float = 0.1,
                    check_frequency: int = -1, suffix: str = '') → None
```

Reveive the statistics (distance, `max_nbor_size` and `env_mat_range`) of the training data.

Parameters

`min_nbor_dist`

The nearest distance between atoms

`graph`

[`tf.Graph`] The graph of the model

`graph_def`

[`tf.GraphDef`] The `graph_def` of the model

```

    table_extrapolate
        The scale of model extrapolation
    table_stride_1
        The uniform stride of the first table
    table_stride_2
        The uniform stride of the second table
    check_frequency
        The overflow check frequency
    suffix
        [str, optional] The suffix of the scope
property explicit_ntypes: bool
    Explicit ntypes with type embedding.
init_variables(graph: Graph, graph_def: GraphDef, suffix: str = '') → None
    Init the embedding net variables with the given dict.
Parameters
    graph
        [tf.Graph] The input frozen model graph
    graph_def
        [tf.GraphDef] The input frozen model graph_def
    suffix
        [str, optional] The suffix of the scope
class deepmd.descriptor.DescriptSeAttenV2(*args, **kwargs)
    Bases: DescriptSeAtten
    Smooth version 2.0 descriptor with attention.
Parameters
    rcut
        The cut-off radius  $r_c$ 
    rcut_smth
        From where the environment matrix should be smoothed  $r_s$ 
    sel
        [list[str]] sel[i] specifies the maximum number of type i atoms in the cut-off radius
    neuron
        [list[int]] Number of neurons in each hidden layers of the embedding net  $\mathcal{N}$ 
    axis_neuron
        Number of the axis neuron  $M_2$  (number of columns of the sub-matrix of the embedding matrix)
    resnet_dt
        Time-step dt in the resnet construction:  $y = x + dt * \phi(Wx + b)$ 
    trainable
        If the weights of embedding net are trainable.
    seed
        Random seed for initializing the network parameters.

```

`type_one_side`
 Try to build `N_types` embedding nets. Otherwise, building `N_types^2` embedding nets

`exclude_types`
`[List[List[int]]]` The excluded pairs of types which have no interaction with each other. For example, `[[0, 1]]` means no interaction between type 0 and type 1.

`set_davg_zero`
 Set the shift of embedding net input to zero.

`activation_function`
 The activation function in the embedding net. Supported options are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”, “gelu_tf”, “None”, “none”.

`precision`
 The precision of the embedding net parameters. Supported options are “default”, “float16”, “float32”, “float64”, “bfloat16”.

`uniform_seed`
 Only for the purpose of backward compatibility, retrieves the old behavior of using the random seed

`attn`
 The length of hidden vector during scale-dot attention computation.

`attn_layer`
 The number of layers in attention mechanism.

`attn_dotr`
 Whether to dot the relative coordinates on the attention weights as a gated scheme.

`attn_mask`
 Whether to mask the diagonal in the attention weights.

`multi_task`
 If the model has multi fitting nets to train.

Attributes

`explicit_ntypes`
 Explicit ntypes with type embedding.

`precision`
 Precision of filter network.

Methods

| | |
|--|---|
| <code>build(coord_, atype_, natoms, box_, mesh, ...)</code> | Build the computational graph for the descriptor. |
| <code>build_type_exclude_mask(exclude_types, ...)</code> | Build the type exclude mask for the attention descriptor. |
| <code>compute_input_stats(data_coord, data_box, ...)</code> | Compute the statistics (avg and std) of the training data. |
| <code>enable_compression(min_nbor_dist, graph, ...)</code> | Reveive the statistics (distance, max_nbor_size and env_mat_range) of the training data. |
| <code>enable_mixed_precision([mixed_prec])</code> | Reveive the mixed precision setting. |
| <code>get_dim_out()</code> | Returns the output dimension of this descriptor. |
| <code>get_dim_rot_mat_1()</code> | Returns the first dimension of the rotation matrix. |
| <code>get_nlist()</code> | Returns neighbor information. |
| <code>get_ntypes()</code> | Returns the number of atom types. |
| <code>get_rcut()</code> | Returns the cut-off radius. |
| <code>get_rot_mat()</code> | Get rotational matrix. |
| <code>get_tensor_names([suffix])</code> | Get names of tensors. |
| <code>init_variables(graph, graph_def[, suffix])</code> | Init the embedding net variables with the given dict. |
| <code>merge_input_stats(stat_dict)</code> | Merge the statistics computed from <code>compute_input_stats</code> to obtain the <code>self.davg</code> and <code>self.dstd</code> . |
| <code>pass_tensors_from_frz_model(descrpt_reshape, ...)</code> | Pass the <code>descrpt_reshape</code> tensor as well as <code>descrpt_deriv</code> tensor from the <code>frz graph_def</code> . |
| <code>prod_force_virial(atom_ener, natoms)</code> | Compute force and virial. |
| <code>register(key)</code> | Register a descriptor plugin. |

```
class deepmd.descriptor.DescriptSeR(*args, **kwargs)
```

Bases: *DescriptSe*

DeepPot-SE constructed from radial information of atomic configurations.

The embedding takes the distance between atoms as input.

Parameters

`rcut`

The cut-off radius

`rcut_smth`

From where the environment matrix should be smoothed

`sel`

`[list[str]]` `sel[i]` specifies the maxmum number of type `i` atoms in the cut-off radius

`neuron`

`[list[int]]` Number of neurons in each hidden layers of the embedding net

`resnet_dt`

Time-step `dt` in the resnet construction: $y = x + dt * \phi(Wx + b)$

`trainable`

If the weights of embedding net are trainable.

seed
Random seed for initializing the network parameters.

type_one_side
Try to build N_{types} embedding nets. Otherwise, building N_{types}^2 embedding nets

exclude_types
`[List[List[int]]]` The excluded pairs of types which have no interaction with each other. For example, `[[0, 1]]` means no interaction between type 0 and type 1.

activation_function
The activation function in the embedding net. Supported options are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”, “gelu_tf”, “None”, “none”.

precision
The precision of the embedding net parameters. Supported options are “default”, “float16”, “float32”, “float64”, “bfloat16”.

uniform_seed
Only for the purpose of backward compatibility, retrieves the old behavior of using the random seed

Attributes

explicit_ntypes
Explicit ntypes with type embedding.

precision
Precision of filter network.

Methods

| | |
|--|---|
| <code>build(coord_, atype_, natoms, box_, mesh, ...)</code> | Build the computational graph for the descriptor. |
| <code>build_type_exclude_mask(exclude_types, ...)</code> | Build the type exclude mask for the descriptor. |
| <code>compute_input_stats(data_coord, data_box, ...)</code> | Compute the statistics (avg and std) of the training data. |
| <code>enable_compression(min_nbor_dist, graph, ...)</code> | Receive the statistics (distance, max_nbor_size and env_mat_range) of the training data. |
| <code>enable_mixed_precision([mixed_prec])</code> | Receive the mixed precision setting. |
| <code>get_dim_out()</code> | Returns the output dimension of this descriptor. |
| <code>get_dim_rot_mat_1()</code> | Returns the first dimension of the rotation matrix. |
| <code>get_nlist()</code> | Returns neighbor information. |
| <code>get_ntypes()</code> | Returns the number of atom types. |
| <code>get_rcut()</code> | Returns the cut-off radius. |
| <code>get_tensor_names([suffix])</code> | Get names of tensors. |
| <code>init_variables(graph, graph_def[, suffix])</code> | Init the embedding net variables with the given dict. |
| <code>merge_input_stats(stat_dict)</code> | Merge the statistics computed from compute_input_stats to obtain the self.davg and self.dstd. |
| <code>pass_tensors_from_frz_model(descrpt_reshape, ...)</code> | Pass the descrpt_reshape tensor as well as descrpt_deriv tensor from the frz graph_def. |
| <code>prod_force_virial(atom_ener, natoms)</code> | Compute force and virial. |
| <code>register(key)</code> | Register a descriptor plugin. |

`build(coord_: Tensor, atype_: Tensor, natoms: Tensor, box_: Tensor, mesh: Tensor, input_dict: dict, reuse: Optional[bool] = None, suffix: str = '') → Tensor`

Build the computational graph for the descriptor.

Parameters

`coord_`
The coordinate of atoms

`atype_`
The type of atoms

`natoms`
The number of atoms. This tensor has the length of Ntypes + 2. `natoms[0]`: number of local atoms, `natoms[1]`: total number of atoms held by this processor, `natoms[i]`: $2 \leq i < \text{Ntypes} + 2$, number of type i atoms

`box_`
[`tf.Tensor`] The box of the system

`mesh`
For historical reasons, only the length of the Tensor matters. if size of mesh == 6, pbc is assumed. if size of mesh == 0, no-pbc is assumed.

`input_dict`
Dictionary for additional inputs

`reuse`
The weights in the networks should be reused when get the variable.

suffix
Name suffix to identify this descriptor

Returns

descriptor
The output descriptor

compute_input_stats(data_coord, data_box, data_atype, natoms_vec, mesh, input_dict, **kwargs)
Compute the statistics (avg and std) of the training data. The input will be normalized by the statistics.

Parameters

data_coord
The coordinates. Can be generated by `deepmd.model.make_stat_input`

data_box
The box. Can be generated by `deepmd.model.make_stat_input`

data_atype
The atom types. Can be generated by `deepmd.model.make_stat_input`

natoms_vec
The vector for the number of atoms of the system and different types of atoms.
Can be generated by `deepmd.model.make_stat_input`

mesh
The mesh for neighbor searching. Can be generated by
`deepmd.model.make_stat_input`

input_dict
Dictionary for additional input

**kwargs
Additional keyword arguments.

enable_compression(min_nbor_dist: float, graph: Graph, graph_def: GraphDef, table_extrapolate: float = 5, table_stride_1: float = 0.01, table_stride_2: float = 0.1, check_frequency: int = -1, suffix: str = '') → None

Reveive the statistics (distance, max_nbor_size and env_mat_range) of the training data.

Parameters

min_nbor_dist
The nearest distance between atoms

graph
[tf.Graph] The graph of the model

graph_def
[tf.GraphDef] The graph_def of the model

table_extrapolate
The scale of model extrapolation

table_stride_1
The uniform stride of the first table

table_stride_2
The uniform stride of the second table

`check_frequency`
The overflow check frequency

`suffix`
[`str`, `optional`] The suffix of the scope

`get_dim_out()`
Returns the output dimension of this descriptor.

`get_nlist()`
Returns neighbor information.

Returns

`nlist`
Neighbor list

`rij`
The relative distance between the neighbor and the center atom.

`sel_a`
The number of neighbors with full information

`sel_r`
The number of neighbors with only radial information

`get_ntypes()`
Returns the number of atom types.

`get_rcut()`
Returns the cut-off radius.

`merge_input_stats(stat_dict)`
Merge the statisitcs computed from `compute_input_stats` to obtain the `self.davg` and `self.dstd`.

Parameters

`stat_dict`
The dict of statisitcs computed from `compute_input_stats`, including:

`sumr`
The sum of radial statisitcs.

`sumn`
The sum of neighbor numbers.

`sumr2`
The sum of square of radial statisitcs.

`prod_force_virial(atom_ener: Tensor, natoms: Tensor) → Tuple[Tensor, Tensor, Tensor]`
Compute force and virial.

Parameters

`atom_ener`
The atomic energy

`natoms`
The number of atoms. This tensor has the length of `Ntypes + 2` `natoms[0]`: number of local atoms `natoms[1]`: total number of atoms held by this processor `natoms[i]`: $2 \leq i < Ntypes+2$, number of type `i` atoms

Returns

force
The force on atoms

virial
The total virial

atom_virial
The atomic virial

class deepmd.descriptor.DescriptSeT(*args, **kwargs)

Bases: *DescriptSe*

DeepPot-SE constructed from all information (both angular and radial) of atomic configurations.

The embedding takes angles between two neighboring atoms as input.

Parameters

rcut
The cut-off radius

rcut_smth
From where the environment matrix should be smoothed

sel
[*list*[*str*]] sel[i] specifies the maxmum number of type i atoms in the cut-off radius

neuron
[*list*[*int*]] Number of neurons in each hidden layers of the embedding net

resnet_dt
Time-step dt in the resnet construction: $y = x + dt * \phi(Wx + b)$

trainable
If the weights of embedding net are trainable.

seed
Random seed for initializing the network parameters.

set_davg_zero
Set the shift of embedding net input to zero.

activation_function
The activation function in the embedding net. Supported options are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”, “gelu_tf”, “None”, “none”.

precision
The precision of the embedding net parameters. Supported options are “default”, “float16”, “float32”, “float64”, “bfloat16”.

uniform_seed
Only for the purpose of backward compatibility, retrieves the old behavior of using the random seed

Attributes

explicit_ntypes
Explicit ntypes with type embedding.

precision
Precision of filter network.

Methods

| | |
|--|---|
| <code>build(coord_, atype_, natoms, box_, mesh, ...)</code> | Build the computational graph for the descriptor. |
| <code>build_type_exclude_mask(exclude_types, ...)</code> | Build the type exclude mask for the descriptor. |
| <code>compute_input_stats(data_coord, data_box, ...)</code> | Compute the statistics (avg and std) of the training data. |
| <code>enable_compression(min_nbor_dist, graph, ...)</code> | Receive the statistics (distance, max_nbor_size and env_mat_range) of the training data. |
| <code>enable_mixed_precision([mixed_prec])</code> | Receive the mixed precision setting. |
| <code>get_dim_out()</code> | Returns the output dimension of this descriptor. |
| <code>get_dim_rot_mat_1()</code> | Returns the first dimension of the rotation matrix. |
| <code>get_nlist()</code> | Returns neighbor information. |
| <code>get_ntypes()</code> | Returns the number of atom types. |
| <code>get_rcut()</code> | Returns the cut-off radius. |
| <code>get_tensor_names([suffix])</code> | Get names of tensors. |
| <code>init_variables(graph, graph_def[, suffix])</code> | Init the embedding net variables with the given dict. |
| <code>merge_input_stats(stat_dict)</code> | Merge the statistics computed from compute_input_stats to obtain the self.davg and self.dstd. |
| <code>pass_tensors_from_frz_model(descrpt_reshape, ...)</code> | Pass the descrpt_reshape tensor as well as descrpt_deriv tensor from the frz graph_def. |
| <code>prod_force_virial(atom_ener, natoms)</code> | Compute force and virial. |
| <code>register(key)</code> | Register a descriptor plugin. |

build(coord_: Tensor, atype_: Tensor, natoms: Tensor, box_: Tensor, mesh: Tensor, input_dict: dict, reuse: Optional[bool] = None, suffix: str = '') → Tensor

Build the computational graph for the descriptor.

Parameters

coord_
The coordinate of atoms

atype_
The type of atoms

natoms
The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 ≤ i < Ntypes+2, number of type i atoms

box_
[tf.Tensor] The box of the system

mesh
For historical reasons, only the length of the Tensor matters. if size of mesh == 6, pbc is assumed. if size of mesh == 0, no-pbc is assumed.

input_dict
Dictionary for additional inputs

reuse
The weights in the networks should be reused when get the variable.

suffix
Name suffix to identify this descriptor

Returns

descriptor
The output descriptor

compute_input_stats(data_coord: list, data_box: list, data_atype: list, natoms_vec: list, mesh: list, input_dict: dict, **kwargs) → None

Compute the statistics (avg and std) of the training data. The input will be normalized by the statistics.

Parameters

data_coord
The coordinates. Can be generated by `deepmd.model.make_stat_input`

data_box
The box. Can be generated by `deepmd.model.make_stat_input`

data_atype
The atom types. Can be generated by `deepmd.model.make_stat_input`

natoms_vec
The vector for the number of atoms of the system and different types of atoms.
Can be generated by `deepmd.model.make_stat_input`

mesh
The mesh for neighbor searching. Can be generated by
`deepmd.model.make_stat_input`

input_dict
Dictionary for additional input

**kwargs
Additional keyword arguments.

enable_compression(min_nbor_dist: float, graph: Graph, graph_def: GraphDef, table_extrapolate: float = 5, table_stride_1: float = 0.01, table_stride_2: float = 0.1, check_frequency: int = -1, suffix: str = '') → None

Reveive the statistics (distance, max_nbor_size and env_mat_range) of the training data.

Parameters

min_nbor_dist
The nearest distance between atoms

graph
[tf.Graph] The graph of the model

graph_def
[tf.GraphDef] The graph_def of the model

table_extrapolate
The scale of model extrapolation

table_stride_1
The uniform stride of the first table

table_stride_2
The uniform stride of the second table

`check_frequency`
The overflow check frequency

`suffix`
[`str`, `optional`] The suffix of the scope

`get_dim_out()` → `int`
Returns the output dimension of this descriptor.

`get_nlist()` → `Tuple`[`Tensor`, `Tensor`, `List`[`int`], `List`[`int`]]
Returns neighbor information.

Returns

`nlist`
Neighbor list

`rij`
The relative distance between the neighbor and the center atom.

`sel_a`
The number of neighbors with full information

`sel_r`
The number of neighbors with only radial information

`get_ntypes()` → `int`
Returns the number of atom types.

`get_rcut()` → `float`
Returns the cut-off radius.

`merge_input_stats(stat_dict)`
Merge the statisitcs computed from `compute_input_stats` to obtain the `self.davg` and `self.dstd`.

Parameters

`stat_dict`
The dict of statisitcs computed from `compute_input_stats`, including:

`sumr`
The sum of radial statisitcs.

`suma`
The sum of relative coord statisitcs.

`sumn`
The sum of neighbor numbers.

`sumr2`
The sum of square of radial statisitcs.

`suma2`
The sum of square of relative coord statisitcs.

`prod_force_virial(atom_ener: Tensor, natoms: Tensor)` → `Tuple`[`Tensor`, `Tensor`, `Tensor`]
Compute force and virial.

Parameters

`atom_ener`
The atomic energy

natoms
 The number of atoms. This tensor has the length of $N_{\text{types}} + 2$ `natoms[0]`: number of local atoms `natoms[1]`: total number of atoms held by this processor `natoms[i]`: $2 \leq i < N_{\text{types}} + 2$, number of type i atoms

Returns

force
 The force on atoms

virial
 The total virial

atom_virial
 The atomic virial

Submodules

deepmd.descriptor.descriptor module

```
class deepmd.descriptor.descriptor.Descriptor(*args, **kwargs)
```

Bases: *PluginVariant*

The abstract class for descriptors. All specific descriptors should be based on this class.

The descriptor \mathcal{D} describes the environment of an atom, which should be a function of coordinates and types of its neighbour atoms.

Notes

Only methods and attributes defined in this class are generally public, that can be called by other classes.

Examples

```
>>> descript = Descriptor(type="se_e2_a", rcut=6., rcut_smth=0.5, sel=[50])
>>> type(descript)
<class 'deepmd.descriptor.se_a.DescriptSeA'>
```

Attributes

explicit_ntypes
 Explicit ntypes with type embedding.

Methods

| | |
|--|---|
| <i>build</i> (coord_, atype_, natoms, box_, mesh, ...) | Build the computational graph for the descriptor. |
| <i>build_type_exclude_mask</i> (exclude_types, ...) | Build the type exclude mask for the descriptor. |
| <i>compute_input_stats</i> (data_coord, data_box, ...) | Compute the statistics (avg and std) of the training data. |
| <i>enable_compression</i> (min_nbor_dist, graph, ...) | Receive the statistics (distance, max_nbor_size and env_mat_range) of the training data. |
| <i>enable_mixed_precision</i> ([mixed_prec]) | Receive the mixed precision setting. |
| <i>get_dim_out</i> () | Returns the output dimension of this descriptor. |
| <i>get_dim_rot_mat_1</i> () | Returns the first dimension of the rotation matrix. |
| <i>get_nlist</i> () | Returns neighbor information. |
| <i>get_ntypes</i> () | Returns the number of atom types. |
| <i>get_rcut</i> () | Returns the cut-off radius. |
| <i>get_tensor_names</i> ([suffix]) | Get names of tensors. |
| <i>init_variables</i> (graph, graph_def[, suffix]) | Init the embedding net variables with the given dict. |
| <i>pass_tensors_from_frz_model</i> (*tensors) | Pass the descript_reshape tensor as well as descript_deriv tensor from the frz graph_def. |
| <i>prod_force_virial</i> (atom_ener, natoms) | Compute force and virial. |
| <i>register</i> (key) | Register a descriptor plugin. |

abstract *build*(coord_: Tensor, atype_: Tensor, natoms: Tensor, box_: Tensor, mesh: Tensor, input_dict: Dict[str, Any], reuse: Optional[bool] = None, suffix: str = '') → Tensor

Build the computational graph for the descriptor.

Parameters

coord_
[tf.Tensor] The coordinate of atoms

atype_
[tf.Tensor] The type of atoms

natoms
[tf.Tensor] The number of atoms. This tensor has the length of Ntypes + 2
natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 ≤ i < Ntypes+2, number of type i atoms

box_
[tf.Tensor] The box of frames

mesh
[tf.Tensor] For historical reasons, only the length of the Tensor matters. if size of mesh == 6, pbc is assumed. if size of mesh == 0, no-pbc is assumed.

input_dict
[dict[str, Any]] Dictionary for additional inputs

reuse
[bool, optional] The weights in the networks should be reused when get the variable.

suffix
[str, optional] Name suffix to identify this descriptor

Returns

descriptor: `tf.Tensor`
The output descriptor

Notes

This method must be implemented, as it's called by other classes.

build_type_exclude_mask(exclude_types: `List[Tuple[int, int]]`, ntypes: `int`, sel: `List[int]`, ndescript: `int`, atype: `Tensor`, shape0: `Tensor`) → `Tensor`

Build the type exclude mask for the descriptor.

Parameters

exclude_types
[`List[Tuple[int, int]]`] The list of excluded types, e.g. [(0, 1), (1, 0)] means the interaction between type 0 and type 1 is excluded.

ntypes
[`int`] The number of types.

sel
[`List[int]`] The list of the number of selected neighbors for each type.

ndescript
[`int`] The number of descriptors for each atom.

atype
[`tf.Tensor`] The type of atoms, with the size of shape0.

shape0
[`tf.Tensor`] The shape of the first dimension of the inputs, which is equal to nsamples * natoms.

Returns

`tf.Tensor`
The type exclude mask, with the shape of (shape0, ndescript), and the precision of GLOBAL_TF_FLOAT_PRECISION. The mask has the value of 1 if the interaction between two types is not excluded, and 0 otherwise.

Notes

To exclude the interaction between two types, the derivative of energy with respect to distances (or angles) between two atoms should be zero[Rafclae60e195-1], i.e.

$$\forall i \in \text{type 1}, j \in \text{type 2}, \frac{\partial E}{\partial r_{ij}} = 0$$

When embedding networks between every two types are built, we can just remove that network. But when type_one_side is enabled, a network may be built for multiple pairs of types. In this case, we need to build a mask to exclude the interaction between two types.

The mask assumes the descriptors are sorted by neighbor type with the fixed number of given sel and each neighbor has the same number of descriptors (for example 4).

References

[1]

```
abstract compute_input_stats(data_coord: List[ndarray], data_box: List[ndarray], data_atype:
                             List[ndarray], natoms_vec: List[ndarray], mesh: List[ndarray],
                             input_dict: Dict[str, List[ndarray]], **kwargs) → None
```

Compute the statisitcs (avg and std) of the training data. The input will be normalized by the statistics.

Parameters

data_coord
 [list[np.ndarray]] The coordinates. Can be generated by `deepmd.model.model_stat.make_stat_input()`

data_box
 [list[np.ndarray]] The box. Can be generated by `deepmd.model.model_stat.make_stat_input()`

data_atype
 [list[np.ndarray]] The atom types. Can be generated by `deepmd.model.model_stat.make_stat_input()`

natoms_vec
 [list[np.ndarray]] The vector for the number of atoms of the system and different types of atoms. Can be generated by `deepmd.model.model_stat.make_stat_input()`

mesh
 [list[np.ndarray]] The mesh for neighbor searching. Can be generated by `deepmd.model.model_stat.make_stat_input()`

input_dict
 [dict[str, list[np.ndarray]]] Dictionary for additional input

****kwargs**
 Additional keyword arguments which may contain `mixed_type` and `real_natoms_vec`.

Notes

This method must be implemented, as it's called by other classes.

```
enable_compression(min_nbor_dist: float, graph: Graph, graph_def: GraphDef, table_extrapolate:
                    float = 5.0, table_stride_1: float = 0.01, table_stride_2: float = 0.1,
                    check_frequency: int = -1, suffix: str = "") → None
```

Reveive the statisitcs (distance, max_nbor_size and env_mat_range) of the training data.

Parameters

min_nbor_dist
 [float] The nearest distance between atoms

graph
 [tf.Graph] The graph of the model

graph_def
 [tf.GraphDef] The graph definition of the model

`table_extrapolate`
 [`float`, default: 5.] The scale of model extrapolation
`table_stride_1`
 [`float`, default: 0.01] The uniform stride of the first table
`table_stride_2`
 [`float`, default: 0.1] The uniform stride of the second table
`check_frequency`
 [`int`, default: -1] The overflow check frequency
`suffix`
 [`str`, optional] The suffix of the scope

Notes

This method is called by others when the descriptor supported compression.

enable_mixed_precision(mixed_prec: `Optional[dict]` = None) → `None`

Reveive the mixed precision setting.

Parameters

`mixed_prec`
 The mixed precision setting used in the embedding net

Notes

This method is called by others when the descriptor supported compression.

property explicit_ntypes: `bool`

Explicit ntypes with type embedding.

abstract get_dim_out() → `int`

Returns the output dimension of this descriptor.

Returns

`int`
 the output dimension of this descriptor

Notes

This method must be implemented, as it's called by other classes.

get_dim_rot_mat_1() → `int`

Returns the first dimension of the rotation matrix. The rotation is of shape dim_1 x 3.

Returns

`int`
 the first dimension of the rotation matrix

get_nlist() → `Tuple[Tensor, Tensor, List[int], List[int]]`

Returns neighbor information.

Returns

`nlist`
[`tf.Tensor`] Neighbor list

`rij`
[`tf.Tensor`] The relative distance between the neighbor and the center atom.

`sel_a`
[`list[int]`] The number of neighbors with full information

`sel_r`
[`list[int]`] The number of neighbors with only radial information

abstract `get_ntypes()` → `int`
Returns the number of atom types.

Returns

`int`
the number of atom types

Notes

This method must be implemented, as it's called by other classes.

abstract `get_rcut()` → `float`
Returns the cut-off radius.

Returns

`float`
the cut-off radius

Notes

This method must be implemented, as it's called by other classes.

`get_tensor_names(suffix: str = '')` → `Tuple[str]`
Get names of tensors.

Parameters

`suffix`
[`str`] The suffix of the scope

Returns

`Tuple[str]`
Names of tensors

init_variables(`graph`: `Graph`, `graph_def`: `GraphDef`, `suffix`: `str` = '') → `None`
Init the embedding net variables with the given dict.

Parameters

`graph`
[`tf.Graph`] The input frozen model graph

`graph_def`
[`tf.GraphDef`] The input frozen model graph_def

suffix
 [str, optional] The suffix of the scope

Notes

This method is called by others when the descriptor supported initialization from the given variables.

pass_tensors_from_frz_model(*tensors: Tensor) → None

Pass the descript_reshape tensor as well as descript_deriv tensor from the frz graph_def.

Parameters

*tensors
 [tf.Tensor] passed tensors

Notes

The number of parameters in the method must be equal to the numbers of returns in *get_tensor_names()*.

abstract prod_force_virial(atom_ener: Tensor, natoms: Tensor) → Tuple[Tensor, Tensor, Tensor]

Compute force and virial.

Parameters

atom_ener
 [tf.Tensor] The atomic energy

natoms
 [tf.Tensor] The number of atoms. This tensor has the length of Ntypes + 2
 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this
 processor natoms[i]: 2 ≤ i < Ntypes+2, number of type i atoms

Returns

force
 [tf.Tensor] The force on atoms

virial
 [tf.Tensor] The total virial

atom_virial
 [tf.Tensor] The atomic virial

static register(key: str) → Callable

Register a descriptor plugin.

Parameters

key
 [str] the key of a descriptor

Returns

Descriptor
 the registered descriptor

Examples

```
>>> @Descriptor.register("some_descrpt")
class SomeDescriptor(Descriptor):
    pass
```

deepmd.descriptor.hybrid module

`class deepmd.descriptor.hybrid.DescriptHybrid(*args, **kwargs)`

Bases: *Descriptor*

Concate a list of descriptors to form a new descriptor.

Parameters

list

[list] Build a descriptor from the concatenation of the list of descriptors.

Attributes

explicit_ntypes

Explicit ntypes with type embedding.

Methods

| | |
|--|--|
| <i>build</i> (coord_, atype_, natoms, box_, mesh, ...) | Build the computational graph for the descriptor. |
| <i>build_type_exclude_mask</i> (exclude_types, ...) | Build the type exclude mask for the descriptor. |
| <i>compute_input_stats</i> (data_coord, data_box, ...) | Compute the statisitcs (avg and std) of the training data. |
| <i>enable_compression</i> (min_nbor_dist, graph, ...) | Reveive the statisitcs (distance, max_nbor_size and env_mat_range) of the training data. |
| <i>enable_mixed_precision</i> ([mixed_prec]) | Reveive the mixed precision setting. |
| <i>get_dim_out</i> () | Returns the output dimension of this descriptor. |
| <i>get_dim_rot_mat_1</i> () | Returns the first dimension of the rotation matrix. |
| <i>get_nlist</i> () | Get the neighbor information of the descriptor, returns the nlist of the descriptor with the largest cut-off radius. |
| <i>get_nlist_i</i> (ii) | Get the neighbor information of the ii-th descriptor. |
| <i>get_ntypes</i> () | Returns the number of atom types. |
| <i>get_rcut</i> () | Returns the cut-off radius. |
| <i>get_tensor_names</i> ([suffix]) | Get names of tensors. |
| <i>init_variables</i> (graph, graph_def[, suffix]) | Init the embedding net variables with the given dict. |
| <i>merge_input_stats</i> (stat_dict) | Merge the statisitcs computed from compute_input_stats to obtain the self.davg and self.dstd. |
| <i>pass_tensors_from_frz_model</i> (*tensors) | Pass the descrpt_reshape tensor as well as descrpt_deriv tensor from the frz graph_def. |
| <i>prod_force_virial</i> (atom_ener, natoms) | Compute force and virial. |
| <i>register</i> (key) | Register a descriptor plugin. |

build(coord_: Tensor, atype_: Tensor, natoms: Tensor, box_: Tensor, mesh: Tensor, input_dict: dict, reuse: Optional[bool] = None, suffix: str = '') → Tensor

Build the computational graph for the descriptor.

Parameters

coord_
The coordinate of atoms

atype_
The type of atoms

natoms
The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 ≤ i < Ntypes+2, number of type i atoms

box_
[tf.Tensor] The box of the system

mesh
For historical reasons, only the length of the Tensor matters. if size of mesh == 6, pbc is assumed. if size of mesh == 0, no-pbc is assumed.

input_dict
Dictionary for additional inputs

reuse
The weights in the networks should be reused when get the variable.

suffix
Name suffix to identify this descriptor

Returns

descriptor
The output descriptor

compute_input_stats(data_coord: list, data_box: list, data_atype: list, natoms_vec: list, mesh: list, input_dict: dict, mixed_type: bool = False, real_natoms_vec: Optional[list] = None, **kwargs) → None

Compute the statistics (avg and std) of the training data. The input will be normalized by the statistics.

Parameters

data_coord
The coordinates. Can be generated by deepmd.model.make_stat_input

data_box
The box. Can be generated by deepmd.model.make_stat_input

data_atype
The atom types. Can be generated by deepmd.model.make_stat_input

natoms_vec
The vector for the number of atoms of the system and different types of atoms. Can be generated by deepmd.model.make_stat_input

mesh
The mesh for neighbor searching. Can be generated by deepmd.model.make_stat_input

`input_dict`
Dictionary for additional input

`mixed_type`
Whether to perform the `mixed_type` mode. If `True`, the input data has the `mixed_type` format (see `doc/model/train_se_atten.md`), in which frames in a system may have different `natoms_vec(s)`, with the same `nloc`.

`real_natoms_vec`
If `mixed_type` is `True`, it takes in the `real_natoms_vec` for each frame.

`**kwargs`
Additional keyword arguments.

`enable_compression`(`min_nbor_dist`: `float`, `graph`: `Graph`, `graph_def`: `GraphDef`, `table_extrapolate`: `float` = 5.0, `table_stride_1`: `float` = 0.01, `table_stride_2`: `float` = 0.1, `check_frequency`: `int` = -1, `suffix`: `str` = "") \rightarrow `None`
Reveive the statisitcs (distance, `max_nbor_size` and `env_mat_range`) of the training data.

Parameters

`min_nbor_dist`
[`float`] The nearest distance between atoms

`graph`
[`tf.Graph`] The graph of the model

`graph_def`
[`tf.GraphDef`] The `graph_def` of the model

`table_extrapolate`
[`float`, default: 5.] The scale of model extrapolation

`table_stride_1`
[`float`, default: 0.01] The uniform stride of the first table

`table_stride_2`
[`float`, default: 0.1] The uniform stride of the second table

`check_frequency`
[`int`, default: -1] The overflow check frequency

`suffix`
[`str`, optional] The suffix of the scope

`enable_mixed_precision`(`mixed_prec`: `Optional[dict]` = `None`) \rightarrow `None`
Reveive the mixed precision setting.

Parameters

`mixed_prec`
The mixed precision setting used in the embedding net

`property explicit_ntypes`: `bool`
Explicit ntypes with type embedding.

`get_dim_out()` \rightarrow `int`
Returns the output dimension of this descriptor.

`get_nlist()` \rightarrow `Tuple`[`Tensor`, `Tensor`, `List[int]`, `List[int]`]
Get the neighbor information of the descriptor, returns the `nlist` of the descriptor with the largest cut-off radius.

Returns

nlist
Neighbor list

rij
The relative distance between the neighbor and the center atom.

sel_a
The number of neighbors with full information

sel_r
The number of neighbors with only radial information

get_nlist_i(ii: `int`) → `Tuple`[`Tensor`, `Tensor`, `List`[`int`], `List`[`int`]]

Get the neighbor information of the ii-th descriptor.

Parameters

ii
[`int`] The index of the descriptor

Returns

nlist
Neighbor list

rij
The relative distance between the neighbor and the center atom.

sel_a
The number of neighbors with full information

sel_r
The number of neighbors with only radial information

get_ntypes() → `int`

Returns the number of atom types.

get_rcut() → `float`

Returns the cut-off radius.

get_tensor_names(suffix: `str` = '') → `Tuple`[`str`]

Get names of tensors.

Parameters

suffix
[`str`] The suffix of the scope

Returns

`Tuple`[`str`]
Names of tensors

init_variables(graph: `Graph`, graph_def: `GraphDef`, suffix: `str` = '') → `None`

Init the embedding net variables with the given dict.

Parameters

graph
[`tf.Graph`] The input frozen model graph

`graph_def`
[`tf.GraphDef`] The input frozen model `graph_def`

`suffix`
[`str`, `optional`] The suffix of the scope

`merge_input_stats`(`stat_dict`)

Merge the statistics computed from `compute_input_stats` to obtain the `self.davg` and `self.dstd`.

Parameters

`stat_dict`
The dict of statistics computed from `compute_input_stats`, including:

`sumr`
The sum of radial statistics.

`suma`
The sum of relative coord statistics.

`sumn`
The sum of neighbor numbers.

`sumr2`
The sum of square of radial statistics.

`suma2`
The sum of square of relative coord statistics.

`pass_tensors_from_frz_model`(*`tensors`: `Tensor`) → `None`

Pass the `descript_reshape` tensor as well as `descript_deriv` tensor from the `frz_graph_def`.

Parameters

*`tensors`
[`tf.Tensor`] passed tensors

`prod_force_virial`(`atom_ener`: `Tensor`, `natoms`: `Tensor`) → `Tuple`[`Tensor`, `Tensor`, `Tensor`]

Compute force and virial.

Parameters

`atom_ener`
The atomic energy

`natoms`
The number of atoms. This tensor has the length of `Ntypes + 2` `natoms[0]`: number of local atoms `natoms[1]`: total number of atoms held by this processor `natoms[i]`: $2 \leq i < Ntypes + 2$, number of type `i` atoms

Returns

`force`
The force on atoms

`virial`
The total virial

`atom_virial`
The atomic virial

deepmd.descriptor.loc_frame module

```
class deepmd.descriptor.loc_frame.DescriptLocFrame(*args, **kwargs)
```

Bases: *Descriptor*

Defines a local frame at each atom, and the compute the descriptor as local coordinates under this frame.

Parameters

rcut

The cut-off radius

sel_a

[list[str]] The length of the list should be the same as the number of atom types in the system. sel_a[i] gives the selected number of type-i neighbors. The full relative coordinates of the neighbors are used by the descriptor.

sel_r

[list[str]] The length of the list should be the same as the number of atom types in the system. sel_r[i] gives the selected number of type-i neighbors. Only relative distance of the neighbors are used by the descriptor. sel_a[i] + sel_r[i] is recommended to be larger than the maximally possible number of type-i neighbors in the cut-off radius.

axis_rule: list[int]

The length should be 6 times of the number of types. - axis_rule[i*6+0]: class of the atom defining the first axis of type-i atom. 0 for neighbors with full coordinates and 1 for neighbors only with relative distance. - axis_rule[i*6+1]: type of the atom defining the first axis of type-i atom. - axis_rule[i*6+2]: index of the axis atom defining the first axis. Note that the neighbors with the same class and type are sorted according to their relative distance. - axis_rule[i*6+3]: class of the atom defining the second axis of type-i atom. 0 for neighbors with full coordinates and 1 for neighbors only with relative distance. - axis_rule[i*6+4]: type of the atom defining the second axis of type-i atom. - axis_rule[i*6+5]: index of the axis atom defining the second axis. Note that the neighbors with the same class and type are sorted according to their relative distance.

Attributes

explicit_ntypes

Explicit ntypes with type embedding.

Methods

| | |
|---|---|
| <code>build(coord_, atype_, natoms, box_, mesh, ...)</code> | Build the computational graph for the descriptor. |
| <code>build_type_exclude_mask(exclude_types, ...)</code> | Build the type exclude mask for the descriptor. |
| <code>compute_input_stats(data_coord, data_box, ...)</code> | Compute the statistics (avg and std) of the training data. |
| <code>enable_compression(min_nbor_dist, graph, ...)</code> | Receive the statistics (distance, max_nbor_size and env_mat_range) of the training data. |
| <code>enable_mixed_precision([mixed_prec])</code> | Receive the mixed precision setting. |
| <code>get_dim_out()</code> | Returns the output dimension of this descriptor. |
| <code>get_dim_rot_mat_1()</code> | Returns the first dimension of the rotation matrix. |
| <code>get_nlist()</code> | Returns |
| <code>get_ntypes()</code> | Returns the number of atom types. |
| <code>get_rcut()</code> | Returns the cut-off radius. |
| <code>get_rot_mat()</code> | Get rotational matrix. |
| <code>get_tensor_names([suffix])</code> | Get names of tensors. |
| <code>init_variables(graph, graph_def[, suffix])</code> | Init the embedding net variables with the given dict. |
| <code>pass_tensors_from_frz_model(*tensors)</code> | Pass the <code>descript_reshape</code> tensor as well as <code>descript_deriv</code> tensor from the <code>frz_graph_def</code> . |
| <code>prod_force_virial(atom_ener, natoms)</code> | Compute force and virial. |
| <code>register(key)</code> | Register a descriptor plugin. |

build(coord_: Tensor, atype_: Tensor, natoms: Tensor, box_: Tensor, mesh: Tensor, input_dict: dict, reuse: Optional[bool] = None, suffix: str = '') → Tensor

Build the computational graph for the descriptor.

Parameters

coord_
The coordinate of atoms

atype_
The type of atoms

natoms
The number of atoms. This tensor has the length of Ntypes + 2: natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 ≤ i < Ntypes+2, number of type i atoms

box_
[tf.Tensor] The box of the system

mesh
For historical reasons, only the length of the Tensor matters. if size of mesh == 6, pbc is assumed. if size of mesh == 0, no-pbc is assumed.

input_dict
Dictionary for additional inputs

reuse
The weights in the networks should be reused when get the variable.

suffix
Name suffix to identify this descriptor

Returns

descriptor
The output descriptor

compute_input_stats(data_coord: list, data_box: list, data_atype: list, natoms_vec: list, mesh: list, input_dict: dict, **kwargs) → None

Compute the statistics (avg and std) of the training data. The input will be normalized by the statistics.

Parameters

data_coord
The coordinates. Can be generated by `deepmd.model.make_stat_input`

data_box
The box. Can be generated by `deepmd.model.make_stat_input`

data_atype
The atom types. Can be generated by `deepmd.model.make_stat_input`

natoms_vec
The vector for the number of atoms of the system and different types of atoms.
Can be generated by `deepmd.model.make_stat_input`

mesh
The mesh for neighbor searching. Can be generated by `deepmd.model.make_stat_input`

input_dict
Dictionary for additional input

****kwargs**
Additional keyword arguments.

get_dim_out() → int
Returns the output dimension of this descriptor.

get_nlist() → Tuple[Tensor, Tensor, List[int], List[int]]

Returns

nlist
Neighbor list

rij
The relative distance between the neighbor and the center atom.

sel_a
The number of neighbors with full information

sel_r
The number of neighbors with only radial information

get_ntypes() → int
Returns the number of atom types.

get_rcut() → float
Returns the cut-off radius.

`get_rot_mat()` → Tensor

Get rotational matrix.

`init_variables(graph: Graph, graph_def: GraphDef, suffix: str = '')` → None

Init the embedding net variables with the given dict.

Parameters

`graph`

[[tf.Graph](#)] The input frozen model graph

`graph_def`

[[tf.GraphDef](#)] The input frozen model graph_def

`suffix`

[[str](#), optional] The suffix of the scope

`prod_force_virial(atom_ener: Tensor, natoms: Tensor)` → [Tuple](#)[Tensor, Tensor, Tensor]

Compute force and virial.

Parameters

`atom_ener`

The atomic energy

`natoms`

The number of atoms. This tensor has the length of Ntypes + 2
natoms[0]: number of local atoms
natoms[1]: total number of atoms held by this processor
natoms[i]: 2 ≤ i < Ntypes+2, number of type i atoms

Returns

force

The force on atoms

virial

The total virial

atom_virial

The atomic virial

deepmd.descriptor.se module

`class deepmd.descriptor.se.DescriptSe(*args, **kwargs)`

Bases: [Descriptor](#)

A base class for smooth version of descriptors.

Notes

All of these descriptors have an environmental matrix and an embedding network ([deepmd.utils.network.embedding_net\(\)](#)), so they can share some similar methods without defining them twice.

Attributes

`embedding_net_variables`

[[dict](#)] initial embedding network variables

`descript_reshape`

[[tf.Tensor](#)] the reshaped descriptor

`descript_deriv`
`[tf.Tensor]` the descriptor derivative
`rij`
`[tf.Tensor]` distances between two atoms
`nlist`
`[tf.Tensor]` the neighbor list

Methods

| | |
|--|--|
| <code>build(coord_, atype_, natoms, box_, mesh, ...)</code> | Build the computational graph for the descriptor. |
| <code>build_type_exclude_mask(exclude_types, ...)</code> | Build the type exclude mask for the descriptor. |
| <code>compute_input_stats(data_coord, data_box, ...)</code> | Compute the statistics (avg and std) of the training data. |
| <code>enable_compression(min_nbor_dist, graph, ...)</code> | Reveive the statistics (distance, max_nbor_size and env_mat_range) of the training data. |
| <code>enable_mixed_precision([mixed_prec])</code> | Reveive the mixed precision setting. |
| <code>get_dim_out()</code> | Returns the output dimension of this descriptor. |
| <code>get_dim_rot_mat_1()</code> | Returns the first dimension of the rotation matrix. |
| <code>get_nlist()</code> | Returns neighbor information. |
| <code>get_ntypes()</code> | Returns the number of atom types. |
| <code>get_rcut()</code> | Returns the cut-off radius. |
| <code>get_tensor_names([suffix])</code> | Get names of tensors. |
| <code>init_variables(graph, graph_def[, suffix])</code> | Init the embedding net variables with the given dict. |
| <code>pass_tensors_from_frz_model(descrpt_reshape, ...)</code> | Pass the descrpt_reshape tensor as well as descrpt_deriv tensor from the frz graph_def. |
| <code>prod_force_virial(atom_ener, natoms)</code> | Compute force and virial. |
| <code>register(key)</code> | Register a descriptor plugin. |

get_tensor_names(suffix: `str` = "") → `Tuple[str]`

Get names of tensors.

Parameters

`suffix`
`[str]` The suffix of the scope

Returns

`Tuple[str]`
 Names of tensors

init_variables(graph: `Graph`, graph_def: `GraphDef`, suffix: `str` = "") → `None`

Init the embedding net variables with the given dict.

Parameters

`graph`
`[tf.Graph]` The input frozen model graph
`graph_def`
`[tf.GraphDef]` The input frozen model graph_def

suffix
 [str, optional] The suffix of the scope

pass_tensors_from_frz_model(descript_reshape: Tensor, descript_deriv: Tensor, rij: Tensor, nlist: Tensor)

Pass the descript_reshape tensor as well as descript_deriv tensor from the frz graph_def.

Parameters

descript_reshape
 The passed descript_reshape tensor

descript_deriv
 The passed descript_deriv tensor

rij
 The passed rij tensor

nlist
 The passed nlist tensor

property precision: DType
 Precision of filter network.

deepmd.descriptor.se_a module

class deepmd.descriptor.se_a.DescriptSeA(*args, **kwargs)

Bases: *DescriptSe*

DeepPot-SE constructed from all information (both angular and radial) of atomic configurations. The embedding takes the distance between atoms as input.

The descriptor $\mathcal{D}^i \in \mathbb{R}^{M_1 \times M_2}$ is given by [1]

$$\mathcal{D}^i = (\mathcal{G}^i)^T \mathcal{R}^i (\mathcal{R}^i)^T \mathcal{G}_{<}^i$$

where $\mathcal{R}^i \in \mathbb{R}^{N \times 4}$ is the coordinate matrix, and each row of \mathcal{R}^i can be constructed as follows

$$(\mathcal{R}^i)_j = \begin{bmatrix} \frac{s(r_{ji})}{r_{ji}} \frac{x_{ji}}{r_{ji}} \\ \frac{s(r_{ji})}{r_{ji}} \frac{y_{ji}}{r_{ji}} \\ \frac{s(r_{ji})}{r_{ji}} \frac{z_{ji}}{r_{ji}} \end{bmatrix}$$

where $\mathbf{R}_{ji} = \mathbf{R}_j - \mathbf{R}_i = (x_{ji}, y_{ji}, z_{ji})$ is the relative coordinate and $r_{ji} = \|\mathbf{R}_{ji}\|$ is its norm. The switching function $s(r)$ is defined as:

$$s(r) = \begin{cases} \frac{1}{r}, & r < r_s \\ \frac{1}{r} \left\{ \left(\frac{r-r_s}{r_c-r_s} \right)^3 \left(-6 \left(\frac{r-r_s}{r_c-r_s} \right)^2 + 15 \frac{r-r_s}{r_c-r_s} - 10 \right) + 1 \right\}, & r_s \leq r < r_c \\ 0, & r \geq r_c \end{cases}$$

Each row of the embedding matrix $\mathcal{G}^i \in \mathbb{R}^{N \times M_1}$ consists of outputs of a embedding network \mathcal{N} of $s(r_{ji})$:

$$(\mathcal{G}^i)_j = \mathcal{N}(s(r_{ji}))$$

$\mathcal{G}_{<}^i \in \mathbb{R}^{N \times M_2}$ takes first M_2 columns of \mathcal{G}^i . The equation of embedding network \mathcal{N} can be found at `deepmd.utils.network.embedding_net()`.

Parameters

| | |
|----------------------------------|--|
| <code>rcut</code> | The cut-off radius r_c |
| <code>rcut_smth</code> | From where the environment matrix should be smoothed r_s |
| <code>sel</code> | <code>[list[str]]</code> <code>sel[i]</code> specifies the maximum number of type <code>i</code> atoms in the cut-off radius |
| <code>neuron</code> | <code>[list[int]]</code> Number of neurons in each hidden layers of the embedding net \mathcal{N} |
| <code>axis_neuron</code> | Number of the axis neuron M_2 (number of columns of the sub-matrix of the embedding matrix) |
| <code>resnet_dt</code> | Time-step <code>dt</code> in the resnet construction: $y = x + dt * \phi(Wx + b)$ |
| <code>trainable</code> | If the weights of embedding net are trainable. |
| <code>seed</code> | Random seed for initializing the network parameters. |
| <code>type_one_side</code> | Try to build <code>N_types</code> embedding nets. Otherwise, building <code>N_types^2</code> embedding nets |
| <code>exclude_types</code> | <code>[List[List[int]]]</code> The excluded pairs of types which have no interaction with each other. For example, <code>[[0, 1]]</code> means no interaction between type 0 and type 1. |
| <code>set_davg_zero</code> | Set the shift of embedding net input to zero. |
| <code>activation_function</code> | The activation function in the embedding net. Supported options are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”, “gelu_tf”, “None”, “none”. |
| <code>precision</code> | The precision of the embedding net parameters. Supported options are “default”, “float16”, “float32”, “float64”, “bfloat16”. |
| <code>uniform_seed</code> | Only for the purpose of backward compatibility, retrieves the old behavior of using the random seed |
| <code>multi_task</code> | If the model has multi fitting nets to train. |

References

[1]

Attributes

explicit_ntypes

Explicit ntypes with type embedding.

precision

Precision of filter network.

Methods

| | |
|--|---|
| <i>build</i> (coord_, atype_, natoms, box_, mesh, ...) | Build the computational graph for the descriptor. |
| <i>build_type_exclude_mask</i> (exclude_types, ...) | Build the type exclude mask for the descriptor. |
| <i>compute_input_stats</i> (data_coord, data_box, ...) | Compute the statistics (avg and std) of the training data. |
| <i>enable_compression</i> (min_nbor_dist, graph, ...) | Reveive the statistics (distance, max_nbor_size and env_mat_range) of the training data. |
| <i>enable_mixed_precision</i> ([mixed_prec]) | Reveive the mixed precision setting. |
| <i>get_dim_out</i> () | Returns the output dimension of this descriptor. |
| <i>get_dim_rot_mat_1</i> () | Returns the first dimension of the rotation matrix. |
| <i>get_nlist</i> () | Returns neighbor information. |
| <i>get_ntypes</i> () | Returns the number of atom types. |
| <i>get_rcut</i> () | Returns the cut-off radius. |
| <i>get_rot_mat</i> () | Get rotational matrix. |
| <i>get_tensor_names</i> ([suffix]) | Get names of tensors. |
| <i>init_variables</i> (graph, graph_def[, suffix]) | Init the embedding net variables with the given dict. |
| <i>merge_input_stats</i> (stat_dict) | Merge the statistics computed from compute_input_stats to obtain the self.davg and self.dstd. |
| <i>pass_tensors_from_frz_model</i> (descript_reshape, ...) | Pass the descript_reshape tensor as well as descript_deriv tensor from the frz graph_def. |
| <i>prod_force_virial</i> (atom_ener, natoms) | Compute force and virial. |
| <i>register</i> (key) | Register a descriptor plugin. |

build(coord_: Tensor, atype_: Tensor, natoms: Tensor, box_: Tensor, mesh: Tensor, input_dict: dict, reuse: Optional[bool] = None, suffix: str = '') → Tensor

Build the computational graph for the descriptor.

Parameters

coord_

The coordinate of atoms

atype_

The type of atoms

natoms

The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number

of local atoms `natoms[1]`: total number of atoms held by this processor `natoms[i]`:
 $2 \leq i < \text{Ntypes} + 2$, number of type i atoms

`box_`
`[tf.Tensor]` The box of the system

`mesh`
 For historical reasons, only the length of the Tensor matters. if size of `mesh == 6`,
 pbc is assumed. if size of `mesh == 0`, no-pbc is assumed.

`input_dict`
 Dictionary for additional inputs

`reuse`
 The weights in the networks should be reused when get the variable.

`suffix`
 Name suffix to identify this descriptor

Returns

descriptor
 The output descriptor

compute_input_stats(`data_coord`: list, `data_box`: list, `data_atype`: list, `natoms_vec`: list, `mesh`: list,
`input_dict`: dict, ****kwargs**) \rightarrow None

Compute the statistics (avg and std) of the training data. The input will be normalized by the statistics.

Parameters

`data_coord`
 The coordinates. Can be generated by `deepmd.model.make_stat_input`

`data_box`
 The box. Can be generated by `deepmd.model.make_stat_input`

`data_atype`
 The atom types. Can be generated by `deepmd.model.make_stat_input`

`natoms_vec`
 The vector for the number of atoms of the system and different types of atoms.
 Can be generated by `deepmd.model.make_stat_input`

`mesh`
 The mesh for neighbor searching. Can be generated by
`deepmd.model.make_stat_input`

`input_dict`
 Dictionary for additional input

****kwargs**
 Additional keyword arguments.

enable_compression(`min_nbor_dist`: float, `graph`: Graph, `graph_def`: GraphDef, `table_extrapolate`:
float = 5, `table_stride_1`: float = 0.01, `table_stride_2`: float = 0.1,
`check_frequency`: int = -1, `suffix`: str = '') \rightarrow None

Reveive the statistics (distance, `max_nbor_size` and `env_mat_range`) of the training data.

Parameters

`min_nbor_dist`
 The nearest distance between atoms

`graph`
[`tf.Graph`] The graph of the model

`graph_def`
[`tf.GraphDef`] The graph_def of the model

`table_extrapolate`
The scale of model extrapolation

`table_stride_1`
The uniform stride of the first table

`table_stride_2`
The uniform stride of the second table

`check_frequency`
The overflow check frequency

`suffix`
[`str`, `optional`] The suffix of the scope

`enable_mixed_precision`(mixed_prec: `Optional[dict]` = None) → `None`
Reveive the mixed precision setting.

Parameters

`mixed_prec`
The mixed precision setting used in the embedding net

`get_dim_out()` → `int`
Returns the output dimension of this descriptor.

`get_dim_rot_mat_1()` → `int`
Returns the first dimension of the rotation matrix. The rotation is of shape dim_1 x 3.

`get_nlist()` → `Tuple`[`Tensor`, `Tensor`, `List[int]`, `List[int]`]
Returns neighbor information.

Returns

`nlist`
Neighbor list

`rij`
The relative distance between the neighbor and the center atom.

`sel_a`
The number of neighbors with full information

`sel_r`
The number of neighbors with only radial information

`get_ntypes()` → `int`
Returns the number of atom types.

`get_rcut()` → `float`
Returns the cut-off radius.

`get_rot_mat()` → `Tensor`
Get rotational matrix.

init_variables(graph: Graph, graph_def: GraphDef, suffix: str = '') → None

Init the embedding net variables with the given dict.

Parameters

graph
[tf.Graph] The input frozen model graph

graph_def
[tf.GraphDef] The input frozen model graph_def

suffix
[str, optional] The suffix of the scope

merge_input_stats(stat_dict)

Merge the statistics computed from compute_input_stats to obtain the self.davg and self.dstd.

Parameters

stat_dict
The dict of statistics computed from compute_input_stats, including:

sumr
The sum of radial statistics.

suma
The sum of relative coord statistics.

sumn
The sum of neighbor numbers.

sumr2
The sum of square of radial statistics.

suma2
The sum of square of relative coord statistics.

prod_force_virial(atom_ener: Tensor, natoms: Tensor) → Tuple[Tensor, Tensor, Tensor]

Compute force and virial.

Parameters

atom_ener
The atomic energy

natoms
The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 ≤ i < Ntypes+2, number of type i atoms

Returns

force
The force on atoms

virial
The total virial

atom_virial
The atomic virial

deepmd.descriptor.se_a_ebd module

```
class deepmd.descriptor.se_a_ebd.DescriptSeAEbd(*args, **kwargs)
```

Bases: *DescriptSeA*

DeepPot-SE descriptor with type embedding approach.

Parameters

rcut

The cut-off radius

rcut_smth

From where the environment matrix should be smoothed

sel

`[list[str]]` sel[i] specifies the maximum number of type i atoms in the cut-off radius

neuron

`[list[int]]` Number of neurons in each hidden layers of the embedding net

axis_neuron

Number of the axis neuron (number of columns of the sub-matrix of the embedding matrix)

resnet_dt

Time-step dt in the resnet construction: $y = x + dt * \phi(Wx + b)$

trainable

If the weights of embedding net are trainable.

seed

Random seed for initializing the network parameters.

type_one_side

Try to build N_{types} embedding nets. Otherwise, building N_{types}^2 embedding nets

type_nchanl

Number of channels for type representation

type_nlayer

Number of hidden layers for the type embedding net (skip connected).

numb_aparam

Number of atomic parameters. If >0 it will be embedded with atom types.

set_davg_zero

Set the shift of embedding net input to zero.

activation_function

The activation function in the embedding net. Supported options are {0}

precision

The precision of the embedding net parameters. Supported options are {1}

exclude_types

`[List[List[int]]]` The excluded pairs of types which have no interaction with each other. For example, `[[0, 1]]` means no interaction between type 0 and type 1.

Attributes

explicit_ntypes

Explicit ntypes with type embedding.

precision

Precision of filter network.

Methods

| | |
|--|---|
| <code>build(coord_, atype_, natoms, box_, mesh, ...)</code> | Build the computational graph for the descriptor. |
| <code>build_type_exclude_mask(exclude_types, ...)</code> | Build the type exclude mask for the descriptor. |
| <code>compute_input_stats(data_coord, data_box, ...)</code> | Compute the statistics (avg and std) of the training data. |
| <code>enable_compression(min_nbor_dist, graph, ...)</code> | Reveive the statistics (distance, max_nbor_size and env_mat_range) of the training data. |
| <code>enable_mixed_precision([mixed_prec])</code> | Reveive the mixed precision setting. |
| <code>get_dim_out()</code> | Returns the output dimension of this descriptor. |
| <code>get_dim_rot_mat_1()</code> | Returns the first dimension of the rotation matrix. |
| <code>get_nlist()</code> | Returns neighbor information. |
| <code>get_ntypes()</code> | Returns the number of atom types. |
| <code>get_rcut()</code> | Returns the cut-off radius. |
| <code>get_rot_mat()</code> | Get rotational matrix. |
| <code>get_tensor_names([suffix])</code> | Get names of tensors. |
| <code>init_variables(graph, graph_def[, suffix])</code> | Init the embedding net variables with the given dict. |
| <code>merge_input_stats(stat_dict)</code> | Merge the statistics computed from compute_input_stats to obtain the self.davg and self.dstd. |
| <code>pass_tensors_from_frz_model(descrpt_reshape, ...)</code> | Pass the descrpt_reshape tensor as well as descrpt_deriv tensor from the frz_graph_def. |
| <code>prod_force_virial(atom_ener, natoms)</code> | Compute force and virial. |
| <code>register(key)</code> | Register a descriptor plugin. |

build(coord_: Tensor, atype_: Tensor, natoms: Tensor, box_: Tensor, mesh: Tensor, input_dict: dict, reuse: Optional[bool] = None, suffix: str = '') → Tensor

Build the computational graph for the descriptor.

Parameters**coord_**

The coordinate of atoms

atype_

The type of atoms

natoms

The number of atoms. This tensor has the length of Ntypes + 2
 natoms[0]: number of local atoms
 natoms[1]: total number of atoms held by this processor
 natoms[i]: 2 ≤ i < Ntypes+2, number of type i atoms

box_

[tf.Tensor] The box of the system

mesh
For historical reasons, only the length of the Tensor matters. if size of mesh == 6, pbc is assumed. if size of mesh == 0, no-pbc is assumed.

input_dict
Dictionary for additional inputs

reuse
The weights in the networks should be reused when get the variable.

suffix
Name suffix to identify this descriptor

Returns

descriptor
The output descriptor

deepmd.descriptor.se_a_ef module

`class deepmd.descriptor.se_a_ef.DescriptSeAEf(*args, **kwargs)`

Bases: *Descriptor*

Smooth edition descriptor with Ef.

Parameters

rcut
The cut-off radius

rcut_smth
From where the environment matrix should be smoothed

sel
`[list[str]]` sel[i] specifies the maximum number of type i atoms in the cut-off radius

neuron
`[list[int]]` Number of neurons in each hidden layers of the embedding net

axis_neuron
Number of the axis neuron (number of columns of the sub-matrix of the embedding matrix)

resnet_dt
Time-step dt in the resnet construction: $y = x + dt * \phi(Wx + b)$

trainable
If the weights of embedding net are trainable.

seed
Random seed for initializing the network parameters.

type_one_side
Try to build N_{types} embedding nets. Otherwise, building N_{types}^2 embedding nets

exclude_types
`[List[List[int]]]` The excluded pairs of types which have no interaction with each other. For example, `[[0, 1]]` means no interaction between type 0 and type 1.

set_davg_zero
Set the shift of embedding net input to zero.

activation_function

The activation function in the embedding net. Supported options are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”, “gelu_tf”, “None”, “none”.

precision

The precision of the embedding net parameters. Supported options are “default”, “float16”, “float32”, “float64”, “bfloat16”.

uniform_seed

Only for the purpose of backward compatibility, retrieves the old behavior of using the random seed

Attributes**explicit_ntypes**

Explicit ntypes with type embedding.

Methods

| | |
|--|---|
| <i>build</i> (coord_, atype_, natoms, box_, mesh, ...) | Build the computational graph for the descriptor. |
| <i>build_type_exclude_mask</i> (exclude_types, ...) | Build the type exclude mask for the descriptor. |
| <i>compute_input_stats</i> (data_coord, data_box, ...) | Compute the statistics (avg and std) of the training data. |
| <i>enable_compression</i> (min_nbor_dist, graph, ...) | Reveive the statistics (distance, max_nbor_size and env_mat_range) of the training data. |
| <i>enable_mixed_precision</i> ([mixed_prec]) | Reveive the mixed precision setting. |
| <i>get_dim_out</i> () | Returns the output dimension of this descriptor. |
| <i>get_dim_rot_mat_1</i> () | Returns the first dimension of the rotation matrix. |
| <i>get_nlist</i> () | Returns neighbor information. |
| <i>get_ntypes</i> () | Returns the number of atom types. |
| <i>get_rcut</i> () | Returns the cut-off radius. |
| <i>get_rot_mat</i> () | Get rotational matrix. |
| <i>get_tensor_names</i> ([suffix]) | Get names of tensors. |
| <i>init_variables</i> (graph, graph_def[, suffix]) | Init the embedding net variables with the given dict. |
| <i>pass_tensors_from_frz_model</i> (*tensors) | Pass the descript_reshape tensor as well as descript_deriv tensor from the frz_graph_def. |
| <i>prod_force_virial</i> (atom_ener, natoms) | Compute force and virial. |
| <i>register</i> (key) | Register a descriptor plugin. |

build(coord_: Tensor, atype_: Tensor, natoms: Tensor, box_: Tensor, mesh: Tensor, input_dict: dict, reuse: Optional[bool] = None, suffix: str = '') → Tensor

Build the computational graph for the descriptor.

Parameters**coord_**

The coordinate of atoms

atype_

The type of atoms

natoms
The number of atoms. This tensor has the length of `Ntypes + 2` `natoms[0]`: number of local atoms `natoms[1]`: total number of atoms held by this processor `natoms[i]`: $2 \leq i < Ntypes+2$, number of type `i` atoms

box_
[`tf.Tensor`] The box of the system

mesh
For historical reasons, only the length of the Tensor matters. if size of mesh == 6, pbc is assumed. if size of mesh == 0, no-pbc is assumed.

input_dict
Dictionary for additional inputs. Should have 'efield'.

reuse
The weights in the networks should be reused when get the variable.

suffix
Name suffix to identify this descriptor

Returns

descriptor
The output descriptor

compute_input_stats(data_coord: list, data_box: list, data_atype: list, natoms_vec: list, mesh: list, input_dict: dict, **kwargs) → None

Compute the statistics (avg and std) of the training data. The input will be normalized by the statistics.

Parameters

data_coord
The coordinates. Can be generated by `deepmd.model.make_stat_input`

data_box
The box. Can be generated by `deepmd.model.make_stat_input`

data_atype
The atom types. Can be generated by `deepmd.model.make_stat_input`

natoms_vec
The vector for the number of atoms of the system and different types of atoms. Can be generated by `deepmd.model.make_stat_input`

mesh
The mesh for neighbor searching. Can be generated by `deepmd.model.make_stat_input`

input_dict
Dictionary for additional input

****kwargs**
Additional keyword arguments.

get_dim_out() → int
Returns the output dimension of this descriptor.

get_dim_rot_mat_1() → int
Returns the first dimension of the rotation matrix. The rotation is of shape `dim_1 x 3`.

`get_nlist()` → `Tuple[Tensor, Tensor, List[int], List[int]]`

Returns neighbor information.

Returns

nlist

Neighbor list

rij

The relative distance between the neighbor and the center atom.

sel_a

The number of neighbors with full information

sel_r

The number of neighbors with only radial information

`get_ntypes()` → `int`

Returns the number of atom types.

`get_rcut()` → `float`

Returns the cut-off radius.

`get_rot_mat()` → `Tensor`

Get rotational matrix.

`prod_force_virial(atom_ener: Tensor, natoms: Tensor)` → `Tuple[Tensor, Tensor, Tensor]`

Compute force and virial.

Parameters

atom_ener

The atomic energy

natoms

The number of atoms. This tensor has the length of `Ntypes + 2` `natoms[0]`: number of local atoms `natoms[1]`: total number of atoms held by this processor `natoms[i]`: $2 \leq i < Ntypes + 2$, number of type *i* atoms

Returns

force

The force on atoms

virial

The total virial

atom_virial

The atomic virial

`class deepmd.descriptor.se_a_ef.DescriptSeAEfLower(*args, **kwargs)`

Bases: `DescriptSeA`

Helper class for implementing `DescriptSeAEf`.

Attributes

explicit_ntypes

Explicit ntypes with type embedding.

precision

Precision of filter network.

Methods

| | |
|--|---|
| <code>build(coord_, atype_, natoms, box_, mesh, ...)</code> | Build the computational graph for the descriptor. |
| <code>build_type_exclude_mask(exclude_types, ...)</code> | Build the type exclude mask for the descriptor. |
| <code>compute_input_stats(data_coord, data_box, ...)</code> | Compute the statistics (avg and std) of the training data. |
| <code>enable_compression(min_nbor_dist, graph, ...)</code> | Receive the statistics (distance, max_nbor_size and env_mat_range) of the training data. |
| <code>enable_mixed_precision([mixed_prec])</code> | Receive the mixed precision setting. |
| <code>get_dim_out()</code> | Returns the output dimension of this descriptor. |
| <code>get_dim_rot_mat_1()</code> | Returns the first dimension of the rotation matrix. |
| <code>get_nlist()</code> | Returns neighbor information. |
| <code>get_ntypes()</code> | Returns the number of atom types. |
| <code>get_rcut()</code> | Returns the cut-off radius. |
| <code>get_rot_mat()</code> | Get rotational matrix. |
| <code>get_tensor_names([suffix])</code> | Get names of tensors. |
| <code>init_variables(graph, graph_def[, suffix])</code> | Init the embedding net variables with the given dict. |
| <code>merge_input_stats(stat_dict)</code> | Merge the statistics computed from compute_input_stats to obtain the self.davg and self.dstd. |
| <code>pass_tensors_from_frz_model(descrpt_reshape, ...)</code> | Pass the descrpt_reshape tensor as well as descrpt_deriv tensor from the frz graph_def. |
| <code>prod_force_virial(atom_ener, natoms)</code> | Compute force and virial. |
| <code>register(key)</code> | Register a descriptor plugin. |

build(coord_, atype_, natoms, box_, mesh, input_dict, suffix='', reuse=None)

Build the computational graph for the descriptor.

Parameters

coord_

The coordinate of atoms

atype_

The type of atoms

natoms

The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: $2 \leq i < \text{Ntypes} + 2$, number of type i atoms

box_

[`tf.Tensor`] The box of the system

mesh

For historical reasons, only the length of the Tensor matters. if size of mesh == 6, pbc is assumed. if size of mesh == 0, no-pbc is assumed.

input_dict

Dictionary for additional inputs

reuse

The weights in the networks should be reused when get the variable.

suffix
Name suffix to identify this descriptor

Returns

descriptor
The output descriptor

compute_input_stats(data_coord, data_box, data_atype, natoms_vec, mesh, input_dict, **kwargs)
Compute the statisitcs (avg and std) of the training data. The input will be normalized by the statistics.

Parameters

data_coord
The coordinates. Can be generated by `deepmd.model.make_stat_input`

data_box
The box. Can be generated by `deepmd.model.make_stat_input`

data_atype
The atom types. Can be generated by `deepmd.model.make_stat_input`

natoms_vec
The vector for the number of atoms of the system and different types of atoms.
Can be generated by `deepmd.model.make_stat_input`

mesh
The mesh for neighbor searching. Can be generated by
`deepmd.model.make_stat_input`

input_dict
Dictionary for additional input

**kwargs
Additional keyword arguments.

deepmd.descriptor.se_a_mask module

class `deepmd.descriptor.se_a_mask.DescriptSeAMask`(*args, **kwargs)

Bases: *DescriptSeA*

DeepPot-SE constructed from all information (both angular and radial) of atomic configurations. The embedding takes the distance between atoms as input.

The descriptor $\mathcal{D}^i \in \mathbb{R}^{M_1 \times M_2}$ is given by [1]

$$\mathcal{D}^i = (\mathcal{G}^i)^T \mathcal{R}^i (\mathcal{R}^i)^T \mathcal{G}_{<}^i$$

where $\mathcal{R}^i \in \mathbb{R}^{N \times 4}$ is the coordinate matrix, and each row of \mathcal{R}^i can be constructed as follows

$$(\mathcal{R}^i)_j = \begin{bmatrix} \frac{s(r_{ji})}{s(r_{ji})x_{ji}} \\ \frac{r_{ji}}{s(r_{ji})y_{ji}} \\ \frac{r_{ji}}{s(r_{ji})z_{ji}} \\ \frac{r_{ji}}{r_{ji}} \end{bmatrix}$$

where $\mathbf{R}_{ji} = \mathbf{R}_j - \mathbf{R}_i = (x_{ji}, y_{ji}, z_{ji})$ is the relative coordinate and $r_{ji} = \|\mathbf{R}_{ji}\|$ is its norm. The switching function $s(r)$ is defined as:

$$s(r) = \begin{cases} \frac{1}{r}, & r < r_s \\ \frac{1}{r} \left\{ \left(\frac{r-r_s}{r_c-r_s} \right)^3 \left(-6 \left(\frac{r-r_s}{r_c-r_s} \right)^2 + 15 \frac{r-r_s}{r_c-r_s} - 10 \right) + 1 \right\}, & r_s \leq r < r_c \\ 0, & r \geq r_c \end{cases}$$

Each row of the embedding matrix $\mathcal{G}^i \in \mathbb{R}^{N \times M_1}$ consists of outputs of an embedding network \mathcal{N} of $s(r_{ji})$:

$$(\mathcal{G}^i)_j = \mathcal{N}(s(r_{ji}))$$

$\mathcal{G}^i_{<} \in \mathbb{R}^{N \times M_2}$ takes first M_2 columns of \mathcal{G}^i . The equation of embedding network \mathcal{N} can be found at `deepmd.utils.network.embedding_net()`. Specially for descriptor `se_a_mask` is a concise implementation of `se_a`. The difference is that `se_a_mask` only considered a non-pbc system. And accept a mask matrix to indicate the atom i in frame j is a real atom or not. (1 means real atom, 0 means ghost atom) Thus `se_a_mask` can accept a variable number of atoms in a frame.

Parameters

- `sel`
[`list[str]`] `sel[i]` specifies the maximum number of type i atoms in the neighbor list.
- `neuron`
[`list[int]`] Number of neurons in each hidden layers of the embedding net \mathcal{N}
- `axis_neuron`
Number of the axis neuron M_2 (number of columns of the sub-matrix of the embedding matrix)
- `resnet_dt`
Time-step dt in the resnet construction: $y = x + dt * \phi(Wx + b)$
- `trainable`
If the weights of embedding net are trainable.
- `seed`
Random seed for initializing the network parameters.
- `type_one_side`
Try to build N_{types} embedding nets. Otherwise, building N_{types}^2 embedding nets
- `exclude_types`
[`List[List[int]]`] The excluded pairs of types which have no interaction with each other. For example, `[[0, 1]]` means no interaction between type 0 and type 1.
- `activation_function`
The activation function in the embedding net. Supported options are {0}
- `precision`
The precision of the embedding net parameters. Supported options are {1}
- `uniform_seed`
Only for the purpose of backward compatibility, retrieves the old behavior of using the random seed

References

[1]

Attributes

explicit_ntypes

Explicit ntypes with type embedding.

precision

Precision of filter network.

Methods

| | |
|--|---|
| <i>build</i> (coord_, atype_, natoms, box_, mesh, ...) | Build the computational graph for the descriptor. |
| <i>build_type_exclude_mask</i> (exclude_types, ...) | Build the type exclude mask for the descriptor. |
| <i>compute_input_stats</i> (data_coord, data_box, ...) | Compute the statistics (avg and std) of the training data. |
| <i>enable_compression</i> (min_nbor_dist, graph, ...) | Reveive the statistics (distance, max_nbor_size and env_mat_range) of the training data. |
| <i>enable_mixed_precision</i> ([mixed_prec]) | Reveive the mixed precision setting. |
| <i>get_dim_out</i> () | Returns the output dimension of this descriptor. |
| <i>get_dim_rot_mat_1</i> () | Returns the first dimension of the rotation matrix. |
| <i>get_nlist</i> () | Returns neighbor information. |
| <i>get_ntypes</i> () | Returns the number of atom types. |
| <i>get_rcut</i> () | Returns the cutoff radius. |
| <i>get_rot_mat</i> () | Get rotational matrix. |
| <i>get_tensor_names</i> ([suffix]) | Get names of tensors. |
| <i>init_variables</i> (graph, graph_def[, suffix]) | Init the embedding net variables with the given dict. |
| <i>merge_input_stats</i> (stat_dict) | Merge the statistics computed from compute_input_stats to obtain the self.davg and self.dstd. |
| <i>pass_tensors_from_frz_model</i> (descript_reshape, ...) | Pass the descript_reshape tensor as well as descript_deriv tensor from the frz graph_def. |
| <i>prod_force_virial</i> (atom_ener, natoms) | Compute force and virial. |
| <i>register</i> (key) | Register a descriptor plugin. |

build(coord_: Tensor, atype_: Tensor, natoms: Tensor, box_: Tensor, mesh: Tensor, input_dict: Dict[str, Any], reuse: Optional[bool] = None, suffix: str = '') → Tensor

Build the computational graph for the descriptor.

Parameters

coord_

The coordinate of atoms

atype_

The type of atoms

natoms

The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number

of local atoms `natoms[1]`: total number of atoms held by this processor `natoms[i]`:
 $2 \leq i < Ntypes+2$, number of type `i` atoms

`box_`
`[tf.Tensor]` The box of the system

`mesh`
 For historical reasons, only the length of the Tensor matters. if size of `mesh == 6`,
 pbc is assumed. if size of `mesh == 0`, no-pbc is assumed.

`input_dict`
 Dictionary for additional inputs

`reuse`
 The weights in the networks should be reused when get the variable.

`suffix`
 Name suffix to identify this descriptor

Returns

descriptor
 The output descriptor

compute_input_stats(`data_coord`: list, `data_box`: list, `data_atype`: list, `natoms_vec`: list, `mesh`: list,
`input_dict`: dict, ****kwargs**) → None

Compute the statistics (avg and std) of the training data. The input will be normalized by the
 statistics.

Parameters

`data_coord`
 The coordinates. Can be generated by `deepmd.model.make_stat_input`

`data_box`
 The box. Can be generated by `deepmd.model.make_stat_input`

`data_atype`
 The atom types. Can be generated by `deepmd.model.make_stat_input`

`natoms_vec`
 The vector for the number of atoms of the system and different types of atoms.
 Can be generated by `deepmd.model.make_stat_input`

`mesh`
 The mesh for neighbor searching. Can be generated by
`deepmd.model.make_stat_input`

`input_dict`
 Dictionary for additional input

****kwargs**
 Additional keyword arguments.

get_rcut() → float
 Returns the cutoff radius.

prod_force_virial(`atom_ener`: Tensor, `natoms`: Tensor) → Tuple[Tensor, Tensor, Tensor]
 Compute force and virial.

Parameters

atom_ener
 The atomic energy

natoms
 The number of atoms. This tensor has the length of $N_{\text{types}} + 2$ `natoms[0]`: number of local atoms `natoms[1]`: total number of atoms held by this processor `natoms[i]`: $2 \leq i < N_{\text{types}} + 2$, number of type i atoms

Returns

force
 The force on atoms

virial
 None for `se_a_mask` op

atom_virial
 None for `se_a_mask` op

deepmd.descriptor.se_atten module

class `deepmd.descriptor.se_atten.DescriptSeAtten(*args, **kwargs)`

Bases: *DescriptSeA*

Smooth version descriptor with attention.

Parameters

rcut
 The cut-off radius r_c

rcut_smth
 From where the environment matrix should be smoothed r_s

sel
`[list[str]]` `sel[i]` specifies the maximum number of type i atoms in the cut-off radius

neuron
`[list[int]]` Number of neurons in each hidden layers of the embedding net \mathcal{N}

axis_neuron
 Number of the axis neuron M_2 (number of columns of the sub-matrix of the embedding matrix)

resnet_dt
 Time-step dt in the resnet construction: $y = x + \text{dt} * \text{phi}(Wx + b)$

trainable
 If the weights of embedding net are trainable.

seed
 Random seed for initializing the network parameters.

type_one_side
 Try to build N_{types} embedding nets. Otherwise, building N_{types}^2 embedding nets

exclude_types
`[List[List[int]]]` The excluded pairs of types which have no interaction with each other. For example, `[[0, 1]]` means no interaction between type 0 and type 1.

set_davg_zero
Set the shift of embedding net input to zero.

activation_function
The activation function in the embedding net. Supported options are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”, “gelu_tf”, “None”, “none”.

precision
The precision of the embedding net parameters. Supported options are “default”, “float16”, “float32”, “float64”, “bfloat16”.

uniform_seed
Only for the purpose of backward compatibility, retrieves the old behavior of using the random seed

attn
The length of hidden vector during scale-dot attention computation.

attn_layer
The number of layers in attention mechanism.

attn_dotr
Whether to dot the relative coordinates on the attention weights as a gated scheme.

attn_mask
Whether to mask the diagonal in the attention weights.

multi_task
If the model has multi fitting nets to train.

stripped_type_embedding
Whether to strip the type embedding into a separated embedding network. Default value will be True in se_attn_v2 descriptor.

smooth_type_embdding
When using stripped type embedding, whether to dot smooth factor on the network output of type embedding to keep the network smooth, instead of setting set_davg_zero to be True. Default value will be True in se_attn_v2 descriptor.

Attributes

explicit_ntypes
Explicit ntypes with type embedding.

precision
Precision of filter network.

Methods

| | |
|--|---|
| <code>build(coord_, atype_, natoms, box_, mesh, ...)</code> | Build the computational graph for the descriptor. |
| <code>build_type_exclude_mask(exclude_types, ...)</code> | Build the type exclude mask for the attention descriptor. |
| <code>compute_input_stats(data_coord, data_box, ...)</code> | Compute the statistics (avg and std) of the training data. |
| <code>enable_compression(min_nbor_dist, graph, ...)</code> | Reveive the statistics (distance, max_nbor_size and env_mat_range) of the training data. |
| <code>enable_mixed_precision([mixed_prec])</code> | Reveive the mixed precision setting. |
| <code>get_dim_out()</code> | Returns the output dimension of this descriptor. |
| <code>get_dim_rot_mat_1()</code> | Returns the first dimension of the rotation matrix. |
| <code>get_nlist()</code> | Returns neighbor information. |
| <code>get_ntypes()</code> | Returns the number of atom types. |
| <code>get_rcut()</code> | Returns the cut-off radius. |
| <code>get_rot_mat()</code> | Get rotational matrix. |
| <code>get_tensor_names([suffix])</code> | Get names of tensors. |
| <code>init_variables(graph, graph_def[, suffix])</code> | Init the embedding net variables with the given dict. |
| <code>merge_input_stats(stat_dict)</code> | Merge the statistics computed from compute_input_stats to obtain the self.davg and self.dstd. |
| <code>pass_tensors_from_frz_model(descrpt_reshape, ...)</code> | Pass the descrpt_reshape tensor as well as descrpt_deriv tensor from the frz graph_def. |
| <code>prod_force_virial(atom_ener, natoms)</code> | Compute force and virial. |
| <code>register(key)</code> | Register a descriptor plugin. |

`build(coord_ : Tensor, atype_ : Tensor, natoms: Tensor, box_ : Tensor, mesh: Tensor, input_dict: dict, reuse: Optional[bool] = None, suffix: str = "") → Tensor`

Build the computational graph for the descriptor.

Parameters

`coord_`
The coordinate of atoms

`atype_`
The type of atoms

`natoms`
The number of atoms. This tensor has the length of Ntypes + 2 `natoms[0]`: number of local atoms `natoms[1]`: total number of atoms held by this processor `natoms[i]`: $2 \leq i < \text{Ntypes} + 2$, number of type i atoms

`box_`
[`tf.Tensor`] The box of the system

`mesh`
For historical reasons, only the length of the Tensor matters. if size of mesh == 6, pbc is assumed. if size of mesh == 0, no-pbc is assumed.

`input_dict`
Dictionary for additional inputs

reuse

The weights in the networks should be reused when get the variable.

suffix

Name suffix to identify this descriptor

Returns

descriptor

The output descriptor

build_type_exclude_mask(exclude_types: List[Tuple[int, int]], ntypes: int, sel: List[int], ndescript: int, atype: Tensor, shape0: Tensor, nei_type_vec: Tensor) → Tensor

Build the type exclude mask for the attention descriptor.

Parameters

exclude_types

[List[Tuple[int, int]]] The list of excluded types, e.g. [(0, 1), (1, 0)] means the interaction between type 0 and type 1 is excluded.

ntypes

[int] The number of types.

sel

[List[int]] The list of the number of selected neighbors for each type.

ndescript

[int] The number of descriptors for each atom.

atype

[tf.Tensor] The type of atoms, with the size of shape0.

shape0

[tf.Tensor] The shape of the first dimension of the inputs, which is equal to nsamples * natoms.

nei_type_vec

[tf.Tensor] The type of neighbors, with the size of (shape0, nnei).

Returns

tf.Tensor

The type exclude mask, with the shape of (shape0, ndescript), and the precision of GLOBAL_TF_FLOAT_PRECISION. The mask has the value of 1 if the interaction between two types is not excluded, and 0 otherwise.

See also:

`deepmd.descriptor.descriptor.Descriptor.build_type_exclude_mask`

Notes

This method has the similar way to build the type exclude mask as `deepmd.descriptor.descriptor.Descriptor.build_type_exclude_mask()`. The mathematical expression has been explained in that method. The difference is that the attention descriptor has provided the type of the neighbors (`idx_j`) that is not in order, so we use it from an extra input.

```
compute_input_stats(data_coord: list, data_box: list, data_atype: list, natoms_vec: list, mesh: list,
                    input_dict: dict, mixed_type: bool = False, real_natoms_vec: Optional[list] =
                    None, **kwargs) → None
```

Compute the statistics (avg and std) of the training data. The input will be normalized by the statistics.

Parameters

`data_coord`

The coordinates. Can be generated by `deepmd.model.make_stat_input`

`data_box`

The box. Can be generated by `deepmd.model.make_stat_input`

`data_atype`

The atom types. Can be generated by `deepmd.model.make_stat_input`

`natoms_vec`

The vector for the number of atoms of the system and different types of atoms. If `mixed_type` is True, this para is blank. See `real_natoms_vec`.

`mesh`

The mesh for neighbor searching. Can be generated by `deepmd.model.make_stat_input`

`input_dict`

Dictionary for additional input

`mixed_type`

Whether to perform the mixed_type mode. If True, the input data has the mixed_type format (see `doc/model/train_se_atten.md`), in which frames in a system may have different `natoms_vec(s)`, with the same `nloc`.

`real_natoms_vec`

If `mixed_type` is True, it takes in the real `natoms_vec` for each frame.

`**kwargs`

Additional keyword arguments.

```
enable_compression(min_nbor_dist: float, graph: Graph, graph_def: GraphDef, table_extrapolate:
                    float = 5, table_stride_1: float = 0.01, table_stride_2: float = 0.1,
                    check_frequency: int = -1, suffix: str = '') → None
```

Reveive the statistics (distance, max_nbor_size and env_mat_range) of the training data.

Parameters

`min_nbor_dist`

The nearest distance between atoms

`graph`

[`tf.Graph`] The graph of the model

`graph_def`

[`tf.GraphDef`] The `graph_def` of the model

```

    table_extrapolate
        The scale of model extrapolation
    table_stride_1
        The uniform stride of the first table
    table_stride_2
        The uniform stride of the second table
    check_frequency
        The overflow check frequency
    suffix
        [str, optional] The suffix of the scope
property explicit_ntypes: bool
    Explicit ntypes with type embedding.
init_variables(graph: Graph, graph_def: GraphDef, suffix: str = '') → None
    Init the embedding net variables with the given dict.
Parameters
    graph
        [tf.Graph] The input frozen model graph
    graph_def
        [tf.GraphDef] The input frozen model graph_def
    suffix
        [str, optional] The suffix of the scope

```

deepmd.descriptor.se_atten_v2 module

```

class deepmd.descriptor.se_atten_v2.DescriptSeAttenV2(*args, **kwargs)
    Bases: DescriptSeAtten
    Smooth version 2.0 descriptor with attention.
Parameters
    rcut
        The cut-off radius  $r_c$ 
    rcut_smth
        From where the environment matrix should be smoothed  $r_s$ 
    sel
        [list[str]] sel[i] specifies the maximum number of type i atoms in the cut-off radius
    neuron
        [list[int]] Number of neurons in each hidden layers of the embedding net  $\mathcal{N}$ 
    axis_neuron
        Number of the axis neuron  $M_2$  (number of columns of the sub-matrix of the embedding matrix)
    resnet_dt
        Time-step dt in the resnet construction:  $y = x + dt * \phi(Wx + b)$ 
    trainable
        If the weights of embedding net are trainable.

```


seed
Random seed for initializing the network parameters.

type_one_side
Try to build N_{types} embedding nets. Otherwise, building N_{types}^2 embedding nets

exclude_types
[List[List[int]]] The excluded pairs of types which have no interaction with each other. For example, `[[0, 1]]` means no interaction between type 0 and type 1.

set_davg_zero
Set the shift of embedding net input to zero.

activation_function
The activation function in the embedding net. Supported options are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”, “gelu_tf”, “None”, “none”.

precision
The precision of the embedding net parameters. Supported options are “default”, “float16”, “float32”, “float64”, “bfloat16”.

uniform_seed
Only for the purpose of backward compatibility, retrieves the old behavior of using the random seed

attn
The length of hidden vector during scale-dot attention computation.

attn_layer
The number of layers in attention mechanism.

attn_dotr
Whether to dot the relative coordinates on the attention weights as a gated scheme.

attn_mask
Whether to mask the diagonal in the attention weights.

multi_task
If the model has multi fitting nets to train.

Attributes

explicit_ntypes
Explicit ntypes with type embedding.

precision
Precision of filter network.

Methods

| | |
|--|---|
| <code>build(coord_, atype_, natoms, box_, mesh, ...)</code> | Build the computational graph for the descriptor. |
| <code>build_type_exclude_mask(exclude_types, ...)</code> | Build the type exclude mask for the attention descriptor. |
| <code>compute_input_stats(data_coord, data_box, ...)</code> | Compute the statistics (avg and std) of the training data. |
| <code>enable_compression(min_nbor_dist, graph, ...)</code> | Reveive the statistics (distance, max_nbor_size and env_mat_range) of the training data. |
| <code>enable_mixed_precision([mixed_prec])</code> | Reveive the mixed precision setting. |
| <code>get_dim_out()</code> | Returns the output dimension of this descriptor. |
| <code>get_dim_rot_mat_1()</code> | Returns the first dimension of the rotation matrix. |
| <code>get_nlist()</code> | Returns neighbor information. |
| <code>get_ntypes()</code> | Returns the number of atom types. |
| <code>get_rcut()</code> | Returns the cut-off radius. |
| <code>get_rot_mat()</code> | Get rotational matrix. |
| <code>get_tensor_names([suffix])</code> | Get names of tensors. |
| <code>init_variables(graph, graph_def[, suffix])</code> | Init the embedding net variables with the given dict. |
| <code>merge_input_stats(stat_dict)</code> | Merge the statistics computed from <code>compute_input_stats</code> to obtain the <code>self.davg</code> and <code>self.dstd</code> . |
| <code>pass_tensors_from_frz_model(descrpt_reshape, ...)</code> | Pass the <code>descrpt_reshape</code> tensor as well as <code>descrpt_deriv</code> tensor from the <code>frz graph_def</code> . |
| <code>prod_force_virial(atom_ener, natoms)</code> | Compute force and virial. |
| <code>register(key)</code> | Register a descriptor plugin. |

deepmd.descriptor.se_r module

```
class deepmd.descriptor.se_r.DescriptSeR(*args, **kwargs)
```

Bases: *DescriptSe*

DeepPot-SE constructed from radial information of atomic configurations.

The embedding takes the distance between atoms as input.

Parameters

`rcut`

The cut-off radius

`rcut_smth`

From where the environment matrix should be smoothed

`sel`

`[list[str]] sel[i]` specifies the maximum number of type `i` atoms in the cut-off radius

`neuron`

`[list[int]]` Number of neurons in each hidden layers of the embedding net

`resnet_dt`

Time-step `dt` in the resnet construction: $y = x + dt * \phi(Wx + b)$

trainable
If the weights of embedding net are trainable.

seed
Random seed for initializing the network parameters.

type_one_side
Try to build N_{types} embedding nets. Otherwise, building N_{types}^2 embedding nets

exclude_types
[`List[List[int]]`] The excluded pairs of types which have no interaction with each other. For example, `[[0, 1]]` means no interaction between type 0 and type 1.

activation_function
The activation function in the embedding net. Supported options are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”, “gelu_tf”, “None”, “none”.

precision
The precision of the embedding net parameters. Supported options are “default”, “float16”, “float32”, “float64”, “bfloat16”.

uniform_seed
Only for the purpose of backward compatibility, retrieves the old behavior of using the random seed

Attributes

explicit_ntypes
Explicit ntypes with type embedding.

precision
Precision of filter network.

Methods

| | |
|--|---|
| <code>build(coord_, atype_, natoms, box_, mesh, ...)</code> | Build the computational graph for the descriptor. |
| <code>build_type_exclude_mask(exclude_types, ...)</code> | Build the type exclude mask for the descriptor. |
| <code>compute_input_stats(data_coord, data_box, ...)</code> | Compute the statistics (avg and std) of the training data. |
| <code>enable_compression(min_nbor_dist, graph, ...)</code> | Receive the statistics (distance, max_nbor_size and env_mat_range) of the training data. |
| <code>enable_mixed_precision([mixed_prec])</code> | Receive the mixed precision setting. |
| <code>get_dim_out()</code> | Returns the output dimension of this descriptor. |
| <code>get_dim_rot_mat_1()</code> | Returns the first dimension of the rotation matrix. |
| <code>get_nlist()</code> | Returns neighbor information. |
| <code>get_ntypes()</code> | Returns the number of atom types. |
| <code>get_rcut()</code> | Returns the cut-off radius. |
| <code>get_tensor_names([suffix])</code> | Get names of tensors. |
| <code>init_variables(graph, graph_def[, suffix])</code> | Init the embedding net variables with the given dict. |
| <code>merge_input_stats(stat_dict)</code> | Merge the statistics computed from compute_input_stats to obtain the self.davg and self.dstd. |
| <code>pass_tensors_from_frz_model(descrpt_reshape, ...)</code> | Pass the descrpt_reshape tensor as well as descrpt_deriv tensor from the frz graph_def. |
| <code>prod_force_virial(atom_ener, natoms)</code> | Compute force and virial. |
| <code>register(key)</code> | Register a descriptor plugin. |

build(coord_: Tensor, atype_: Tensor, natoms: Tensor, box_: Tensor, mesh: Tensor, input_dict: dict, reuse: Optional[bool] = None, suffix: str = '') → Tensor

Build the computational graph for the descriptor.

Parameters

coord_
The coordinate of atoms

atype_
The type of atoms

natoms
The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 ≤ i < Ntypes+2, number of type i atoms

box_
[tf.Tensor] The box of the system

mesh
For historical reasons, only the length of the Tensor matters. if size of mesh == 6, pbc is assumed. if size of mesh == 0, no-pbc is assumed.

input_dict
Dictionary for additional inputs

reuse
The weights in the networks should be reused when get the variable.

suffix
Name suffix to identify this descriptor

Returns

descriptor
The output descriptor

compute_input_stats(data_coord, data_box, data_atype, natoms_vec, mesh, input_dict, **kwargs)
Compute the statistics (avg and std) of the training data. The input will be normalized by the statistics.

Parameters

data_coord
The coordinates. Can be generated by `deepmd.model.make_stat_input`

data_box
The box. Can be generated by `deepmd.model.make_stat_input`

data_atype
The atom types. Can be generated by `deepmd.model.make_stat_input`

natoms_vec
The vector for the number of atoms of the system and different types of atoms.
Can be generated by `deepmd.model.make_stat_input`

mesh
The mesh for neighbor searching. Can be generated by
`deepmd.model.make_stat_input`

input_dict
Dictionary for additional input

**kwargs
Additional keyword arguments.

enable_compression(min_nbor_dist: float, graph: Graph, graph_def: GraphDef, table_extrapolate: float = 5, table_stride_1: float = 0.01, table_stride_2: float = 0.1, check_frequency: int = -1, suffix: str = '') → None

Reveive the statistics (distance, max_nbor_size and env_mat_range) of the training data.

Parameters

min_nbor_dist
The nearest distance between atoms

graph
[tf.Graph] The graph of the model

graph_def
[tf.GraphDef] The graph_def of the model

table_extrapolate
The scale of model extrapolation

table_stride_1
The uniform stride of the first table

table_stride_2
The uniform stride of the second table

`check_frequency`
The overflow check frequency

`suffix`
[`str`, `optional`] The suffix of the scope

`get_dim_out()`
Returns the output dimension of this descriptor.

`get_nlist()`
Returns neighbor information.

Returns

`nlist`
Neighbor list

`rij`
The relative distance between the neighbor and the center atom.

`sel_a`
The number of neighbors with full information

`sel_r`
The number of neighbors with only radial information

`get_ntypes()`
Returns the number of atom types.

`get_rcut()`
Returns the cut-off radius.

`merge_input_stats(stat_dict)`
Merge the statisitcs computed from `compute_input_stats` to obtain the `self.davg` and `self.dstd`.

Parameters

`stat_dict`
The dict of statisitcs computed from `compute_input_stats`, including:

`sumr`
The sum of radial statisitcs.

`sumn`
The sum of neighbor numbers.

`sumr2`
The sum of square of radial statisitcs.

`prod_force_virial(atom_ener: Tensor, natoms: Tensor) → Tuple[Tensor, Tensor, Tensor]`
Compute force and virial.

Parameters

`atom_ener`
The atomic energy

`natoms`
The number of atoms. This tensor has the length of `Ntypes + 2` `natoms[0]`: number of local atoms `natoms[1]`: total number of atoms held by this processor `natoms[i]`: $2 \leq i < Ntypes+2$, number of type `i` atoms

Returns

force
The force on atoms

virial
The total virial

atom_virial
The atomic virial

deepmd.descriptor.se_t module

`class deepmd.descriptor.se_t.DescriptSeT(*args, **kwargs)`

Bases: *DescriptSe*

DeepPot-SE constructed from all information (both angular and radial) of atomic configurations.

The embedding takes angles between two neighboring atoms as input.

Parameters

rcut
The cut-off radius

rcut_smth
From where the environment matrix should be smoothed

sel
[`list[str]`] `sel[i]` specifies the maximum number of type `i` atoms in the cut-off radius

neuron
[`list[int]`] Number of neurons in each hidden layers of the embedding net

resnet_dt
Time-step `dt` in the resnet construction: $y = x + dt * \phi(Wx + b)$

trainable
If the weights of embedding net are trainable.

seed
Random seed for initializing the network parameters.

set_davg_zero
Set the shift of embedding net input to zero.

activation_function
The activation function in the embedding net. Supported options are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”, “gelu_tf”, “None”, “none”.

precision
The precision of the embedding net parameters. Supported options are “default”, “float16”, “float32”, “float64”, “bfloat16”.

uniform_seed
Only for the purpose of backward compatibility, retrieves the old behavior of using the random seed

Attributes

explicit_ntypes
Explicit ntypes with type embedding.

precision

Precision of filter network.

Methods

| | |
|--|---|
| <i>build</i> (coord_, atype_, natoms, box_, mesh, ...) | Build the computational graph for the descriptor. |
| <i>build_type_exclude_mask</i> (exclude_types, ...) | Build the type exclude mask for the descriptor. |
| <i>compute_input_stats</i> (data_coord, data_box, ...) | Compute the statistics (avg and std) of the training data. |
| <i>enable_compression</i> (min_nbor_dist, graph, ...) | Reveive the statistics (distance, max_nbor_size and env_mat_range) of the training data. |
| <i>enable_mixed_precision</i> ([mixed_prec]) | Reveive the mixed precision setting. |
| <i>get_dim_out</i> () | Returns the output dimension of this descriptor. |
| <i>get_dim_rot_mat_1</i> () | Returns the first dimension of the rotation matrix. |
| <i>get_nlist</i> () | Returns neighbor information. |
| <i>get_ntypes</i> () | Returns the number of atom types. |
| <i>get_rcut</i> () | Returns the cut-off radius. |
| <i>get_tensor_names</i> ([suffix]) | Get names of tensors. |
| <i>init_variables</i> (graph, graph_def[, suffix]) | Init the embedding net variables with the given dict. |
| <i>merge_input_stats</i> (stat_dict) | Merge the statistics computed from compute_input_stats to obtain the self.davg and self.dstd. |
| <i>pass_tensors_from_frz_model</i> (descript_reshape, ...) | Pass the descript_reshape tensor as well as descript_deriv tensor from the frz_graph_def. |
| <i>prod_force_virial</i> (atom_ener, natoms) | Compute force and virial. |
| <i>register</i> (key) | Register a descriptor plugin. |

build(coord_: Tensor, atype_: Tensor, natoms: Tensor, box_: Tensor, mesh: Tensor, input_dict: dict, reuse: Optional[bool] = None, suffix: str = '') → Tensor

Build the computational graph for the descriptor.

Parameters

coord_

The coordinate of atoms

atype_

The type of atoms

natoms

The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 ≤ i < Ntypes+2, number of type i atoms

box_

[tf.Tensor] The box of the system

mesh

For historical reasons, only the length of the Tensor matters. if size of mesh == 6, pbc is assumed. if size of mesh == 0, no-pbc is assumed.

`input_dict`
 Dictionary for additional inputs

`reuse`
 The weights in the networks should be reused when get the variable.

`suffix`
 Name suffix to identify this descriptor

Returns

descriptor
 The output descriptor

compute_input_stats(data_coord: list, data_box: list, data_atype: list, natoms_vec: list, mesh: list, input_dict: dict, **kwargs) → None

Compute the statisitcs (avg and std) of the training data. The input will be normalized by the statistics.

Parameters

`data_coord`
 The coordinates. Can be generated by `deepmd.model.make_stat_input`

`data_box`
 The box. Can be generated by `deepmd.model.make_stat_input`

`data_atype`
 The atom types. Can be generated by `deepmd.model.make_stat_input`

`natoms_vec`
 The vector for the number of atoms of the system and different types of atoms.
 Can be generated by `deepmd.model.make_stat_input`

`mesh`
 The mesh for neighbor searching. Can be generated by `deepmd.model.make_stat_input`

`input_dict`
 Dictionary for additional input

`**kwargs`
 Additional keyword arguments.

enable_compression(min_nbor_dist: float, graph: Graph, graph_def: GraphDef, table_extrapolate: float = 5, table_stride_1: float = 0.01, table_stride_2: float = 0.1, check_frequency: int = -1, suffix: str = '') → None

Reveive the statisitcs (distance, max_nbor_size and env_mat_range) of the training data.

Parameters

`min_nbor_dist`
 The nearest distance between atoms

`graph`
 [tf.Graph] The graph of the model

`graph_def`
 [tf.GraphDef] The graph_def of the model

`table_extrapolate`
 The scale of model extrapolation

`table_stride_1`
The uniform stride of the first table

`table_stride_2`
The uniform stride of the second table

`check_frequency`
The overflow check frequency

`suffix`
[`str`, `optional`] The suffix of the scope

`get_dim_out()` → `int`

Returns the output dimension of this descriptor.

`get_nlist()` → `Tuple`[`Tensor`, `Tensor`, `List`[`int`], `List`[`int`]]

Returns neighbor information.

Returns

`nlist`
Neighbor list

`rij`
The relative distance between the neighbor and the center atom.

`sel_a`
The number of neighbors with full information

`sel_r`
The number of neighbors with only radial information

`get_ntypes()` → `int`

Returns the number of atom types.

`get_rcut()` → `float`

Returns the cut-off radius.

`merge_input_stats`(`stat_dict`)

Merge the statisitcs computed from `compute_input_stats` to obtain the `self.davg` and `self.dstd`.

Parameters

`stat_dict`
The dict of statisitcs computed from `compute_input_stats`, including:

`sumr`
The sum of radial statisitcs.

`suma`
The sum of relative coord statisitcs.

`sumn`
The sum of neighbor numbers.

`sumr2`
The sum of square of radial statisitcs.

`suma2`
The sum of square of relative coord statisitcs.

`prod_force_virial(atom_ener: Tensor, natoms: Tensor) → Tuple[Tensor, Tensor, Tensor]`

Compute force and virial.

Parameters

`atom_ener`

The atomic energy

`natoms`

The number of atoms. This tensor has the length of `Ntypes + 2` `natoms[0]`: number of local atoms `natoms[1]`: total number of atoms held by this processor `natoms[i]`: $2 \leq i < Ntypes + 2$, number of type `i` atoms

Returns

`force`

The force on atoms

`virial`

The total virial

`atom_virial`

The atomic virial

deepmd.entrypoints package

Submodule that contains all the DeePMD-Kit entry point scripts.

`deepmd.entrypoints.compress(*, input: str, output: str, extrapolate: int, step: float, frequency: str, checkpoint_folder: str, training_script: str, mpi_log: str, log_path: Optional[str], log_level: int, **kwargs)`

Compress model.

The table is composed of fifth-order polynomial coefficients and is assembled from two sub-tables. The first table takes the step parameter as the domain's uniform step size, while the second table takes `10 * step` as its uniform step size. The range of the first table is automatically detected by the code, while the second table ranges from the first table's upper boundary(`upper`) to the `extrapolate(parameter) * upper`.

Parameters

`input`

[`str`] frozen model file to compress

`output`

[`str`] compressed model filename

`extrapolate`

[`int`] scale of model extrapolation

`step`

[`float`] uniform step size of the tabulation's first table

`frequency`

[`str`] frequency of tabulation overflow check

`checkpoint_folder`

[`str`] training checkpoint folder for freezing

`training_script`

[`str`] training script of the input frozen model

`mpi_log`
 [`str`] mpi logging mode for training

`log_path`
 [`Optional[str]`] if speccified log will be written to this file

`log_level`
 [`int`] logging level

`**kwargs`
 additional arguments

`deepmd.entrypoints.convert(*, FROM: str, input_model: str, output_model: str, **kwargs)`

`deepmd.entrypoints.doc_train_input(*, out_type: str = 'rst', **kwargs)`

Print out trining input arguments to console.

`deepmd.entrypoints.freeze(*, checkpoint_folder: str, output: str, node_names: Optional[str] = None, nvnmd_weight: Optional[str] = None, united_model: bool = False, **kwargs)`

Freeze the graph in supplied folder.

Parameters

`checkpoint_folder`
 [`str`] location of the folder with model

`output`
 [`str`] output file name

`node_names`
 [`Optional[str]`, `optional`] names of nodes to output, by default None

`nvnmd_weight`
 [`Optional[str]`, `optional`] nvnmd weight file

`united_model`
 [`bool`] when in multi-task mode, freeze all nodes into one unit model

`**kwargs`
 other arguments

`deepmd.entrypoints.make_model_devi(*, models: list, system: str, set_prefix: str, output: str, frequency: int, real_error: bool = False, **kwargs)`

Make model deviation calculation.

Parameters

`models`
 [`list`] A list of paths of models to use for making model deviation

`system`
 [`str`] The path of system to make model deviation calculation

`set_prefix`
 [`str`] The set prefix of the system

`output`
 [`str`] The output file for model deviation results

`frequency`
 [`int`] The number of steps that elapse between writing coordinates in a trajectory by

a MD engine (such as Gromacs / Lammmps). This paramter is used to determine the index in the output file.

`real_error`
`[bool, default: False]` If True, calculate the RMS real error instead of model deviation.

`**kwargs`
 Arbitrary keyword arguments.

`deepmd.entrypoints.neighbor_stat(*, system: str, rcut: float, type_map: List[str], one_type: bool = False, **kwargs)`

Calculate neighbor statistics.

Parameters

`system`
`[str]` system to stat

`rcut`
`[float]` cutoff radius

`type_map`
`[list[str]]` type map

`one_type`
`[bool, optional, default=False]` treat all types as a single type

`**kwargs`
 additional arguments

Examples

```
>>> neighbor_stat(system='.', rcut=6., type_map=["C", "H", "O", "N", "P", "S", "Mg", "Na", "HW",
↪ "O", "OW", "mNa", "mCl", "mC", "mH", "mMg", "mN", "mO", "mP"])
min_nbor_dist: 0.6599510670195264
max_nbor_size: [23, 26, 19, 16, 2, 2, 1, 1, 72, 37, 5, 0, 31, 29, 1, 21, 20, 5]
```

`deepmd.entrypoints.test(*, model: str, system: str, datafile: str, set_prefix: str, numb_test: int, rand_seed: Optional[int], shuffle_test: bool, detail_file: str, atomic: bool, **kwargs)`

Test model predictions.

Parameters

`model`
`[str]` path where model is stored

`system`
`[str]` system directory

`datafile`
`[str]` the path to the list of systems to test

`set_prefix`
`[str]` string prefix of set

`numb_test`
`[int]` munber of tests to do. 0 means all data.

```
    rand_seed
        [Optional[int]] seed for random generator

    shuffle_test
        [bool] whether to shuffle tests

    detail_file
        [Optional[str]] file where test details will be output

    atomic
        [bool] whether per atom quantities should be computed

    **kwargs
        additional arguments

    Raises
        RuntimeError
            if no valid system was found

deepmd.entrypoints.train_dp(*, INPUT: str, init_model: Optional[str], restart: Optional[str], output:
    str, init_frz_model: str, mpi_log: str, log_level: int, log_path:
    Optional[str], is_compress: bool = False, skip_neighbor_stat: bool =
    False, finetune: Optional[str] = None, **kwargs)
```

Run DeePMD model training.

Parameters

```
    INPUT
        [str] json/yaml control file

    init_model
        [Optional[str]] path to checkpoint folder or None

    restart
        [Optional[str]] path to checkpoint folder or None

    output
        [str] path for dump file with arguments

    init_frz_model
        [str] path to frozen model or None

    mpi_log
        [str] mpi logging mode

    log_level
        [int] logging level defined by int 0-3

    log_path
        [Optional[str]] logging file path or None if logs are to be output only to stdout

    is_compress
        [bool] indicates whether in the model compress mode

    skip_neighbor_stat
        [bool, default=False] skip checking neighbor statistics

    finetune
        [Optional[str]] path to pretrained model or None

    **kwargs
        additional arguments
```

Raises

`RuntimeError`

if distributed training job name is wrong

```
deepmd.entrypoints.transfer(*, old_model: str, raw_model: str, output: str, **kwargs)
```

Transfer operation from old from graph to new prepared raw graph.

Parameters

`old_model`

[`str`] frozen old graph model

`raw_model`

[`str`] new model that will accept ops from old model

`output`

[`str`] new model with transfered parameters will be saved to this location

`**kwargs`

additional arguments

Submodules

`deepmd.entrypoints.compress` module

Compress a model, which including tabulating the embedding-net.

```
deepmd.entrypoints.compress.compress(*, input: str, output: str, extrapolate: int, step: float,
                                     frequency: str, checkpoint_folder: str, training_script: str,
                                     mpi_log: str, log_path: Optional[str], log_level: int, **kwargs)
```

Compress model.

The table is composed of fifth-order polynomial coefficients and is assembled from two sub-tables. The first table takes the step parameter as the domain's uniform step size, while the second table takes 10 * step as it's uniform step size. The range of the first table is automatically detected by the code, while the second table ranges from the first table's upper boundary(upper) to the extrapolate(parameter) * upper.

Parameters

`input`

[`str`] frozen model file to compress

`output`

[`str`] compressed model filename

`extrapolate`

[`int`] scale of model extrapolation

`step`

[`float`] uniform step size of the tabulation's first table

`frequency`

[`str`] frequency of tabulation overflow check

`checkpoint_folder`

[`str`] training checkpoint folder for freezing

`training_script`

[`str`] training script of the input frozen model

`mpi_log`
 [`str`] mpi logging mode for training

`log_path`
 [`Optional[str]`] if speccified log will be written to this file

`log_level`
 [`int`] logging level

`**kwargs`
 additional arguments

deepmd.entrypoints.convert module

`deepmd.entrypoints.convert.convert(*, FROM: str, input_model: str, output_model: str, **kwargs)`

deepmd.entrypoints.doc module

Module that prints train input arguments docstrings.

`deepmd.entrypoints.doc.doc_train_input(*, out_type: str = 'rst', **kwargs)`
 Print out trining input arguments to console.

deepmd.entrypoints.freeze module

Script for freezing TF trained graph so it can be used with LAMMPS and i-PI.

References

<https://blog.metaflow.fr/tensorflow-how-to-freeze-a-model-and-serve-it-with-a-python-api-d4f3596b3adc>

`deepmd.entrypoints.freeze.freeze(*, checkpoint_folder: str, output: str, node_names: Optional[str] = None, nvnmd_weight: Optional[str] = None, united_model: bool = False, **kwargs)`

Freeze the graph in supplied folder.

Parameters

`checkpoint_folder`
 [`str`] location of the folder with model

`output`
 [`str`] output file name

`node_names`
 [`Optional[str]`, `optional`] names of nodes to output, by default None

`nvnmd_weight`
 [`Optional[str]`, `optional`] nvnmd weight file

`united_model`
 [`bool`] when in multi-task mode, freeze all nodes into one unit model


```

    **kwargs
    other arguments

```

deepmd.entrypoints.ipi module

Use dp_ipi inside the Python package.

```

deepmd.entrypoints.ipi.dp_ipi()
dp_ipi.

```

deepmd.entrypoints.main module

DeePMD-Kit entry point module.

```

deepmd.entrypoints.main.get_ll(log_level: str) → int

```

Convert string to python logging level.

Parameters

```

    log_level
    [str] allowed input values are: DEBUG, INFO, WARNING, ERROR, 3, 2, 1, 0

```

Returns

```

    int
    one of python logging module log levels - 10, 20, 30 or 40

```

```

deepmd.entrypoints.main.main(args: Optional[Union[List[str], Namespace]] = None)

```

DeePMD-Kit entry point.

Parameters

```

    args
    [List[str] or argparse.Namespace, optional] list of command line arguments,
    used to avoid calling from the subprocess, as it is quite slow to import tensorflow;
    if Namespace is given, it will be used directly

```

Raises

```

    RuntimeError
    if no command was input

```

```

deepmd.entrypoints.main.main_parser() → ArgumentParser

```

DeePMD-Kit commandline options argument parser.

Returns

```

    argparse.ArgumentParser
    main parser of DeePMD-kit

```

```

deepmd.entrypoints.main.parse_args(args: Optional[List[str]] = None) → Namespace

```

Parse arguments and convert argument strings to objects.

Parameters

```

    args
    [List[str]] list of command line arguments, main purpose is testing default option
    None takes arguments from sys.argv

```

Returns

```
argparse.Namespace
the populated namespace
```

deepmd.entrypoints.neighbor_stat module

```
deepmd.entrypoints.neighbor_stat.neighbor_stat(*, system: str, rcut: float, type_map: List[str],
                                                one_type: bool = False, **kwargs)
```

Calculate neighbor statistics.

Parameters

```
system
    [str] system to stat
rcut
    [float] cutoff radius
type_map
    [list[str]] type map
one_type
    [bool, optional, default=False] treat all types as a single type
**kwargs
    additional arguments
```

Examples

```
>>> neighbor_stat(system='.', rcut=6., type_map=["C", "H", "O", "N", "P", "S", "Mg", "Na", "HW
↪", "OW", "mNa", "mCl", "mC", "mH", "mMg", "mN", "mO", "mP"])
min_nbor_dist: 0.6599510670195264
max_nbor_size: [23, 26, 19, 16, 2, 2, 1, 1, 72, 37, 5, 0, 31, 29, 1, 21, 20, 5]
```

deepmd.entrypoints.test module

Test trained DeePMD model.

```
deepmd.entrypoints.test.test(*, model: str, system: str, datafile: str, set_prefix: str, numb_test: int,
                             rand_seed: Optional[int], shuffle_test: bool, detail_file: str, atomic: bool,
                             **kwargs)
```

Test model predictions.

Parameters

```
model
    [str] path where model is stored
system
    [str] system directory
datafile
    [str] the path to the list of systems to test
set_prefix
    [str] string prefix of set
```

`numb_test`
 [`int`] number of tests to do. 0 means all data.
`rand_seed`
 [`Optional[int]`] seed for random generator
`shuffle_test`
 [`bool`] whether to shuffle tests
`detail_file`
 [`Optional[str]`] file where test details will be output
`atomic`
 [`bool`] whether per atom quantities should be computed
`**kwargs`
 additional arguments
 Raises
 `RuntimeError`
 if no valid system was found

deepmd.entrypoints.train module

DeePMD training entrypoint script.

Can handle local or distributed training.

```
deepmd.entrypoints.train.train(*, INPUT: str, init_model: Optional[str], restart: Optional[str], output:
                               str, init_frz_model: str, mpi_log: str, log_level: int, log_path:
                               Optional[str], is_compress: bool = False, skip_neighbor_stat: bool =
                               False, finetune: Optional[str] = None, **kwargs)
```

Run DeePMD model training.

Parameters

`INPUT`
 [`str`] json/yaml control file
`init_model`
 [`Optional[str]`] path to checkpoint folder or None
`restart`
 [`Optional[str]`] path to checkpoint folder or None
`output`
 [`str`] path for dump file with arguments
`init_frz_model`
 [`str`] path to frozen model or None
`mpi_log`
 [`str`] mpi logging mode
`log_level`
 [`int`] logging level defined by int 0-3
`log_path`
 [`Optional[str]`] logging file path or None if logs are to be output only to stdout

`is_compress`
 [`bool`] indicates whether in the model compress mode

`skip_neighbor_stat`
 [`bool`, default=False] skip checking neighbor statistics

`finetune`
 [`Optional[str]`] path to pretrained model or None

`**kwargs`
 additional arguments

Raises

`RuntimeError`
 if distributed training job name is wrong

deepmd.entrypoints.transfer module

Module used for transferring parameters between models.

`deepmd.entrypoints.transfer.transfer(*, old_model: str, raw_model: str, output: str, **kwargs)`

Transfer operation from old from graph to new prepared raw graph.

Parameters

`old_model`
 [`str`] frozen old graph model

`raw_model`
 [`str`] new model that will accept ops from old model

`output`
 [`str`] new model with transfered parameters will be saved to this location

`**kwargs`
 additional arguments

deepmd.fit package

`class deepmd.fit.DOSFitting(*args, **kwargs)`

Bases: *Fitting*

Fitting the density of states (DOS) of the system. The energy should be shifted by the fermi level.

Parameters

`descript`
 The descriptor \mathcal{D}

`neuron`
 Number of neurons N in each hidden layer of the fitting net

`resnet_dt`
 Time-step dt in the resnet construction: $y = x + dt * \phi(Wx + b)$

`numb_fparam`
 Number of frame parameter

`numb_aparam`
 Number of atomic parameter

! numb_dos (added)
 Number of gridpoints on which the DOS is evaluated (NEDOS in VASP)

rcond
 The condition number for the regression of atomic energy.

trainable
 If the weights of fitting net are trainable. Suppose that we have N_l hidden layers in the fitting net, this list is of length $N_l + 1$, specifying if the hidden layers and the output layer are trainable.

seed
 Random seed for initializing the network parameters.

activation_function
 The activation function ϕ in the embedding net. Supported options are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”, “gelu_tf”, “None”, “none”.

precision
 The precision of the embedding net parameters. Supported options are “default”, “float16”, “float32”, “float64”, “bfloat16”.

uniform_seed
 Only for the purpose of backward compatibility, retrieves the old behavior of using the random seed

layer_name
`[list[Optional[str]], optional]` The name of the each layer. If two layers, either in the same fitting or different fittings, have the same name, they will share the same neural network parameters.

use_aparam_as_mask: bool, optional
 If True, the atomic parameters will be used as a mask that determines the atom is real/virtual. And the aparam will not be used as the atomic parameters for embedding.

Attributes

precision
 Precision of fitting network.

Methods

| | |
|--|---|
| <code>build(inputs, natoms[, input_dict, reuse, ...])</code> | Build the computational graph for fitting net. |
| <code>compute_input_stats(all_stat[, protection])</code> | Compute the input statistics. |
| <code>compute_output_stats(all_stat[, mixed_type])</code> | Compute the output statistics. |
| <code>enable_mixed_precision([mixed_prec])</code> | Reveive the mixed precision setting. |
| <code>get_loss(loss, lr)</code> | Get the loss function. |
| <code>get_numb_aparam()</code> | Get the number of atomic parameters. |
| <code>get_numb_dos()</code> | Get the number of gridpoints in energy space. |
| <code>get_numb_fparam()</code> | Get the number of frame parameters. |
| <code>init_variables(graph, graph_def[, suffix])</code> | Init the fitting net variables with the given dict. |
| <code>register(key)</code> | Register a Fitting plugin. |

build(inputs: Tensor, natoms: Tensor, input_dict: `Optional[dict] = None`, reuse: `Optional[bool] = None`, suffix: `str = ''`) \rightarrow Tensor
 Build the computational graph for fitting net.

Parameters

inputs

The input descriptor

input_dict

Additional dict for inputs. if `numb_fparam > 0`, should have `input_dict['fparam']`
if `numb_aparam > 0`, should have `input_dict['aparam']`

natoms

The number of atoms. This tensor has the length of `Ntypes + 2` `natoms[0]`: number of local atoms `natoms[1]`: total number of atoms held by this processor `natoms[i]`: $2 \leq i < Ntypes+2$, number of type `i` atoms

reuse

The weights in the networks should be reused when get the variable.

suffix

Name suffix to identify this descriptor

Returns

ener

The system energy

compute_input_stats(all_stat: dict, protection: float = 0.01) → None

Compute the input statistics.

Parameters

all_stat

if `numb_fparam > 0` must have `all_stat['fparam']` if `numb_aparam > 0` must have `all_stat['aparam']` can be prepared by `model.make_stat_input`

protection

Divided-by-zero protection

compute_output_stats(all_stat: dict, mixed_type: bool = False) → None

Compute the output statistics.

Parameters

all_stat

must have the following components: `all_stat['dos']` of shape `n_sys x n_batch x n_frame x numb_dos` can be prepared by `model.make_stat_input`

mixed_type

Whether to perform the mixed_type mode. If True, the input data has the mixed_type format (see doc/model/train_se_atten.md), in which frames in a system may have different `natoms_vec(s)`, with the same `nloc`.

enable_mixed_precision(mixed_prec: Optional[dict] = None) → None

Reveive the mixed precision setting.

Parameters

mixed_prec

The mixed precision setting used in the embedding net

get_loss(loss: dict, lr) → Loss

Get the loss function.

Parameters

`loss`
 [dict] the loss dict

`lr`
 [LearningRateExp] the learning rate

Returns

`Loss`
 the loss function

`get_numb_aparam() → int`
 Get the number of atomic parameters.

`get_numb_dos() → int`
 Get the number of gridpoints in energy space.

`get_numb_fparam() → int`
 Get the number of frame parameters.

`init_variables(graph: Graph, graph_def: GraphDef, suffix: str = '') → None`
 Init the fitting net variables with the given dict.

Parameters

`graph`
 [tf.Graph] The input frozen model graph

`graph_def`
 [tf.GraphDef] The input frozen model graph_def

`suffix`
 [str] suffix to name scope

`class deepmd.fit.DipoleFittingSeA(*args, **kwargs)`
 Bases: *Fitting*

Fit the atomic dipole with descriptor se_a.

Parameters

`descript`
 [tf.Tensor] The descriptor

`neuron`
 [List[int]] Number of neurons in each hidden layer of the fitting net

`resnet_dt`
 [bool] Time-step dt in the resnet construction: $y = x + dt * \phi(Wx + b)$

`sel_type`
 [List[int]] The atom types selected to have an atomic dipole prediction. If is None, all atoms are selected.

`seed`
 [int] Random seed for initializing the network parameters.

`activation_function`
 [str] The activation function in the embedding net. Supported options are "relu", "relu6", "softplus", "sigmoid", "tanh", "gelu", "gelu_tf", "None", "none".

precision

[[str](#)] The precision of the embedding net parameters. Supported options are “default”, “float16”, “float32”, “float64”, “bfloat16”.

uniform_seed

Only for the purpose of backward compatibility, retrieves the old behavior of using the random seed

Attributes

precision

Precision of fitting network.

Methods

| | |
|--|---|
| <i>build</i> (input_d, rot_mat, natoms[, ...]) | Build the computational graph for fitting net. |
| <i>enable_mixed_precision</i> ([mixed_prec]) | Reveive the mixed precision setting. |
| <i>get_loss</i> (loss, lr) | Get the loss function. |
| <i>get_out_size</i> () | Get the output size. |
| <i>get_sel_type</i> () | Get selected type. |
| <i>init_variables</i> (graph, graph_def[, suffix]) | Init the fitting net variables with the given dict. |
| <i>register</i> (key) | Register a Fitting plugin. |

build(input_d: Tensor, rot_mat: Tensor, natoms: Tensor, input_dict: [Optional\[dict\]](#) = None, reuse: [Optional\[bool\]](#) = None, suffix: [str](#) = '') → Tensor

Build the computational graph for fitting net.

Parameters

input_d

The input descriptor

rot_mat

The rotation matrix from the descriptor.

natoms

The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 ≤ i < Ntypes+2, number of type i atoms

input_dict

Additional dict for inputs.

reuse

The weights in the networks should be reused when get the variable.

suffix

Name suffix to identify this descriptor

Returns

[*dipole*](#)

The atomic dipole.

enable_mixed_precision(mixed_prec: [Optional\[dict\]](#) = None) → None

Reveive the mixed precision setting.

Parameters

`mixed_prec`
The mixed precision setting used in the embedding net

`get_loss(loss: dict, lr) → Loss`
Get the loss function.

Parameters

- `loss`
[dict] the loss dict
- `lr`
[LearningRateExp] the learning rate

Returns

- Loss**
the loss function

`get_out_size() → int`
Get the output size. Should be 3.

`get_sel_type() → int`
Get selected type.

`init_variables(graph: Graph, graph_def: GraphDef, suffix: str = '') → None`
Init the fitting net variables with the given dict.

Parameters

- `graph`
[tf.Graph] The input frozen model graph
- `graph_def`
[tf.GraphDef] The input frozen model graph_def
- `suffix`
[str] suffix to name scope

class deepmd.fit.EnerFitting(*args, **kwargs)

Bases: *Fitting*

Fitting the energy of the system. The force and the virial can also be trained.

The potential energy E is a fitting network function of the descriptor \mathcal{D} :

$$E(\mathcal{D}) = \mathcal{L}^{(n)} \circ \mathcal{L}^{(n-1)} \circ \dots \circ \mathcal{L}^{(1)} \circ \mathcal{L}^{(0)}$$

The first n hidden layers $\mathcal{L}^{(0)}, \dots, \mathcal{L}^{(n-1)}$ are given by

$$y = \mathcal{L}(x; w, b) = \phi(x^T w + b)$$

where $x \in \mathbb{R}^{N_1}$ is the input vector and $y \in \mathbb{R}^{N_2}$ is the output vector. $w \in \mathbb{R}^{N_1 \times N_2}$ and $b \in \mathbb{R}^{N_2}$ are weights and biases, respectively, both of which are trainable if `trainable[i]` is True. ϕ is the activation function.

The output layer $\mathcal{L}^{(n)}$ is given by

$$y = \mathcal{L}^{(n)}(x; w, b) = x^T w + b$$

where $x \in \mathbb{R}^{N_{n-1}}$ is the input vector and $y \in \mathbb{R}$ is the output scalar. $w \in \mathbb{R}^{N_{n-1}}$ and $b \in \mathbb{R}$ are weights and bias, respectively, both of which are trainable if `trainable[n]` is True.

Parameters

- descript**
The descriptor \mathcal{D}
- neuron**
Number of neurons N in each hidden layer of the fitting net
- resnet_dt**
Time-step dt in the resnet construction: $y = x + dt * \phi(Wx + b)$
- numb_fparam**
Number of frame parameter
- numb_aparam**
Number of atomic parameter
- rcond**
The condition number for the regression of atomic energy.
- tot_ener_zero**
Force the total energy to zero. Useful for the charge fitting.
- trainable**
If the weights of fitting net are trainable. Suppose that we have N_l hidden layers in the fitting net, this list is of length $N_l + 1$, specifying if the hidden layers and the output layer are trainable.
- seed**
Random seed for initializing the network parameters.
- atom_ener**
Specifying atomic energy contribution in vacuum. The `set_davg_zero` key in the descriptor should be set.
- activation_function**
The activation function ϕ in the embedding net. Supported options are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”, “gelu_tf”, “None”, “none”.
- precision**
The precision of the embedding net parameters. Supported options are “default”, “float16”, “float32”, “float64”, “bfloat16”.
- uniform_seed**
Only for the purpose of backward compatibility, retrieves the old behavior of using the random seed
- layer_name**
[`list[Optional[str]]`, `optional`] The name of the each layer. If two layers, either in the same fitting or different fittings, have the same name, they will share the same neural network parameters.
- use_aparam_as_mask**: bool, optional
If True, the atomic parameters will be used as a mask that determines the atom is real/virtual. And the aparam will not be used as the atomic parameters for embedding.

Attributes

- precision**
Precision of fitting network.

Methods

| | |
|---|--|
| <i>build</i> (inputs, natoms[, input_dict, reuse, ...]) | Build the computational graph for fitting net. |
| <i>change_energy_bias</i> (data, frozen_model, ...) | Change the energy bias according to the input data and the pretrained model. |
| <i>compute_input_stats</i> (all_stat[, protection]) | Compute the input statistics. |
| <i>compute_output_stats</i> (all_stat[, mixed_type]) | Compute the output statistics. |
| <i>enable_mixed_precision</i> ([mixed_prec]) | Reveive the mixed precision setting. |
| <i>get_loss</i> (loss, lr) | Get the loss function. |
| <i>get_numb_aparam</i> () | Get the number of atomic parameters. |
| <i>get_numb_fparam</i> () | Get the number of frame parameters. |
| <i>init_variables</i> (graph, graph_def[, suffix]) | Init the fitting net variables with the given dict. |
| <i>register</i> (key) | Register a Fitting plugin. |

build(inputs: Tensor, natoms: Tensor, input_dict: [Optional\[dict\]](#) = None, reuse: [Optional\[bool\]](#) = None, suffix: [str](#) = '') → Tensor

Build the computational graph for fitting net.

Parameters

inputs

The input descriptor

input_dict

Additional dict for inputs. if num_b_fparam > 0, should have input_dict['fparam']
if num_b_aparam > 0, should have input_dict['aparam']

natoms

The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 ≤ i < Ntypes+2, number of type i atoms

reuse

The weights in the networks should be reused when get the variable.

suffix

Name suffix to identify this descriptor

Returns

ener

The system energy

change_energy_bias(data, frozen_model, origin_type_map, full_type_map, bias_shift='delta', ntest=10) → [None](#)

Change the energy bias according to the input data and the pretrained model.

Parameters

data

[[DeepmdDataSystem](#)] The training data.

frozen_model

[[str](#)] The path file of frozen model.

origin_type_map

[[list](#)] The original type_map in dataset, they are targets to change the energy bias.

`full_type_map`
[`str`] The full type_map in pretrained model

`bias_shift`
[`str`] The mode for changing energy bias : ['delta', 'statistic'] 'delta' : perform predictions on energies of target dataset,
and do least square on the errors to obtain the target shift as bias.
'statistic' : directly use the statistic energy bias in the target dataset.

`n_test`
[`int`] The number of test samples in a system to change the energy bias.

`compute_input_stats`(all_stat: `dict`, protection: `float` = 0.01) → `None`

Compute the input statistics.

Parameters

`all_stat`
if `numb_fparam` > 0 must have `all_stat['fparam']` if `numb_aparam` > 0 must have `all_stat['aparam']` can be prepared by `model.make_stat_input`

`protection`
Divided-by-zero protection

`compute_output_stats`(all_stat: `dict`, mixed_type: `bool` = False) → `None`

Compute the output statistics.

Parameters

`all_stat`
must have the following components: `all_stat['energy']` of shape `n_sys x n_batch x n_frame` can be prepared by `model.make_stat_input`

`mixed_type`
Whether to perform the mixed_type mode. If True, the input data has the mixed_type format (see `doc/model/train_se_atten.md`), in which frames in a system may have different `natoms_vec(s)`, with the same `nloc`.

`enable_mixed_precision`(mixed_prec: `Optional[dict]` = None) → `None`

Reveive the mixed precision setting.

Parameters

`mixed_prec`
The mixed precision setting used in the embedding net

`get_loss`(loss: `dict`, lr) → `Loss`

Get the loss function.

Parameters

`loss`
[`dict`] The loss function parameters.

`lr`
[`LearningRateExp`] The learning rate.

Returns

`Loss`
The loss function.

`get_numb_aparam()` → `int`

Get the number of atomic parameters.

`get_numb_fparam()` → `int`

Get the number of frame parameters.

`init_variables(graph: Graph, graph_def: GraphDef, suffix: str = '')` → `None`

Init the fitting net variables with the given dict.

Parameters

`graph`

[`tf.Graph`] The input frozen model graph

`graph_def`

[`tf.GraphDef`] The input frozen model graph_def

`suffix`

[`str`] suffix to name scope

`class deepmd.fit.Fitting(*args, **kwargs)`

Bases: *PluginVariant*

Attributes

precision

Precision of fitting network.

Methods

| | |
|--|---|
| <i>get_loss</i> (loss, lr) | Get the loss function. |
| <i>init_variables</i> (graph, graph_def[, suffix]) | Init the fitting net variables with the given dict. |
| <i>register</i> (key) | Register a Fitting plugin. |

abstract `get_loss(loss: dict, lr)` → `Loss`

Get the loss function.

Parameters

`loss`

[`dict`] the loss dict

`lr`

[`LearningRateExp`] the learning rate

Returns

Loss

the loss function

`init_variables(graph: Graph, graph_def: GraphDef, suffix: str = '')` → `None`

Init the fitting net variables with the given dict.

Parameters

`graph`

[`tf.Graph`] The input frozen model graph

`graph_def`

[`tf.GraphDef`] The input frozen model graph_def

suffix
 [str] suffix to name scope

Notes

This method is called by others when the fitting supported initialization from the given variables.

property precision: DType

Precision of fitting network.

static register(key: str) → Callable

Register a Fitting plugin.

Parameters

key
 [str] the key of a Fitting

Returns

Fitting
 the registered Fitting

Examples

```
>>> @Fitting.register("some_fitting")
class SomeFitting(Fitting):
    pass
```

```
class deepmd.fit.GlobalPolarFittingSeA(descrpt: Tensor, neuron: List[int] = [120, 120, 120],
                                       resnet_dt: bool = True, sel_type: Optional[List[int]] = None,
                                       fit_diag: bool = True, scale: Optional[List[float]] = None,
                                       diag_shift: Optional[List[float]] = None, seed: Optional[int]
                                       = None, activation_function: str = 'tanh', precision: str =
                                       'default')
```

Bases: `object`

Fit the system polarizability with descriptor se_a.

Parameters

descrpt
 [tf.Tensor] The descriptor

neuron
 [List[int]] Number of neurons in each hidden layer of the fitting net

resnet_dt
 [bool] Time-step dt in the resnet construction: $y = x + dt * \phi(Wx + b)$

sel_type
 [List[int]] The atom types selected to have an atomic polarizability prediction

fit_diag
 [bool] Fit the diagonal part of the rotational invariant polarizability matrix, which will be converted to normal polarizability matrix by contracting with the rotation matrix.

scale
 [List[float]] The output of the fitting net (polarizability matrix) for type i atom will be scaled by scale[i]

diag_shift
 [List[float]] The diagonal part of the polarizability matrix of type i will be shifted by diag_shift[i]. The shift operation is carried out after scale.

seed
 [int] Random seed for initializing the network parameters.

activation_function
 [str] The activation function in the embedding net. Supported options are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”, “gelu_tf”, “None”, “none”.

precision
 [str] The precision of the embedding net parameters. Supported options are “default”, “float16”, “float32”, “float64”, “bfloat16”.

Methods

| | |
|--|---|
| <i>build</i> (input_d, rot_mat, natoms[, ...]) | Build the computational graph for fitting net. |
| <i>enable_mixed_precision</i> ([mixed_prec]) | Reveive the mixed precision setting. |
| <i>get_loss</i> (loss, lr) | Get the loss function. |
| <i>get_out_size</i> () | Get the output size. |
| <i>get_sel_type</i> () | Get selected atom types. |
| <i>init_variables</i> (graph, graph_def[, suffix]) | Init the fitting net variables with the given dict. |

build(input_d, rot_mat, natoms, input_dict: Optional[dict] = None, reuse=None, suffix='') → Tensor

Build the computational graph for fitting net.

Parameters

input_d
 The input descriptor

rot_mat
 The rotation matrix from the descriptor.

natoms
 The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 ≤ i < Ntypes+2, number of type i atoms

input_dict
 Additional dict for inputs.

reuse
 The weights in the networks should be reused when get the variable.

suffix
 Name suffix to identify this descriptor

Returns

polar
 The system polarizability

`enable_mixed_precision(mixed_prec: Optional[dict] = None) → None`

Reveive the mixed precision setting.

Parameters

`mixed_prec`

The mixed precision setting used in the embedding net

`get_loss(loss: dict, lr) → Loss`

Get the loss function.

Parameters

`loss`

[dict] the loss dict

`lr`

[LearningRateExp] the learning rate

Returns

Loss

the loss function

`get_out_size() → int`

Get the output size. Should be 9.

`get_sel_type() → int`

Get selected atom types.

`init_variables(graph: Graph, graph_def: GraphDef, suffix: str = "") → None`

Init the fitting net variables with the given dict.

Parameters

`graph`

[tf.Graph] The input frozen model graph

`graph_def`

[tf.GraphDef] The input frozen model graph_def

`suffix`

[str] suffix to name scope

`class deepmd.fit.PolarFittingSeA(*args, **kwargs)`

Bases: *Fitting*

Fit the atomic polarizability with descriptor se_a.

Parameters

`descript`

[tf.Tensor] The descriptior

`neuron`

[List[int]] Number of neurons in each hidden layer of the fitting net

`resnet_dt`

[bool] Time-step dt in the resnet construction: $y = x + dt * \phi(Wx + b)$

`sel_type`

[List[int]] The atom types selected to have an atomic polarizability prediction. If is None, all atoms are selected.

fit_diag
`[bool]` Fit the diagonal part of the rotational invariant polarizability matrix, which will be converted to normal polarizability matrix by contracting with the rotation matrix.

scale
`[List[float]]` The output of the fitting net (polarizability matrix) for type *i* atom will be scaled by `scale[i]`

diag_shift
`[List[float]]` The diagonal part of the polarizability matrix of type *i* will be shifted by `diag_shift[i]`. The shift operation is carried out after scale.

seed
`[int]` Random seed for initializing the network parameters.

activation_function
`[str]` The activation function in the embedding net. Supported options are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”, “gelu_tf”, “None”, “none”.

precision
`[str]` The precision of the embedding net parameters. Supported options are “default”, “float16”, “float32”, “float64”, “bfloat16”.

uniform_seed
 Only for the purpose of backward compatibility, retrieves the old behavior of using the random seed

Attributes

precision
 Precision of fitting network.

Methods

| | |
|--|---|
| <code>build(input_d, rot_mat, natoms[, ...])</code> | Build the computational graph for fitting net. |
| <code>compute_input_stats(all_stat[, protection])</code> | Compute the input statistics. |
| <code>enable_mixed_precision([mixed_prec])</code> | Reveive the mixed precision setting. |
| <code>get_loss(loss, lr)</code> | Get the loss function. |
| <code>get_out_size()</code> | Get the output size. |
| <code>get_sel_type()</code> | Get selected atom types. |
| <code>init_variables(graph, graph_def[, suffix])</code> | Init the fitting net variables with the given dict. |
| <code>register(key)</code> | Register a Fitting plugin. |

build(input_d: Tensor, rot_mat: Tensor, natoms: Tensor, input_dict: `Optional[dict]` = None, reuse: `Optional[bool]` = None, suffix: `str` = “”)

Build the computational graph for fitting net.

Parameters

input_d
 The input descriptor

rot_mat
 The rotation matrix from the descriptor.

natoms
 The number of atoms. This tensor has the length of Ntypes + 2 `natoms[0]`: number

of local atoms natoms[1]: total number of atoms held by this processor natoms[i]:
2 <= i < Ntypes+2, number of type i atoms

input_dict

Additional dict for inputs.

reuse

The weights in the networks should be reused when get the variable.

suffix

Name suffix to identify this descriptor

Returns

atomic_polar

The atomic polarizability

compute_input_stats(all_stat, protection=0.01)

Compute the input statistics.

Parameters

all_stat

Dictionary of inputs. can be prepared by model.make_stat_input

protection

Divided-by-zero protection

enable_mixed_precision(mixed_prec: [Optional\[dict\]](#) = None) → [None](#)

Reveive the mixed precision setting.

Parameters

mixed_prec

The mixed precision setting used in the embedding net

get_loss(loss: [dict](#), lr) → [Loss](#)

Get the loss function.

get_out_size() → [int](#)

Get the output size. Should be 9.

get_sel_type() → [List\[int\]](#)

Get selected atom types.

init_variables(graph: Graph, graph_def: GraphDef, suffix: [str](#) = "") → [None](#)

Init the fitting net variables with the given dict.

Parameters

graph

[\[tf.Graph\]](#) The input frozen model graph

graph_def

[\[tf.GraphDef\]](#) The input frozen model graph_def

suffix

[\[str\]](#) suffix to name scope

Submodules

deepmd.fit.dipole module

`class deepmd.fit.dipole.DipoleFittingSeA(*args, **kwargs)`

Bases: *Fitting*

Fit the atomic dipole with descriptor se_a.

Parameters

descript

[`tf.Tensor`] The descriptor

neuron

[`List[int]`] Number of neurons in each hidden layer of the fitting net

resnet_dt

[`bool`] Time-step dt in the resnet construction: $y = x + dt * \phi(Wx + b)$

sel_type

[`List[int]`] The atom types selected to have an atomic dipole prediction. If is None, all atoms are selected.

seed

[`int`] Random seed for initializing the network parameters.

activation_function

[`str`] The activation function in the embedding net. Supported options are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”, “gelu_tf”, “None”, “none”.

precision

[`str`] The precision of the embedding net parameters. Supported options are “default”, “float16”, “float32”, “float64”, “bfloat16”.

uniform_seed

Only for the purpose of backward compatibility, retrieves the old behavior of using the random seed

Attributes

precision

Precision of fitting network.

Methods

| | |
|---|---|
| <code>build(input_d, rot_mat, natoms[, ...])</code> | Build the computational graph for fitting net. |
| <code>enable_mixed_precision([mixed_prec])</code> | Reveive the mixed precision setting. |
| <code>get_loss(loss, lr)</code> | Get the loss function. |
| <code>get_out_size()</code> | Get the output size. |
| <code>get_sel_type()</code> | Get selected type. |
| <code>init_variables(graph, graph_def[, suffix])</code> | Init the fitting net variables with the given dict. |
| <code>register(key)</code> | Register a Fitting plugin. |

build(input_d: `Tensor`, rot_mat: `Tensor`, natoms: `Tensor`, input_dict: `Optional[dict]` = None, reuse: `Optional[bool]` = None, suffix: `str` = '') → `Tensor`

Build the computational graph for fitting net.

Parameters

input_d

The input descriptor

rot_mat

The rotation matrix from the descriptor.

natoms

The number of atoms. This tensor has the length of `Ntypes + 2` `natoms[0]`: number of local atoms `natoms[1]`: total number of atoms held by this processor `natoms[i]`: $2 \leq i < Ntypes+2$, number of type `i` atoms

input_dict

Additional dict for inputs.

reuse

The weights in the networks should be reused when get the variable.

suffix

Name suffix to identify this descriptor

Returns

dipole

The atomic dipole.

enable_mixed_precision(mixed_prec: `Optional[dict] = None`) → `None`

Reveive the mixed precision setting.

Parameters

mixed_prec

The mixed precision setting used in the embedding net

get_loss(loss: `dict`, lr) → `Loss`

Get the loss function.

Parameters

loss`[dict]` the loss dict**lr**`[LearningRateExp]` the learning rate

Returns

Loss

the loss function

get_out_size() → `int`

Get the output size. Should be 3.

get_sel_type() → `int`

Get selected type.

init_variables(graph: `Graph`, graph_def: `GraphDef`, suffix: `str = ''`) → `None`

Init the fitting net variables with the given dict.

Parameters

graph`[tf.Graph]` The input frozen model graph

graph_def
 [tf.GraphDef] The input frozen model graph_def

suffix
 [str] suffix to name scope

deepmd.fit.dos module

class deepmd.fit.dos.DOSFitting(*args, **kwargs)

Bases: *Fitting*

Fitting the density of states (DOS) of the system. The energy should be shifted by the fermi level.

Parameters

descript
 The descriptor \mathcal{D}

neuron
 Number of neurons N in each hidden layer of the fitting net

resnet_dt
 Time-step dt in the resnet construction: $y = x + dt * \phi(Wx + b)$

numb_fparam
 Number of frame parameter

numb_aparam
 Number of atomic parameter

! numb_dos (added)
 Number of gridpoints on which the DOS is evaluated (NEDOS in VASP)

rcond
 The condition number for the regression of atomic energy.

trainable
 If the weights of fitting net are trainable. Suppose that we have N_l hidden layers in the fitting net, this list is of length $N_l + 1$, specifying if the hidden layers and the output layer are trainable.

seed
 Random seed for initializing the network parameters.

activation_function
 The activation function ϕ in the embedding net. Supported options are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”, “gelu_tf”, “None”, “none”.

precision
 The precision of the embedding net parameters. Supported options are “default”, “float16”, “float32”, “float64”, “bfloat16”.

uniform_seed
 Only for the purpose of backward compatibility, retrieves the old behavior of using the random seed

layer_name
 [list[Optional[str]], optional] The name of the each layer. If two layers, either in the same fitting or different fittings, have the same name, they will share the same neural network parameters.

`use_aparam_as_mask`: bool, optional
 If True, the atomic parameters will be used as a mask that determines the atom is real/virtual. And the aparam will not be used as the atomic parameters for embedding.

Attributes

precision
 Precision of fitting network.

Methods

| | |
|--|---|
| <code>build(inputs, natoms[, input_dict, reuse, ...])</code> | Build the computational graph for fitting net. |
| <code>compute_input_stats(all_stat[, protection])</code> | Compute the input statistics. |
| <code>compute_output_stats(all_stat[, mixed_type])</code> | Compute the output statistics. |
| <code>enable_mixed_precision([mixed_prec])</code> | Reveive the mixed precision setting. |
| <code>get_loss(loss, lr)</code> | Get the loss function. |
| <code>get_numb_aparam()</code> | Get the number of atomic parameters. |
| <code>get_numb_dos()</code> | Get the number of gridpoints in energy space. |
| <code>get_numb_fparam()</code> | Get the number of frame parameters. |
| <code>init_variables(graph, graph_def[, suffix])</code> | Init the fitting net variables with the given dict. |
| <code>register(key)</code> | Register a Fitting plugin. |

build(inputs: Tensor, natoms: Tensor, input_dict: Optional[dict] = None, reuse: Optional[bool] = None, suffix: str = '') → Tensor

Build the computational graph for fitting net.

Parameters

`inputs`
 The input descriptor

`input_dict`
 Additional dict for inputs. if `numb_fparam > 0`, should have `input_dict['fparam']`
 if `numb_aparam > 0`, should have `input_dict['aparam']`

`natoms`
 The number of atoms. This tensor has the length of `Ntypes + 2` `natoms[0]`: number of local atoms `natoms[1]`: total number of atoms held by this processor `natoms[i]`: $2 \leq i < Ntypes+2$, number of type `i` atoms

`reuse`
 The weights in the networks should be reused when get the variable.

`suffix`
 Name suffix to identify this descriptor

Returns

ener
 The system energy

compute_input_stats(all_stat: dict, protection: float = 0.01) → None

Compute the input statistics.

Parameters

`all_stat`
 if `numb_fparam > 0` must have `all_stat['fparam']` if `numb_aparam > 0` must have `all_stat['aparam']` can be prepared by `model.make_stat_input`

`protection`
 Divided-by-zero protection

`compute_output_stats`(`all_stat`: `dict`, `mixed_type`: `bool` = `False`) → `None`
 Compute the output statistics.

Parameters

`all_stat`
 must have the following components: `all_stat['dos']` of shape `n_sys x n_batch x n_frame x numb_dos` can be prepared by `model.make_stat_input`

`mixed_type`
 Whether to perform the `mixed_type` mode. If `True`, the input data has the `mixed_type` format (see `doc/model/train_se_atten.md`), in which frames in a system may have different `natoms_vec(s)`, with the same `nloc`.

`enable_mixed_precision`(`mixed_prec`: `Optional[dict]` = `None`) → `None`
 Receive the mixed precision setting.

Parameters

`mixed_prec`
 The mixed precision setting used in the embedding net

`get_loss`(`loss`: `dict`, `lr`) → `Loss`
 Get the loss function.

Parameters

`loss`
`[dict]` the loss dict

`lr`
`[LearningRateExp]` the learning rate

Returns

`Loss`
 the loss function

`get_numb_aparam`() → `int`
 Get the number of atomic parameters.

`get_numb_dos`() → `int`
 Get the number of gridpoints in energy space.

`get_numb_fparam`() → `int`
 Get the number of frame parameters.

`init_variables`(`graph`: `Graph`, `graph_def`: `GraphDef`, `suffix`: `str` = `''`) → `None`
 Init the fitting net variables with the given dict.

Parameters

`graph`
`[tf.Graph]` The input frozen model graph

```

graph_def
    [tf.GraphDef] The input frozen model graph_def
suffix
    [str] suffix to name scope

```

deepmd.fit.ener module

```
class deepmd.fit.ener.EnerFitting(*args, **kwargs)
```

Bases: *Fitting*

Fitting the energy of the system. The force and the virial can also be trained.

The potential energy E is a fitting network function of the descriptor \mathcal{D} :

$$E(\mathcal{D}) = \mathcal{L}^{(n)} \circ \mathcal{L}^{(n-1)} \circ \dots \circ \mathcal{L}^{(1)} \circ \mathcal{L}^{(0)}$$

The first n hidden layers $\mathcal{L}^{(0)}, \dots, \mathcal{L}^{(n-1)}$ are given by

$$y = \mathcal{L}(x; w, b) = \phi(x^T w + b)$$

where $x \in \mathbb{R}^{N_1}$ is the input vector and $y \in \mathbb{R}^{N_2}$ is the output vector. $w \in \mathbb{R}^{N_1 \times N_2}$ and $b \in \mathbb{R}^{N_2}$ are weights and biases, respectively, both of which are trainable if `trainable[i]` is True. ϕ is the activation function.

The output layer $\mathcal{L}^{(n)}$ is given by

$$y = \mathcal{L}^{(n)}(x; w, b) = x^T w + b$$

where $x \in \mathbb{R}^{N_{n-1}}$ is the input vector and $y \in \mathbb{R}$ is the output scalar. $w \in \mathbb{R}^{N_{n-1}}$ and $b \in \mathbb{R}$ are weights and bias, respectively, both of which are trainable if `trainable[n]` is True.

Parameters

descript

The descriptor \mathcal{D}

neuron

Number of neurons N in each hidden layer of the fitting net

resnet_dt

Time-step dt in the resnet construction: $y = x + dt * \phi(Wx + b)$

numb_fparam

Number of frame parameter

numb_aparam

Number of atomic parameter

rcond

The condition number for the regression of atomic energy.

tot_ener_zero

Force the total energy to zero. Useful for the charge fitting.

trainable

If the weights of fitting net are trainable. Suppose that we have N_l hidden layers in the fitting net, this list is of length $N_l + 1$, specifying if the hidden layers and the output layer are trainable.

- seed**
Random seed for initializing the network parameters.
- atom_ener**
Specifying atomic energy contribution in vacuum. The `set_davg_zero` key in the descriptor should be set.
- activation_function**
The activation function ϕ in the embedding net. Supported options are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”, “gelu_tf”, “None”, “none”.
- precision**
The precision of the embedding net parameters. Supported options are “default”, “float16”, “float32”, “float64”, “bfloat16”.
- uniform_seed**
Only for the purpose of backward compatibility, retrieves the old behavior of using the random seed
- layer_name**
[`list`[`Optional`[`str`]], `optional`] The name of the each layer. If two layers, either in the same fitting or different fittings, have the same name, they will share the same neural network parameters.
- use_aparam_as_mask**: `bool`, `optional`
If True, the atomic parameters will be used as a mask that determines the atom is real/virtual. And the aparam will not be used as the atomic parameters for embedding.

Attributes

- precision**
Precision of fitting network.

Methods

| | |
|---|--|
| <code>build</code> (inputs, natoms[, input_dict, reuse, ...]) | Build the computational graph for fitting net. |
| <code>change_energy_bias</code> (data, frozen_model, ...) | Change the energy bias according to the input data and the pretrained model. |
| <code>compute_input_stats</code> (all_stat[, protection]) | Compute the input statistics. |
| <code>compute_output_stats</code> (all_stat[, mixed_type]) | Compute the output statistics. |
| <code>enable_mixed_precision</code> ([mixed_prec]) | Reveive the mixed precision setting. |
| <code>get_loss</code> (loss, lr) | Get the loss function. |
| <code>get_numb_aparam</code> () | Get the number of atomic parameters. |
| <code>get_numb_fparam</code> () | Get the number of frame parameters. |
| <code>init_variables</code> (graph, graph_def[, suffix]) | Init the fitting net variables with the given dict. |
| <code>register</code> (key) | Register a Fitting plugin. |

build(inputs: Tensor, natoms: Tensor, input_dict: `Optional`[dict] = None, reuse: `Optional`[bool] = None, suffix: `str` = '') → Tensor

Build the computational graph for fitting net.

Parameters

- inputs**
The input descriptor

input_dict
Additional dict for inputs. if `numb_fparam > 0`, should have `input_dict['fparam']`
if `numb_aparam > 0`, should have `input_dict['aparam']`

natoms
The number of atoms. This tensor has the length of `Ntypes + 2` `natoms[0]`: number of local atoms `natoms[1]`: total number of atoms held by this processor `natoms[i]`: $2 \leq i < Ntypes+2$, number of type `i` atoms

reuse
The weights in the networks should be reused when get the variable.

suffix
Name suffix to identify this descriptor

Returns

ener
The system energy

change_energy_bias(data, frozen_model, origin_type_map, full_type_map, bias_shift='delta', ntest=10) → `None`

Change the energy bias according to the input data and the pretrained model.

Parameters

data
[`DeepmdDataSystem`] The training data.

frozen_model
[`str`] The path file of frozen model.

origin_type_map
[`list`] The original type_map in dataset, they are targets to change the energy bias.

full_type_map
[`str`] The full type_map in pretrained model

bias_shift
[`str`] The mode for changing energy bias : ['delta', 'statistic'] 'delta' : perform predictions on energies of target dataset,
and do least square on the errors to obtain the target shift as bias.
'statistic' : directly use the statistic energy bias in the target dataset.

ntest
[`int`] The number of test samples in a system to change the energy bias.

compute_input_stats(all_stat: `dict`, protection: `float` = 0.01) → `None`

Compute the input statistics.

Parameters

all_stat
if `numb_fparam > 0` must have `all_stat['fparam']` if `numb_aparam > 0` must have `all_stat['aparam']` can be prepared by `model.make_stat_input`

protection
Divided-by-zero protection

compute_output_stats(all_stat: [dict](#), mixed_type: [bool](#) = False) → [None](#)

Compute the output statistics.

Parameters

all_stat
must have the following components: all_stat['energy'] of shape n_sys x n_batch x n_frame can be prepared by model.make_stat_input

mixed_type
Whether to perform the mixed_type mode. If True, the input data has the mixed_type format (see doc/model/train_se_atten.md), in which frames in a system may have different natoms_vec(s), with the same nloc.

enable_mixed_precision(mixed_prec: [Optional\[dict\]](#) = None) → [None](#)

Reveive the mixed precision setting.

Parameters

mixed_prec
The mixed precision setting used in the embedding net

get_loss(loss: [dict](#), lr) → [Loss](#)

Get the loss function.

Parameters

loss
[[dict](#)] The loss function parameters.

lr
[[LearningRateExp](#)] The learning rate.

Returns

Loss
The loss function.

get_numb_aparam() → [int](#)

Get the number of atomic parameters.

get_numb_fparam() → [int](#)

Get the number of frame parameters.

init_variables(graph: [Graph](#), graph_def: [GraphDef](#), suffix: [str](#) = "") → [None](#)

Init the fitting net variables with the given dict.

Parameters

graph
[[tf.Graph](#)] The input frozen model graph

graph_def
[[tf.GraphDef](#)] The input frozen model graph_def

suffix
[[str](#)] suffix to name scope

deepmd.fit.fitting module

```
class deepmd.fit.fitting.Fitting(*args, **kwargs)
```

Bases: *PluginVariant*

Attributes

precision

Precision of fitting network.

Methods

| | |
|--|---|
| <i>get_loss</i> (loss, lr) | Get the loss function. |
| <i>init_variables</i> (graph, graph_def[, suffix]) | Init the fitting net variables with the given dict. |
| <i>register</i> (key) | Register a Fitting plugin. |

```
abstract get_loss(loss: dict, lr) → Loss
```

Get the loss function.

Parameters

loss

[dict] the loss dict

lr

[LearningRateExp] the learning rate

Returns

Loss

the loss function

```
init_variables(graph: Graph, graph_def: GraphDef, suffix: str = "") → None
```

Init the fitting net variables with the given dict.

Parameters

graph

[tf.Graph] The input frozen model graph

graph_def

[tf.GraphDef] The input frozen model graph_def

suffix

[str] suffix to name scope

Notes

This method is called by others when the fitting supported initialization from the given variables.

```
property precision: DType
```

Precision of fitting network.

```
static register(key: str) → Callable
```

Register a Fitting plugin.

Parameters

key
 [str] the key of a Fitting

Returns

Fitting
 the registered Fitting

Examples

```
>>> @Fitting.register("some_fitting")
      class SomeFitting(Fitting):
          pass
```

deepmd.fit.polar module

```
class deepmd.fit.polar.GlobalPolarFittingSeA(descrpt: Tensor, neuron: List[int] = [120, 120, 120],
                                             resnet_dt: bool = True, sel_type: Optional[List[int]]
                                             = None, fit_diag: bool = True, scale:
                                             Optional[List[float]] = None, diag_shift:
                                             Optional[List[float]] = None, seed: Optional[int] =
                                             None, activation_function: str = 'tanh', precision: str
                                             = 'default')
```

Bases: `object`

Fit the system polarizability with descriptor `se_a`.

Parameters

descrpt
 [tf.Tensor] The descriptor

neuron
 [List[int]] Number of neurons in each hidden layer of the fitting net

resnet_dt
 [bool] Time-step dt in the resnet construction: $y = x + dt * \phi(Wx + b)$

sel_type
 [List[int]] The atom types selected to have an atomic polarizability prediction

fit_diag
 [bool] Fit the diagonal part of the rotational invariant polarizability matrix, which will be converted to normal polarizability matrix by contracting with the rotation matrix.

scale
 [List[float]] The output of the fitting net (polarizability matrix) for type *i* atom will be scaled by `scale[i]`

diag_shift
 [List[float]] The diagonal part of the polarizability matrix of type *i* will be shifted by `diag_shift[i]`. The shift operation is carried out after scale.

seed
 [int] Random seed for initializing the network parameters.

`activation_function`

[`str`] The activation function in the embedding net. Supported options are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”, “gelu_tf”, “None”, “none”.

`precision`

[`str`] The precision of the embedding net parameters. Supported options are “default”, “float16”, “float32”, “float64”, “bfloat16”.

Methods

| | |
|---|---|
| <code>build(input_d, rot_mat, natoms[, ...])</code> | Build the computational graph for fitting net. |
| <code>enable_mixed_precision([mixed_prec])</code> | Reveive the mixed precision setting. |
| <code>get_loss(loss, lr)</code> | Get the loss function. |
| <code>get_out_size()</code> | Get the output size. |
| <code>get_sel_type()</code> | Get selected atom types. |
| <code>init_variables(graph, graph_def[, suffix])</code> | Init the fitting net variables with the given dict. |

build(input_d, rot_mat, natoms, input_dict: `Optional[dict]` = None, reuse=None, suffix='') → Tensor

Build the computational graph for fitting net.

Parameters

`input_d`

The input descriptor

`rot_mat`

The rotation matrix from the descriptor.

`natoms`

The number of atoms. This tensor has the length of Ntypes + 2 `natoms[0]`: number of local atoms `natoms[1]`: total number of atoms held by this processor `natoms[i]`: $2 \leq i < \text{Ntypes} + 2$, number of type *i* atoms

`input_dict`

Additional dict for inputs.

`reuse`

The weights in the networks should be reused when get the variable.

`suffix`

Name suffix to identify this descriptor

Returns

polar

The system polarizability

enable_mixed_precision(mixed_prec: `Optional[dict]` = None) → None

Reveive the mixed precision setting.

Parameters

`mixed_prec`

The mixed precision setting used in the embedding net

`get_loss(loss: dict, lr) → Loss`

Get the loss function.

Parameters

loss

[dict] the loss dict

lr

[LearningRateExp] the learning rate

Returns

Loss

the loss function

`get_out_size() → int`

Get the output size. Should be 9.

`get_sel_type() → int`

Get selected atom types.

`init_variables(graph: Graph, graph_def: GraphDef, suffix: str = '') → None`

Init the fitting net variables with the given dict.

Parameters

graph

[tf.Graph] The input frozen model graph

graph_def

[tf.GraphDef] The input frozen model graph_def

suffix

[str] suffix to name scope

`class deepmd.fit.polar.PolarFittingSeA(*args, **kwargs)`

Bases: *Fitting*

Fit the atomic polarizability with descriptor se_a.

Parameters

descript

[tf.Tensor] The descriptor

neuron

[List[int]] Number of neurons in each hidden layer of the fitting net

resnet_dt

[bool] Time-step dt in the resnet construction: $y = x + dt * \phi(Wx + b)$

sel_type

[List[int]] The atom types selected to have an atomic polarizability prediction. If is None, all atoms are selected.

fit_diag

[bool] Fit the diagonal part of the rotational invariant polarizability matrix, which will be converted to normal polarizability matrix by contracting with the rotation matrix.

scale
`[List[float]]` The output of the fitting net (polarizability matrix) for type *i* atom will be scaled by `scale[i]`

diag_shift
`[List[float]]` The diagonal part of the polarizability matrix of type *i* will be shifted by `diag_shift[i]`. The shift operation is carried out after scale.

seed
`[int]` Random seed for initializing the network parameters.

activation_function
`[str]` The activation function in the embedding net. Supported options are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”, “gelu_tf”, “None”, “none”.

precision
`[str]` The precision of the embedding net parameters. Supported options are “default”, “float16”, “float32”, “float64”, “bfloat16”.

uniform_seed
 Only for the purpose of backward compatibility, retrieves the old behavior of using the random seed

Attributes

precision
 Precision of fitting network.

Methods

| | |
|--|---|
| <code>build(input_d, rot_mat, natoms[, ...])</code> | Build the computational graph for fitting net. |
| <code>compute_input_stats(all_stat[, protection])</code> | Compute the input statistics. |
| <code>enable_mixed_precision([mixed_prec])</code> | Reveive the mixed precision setting. |
| <code>get_loss(loss, lr)</code> | Get the loss function. |
| <code>get_out_size()</code> | Get the output size. |
| <code>get_sel_type()</code> | Get selected atom types. |
| <code>init_variables(graph, graph_def[, suffix])</code> | Init the fitting net variables with the given dict. |
| <code>register(key)</code> | Register a Fitting plugin. |

build(input_d: Tensor, rot_mat: Tensor, natoms: Tensor, input_dict: `Optional[dict]` = None, reuse: `Optional[bool]` = None, suffix: `str` = “”)

Build the computational graph for fitting net.

Parameters

input_d
 The input descriptor

rot_mat
 The rotation matrix from the descriptor.

natoms
 The number of atoms. This tensor has the length of `Ntypes + 2` `natoms[0]`: number of local atoms `natoms[1]`: total number of atoms held by this processor `natoms[i]`: $2 \leq i < Ntypes+2$, number of type *i* atoms

input_dict
 Additional dict for inputs.

reuse

The weights in the networks should be reused when get the variable.

suffix

Name suffix to identify this descriptor

Returns

atomic_polar

The atomic polarizability

compute_input_stats(all_stat, protection=0.01)

Compute the input statistics.

Parameters

all_stat

Dictionary of inputs. can be prepared by model.make_stat_input

protection

Divided-by-zero protection

enable_mixed_precision(mixed_prec: Optional[dict] = None) → None

Reveive the mixed precision setting.

Parameters

mixed_prec

The mixed precision setting used in the embedding net

get_loss(loss: dict, lr) → Loss

Get the loss function.

get_out_size() → int

Get the output size. Should be 9.

get_sel_type() → List[int]

Get selected atom types.

init_variables(graph: Graph, graph_def: GraphDef, suffix: str = '') → None

Init the fitting net variables with the given dict.

Parameters

graph

[tf.Graph] The input frozen model graph

graph_def

[tf.GraphDef] The input frozen model graph_def

suffix

[str] suffix to name scope

deepmd.infer package

Submodule containing all the implemented potentials.

```
class deepmd.infer.DeepDOS(model_file: Path, load_prefix: str = 'load', default_tf_graph: bool = False,
                           auto_batch_size: Union[bool, int, AutoBatchSize] = True)
```

Bases: *DeepEval*

Constructor.

Parameters

model_file
[Path] The name of the frozen model file.

load_prefix: str
The prefix in the load computational graph

default_tf_graph
[bool] If uses the default tf graph, otherwise build a new tf graph for evaluation

auto_batch_size
[bool or int or AutomaticBatchSize, default: True] If True, automatic batch size will be used. If int, it will be used as the initial batch size.

Warning: For developers: DeepTensor initializer must be called at the end after self.tensors are modified because it uses the data in self.tensors dict. Do not change the order!

Attributes

model_type
Get type of model.

model_version
Get version of model.

sess
Get TF session.

Methods

| | |
|--|--|
| <code>eval(coords, cells, atom_types[, atomic, ...])</code> | Evaluate the dos, atom_dos by using this model. |
| <code>eval_descriptor(coords, cells, atom_types[, ...])</code> | Evaluate descriptors by using this DP. |
| <code>eval_typeebd()</code> | Evaluate output of type embedding network by using this model. |
| <code>get_dim_aparam()</code> | Get the number (dimension) of atomic parameters of this DP. |
| <code>get_dim_fparam()</code> | Get the number (dimension) of frame parameters of this DP. |
| <code>get_ntypes()</code> | Get the number of atom types of this model. |
| <code>get_numb_dos()</code> | Get the length of DOS output of this DP model. |
| <code>get_rcut()</code> | Get the cut-off radius of this model. |
| <code>get_sel_type()</code> | Unsupported in this model. |
| <code>get_type_map()</code> | Get the type map (element name of the atom types) of this model. |
| <code>make_natoms_vec(atom_types[, mixed_type])</code> | Make the natom vector used by deepmd-kit. |
| <code>reverse_map(vec, imap)</code> | Reverse mapping of a vector according to the index map. |
| <code>sort_input(coord, atom_type[, sel_atoms, ...])</code> | Sort atoms in the system according their types. |

eval(coords: `ndarray`, cells: `ndarray`, atom_types: `List[int]`, atomic: `bool` = False, fparam: `Optional[ndarray]` = None, aparam: `Optional[ndarray]` = None, mixed_type: `bool` = False) → `Tuple[ndarray, ...]`

Evaluate the dos, atom_dos by using this model.

Parameters

coords

The coordinates of atoms. The array should be of size nframes x natoms x 3

cells

The cell of the region. If None then non-PBC is assumed, otherwise using PBC. The array should be of size nframes x 9

atom_types

The atom types The list should contain natoms ints

atomic

Calculate the atomic energy and virial

fparam

The frame parameter. The array can be of size : - nframes x dim_fparam. - dim_fparam. Then all frames are assumed to be provided with the same fparam.

aparam

The atomic parameter The array can be of size : - nframes x natoms x dim_aparam. - natoms x dim_aparam. Then all frames are assumed to be provided with the same aparam. - dim_aparam. Then all frames and atoms are provided with the same aparam.

mixed_type

Whether to perform the mixed_type mode. If True, the input data has the mixed_type format (see doc/model/train_se_atten.md), in which frames in a system may have different natoms_vec(s), with the same nloc.

Returns

dos

The electron density of state.

atom_dos

The atom-sited density of state. Only returned when `atomic == True`

eval_descriptor(coords: `ndarray`, cells: `ndarray`, atom_types: `List[int]`, fparam: `Optional[ndarray]` = None, aparam: `Optional[ndarray]` = None, efield: `Optional[ndarray]` = None, mixed_type: `bool` = False) → `array`

Evaluate descriptors by using this DP.

Parameters

coords

The coordinates of atoms. The array should be of size `nframes x natoms x 3`

cells

The cell of the region. If None then non-PBC is assumed, otherwise using PBC. The array should be of size `nframes x 9`

atom_types

The atom types The list should contain `natoms` ints

fparam

The frame parameter. The array can be of size : - `nframes x dim_fparam`. - `dim_fparam`. Then all frames are assumed to be provided with the same fparam.

aparam

The atomic parameter The array can be of size : - `nframes x natoms x dim_aparam`. - `natoms x dim_aparam`. Then all frames are assumed to be provided with the same aparam. - `dim_aparam`. Then all frames and atoms are provided with the same aparam.

efield

The external field on atoms. The array should be of size `nframes x natoms x 3`

mixed_type

Whether to perform the mixed_type mode. If True, the input data has the mixed_type format (see `doc/model/train_se_atten.md`), in which frames in a system may have different `natoms_vec(s)`, with the same `nloc`.

Returns

descriptor

Descriptors.

get_dim_aparam() → `int`

Get the number (dimension) of atomic parameters of this DP.

get_dim_fparam() → `int`

Get the number (dimension) of frame parameters of this DP.

get_ntypes() → `int`

Get the number of atom types of this model.

get_numb_dos() → `int`

Get the length of DOS output of this DP model.

`get_rcut()` → `float`

Get the cut-off radius of this model.

`get_sel_type()` → `List[int]`

Unsupported in this model.

`get_type_map()` → `List[str]`

Get the type map (element name of the atom types) of this model.

`load_prefix:` `str`

```
class deepmd.infer.DeepDipole(model_file: Path, load_prefix: str = 'load', default_tf_graph: bool =
                               False)
```

Bases: *DeepTensor*

Constructor.

Parameters

`model_file`

[`Path`] The name of the frozen model file.

`load_prefix:` `str`

The prefix in the load computational graph

`default_tf_graph`

[`bool`] If uses the default tf graph, otherwise build a new tf graph for evaluation

Warning: For developers: DeepTensor initializer must be called at the end after `self.tensors` are modified because it uses the data in `self.tensors` dict. Do not change the order!

Attributes

`model_type`

Get type of model.

`model_version`

Get version of model.

`sess`

Get TF session.

Methods

| | |
|---|--|
| <code>eval(coords, cells, atom_types[, atomic, ...])</code> | Evaluate the model. |
| <code>eval_full(coords, cells, atom_types[, ...])</code> | Evaluate the model with interface similar to the energy model. |
| <code>eval_typeebd()</code> | Evaluate output of type embedding network by using this model. |
| <code>get_dim_aparam()</code> | Unsupported in this model. |
| <code>get_dim_fparam()</code> | Unsupported in this model. |
| <code>get_ntypes()</code> | Get the number of atom types of this model. |
| <code>get_rcut()</code> | Get the cut-off radius of this model. |
| <code>get_sel_type()</code> | Get the selected atom types of this model. |
| <code>get_type_map()</code> | Get the type map (element name of the atom types) of this model. |
| <code>make_natoms_vec(atom_types[, mixed_type])</code> | Make the natom vector used by deepmd-kit. |
| <code>reverse_map(vec, imap)</code> | Reverse mapping of a vector according to the index map. |
| <code>sort_input(coord, atom_type[, sel_atoms, ...])</code> | Sort atoms in the system according their types. |

`get_dim_aparam()` → `int`

Unsupported in this model.

`get_dim_fparam()` → `int`

Unsupported in this model.

`load_prefix:` `str`

```
class deepmd.infer.DeepEval(model_file: Path, load_prefix: str = 'load', default_tf_graph: bool =
                             False, auto_batch_size: Union[bool, int, AutoBatchSize] = False)
```

Bases: `object`

Common methods for DeepPot, DeepWFC, DeepPolar, ...

Parameters

`model_file`

[`Path`] The name of the frozen model file.

`load_prefix:` `str`

The prefix in the load computational graph

`default_tf_graph`

[`bool`] If uses the default tf graph, otherwise build a new tf graph for evaluation

`auto_batch_size`

[`bool` or `int` or `AutomaticBatchSize`, default: `False`] If True, automatic batch size will be used. If int, it will be used as the initial batch size.

Attributes

`model_type`

Get type of model.

`model_version`

Get version of model.

`sess`

Get TF session.

Methods

| | |
|---|--|
| <code>eval_typeebd()</code> | Evaluate output of type embedding network by using this model. |
| <code>make_natoms_vec(atom_types[, mixed_type])</code> | Make the natom vector used by deepmd-kit. |
| <code>reverse_map(vec, imap)</code> | Reverse mapping of a vector according to the index map. |
| <code>sort_input(coord, atom_type[, sel_atoms, ...])</code> | Sort atoms in the system according their types. |

`eval_typeebd()` → `ndarray`

Evaluate output of type embedding network by using this model.

Returns

`np.ndarray`

The output of type embedding network. The shape is `[ntypes, o_size]`, where `ntypes` is the number of types, and `o_size` is the number of nodes in the output layer.

Raises

`KeyError`

If the model does not enable type embedding.

See also:

`deepmd.utils.type_embed.TypeEmbedNet`

The type embedding network.

Examples

Get the output of type embedding network of graph.pb:

```
>>> from deepmd.infer import DeepPotential
>>> dp = DeepPotential('graph.pb')
>>> dp.eval_typeebd()
```

`load_prefix:` `str`

`make_natoms_vec(atom_types: ndarray, mixed_type: bool = False)` → `ndarray`

Make the natom vector used by deepmd-kit.

Parameters

`atom_types`

The type of atoms

`mixed_type`

Whether to perform the mixed_type mode. If True, the input data has the mixed_type format (see doc/model/train_se_atten.md), in which frames in a system may have different natoms_vec(s), with the same nloc.

Returns

`natoms`

The number of atoms. This tensor has the length of `Ntypes + 2` `natoms[0]`: number of local atoms `natoms[1]`: total number of atoms held by this processor `natoms[i]`: $2 \leq i < Ntypes+2$, number of type `i` atoms

property `model_type`: `str`

Get type of model.

:type:str

property `model_version`: `str`

Get version of model.

Returns

`str`

version of model

static `reverse_map`(`vec`: `ndarray`, `imap`: `List[int]`) \rightarrow `ndarray`

Reverse mapping of a vector according to the index map.

Parameters

`vec`

Input vector. Be of shape `[nframes, natoms, -1]`

`imap`

Index map. Be of shape `[natoms]`

Returns

`vec_out`

Reverse mapped vector.

property `sess`: `Session`

Get TF session.

static `sort_input`(`coord`: `ndarray`, `atom_type`: `ndarray`, `sel_atoms`: `Optional[List[int]]` = `None`,
`mixed_type`: `bool` = `False`)

Sort atoms in the system according their types.

Parameters

`coord`

The coordinates of atoms. Should be of shape `[nframes, natoms, 3]`

`atom_type`

The type of atoms Should be of shape `[natoms]`

`sel_atoms`

The selected atoms by type

`mixed_type`

Whether to perform the `mixed_type` mode. If `True`, the input data has the `mixed_type` format (see `doc/model/train_se_atten.md`), in which frames in a system may have different `natoms_vec(s)`, with the same `nloc`.

Returns

`coord_out`

The coordinates after sorting

`atom_type_out`

The atom types after sorting

`idx_map`

The index mapping from the input to the output. For example `coord_out = coord[:,idx_map,:]`

sel_atom_type

Only output if sel_atoms is not None The sorted selected atom types

sel_idx_map

Only output if sel_atoms is not None The index mapping from the selected atoms to sorted selected atoms.

```
class deepmd.infer.DeepGlobalPolar(model_file: str, load_prefix: str = 'load', default_tf_graph: bool
                                   = False)
```

Bases: *DeepTensor*

Constructor.

Parameters

model_file

[str] The name of the frozen model file.

load_prefix: str

The prefix in the load computational graph

default_tf_graph

[bool] If uses the default tf graph, otherwise build a new tf graph for evaluation

Attributes

model_type

Get type of model.

model_version

Get version of model.

sess

Get TF session.

Methods

| | |
|--|--|
| <i>eval</i> (coords, cells, atom_types[, atomic, ...]) | Evaluate the model. |
| <i>eval_full</i> (coords, cells, atom_types[, ...]) | Evaluate the model with interface similar to the energy model. |
| <i>eval_typeebd</i> () | Evaluate output of type embedding network by using this model. |
| <i>get_dim_aparam</i> () | Unsupported in this model. |
| <i>get_dim_fparam</i> () | Unsupported in this model. |
| <i>get_ntypes</i> () | Get the number of atom types of this model. |
| <i>get_rcut</i> () | Get the cut-off radius of this model. |
| <i>get_sel_type</i> () | Get the selected atom types of this model. |
| <i>get_type_map</i> () | Get the type map (element name of the atom types) of this model. |
| <i>make_natoms_vec</i> (atom_types[, mixed_type]) | Make the natom vector used by deepmd-kit. |
| <i>reverse_map</i> (vec, imap) | Reverse mapping of a vector according to the index map. |
| <i>sort_input</i> (coord, atom_type[, sel_atoms, ...]) | Sort atoms in the system according their types. |

```
eval(coords: ndarray, cells: ndarray, atom_types: List[int], atomic: bool = False, fparam:
Optional[ndarray] = None, aparam: Optional[ndarray] = None, efield: Optional[ndarray] =
None) → ndarray
```

Evaluate the model.

Parameters

coords

The coordinates of atoms. The array should be of size nframes x natoms x 3

cells

The cell of the region. If None then non-PBC is assumed, otherwise using PBC. The array should be of size nframes x 9

atom_types

The atom types The list should contain natoms ints

atomic

Not used in this model

fparam

Not used in this model

aparam

Not used in this model

efield

Not used in this model

Returns

tensor

The returned tensor If atomic == False then of size nframes x variable_dof else of size nframes x natoms x variable_dof

`get_dim_aparam()` → `int`

Unsupported in this model.

`get_dim_fparam()` → `int`

Unsupported in this model.

`load_prefix:` `str`

```
class deepmd.infer.DeepPolar(model_file: Path, load_prefix: str = 'load', default_tf_graph: bool = False)
```

Bases: *DeepTensor*

Constructor.

Parameters

model_file

[Path] The name of the frozen model file.

load_prefix: str

The prefix in the load computational graph

default_tf_graph

[bool] If uses the default tf graph, otherwise build a new tf graph for evaluation

Warning: For developers: DeepTensor initializer must be called at the end after self.tensors are modified because it uses the data in self.tensors dict. Do not change the order!

Attributes

model_type
Get type of model.

model_version
Get version of model.

sess
Get TF session.

Methods

| | |
|---|--|
| <code>eval(coords, cells, atom_types[, atomic, ...])</code> | Evaluate the model. |
| <code>eval_full(coords, cells, atom_types[, ...])</code> | Evaluate the model with interface similar to the energy model. |
| <code>eval_typeebd()</code> | Evaluate output of type embedding network by using this model. |
| <code>get_dim_aparam()</code> | Unsupported in this model. |
| <code>get_dim_fparam()</code> | Unsupported in this model. |
| <code>get_ntypes()</code> | Get the number of atom types of this model. |
| <code>get_rcut()</code> | Get the cut-off radius of this model. |
| <code>get_sel_type()</code> | Get the selected atom types of this model. |
| <code>get_type_map()</code> | Get the type map (element name of the atom types) of this model. |
| <code>make_natoms_vec(atom_types[, mixed_type])</code> | Make the natom vector used by deepmd-kit. |
| <code>reverse_map(vec, imap)</code> | Reverse mapping of a vector according to the index map. |
| <code>sort_input(coord, atom_type[, sel_atoms, ...])</code> | Sort atoms in the system according their types. |

`get_dim_aparam() → int`
Unsupported in this model.

`get_dim_fparam() → int`
Unsupported in this model.

load_prefix: `str`

class `deepmd.infer.DeepPot(model_file: Path, load_prefix: str = 'load', default_tf_graph: bool = False, auto_batch_size: Union[bool, int, AutoBatchSize] = True)`

Bases: *DeepEval*

Constructor.

Parameters

model_file
[Path] The name of the frozen model file.

load_prefix: `str`
The prefix in the load computational graph

default_tf_graph
[bool] If uses the default tf graph, otherwise build a new tf graph for evaluation

`auto_batch_size`
[bool or int or AutomaticBatchSize, default: True] If True, automatic batch size will be used. If int, it will be used as the initial batch size.

Warning: For developers: DeepTensor initializer must be called at the end after self.tensors are modified because it uses the data in self.tensors dict. Do not change the order!

Examples

```
>>> from deepmd.infer import DeepPot
>>> import numpy as np
>>> dp = DeepPot('graph.pb')
>>> coord = np.array([[1,0,0], [0,0,1.5], [1,0,3]]).reshape([1, -1])
>>> cell = np.diag(10 * np.ones(3)).reshape([1, -1])
>>> atype = [1,0,1]
>>> e, f, v = dp.eval(coord, cell, atype)
```

where e, f and v are predicted energy, force and virial of the system, respectively.

Attributes

model_type
Get type of model.

model_version
Get version of model.

sess
Get TF session.

Methods

| | |
|--|--|
| <code>eval(coords, cells, atom_types[, atomic, ...])</code> | Evaluate the energy, force and virial by using this DP. |
| <code>eval_descriptor(coords, cells, atom_types[, ...])</code> | Evaluate descriptors by using this DP. |
| <code>eval_typeebd()</code> | Evaluate output of type embedding network by using this model. |
| <code>get_descriptor_type()</code> | Get the descriptor type of this model. |
| <code>get_dim_aparam()</code> | Get the number (dimension) of atomic parameters of this DP. |
| <code>get_dim_fparam()</code> | Get the number (dimension) of frame parameters of this DP. |
| <code>get_ntypes()</code> | Get the number of atom types of this model. |
| <code>get_ntypes_spin()</code> | Get the number of spin atom types of this model. |
| <code>get_rcut()</code> | Get the cut-off radius of this model. |
| <code>get_sel_type()</code> | Unsupported in this model. |
| <code>get_type_map()</code> | Get the type map (element name of the atom types) of this model. |
| <code>make_natoms_vec(atom_types[, mixed_type])</code> | Make the natom vector used by deepmd-kit. |
| <code>reverse_map(vec, imap)</code> | Reverse mapping of a vector according to the index map. |
| <code>sort_input(coord, atom_type[, sel_atoms, ...])</code> | Sort atoms in the system according their types. |

eval(coords: `ndarray`, cells: `ndarray`, atom_types: `List[int]`, atomic: `bool` = False, fparam: `Optional[ndarray]` = None, aparam: `Optional[ndarray]` = None, efield: `Optional[ndarray]` = None, mixed_type: `bool` = False) → `Tuple[ndarray, ...]`

Evaluate the energy, force and virial by using this DP.

Parameters

coords

The coordinates of atoms. The array should be of size nframes x natoms x 3

cells

The cell of the region. If None then non-PBC is assumed, otherwise using PBC. The array should be of size nframes x 9

atom_types

The atom types The list should contain natoms ints

atomic

Calculate the atomic energy and virial

fparam

The frame parameter. The array can be of size : - nframes x dim_fparam. - dim_fparam. Then all frames are assumed to be provided with the same fparam.

aparam

The atomic parameter The array can be of size : - nframes x natoms x dim_aparam. - natoms x dim_aparam. Then all frames are assumed to be provided with the same aparam. - dim_aparam. Then all frames and atoms are provided with the same aparam.

efield

The external field on atoms. The array should be of size nframes x natoms x 3

mixed_type

Whether to perform the mixed_type mode. If True, the input data has the mixed_type format (see doc/model/train_se_atten.md), in which frames in a system may have different natoms_vec(s), with the same nloc.

Returns

energy

The system energy.

force

The force on each atom

virial

The virial

atom_energy

The atomic energy. Only returned when atomic == True

atom_virial

The atomic virial. Only returned when atomic == True

eval_descriptor(coords: ndarray, cells: ndarray, atom_types: List[int], fparam: Optional[ndarray] = None, aparam: Optional[ndarray] = None, efield: Optional[ndarray] = None, mixed_type: bool = False) → array

Evaluate descriptors by using this DP.

Parameters

coords

The coordinates of atoms. The array should be of size nframes x natoms x 3

cells

The cell of the region. If None then non-PBC is assumed, otherwise using PBC. The array should be of size nframes x 9

atom_types

The atom types The list should contain natoms ints

fparam

The frame parameter. The array can be of size : - nframes x dim_fparam. - dim_fparam. Then all frames are assumed to be provided with the same fparam.

aparam

The atomic parameter The array can be of size : - nframes x natoms x dim_aparam. - natoms x dim_aparam. Then all frames are assumed to be provided with the same aparam. - dim_aparam. Then all frames and atoms are provided with the same aparam.

efield

The external field on atoms. The array should be of size nframes x natoms x 3

mixed_type

Whether to perform the mixed_type mode. If True, the input data has the mixed_type format (see doc/model/train_se_atten.md), in which frames in a system may have different natoms_vec(s), with the same nloc.

Returns

descriptor

Descriptors.

`get_descriptor_type() → List[int]`

Get the descriptor type of this model.

`get_dim_aparam() → int`

Get the number (dimension) of atomic parameters of this DP.

`get_dim_fparam() → int`

Get the number (dimension) of frame parameters of this DP.

`get_ntypes() → int`

Get the number of atom types of this model.

`get_ntypes_spin()`

Get the number of spin atom types of this model.

`get_rcut() → float`

Get the cut-off radius of this model.

`get_sel_type() → List[int]`

Unsupported in this model.

`get_type_map() → List[str]`

Get the type map (element name of the atom types) of this model.

`load_prefix: str`

`deepmd.infer.DeepPotential(model_file: Union[str, Path], load_prefix: str = 'load', default_tf_graph: bool = False) → Union[DeepDipole, DeepGlobalPolar, DeepPolar, DeepPot, DeepDOS, DeepWFC]`

Factory function that will initialize appropriate potential read from `model_file`.

Parameters

`model_file`

[`str`] The name of the frozen model file.

`load_prefix`

[`str`] The prefix in the load computational graph

`default_tf_graph`

[`bool`] If uses the default tf graph, otherwise build a new tf graph for evaluation

Returns

`Union[DeepDipole, DeepGlobalPolar, DeepPolar, DeepPot, DeepWFC]`

one of the available potentials

Raises

`RuntimeError`

if model file does not correspond to any implemented potential

`class deepmd.infer.DeepWFC(model_file: Path, load_prefix: str = 'load', default_tf_graph: bool = False)`

Bases: `DeepTensor`

Constructor.

Parameters

`model_file`

[`Path`] The name of the frozen model file.

`load_prefix`: str
The prefix in the load computational graph

`default_tf_graph`
[bool] If uses the default tf graph, otherwise build a new tf graph for evaluation

Warning: For developers: DeepTensor initializer must be called at the end after `self.tensors` are modified because it uses the data in `self.tensors` dict. Do not change the order!

Attributes

`model_type`
Get type of model.

`model_version`
Get version of model.

`sess`
Get TF session.

Methods

| | |
|---|--|
| <code>eval(coords, cells, atom_types[, atomic, ...])</code> | Evaluate the model. |
| <code>eval_full(coords, cells, atom_types[, ...])</code> | Evaluate the model with interface similar to the energy model. |
| <code>eval_typeebd()</code> | Evaluate output of type embedding network by using this model. |
| <code>get_dim_aparam()</code> | Unsupported in this model. |
| <code>get_dim_fparam()</code> | Unsupported in this model. |
| <code>get_ntypes()</code> | Get the number of atom types of this model. |
| <code>get_rcut()</code> | Get the cut-off radius of this model. |
| <code>get_sel_type()</code> | Get the selected atom types of this model. |
| <code>get_type_map()</code> | Get the type map (element name of the atom types) of this model. |
| <code>make_natoms_vec(atom_types[, mixed_type])</code> | Make the natom vector used by deepmd-kit. |
| <code>reverse_map(vec, imap)</code> | Reverse mapping of a vector according to the index map. |
| <code>sort_input(coord, atom_type[, sel_atoms, ...])</code> | Sort atoms in the system according their types. |

`get_dim_aparam() → int`
Unsupported in this model.

`get_dim_fparam() → int`
Unsupported in this model.

`load_prefix`: str

```
class deepmd.infer.DipoleChargeModifier(model_name: str, model_charge_map: List[float],
                                         sys_charge_map: List[float], ewald_h: float = 1,
                                         ewald_beta: float = 1)
```

Bases: *DeepDipole*

Parameters

`model_name`
The model file for the DeepDipole model

`model_charge_map`
Gives the amount of charge for the wfcc

`sys_charge_map`
Gives the amount of charge for the real atoms

`ewald_h`
Grid spacing of the reciprocal part of Ewald sum. Unit: Å

`ewald_beta`
Splitting parameter of the Ewald sum. Unit: Å⁻¹

Attributes

`model_type`
Get type of model.

`model_version`
Get version of model.

`sess`
Get TF session.

Methods

| | |
|---|---|
| <code>build_fv_graph()</code> | Build the computational graph for the force and virial inference. |
| <code>eval(coord, box, atype[, eval_fv])</code> | Evaluate the modification. |
| <code>eval_full(coords, cells, atom_types[, ...])</code> | Evaluate the model with interface similar to the energy model. |
| <code>eval_typeebd()</code> | Evaluate output of type embedding network by using this model. |
| <code>get_dim_apham()</code> | Unsupported in this model. |
| <code>get_dim_fparam()</code> | Unsupported in this model. |
| <code>get_ntypes()</code> | Get the number of atom types of this model. |
| <code>get_rcut()</code> | Get the cut-off radius of this model. |
| <code>get_sel_type()</code> | Get the selected atom types of this model. |
| <code>get_type_map()</code> | Get the type map (element name of the atom types) of this model. |
| <code>make_natoms_vec(atom_types[, mixed_type])</code> | Make the natom vector used by deepmd-kit. |
| <code>modify_data(data, data_sys)</code> | Modify data. |
| <code>reverse_map(vec, imap)</code> | Reverse mapping of a vector according to the index map. |
| <code>sort_input(coord, atom_type[, sel_atoms, ...])</code> | Sort atoms in the system according their types. |

`build_fv_graph()` → Tensor

Build the computational graph for the force and virial inference.

`eval`(coord: ndarray, box: ndarray, atype: ndarray, eval_fv: bool = True) → Tuple[ndarray, ndarray, ndarray]

Evaluate the modification.

Parameters

`coord`
The coordinates of atoms

`box`
The simulation region. PBC is assumed

`atype`
The atom types

`eval_fv`
Evaluate force and virial

Returns

`tot_e`
The energy modification

`tot_f`
The force modification

`tot_v`
The virial modification

`load_prefix`: `str`

`modify_data`(data: `dict`, data_sys: `DeepmdData`) \rightarrow `None`

Modify data.

Parameters

`data`
Internal data of `DeepmdData`. Be a dict, has the following keys - `coord` coordinates - `box` simulation box - `type` atom types - `find_energy` tells if data has energy - `find_force` tells if data has force - `find_virial` tells if data has virial - `energy` energy - `force` force - `virial` virial

`data_sys`
[`DeepmdData`] The data system.

`class deepmd.infer.EwaldRecp`(hh, beta)

Bases: `object`

Evaluate the reciprocal part of the Ewald sum.

Methods

| | |
|--|-----------|
| <code>eval</code> (coord, charge, box) | Evaluate. |
|--|-----------|

`eval`(coord: `ndarray`, charge: `ndarray`, box: `ndarray`) \rightarrow `Tuple`[`ndarray`, `ndarray`, `ndarray`]

Evaluate.

Parameters

`coord`
The coordinates of atoms

`charge`
The atomic charge

box
The simulation region. PBC is assumed

Returns

e
The energy

f
The force

v
The virial

```
deepmd.infer.calc_model_devi(coord, box, atype, models, fname=None, frequency=1,
                             mixed_type=False, fparam: Optional[ndarray] = None, aparam:
                             Optional[ndarray] = None, real_data: Optional[dict] = None)
```

Python interface to calculate model deviation.

Parameters

coord
[`numpy.ndarray`, n_frames x n_atoms x 3] Coordinates of system to calculate

box
[`numpy.ndarray` or `None`, n_frames x 3 x 3] Box to specify periodic boundary condition. If `None`, no pbc will be used

atype
[`numpy.ndarray`, n_atoms x 1] Atom types

models
[list of *DeepPot* models] Models used to evaluate deviation

fname
[`str` or `None`] File to dump results, default `None`

frequency
[`int`] Steps between frames (if the system is given by molecular dynamics engine), default 1

mixed_type
[`bool`] Whether the input atype is in mixed_type format or not

fparam
[`numpy.ndarray`] frame specific parameters

aparam
[`numpy.ndarray`] atomic specific parameters

real_data
[`dict`, optional] real data to calculate RMS real error

Returns

model_devi
[`numpy.ndarray`, n_frames x 8] Model deviation results. The first column is index of steps, the other 7 columns are max_devi_v, min_devi_v, avg_devi_v, max_devi_f, min_devi_f, avg_devi_f, devi_e.

Examples

```
>>> from deepmd.infer import calc_model_devi
>>> from deepmd.infer import DeepPot as DP
>>> import numpy as np
>>> coord = np.array([[1,0,0], [0,0,1.5], [1,0,3]]).reshape([1, -1])
>>> cell = np.diag(10 * np.ones(3)).reshape([1, -1])
>>> atype = [1,0,1]
>>> graphs = [DP("graph.000.pb"), DP("graph.001.pb")]
>>> model_devi = calc_model_devi(coord, cell, atype, graphs)
```

Submodules

deepmd.infer.data_modifier module

```
class deepmd.infer.data_modifier.DipoleChargeModifier(model_name: str, model_charge_map:
List[float], sys_charge_map: List[float],
ewald_h: float = 1, ewald_beta: float = 1)
```

Bases: *DeepDipole*

Parameters

model_name
The model file for the DeepDipole model

model_charge_map
Gives the amount of charge for the wfcc

sys_charge_map
Gives the amount of charge for the real atoms

ewald_h
Grid spacing of the reciprocal part of Ewald sum. Unit: Å

ewald_beta
Splitting parameter of the Ewald sum. Unit: Å⁻¹

Attributes

model_type
Get type of model.

model_version
Get version of model.

sess
Get TF session.

Methods

| | |
|---|---|
| <code>build_fv_graph()</code> | Build the computational graph for the force and virial inference. |
| <code>eval(coord, box, atype[, eval_fv])</code> | Evaluate the modification. |
| <code>eval_full(coords, cells, atom_types[, ...])</code> | Evaluate the model with interface similar to the energy model. |
| <code>eval_typeebd()</code> | Evaluate output of type embedding network by using this model. |
| <code>get_dim_aparam()</code> | Unsupported in this model. |
| <code>get_dim_fparam()</code> | Unsupported in this model. |
| <code>get_ntypes()</code> | Get the number of atom types of this model. |
| <code>get_rcut()</code> | Get the cut-off radius of this model. |
| <code>get_sel_type()</code> | Get the selected atom types of this model. |
| <code>get_type_map()</code> | Get the type map (element name of the atom types) of this model. |
| <code>make_natoms_vec(atom_types[, mixed_type])</code> | Make the natom vector used by deepmd-kit. |
| <code>modify_data(data, data_sys)</code> | Modify data. |
| <code>reverse_map(vec, imap)</code> | Reverse mapping of a vector according to the index map. |
| <code>sort_input(coord, atom_type[, sel_atoms, ...])</code> | Sort atoms in the system according their types. |

`build_fv_graph()` → Tensor

Build the computational graph for the force and virial inference.

`eval(coord: ndarray, box: ndarray, atype: ndarray, eval_fv: bool = True)` → Tuple[ndarray, ndarray, ndarray]

Evaluate the modification.

Parameters

`coord`

The coordinates of atoms

`box`

The simulation region. PBC is assumed

`atype`

The atom types

`eval_fv`

Evaluate force and virial

Returns

`tot_e`

The energy modification

`tot_f`

The force modification

`tot_v`

The virial modification

`load_prefix: str`

`modify_data(data: dict, data_sys: DeepmdData) → None`

Modify data.

Parameters

`data`

Internal data of DeepmdData. Be a dict, has the following keys - coord coordinates - box simulation box - type atom types - find_energy tells if data has energy - find_force tells if data has force - find_virial tells if data has virial - energy energy - force force - virial virial

`data_sys`

[DeepmdData] The data system.

deepmd.infer.deep_dipole module

```
class deepmd.infer.deep_dipole.DeepDipole(model_file: Path, load_prefix: str = 'load',
                                           default_tf_graph: bool = False)
```

Bases: *DeepTensor*

Constructor.

Parameters

`model_file`

[Path] The name of the frozen model file.

`load_prefix: str`

The prefix in the load computational graph

`default_tf_graph`

[bool] If uses the default tf graph, otherwise build a new tf graph for evaluation

Warning: For developers: DeepTensor initializer must be called at the end after self.tensors are modified because it uses the data in self.tensors dict. Do not change the order!

Attributes

`model_type`

Get type of model.

`model_version`

Get version of model.

`sess`

Get TF session.

Methods

| | |
|---|--|
| <code>eval(coords, cells, atom_types[, atomic, ...])</code> | Evaluate the model. |
| <code>eval_full(coords, cells, atom_types[, ...])</code> | Evaluate the model with interface similar to the energy model. |
| <code>eval_typeebd()</code> | Evaluate output of type embedding network by using this model. |
| <code>get_dim_aparam()</code> | Unsupported in this model. |
| <code>get_dim_fparam()</code> | Unsupported in this model. |
| <code>get_ntypes()</code> | Get the number of atom types of this model. |
| <code>get_rcut()</code> | Get the cut-off radius of this model. |
| <code>get_sel_type()</code> | Get the selected atom types of this model. |
| <code>get_type_map()</code> | Get the type map (element name of the atom types) of this model. |
| <code>make_natoms_vec(atom_types[, mixed_type])</code> | Make the natom vector used by deepmd-kit. |
| <code>reverse_map(vec, imap)</code> | Reverse mapping of a vector according to the index map. |
| <code>sort_input(coord, atom_type[, sel_atoms, ...])</code> | Sort atoms in the system according their types. |

`get_dim_aparam()` → `int`

Unsupported in this model.

`get_dim_fparam()` → `int`

Unsupported in this model.

`load_prefix:` `str`

deepmd.infer.deep_dos module

```
class deepmd.infer.deep_dos.DeepDOS(model_file: Path, load_prefix: str = 'load', default_tf_graph:
    bool = False, auto_batch_size: Union[bool, int, AutomaticBatchSize]
    = True)
```

Bases: *DeepEval*

Constructor.

Parameters

`model_file`

[`Path`] The name of the frozen model file.

`load_prefix:` `str`

The prefix in the load computational graph

`default_tf_graph`

[`bool`] If uses the default tf graph, otherwise build a new tf graph for evaluation

`auto_batch_size`

[`bool` or `int` or `AutomaticBatchSize`, default: `True`] If `True`, automatic batch size will be used. If `int`, it will be used as the initial batch size.

Warning: For developers: DeepTensor initializer must be called at the end after `self.tensors` are modified because it uses the data in `self.tensors` dict. Do not change the order!

Attributes

model_type
Get type of model.

model_version
Get version of model.

sess
Get TF session.

Methods

| | |
|---|--|
| <i>eval</i> (coords, cells, atom_types[, atomic, ...]) | Evaluate the dos, atom_dos by using this model. |
| <i>eval_descriptor</i> (coords, cells, atom_types[, ...]) | Evaluate descriptors by using this DP. |
| <i>eval_typeebd</i> () | Evaluate output of type embedding network by using this model. |
| <i>get_dim_aparam</i> () | Get the number (dimension) of atomic parameters of this DP. |
| <i>get_dim_fparam</i> () | Get the number (dimension) of frame parameters of this DP. |
| <i>get_ntypes</i> () | Get the number of atom types of this model. |
| <i>get_numb_dos</i> () | Get the length of DOS output of this DP model. |
| <i>get_rcut</i> () | Get the cut-off radius of this model. |
| <i>get_sel_type</i> () | Unsupported in this model. |
| <i>get_type_map</i> () | Get the type map (element name of the atom types) of this model. |
| <i>make_natoms_vec</i> (atom_types[, mixed_type]) | Make the natom vector used by deepmd-kit. |
| <i>reverse_map</i> (vec, imap) | Reverse mapping of a vector according to the index map. |
| <i>sort_input</i> (coord, atom_type[, sel_atoms, ...]) | Sort atoms in the system according their types. |

eval(coords: ndarray, cells: ndarray, atom_types: List[int], atomic: bool = False, fparam: Optional[ndarray] = None, aparam: Optional[ndarray] = None, mixed_type: bool = False) → Tuple[ndarray, ...]

Evaluate the dos, atom_dos by using this model.

Parameters

coords
The coordinates of atoms. The array should be of size nframes x natoms x 3

cells
The cell of the region. If None then non-PBC is assumed, otherwise using PBC. The array should be of size nframes x 9

atom_types
The atom types The list should contain natoms ints

atomic
Calculate the atomic energy and virial

fparam
The frame parameter. The array can be of size : - nframes x dim_fparam. - dim_fparam. Then all frames are assumed to be provided with the same fparam.

aparam

The atomic parameter The array can be of size : - nframes x natoms x dim_aparam.
- natoms x dim_aparam. Then all frames are assumed to be provided with the same
aparam. - dim_aparam. Then all frames and atoms are provided with the same
aparam.

mixed_type

Whether to perform the mixed_type mode. If True, the input data has the
mixed_type format (see doc/model/train_se_atten.md), in which frames in a sys-
tem may have different natoms_vec(s), with the same nloc.

Returns

dos

The electron density of state.

atom_dos

The atom-sited density of state. Only returned when atomic == True

eval_descriptor(coords: `ndarray`, cells: `ndarray`, atom_types: `List[int]`, fparam: `Optional[ndarray]`
= None, aparam: `Optional[ndarray]` = None, efield: `Optional[ndarray]` = None,
mixed_type: `bool` = False) → array

Evaluate descriptors by using this DP.

Parameters

coords

The coordinates of atoms. The array should be of size nframes x natoms x 3

cells

The cell of the region. If None then non-PBC is assumed, otherwise using PBC. The
array should be of size nframes x 9

atom_types

The atom types The list should contain natoms ints

fparam

The frame parameter. The array can be of size : - nframes x dim_fparam. -
dim_fparam. Then all frames are assumed to be provided with the same fparam.

aparam

The atomic parameter The array can be of size : - nframes x natoms x dim_aparam.
- natoms x dim_aparam. Then all frames are assumed to be provided with the same
aparam. - dim_aparam. Then all frames and atoms are provided with the same
aparam.

efield

The external field on atoms. The array should be of size nframes x natoms x 3

mixed_type

Whether to perform the mixed_type mode. If True, the input data has the
mixed_type format (see doc/model/train_se_atten.md), in which frames in a sys-
tem may have different natoms_vec(s), with the same nloc.

Returns

descriptor

Descriptors.

get_dim_aparam() → int

Get the number (dimension) of atomic parameters of this DP.

`get_dim_fparam() → int`

Get the number (dimension) of frame parameters of this DP.

`get_ntypes() → int`

Get the number of atom types of this model.

`get_numb_dos() → int`

Get the length of DOS output of this DP model.

`get_rcut() → float`

Get the cut-off radius of this model.

`get_sel_type() → List[int]`

Unsupported in this model.

`get_type_map() → List[str]`

Get the type map (element name of the atom types) of this model.

`load_prefix: str`

deepmd.infer.deep_eval module

```
class deepmd.infer.deep_eval.DeepEval(model_file: Path, load_prefix: str = 'load', default_tf_graph:
    bool = False, auto_batch_size: Union[bool, int,
    AutoBatchSize] = False)
```

Bases: `object`

Common methods for DeepPot, DeepWFC, DeepPolar, ...

Parameters

`model_file`

[Path] The name of the frozen model file.

`load_prefix: str`

The prefix in the load computational graph

`default_tf_graph`

[bool] If uses the default tf graph, otherwise build a new tf graph for evaluation

`auto_batch_size`

[bool or int or AutomaticBatchSize, default: False] If True, automatic batch size will be used. If int, it will be used as the initial batch size.

Attributes

`model_type`

Get type of model.

`model_version`

Get version of model.

`sess`

Get TF session.

Methods

| | |
|---|--|
| <code>eval_typeebd()</code> | Evaluate output of type embedding network by using this model. |
| <code>make_natoms_vec(atom_types[, mixed_type])</code> | Make the natom vector used by deepmd-kit. |
| <code>reverse_map(vec, imap)</code> | Reverse mapping of a vector according to the index map. |
| <code>sort_input(coord, atom_type[, sel_atoms, ...])</code> | Sort atoms in the system according their types. |

`eval_typeebd()` → `ndarray`

Evaluate output of type embedding network by using this model.

Returns

`np.ndarray`

The output of type embedding network. The shape is `[ntypes, o_size]`, where `ntypes` is the number of types, and `o_size` is the number of nodes in the output layer.

Raises

`KeyError`

If the model does not enable type embedding.

See also:

`deepmd.utils.type_embed.TypeEmbedNet`

The type embedding network.

Examples

Get the output of type embedding network of graph.pb:

```
>>> from deepmd.infer import DeepPotential
>>> dp = DeepPotential('graph.pb')
>>> dp.eval_typeebd()
```

`load_prefix:` `str`

`make_natoms_vec(atom_types: ndarray, mixed_type: bool = False)` → `ndarray`

Make the natom vector used by deepmd-kit.

Parameters

`atom_types`

The type of atoms

`mixed_type`

Whether to perform the mixed_type mode. If True, the input data has the mixed_type format (see doc/model/train_se_atten.md), in which frames in a system may have different natoms_vec(s), with the same nloc.

Returns

`natoms`

The number of atoms. This tensor has the length of `Ntypes + 2` `natoms[0]`: number of local atoms `natoms[1]`: total number of atoms held by this processor `natoms[i]`: $2 \leq i < Ntypes+2$, number of type `i` atoms

property `model_type`: `str`

Get type of model.

:type:str

property `model_version`: `str`

Get version of model.

Returns

`str`

version of model

static `reverse_map`(`vec`: `ndarray`, `imap`: `List[int]`) \rightarrow `ndarray`

Reverse mapping of a vector according to the index map.

Parameters

`vec`

Input vector. Be of shape `[nframes, natoms, -1]`

`imap`

Index map. Be of shape `[natoms]`

Returns

`vec_out`

Reverse mapped vector.

property `sess`: `Session`

Get TF session.

static `sort_input`(`coord`: `ndarray`, `atom_type`: `ndarray`, `sel_atoms`: `Optional[List[int]]` = `None`,
`mixed_type`: `bool` = `False`)

Sort atoms in the system according their types.

Parameters

`coord`

The coordinates of atoms. Should be of shape `[nframes, natoms, 3]`

`atom_type`

The type of atoms Should be of shape `[natoms]`

`sel_atoms`

The selected atoms by type

`mixed_type`

Whether to perform the `mixed_type` mode. If `True`, the input data has the `mixed_type` format (see `doc/model/train_se_atten.md`), in which frames in a system may have different `natoms_vec(s)`, with the same `nloc`.

Returns

`coord_out`

The coordinates after sorting

`atom_type_out`

The atom types after sorting

`idx_map`

The index mapping from the input to the output. For example `coord_out = coord[:,idx_map,:]`

sel_atom_type
Only output if sel_atoms is not None The sorted selected atom types

sel_idx_map
Only output if sel_atoms is not None The index mapping from the selected atoms to sorted selected atoms.

deepmd.infer.deep_polar module

```
class deepmd.infer.deep_polar.DeepGlobalPolar(model_file: str, load_prefix: str = 'load',
                                              default_tf_graph: bool = False)
```

Bases: *DeepTensor*

Constructor.

Parameters

model_file
[str] The name of the frozen model file.

load_prefix: str
The prefix in the load computational graph

default_tf_graph
[bool] If uses the default tf graph, otherwise build a new tf graph for evaluation

Attributes

model_type
Get type of model.

model_version
Get version of model.

sess
Get TF session.

Methods

| | |
|--|--|
| <i>eval</i> (coords, cells, atom_types[, atomic, ...]) | Evaluate the model. |
| <i>eval_full</i> (coords, cells, atom_types[, ...]) | Evaluate the model with interface similar to the energy model. |
| <i>eval_typeebd</i> () | Evaluate output of type embedding network by using this model. |
| <i>get_dim_aparam</i> () | Unsupported in this model. |
| <i>get_dim_fparam</i> () | Unsupported in this model. |
| <i>get_ntypes</i> () | Get the number of atom types of this model. |
| <i>get_rcut</i> () | Get the cut-off radius of this model. |
| <i>get_sel_type</i> () | Get the selected atom types of this model. |
| <i>get_type_map</i> () | Get the type map (element name of the atom types) of this model. |
| <i>make_natoms_vec</i> (atom_types[, mixed_type]) | Make the natom vector used by deepmd-kit. |
| <i>reverse_map</i> (vec, imap) | Reverse mapping of a vector according to the index map. |
| <i>sort_input</i> (coord, atom_type[, sel_atoms, ...]) | Sort atoms in the system according their types. |

```
eval(coords: ndarray, cells: ndarray, atom_types: List[int], atomic: bool = False, fparam:
Optional[ndarray] = None, aparam: Optional[ndarray] = None, efield: Optional[ndarray] =
None) → ndarray
```

Evaluate the model.

Parameters

coords

The coordinates of atoms. The array should be of size nframes x natoms x 3

cells

The cell of the region. If None then non-PBC is assumed, otherwise using PBC. The array should be of size nframes x 9

atom_types

The atom types The list should contain natoms ints

atomic

Not used in this model

fparam

Not used in this model

aparam

Not used in this model

efield

Not used in this model

Returns

tensor

The returned tensor If atomic == False then of size nframes x variable_dof else of size nframes x natoms x variable_dof

```
get_dim_aparam() → int
```

Unsupported in this model.

```
get_dim_fparam() → int
```

Unsupported in this model.

```
load_prefix: str
```

```
class deepmd.infer.deep_polar.DeepPolar(model_file: Path, load_prefix: str = 'load',
                                         default_tf_graph: bool = False)
```

Bases: *DeepTensor*

Constructor.

Parameters

model_file

[Path] The name of the frozen model file.

load_prefix: str

The prefix in the load computational graph

default_tf_graph

[bool] If uses the default tf graph, otherwise build a new tf graph for evaluation

Warning: For developers: DeepTensor initializer must be called at the end after self.tensors are modified because it uses the data in self.tensors dict. Do not change the order!

Attributes

model_type
Get type of model.

model_version
Get version of model.

sess
Get TF session.

Methods

| | |
|---|--|
| <code>eval(coords, cells, atom_types[, atomic, ...])</code> | Evaluate the model. |
| <code>eval_full(coords, cells, atom_types[, ...])</code> | Evaluate the model with interface similar to the energy model. |
| <code>eval_typeebd()</code> | Evaluate output of type embedding network by using this model. |
| <code>get_dim_aparam()</code> | Unsupported in this model. |
| <code>get_dim_fparam()</code> | Unsupported in this model. |
| <code>get_ntypes()</code> | Get the number of atom types of this model. |
| <code>get_rcut()</code> | Get the cut-off radius of this model. |
| <code>get_sel_type()</code> | Get the selected atom types of this model. |
| <code>get_type_map()</code> | Get the type map (element name of the atom types) of this model. |
| <code>make_natoms_vec(atom_types[, mixed_type])</code> | Make the natom vector used by deepmd-kit. |
| <code>reverse_map(vec, imap)</code> | Reverse mapping of a vector according to the index map. |
| <code>sort_input(coord, atom_type[, sel_atoms, ...])</code> | Sort atoms in the system according their types. |

`get_dim_aparam() → int`
Unsupported in this model.

`get_dim_fparam() → int`
Unsupported in this model.

`load_prefix: str`

deepmd.infer.deep_pot module

```
class deepmd.infer.deep_pot.DeepPot(model_file: Path, load_prefix: str = 'load', default_tf_graph:
    bool = False, auto_batch_size: Union[bool, int, AutoBatchSize]
    = True)
```

Bases: *DeepEval*

Constructor.

Parameters

model_file
[Path] The name of the frozen model file.

load_prefix: str
The prefix in the load computational graph

default_tf_graph
[bool] If uses the default tf graph, otherwise build a new tf graph for evaluation

auto_batch_size
[bool or int or AutomaticBatchSize, default: True] If True, automatic batch size will be used. If int, it will be used as the initial batch size.

Warning: For developers: DeepTensor initializer must be called at the end after self.tensors are modified because it uses the data in self.tensors dict. Do not change the order!

Examples

```
>>> from deepmd.infer import DeepPot
>>> import numpy as np
>>> dp = DeepPot('graph.pb')
>>> coord = np.array([[1,0,0], [0,0,1.5], [1,0,3]]).reshape([1, -1])
>>> cell = np.diag(10 * np.ones(3)).reshape([1, -1])
>>> atype = [1,0,1]
>>> e, f, v = dp.eval(coord, cell, atype)
```

where e, f and v are predicted energy, force and virial of the system, respectively.

Attributes

model_type
Get type of model.

model_version
Get version of model.

sess
Get TF session.

Methods

| | |
|--|--|
| <code>eval(coords, cells, atom_types[, atomic, ...])</code> | Evaluate the energy, force and virial by using this DP. |
| <code>eval_descriptor(coords, cells, atom_types[, ...])</code> | Evaluate descriptors by using this DP. |
| <code>eval_typeebd()</code> | Evaluate output of type embedding network by using this model. |
| <code>get_descriptor_type()</code> | Get the descriptor type of this model. |
| <code>get_dim_aparam()</code> | Get the number (dimension) of atomic parameters of this DP. |
| <code>get_dim_fparam()</code> | Get the number (dimension) of frame parameters of this DP. |
| <code>get_ntypes()</code> | Get the number of atom types of this model. |
| <code>get_ntypes_spin()</code> | Get the number of spin atom types of this model. |
| <code>get_rcut()</code> | Get the cut-off radius of this model. |
| <code>get_sel_type()</code> | Unsupported in this model. |
| <code>get_type_map()</code> | Get the type map (element name of the atom types) of this model. |
| <code>make_natoms_vec(atom_types[, mixed_type])</code> | Make the natom vector used by deepmd-kit. |
| <code>reverse_map(vec, imap)</code> | Reverse mapping of a vector according to the index map. |
| <code>sort_input(coord, atom_type[, sel_atoms, ...])</code> | Sort atoms in the system according their types. |

eval(coords: `ndarray`, cells: `ndarray`, atom_types: `List[int]`, atomic: `bool` = False, fparam: `Optional[ndarray]` = None, aparam: `Optional[ndarray]` = None, efield: `Optional[ndarray]` = None, mixed_type: `bool` = False) → `Tuple[ndarray, ...]`

Evaluate the energy, force and virial by using this DP.

Parameters

coords

The coordinates of atoms. The array should be of size nframes x natoms x 3

cells

The cell of the region. If None then non-PBC is assumed, otherwise using PBC. The array should be of size nframes x 9

atom_types

The atom types The list should contain natoms ints

atomic

Calculate the atomic energy and virial

fparam

The frame parameter. The array can be of size : - nframes x dim_fparam. - dim_fparam. Then all frames are assumed to be provided with the same fparam.

aparam

The atomic parameter The array can be of size : - nframes x natoms x dim_aparam. - natoms x dim_aparam. Then all frames are assumed to be provided with the same aparam. - dim_aparam. Then all frames and atoms are provided with the same aparam.

efield

The external field on atoms. The array should be of size nframes x natoms x 3

mixed_type

Whether to perform the mixed_type mode. If True, the input data has the mixed_type format (see doc/model/train_se_atten.md), in which frames in a system may have different natoms_vec(s), with the same nloc.

Returns

energy

The system energy.

force

The force on each atom

virial

The virial

atom_energy

The atomic energy. Only returned when atomic == True

atom_virial

The atomic virial. Only returned when atomic == True

eval_descriptor(coords: ndarray, cells: ndarray, atom_types: List[int], fparam: Optional[ndarray] = None, aparam: Optional[ndarray] = None, efield: Optional[ndarray] = None, mixed_type: bool = False) → array

Evaluate descriptors by using this DP.

Parameters

coords

The coordinates of atoms. The array should be of size nframes x natoms x 3

cells

The cell of the region. If None then non-PBC is assumed, otherwise using PBC. The array should be of size nframes x 9

atom_types

The atom types The list should contain natoms ints

fparam

The frame parameter. The array can be of size : - nframes x dim_fparam. - dim_fparam. Then all frames are assumed to be provided with the same fparam.

aparam

The atomic parameter The array can be of size : - nframes x natoms x dim_aparam. - natoms x dim_aparam. Then all frames are assumed to be provided with the same aparam. - dim_aparam. Then all frames and atoms are provided with the same aparam.

efield

The external field on atoms. The array should be of size nframes x natoms x 3

mixed_type

Whether to perform the mixed_type mode. If True, the input data has the mixed_type format (see doc/model/train_se_atten.md), in which frames in a system may have different natoms_vec(s), with the same nloc.

Returns

descriptor

Descriptors.

```

get_descriptor_type() → List[int]
    Get the descriptor type of this model.

get_dim_aparam() → int
    Get the number (dimension) of atomic parameters of this DP.

get_dim_fparam() → int
    Get the number (dimension) of frame parameters of this DP.

get_ntypes() → int
    Get the number of atom types of this model.

get_ntypes_spin()
    Get the number of spin atom types of this model.

get_rcut() → float
    Get the cut-off radius of this model.

get_sel_type() → List[int]
    Unsupported in this model.

get_type_map() → List[str]
    Get the type map (element name of the atom types) of this model.

load_prefix: str

```

deepmd.infer.deep_tensor module

```

class deepmd.infer.deep_tensor.DeepTensor(model_file: Path, load_prefix: str = 'load',
                                           default_tf_graph: bool = False)

```

Bases: *DeepEval*

Evaluates a tensor model.

Parameters

- `model_file`: str
The name of the frozen model file.
- `load_prefix`: str
The prefix in the load computational graph
- `default_tf_graph`
[bool] If uses the default tf graph, otherwise build a new tf graph for evaluation

Attributes

- `model_type`
Get type of model.
- `model_version`
Get version of model.
- `sess`
Get TF session.

Methods

| | |
|---|--|
| <code>eval(coords, cells, atom_types[, atomic, ...])</code> | Evaluate the model. |
| <code>eval_full(coords, cells, atom_types[, ...])</code> | Evaluate the model with interface similar to the energy model. |
| <code>eval_typeebd()</code> | Evaluate output of type embedding network by using this model. |
| <code>get_dim_aparam()</code> | Get the number (dimension) of atomic parameters of this DP. |
| <code>get_dim_fparam()</code> | Get the number (dimension) of frame parameters of this DP. |
| <code>get_ntypes()</code> | Get the number of atom types of this model. |
| <code>get_rcut()</code> | Get the cut-off radius of this model. |
| <code>get_sel_type()</code> | Get the selected atom types of this model. |
| <code>get_type_map()</code> | Get the type map (element name of the atom types) of this model. |
| <code>make_natoms_vec(atom_types[, mixed_type])</code> | Make the natom vector used by deepmd-kit. |
| <code>reverse_map(vec, imap)</code> | Reverse mapping of a vector according to the index map. |
| <code>sort_input(coord, atom_type[, sel_atoms, ...])</code> | Sort atoms in the system according their types. |

eval(coords: `ndarray`, cells: `ndarray`, atom_types: `List[int]`, atomic: `bool` = True, fparam: `Optional[ndarray]` = None, aparam: `Optional[ndarray]` = None, efield: `Optional[ndarray]` = None, mixed_type: `bool` = False) → `ndarray`

Evaluate the model.

Parameters

coords

The coordinates of atoms. The array should be of size nframes x natoms x 3

cells

The cell of the region. If None then non-PBC is assumed, otherwise using PBC. The array should be of size nframes x 9

atom_types

The atom types The list should contain natoms ints

atomic

If True (default), return the atomic tensor Otherwise return the global tensor

fparam

Not used in this model

aparam

Not used in this model

efield

Not used in this model

mixed_type

Whether to perform the mixed_type mode. If True, the input data has the mixed_type format (see doc/model/train_se_atten.md), in which frames in a system may have different natoms_vec(s), with the same nloc.

Returns

tensor

The returned tensor If `atomic == False` then of size `nframes x output_dim` else of size `nframes x natoms x output_dim`

eval_full(coords: `ndarray`, cells: `ndarray`, atom_types: `List[int]`, atomic: `bool` = `False`, fparam: `Optional[array]` = `None`, aparam: `Optional[array]` = `None`, efield: `Optional[array]` = `None`, mixed_type: `bool` = `False`) → `Tuple[ndarray, ...]`

Evaluate the model with interface similar to the energy model. Will return global tensor, component-wise force and virial and optionally atomic tensor and atomic virial.

Parameters

coords

The coordinates of atoms. The array should be of size `nframes x natoms x 3`

cells

The cell of the region. If `None` then non-PBC is assumed, otherwise using PBC. The array should be of size `nframes x 9`

atom_types

The atom types The list should contain `natoms` ints

atomic

Whether to calculate atomic tensor and virial

fparam

Not used in this model

aparam

Not used in this model

efield

Not used in this model

mixed_type

Whether to perform the `mixed_type` mode. If `True`, the input data has the `mixed_type` format (see `doc/model/train_se_atten.md`), in which frames in a system may have different `natoms_vec(s)`, with the same `nloc`.

Returns

tensor

The global tensor. shape: `[nframes x nout]`

force

The component-wise force (negative derivative) on each atom. shape: `[nframes x nout x natoms x 3]`

virial

The component-wise virial of the tensor. shape: `[nframes x nout x 9]`

atom_tensor

The atomic tensor. Only returned when `atomic == True` shape: `[nframes x natoms x nout]`

atom_virial

The atomic virial. Only returned when `atomic == True` shape: `[nframes x nout x natoms x 9]`

get_dim_aparam() → `int`

Get the number (dimension) of atomic parameters of this DP.

`get_dim_fparam() → int`

Get the number (dimension) of frame parameters of this DP.

`get_ntypes() → int`

Get the number of atom types of this model.

`get_rcut() → float`

Get the cut-off radius of this model.

`get_sel_type() → List[int]`

Get the selected atom types of this model.

`get_type_map() → List[str]`

Get the type map (element name of the atom types) of this model.

`load_prefix: str`

```
tensors = {'t_box': 't_box:0', 't_coord': 't_coord:0', 't_mesh': 't_mesh:0',
't_natoms': 't_natoms:0', 't_ntypes': 'descript_attr/ntypes:0', 't_output_dim':
'model_attr/output_dim:0', 't_rcut': 'descript_attr/rcut:0', 't_sel_type':
'model_attr/sel_type:0', 't_tmap': 'model_attr/tmap:0', 't_type': 't_type:0'}
```

deepmd.infer.deep_wfc module

```
class deepmd.infer.deep_wfc.DeepWFC(model_file: Path, load_prefix: str = 'load', default_tf_graph:
    bool = False)
```

Bases: *DeepTensor*

Constructor.

Parameters

`model_file`

[Path] The name of the frozen model file.

`load_prefix: str`

The prefix in the load computational graph

`default_tf_graph`

[bool] If uses the default tf graph, otherwise build a new tf graph for evaluation

Warning: For developers: DeepTensor initializer must be called at the end after self.tensors are modified because it uses the data in self.tensors dict. Do not change the order!

Attributes

`model_type`

Get type of model.

`model_version`

Get version of model.

`sess`

Get TF session.

Methods

| | |
|---|--|
| <code>eval(coords, cells, atom_types[, atomic, ...])</code> | Evaluate the model. |
| <code>eval_full(coords, cells, atom_types[, ...])</code> | Evaluate the model with interface similar to the energy model. |
| <code>eval_typeebd()</code> | Evaluate output of type embedding network by using this model. |
| <code>get_dim_aparam()</code> | Unsupported in this model. |
| <code>get_dim_fparam()</code> | Unsupported in this model. |
| <code>get_ntypes()</code> | Get the number of atom types of this model. |
| <code>get_rcut()</code> | Get the cut-off radius of this model. |
| <code>get_sel_type()</code> | Get the selected atom types of this model. |
| <code>get_type_map()</code> | Get the type map (element name of the atom types) of this model. |
| <code>make_natoms_vec(atom_types[, mixed_type])</code> | Make the natom vector used by deepmd-kit. |
| <code>reverse_map(vec, imap)</code> | Reverse mapping of a vector according to the index map. |
| <code>sort_input(coord, atom_type[, sel_atoms, ...])</code> | Sort atoms in the system according their types. |

`get_dim_aparam() → int`
 Unsupported in this model.

`get_dim_fparam() → int`
 Unsupported in this model.

`load_prefix: str`

deepmd.infer.ewald_recip module

`class deepmd.infer.ewald_recip.EwaldRecp(hh, beta)`

Bases: `object`

Evaluate the reciprocal part of the Ewald sum.

Methods

| | |
|---------------------------------------|-----------|
| <code>eval(coord, charge, box)</code> | Evaluate. |
|---------------------------------------|-----------|

`eval(coord: ndarray, charge: ndarray, box: ndarray) → Tuple[ndarray, ndarray, ndarray]`

Evaluate.

Parameters

`coord`
 The coordinates of atoms

`charge`
 The atomic charge

`box`
 The simulation region. PBC is assumed

Returns

e
The energy

f
The force

v
The virial

deepmd.infer.model_devi module

```
deepmd.infer.model_devi.calc_model_devi(coord, box, atype, models, fname=None, frequency=1,
                                         mixed_type=False, fparam: Optional[ndarray] = None,
                                         aparam: Optional[ndarray] = None, real_data:
                                         Optional[dict] = None)
```

Python interface to calculate model deviation.

Parameters

coord
[`numpy.ndarray`, n_frames x n_atoms x 3] Coordinates of system to calculate

box
[`numpy.ndarray` or `None`, n_frames x 3 x 3] Box to specify periodic boundary condition. If `None`, no pbc will be used

atype
[`numpy.ndarray`, n_atoms x 1] Atom types

models
[`list` of DeepPot models] Models used to evaluate deviation

fname
[`str` or `None`] File to dump results, default `None`

frequency
[`int`] Steps between frames (if the system is given by molecular dynamics engine), default 1

mixed_type
[`bool`] Whether the input atype is in mixed_type format or not

fparam
[`numpy.ndarray`] frame specific parameters

aparam
[`numpy.ndarray`] atomic specific parameters

real_data
[`dict`, `optional`] real data to calculate RMS real error

Returns

model_devi
[`numpy.ndarray`, n_frames x 8] Model deviation results. The first column is index of steps, the other 7 columns are max_devi_v, min_devi_v, avg_devi_v, max_devi_f, min_devi_f, avg_devi_f, devi_e.

Examples

```

>>> from deepmd.infer import calc_model_devi
>>> from deepmd.infer import DeepPot as DP
>>> import numpy as np
>>> coord = np.array([[1,0,0], [0,0,1.5], [1,0,3]]).reshape([1, -1])
>>> cell = np.diag(10 * np.ones(3)).reshape([1, -1])
>>> atype = [1,0,1]
>>> graphs = [DP("graph.000.pb"), DP("graph.001.pb")]
>>> model_devi = calc_model_devi(coord, cell, atype, graphs)

```

`deepmd.infer.model_devi.calc_model_devi_e`(es: `ndarray`, real_e: `Optional[ndarray]` = None) → `ndarray`

Calculate model deviation of total energy per atom.

Here we don't use the atomic energy, as the decomposition of energy is arbitrary and not unique. There is no fitting target for atomic energy.

Parameters

es

[`numpy.ndarray`] size of 'n_models x n_frames x 1

real_e

[`numpy.ndarray`] real energy, size of n_frames x 1. If given, the RMS real error is calculated instead.

Returns

max_devi_e

[`numpy.ndarray`] maximum deviation of energy

`deepmd.infer.model_devi.calc_model_devi_f`(fs: `ndarray`, real_f: `Optional[ndarray]` = None) → `Tuple[ndarray]`

Calculate model deviation of force.

Parameters

fs

[`numpy.ndarray`] size of n_models x n_frames x n_atoms x 3

real_f

[`numpy.ndarray` or `None`] real force, size of n_frames x n_atoms x 3. If given, the RMS real error is calculated instead.

Returns

max_devi_f

[`numpy.ndarray`] maximum deviation of force in all atoms

min_devi_f

[`numpy.ndarray`] minimum deviation of force in all atoms

avg_devi_f

[`numpy.ndarray`] average deviation of force in all atoms

`deepmd.infer.model_devi.calc_model_devi_v`(vs: `ndarray`, real_v: `Optional[ndarray]` = None) → `Tuple[ndarray]`

Calculate model deviation of virial.

Parameters

vs
[`numpy.ndarray`] size of `n_models` x `n_frames` x 9

real_v
[`numpy.ndarray`] real virial, size of `n_frames` x 9. If given, the RMS real error is calculated instead.

Returns

max_devi_v
[`numpy.ndarray`] maximum deviation of virial in 9 elements

min_devi_v
[`numpy.ndarray`] minimum deviation of virial in 9 elements

avg_devi_v
[`numpy.ndarray`] average deviation of virial in 9 elements

`deepmd.infer.model_devi.make_model_devi(*, models: list, system: str, set_prefix: str, output: str, frequency: int, real_error: bool = False, **kwargs)`

Make model deviation calculation.

Parameters

models
[`list`] A list of paths of models to use for making model deviation

system
[`str`] The path of system to make model deviation calculation

set_prefix
[`str`] The set prefix of the system

output
[`str`] The output file for model deviation results

frequency
[`int`] The number of steps that elapse between writing coordinates in a trajectory by a MD engine (such as Gromacs / Lammmps). This paramter is used to determine the index in the output file.

real_error
[`bool`, default: `False`] If True, calculate the RMS real error instead of model deviation.

**kwargs
Arbitrary keyword arguments.

`deepmd.infer.model_devi.write_model_devi_out(devi: ndarray, fname: str, header: str = "")`

Write output of model deviation.

Parameters

devi
[`numpy.ndarray`] the first column is the steps index

fname
[`str`] the file name to dump

header
[`str`, default=""] the header to dump

deepmd.loggers package

Module taking care of logging duties.

`deepmd.loggers.set_log_handles`(level: `int`, log_path: `Optional[Path]` = `None`, mpi_log: `Optional[str]` = `None`)

Set desired level for package loggers and add file handlers.

Parameters

level

[`int`] logging level

log_path

[`Optional[str]`] path to log file, if `None` logs will be send only to console. If the parent directory does not exist it will be automatically created, by default `None`

mpi_log

[`Optional[str]`, `optional`] mpi log type. Has three options. master will output logs to file and console only from rank==0. collect will write messages from all ranks to one file opened under rank==0 and to console. workers will open one log file for each worker designated by its rank, console behaviour is the same as for collect. If this argument is specified, package 'mpi4py' must be already installed. by default `None`

Raises

RuntimeError

If the argument `mpi_log` is specified, package `mpi4py` is not installed.

Notes

Logging levels:

| | our notation | python logging | tensorflow cpp | OpenMP |
|---------|--------------|----------------|----------------|----------------|
| debug | 10 | 10 | 0 | 1/on/true/yes |
| info | 20 | 20 | 1 | 0/off/false/no |
| warning | 30 | 30 | 2 | 0/off/false/no |
| error | 40 | 40 | 3 | 0/off/false/no |

References

<https://groups.google.com/g/mpi4py/c/SaNzc8bdj6U> <https://stackoverflow.com/questions/35869137/avoid-tensorflow-print-on-standard-error>
<https://stackoverflow.com/questions/56085015/suppress-openmp-debug-messages-when-running-tensorflow-on-cpu>

Submodules

deepmd.loggers.loggers module

Logger initialization for package.

```
deepmd.loggers.loggers.set_log_handles(level: int, log_path: Optional[Path] = None, mpi_log:
                                     Optional[str] = None)
```

Set desired level for package loggers and add file handlers.

Parameters

level

[int] logging level

log_path

[Optional[str]] path to log file, if None logs will be send only to console. If the parent directory does not exist it will be automatically created, by default None

mpi_log

[Optional[str], optional] mpi log type. Has three options. master will output logs to file and console only from rank==0. collect will write messages from all ranks to one file opened under rank==0 and to console. workers will open one log file for each worker designated by its rank, console behaviour is the same as for collect. If this argument is specified, package 'mpi4py' must be already installed. by default None

Raises

RuntimeError

If the argument mpi_log is specified, package mpi4py is not installed.

Notes

Logging levels:

| | our notation | python logging | tensorflow cpp | OpenMP |
|---------|--------------|----------------|----------------|----------------|
| debug | 10 | 10 | 0 | 1/on/true/yes |
| info | 20 | 20 | 1 | 0/off/false/no |
| warning | 30 | 30 | 2 | 0/off/false/no |
| error | 40 | 40 | 3 | 0/off/false/no |

References

<https://groups.google.com/g/mpi4py/c/SaNzc8bdj6U>

[avoid-tensorflow-print-on-standard-error](https://groups.google.com/g/mpi4py/c/SaNzc8bdj6U/avoid-tensorflow-print-on-standard-error)

[suppress-openmp-debug-messages-when-running-tensorflow-on-cpu](https://groups.google.com/g/mpi4py/c/SaNzc8bdj6U/suppress-openmp-debug-messages-when-running-tensorflow-on-cpu)

<https://stackoverflow.com/questions/35869137/>

<https://stackoverflow.com/questions/56085015/>

deepmd.loss package

```
class deepmd.loss.DOSLoss(starter_learning_rate: float, numb_dos: int = 500, start_pref_dos: float =
    1.0, limit_pref_dos: float = 1.0, start_pref_cdf: float = 1000, limit_pref_cdf:
    float = 1.0, start_pref_adof: float = 0.0, limit_pref_adof: float = 0.0,
    start_pref_acdf: float = 0.0, limit_pref_acdf: float = 0.0, protect_value:
    float = 1e-08, log_fit: bool = False, **kwargs)
```

Bases: *Loss*

Loss function for DeepDOS models.

Methods

| | |
|---|--------------------------------|
| <i>build</i> (learning_rate, natoms, model_dict, ...) | Build the loss function graph. |
| <i>eval</i> (sess, feed_dict, natoms) | Eval the loss function. |

build(learning_rate, natoms, model_dict, label_dict, suffix)

Build the loss function graph.

Parameters

learning_rate

[*tf.Tensor*] learning rate

natoms

[*tf.Tensor*] number of atoms

model_dict

[*dict*[*str*, *tf.Tensor*]] A dictionary that maps model keys to tensors

label_dict

[*dict*[*str*, *tf.Tensor*]] A dictionary that maps label keys to tensors

suffix

[*str*] suffix

Returns

tf.Tensor

the total squared loss

dict[*str*, *tf.Tensor*]

A dictionary that maps loss keys to more loss tensors

eval(sess, feed_dict, natoms)

Eval the loss function.

Parameters

sess

[*tf.Session*] TensorFlow session

feed_dict

[*dict*[*tf.placeholder*, *tf.Tensor*]] A dictionary that maps graph elements to values

natoms

[*tf.Tensor*] number of atoms

Returns

dict

A dictionary that maps keys to values. It should contain key `natoms`

```
class deepmd.loss.EnerDipoleLoss(starter_learning_rate: float, start_pref_e: float = 0.1, limit_pref_e:
                                float = 1.0, start_pref_ed: float = 1.0, limit_pref_ed: float = 1.0)
```

Bases: *Loss*

Methods

| | |
|---|--------------------------------|
| <i>build</i> (learning_rate, natoms, model_dict, ...) | Build the loss function graph. |
| <i>eval</i> (sess, feed_dict, natoms) | Eval the loss function. |

build(learning_rate, natoms, model_dict, label_dict, suffix)

Build the loss function graph.

Parameters

learning_rate

[**tf.Tensor**] learning rate

natoms

[**tf.Tensor**] number of atoms

model_dict

[**dict**[**str**, **tf.Tensor**]] A dictionary that maps model keys to tensors

label_dict

[**dict**[**str**, **tf.Tensor**]] A dictionary that maps label keys to tensors

suffix

[**str**] suffix

Returns

tf.Tensor

the total squared loss

dict[**str**, **tf.Tensor**]

A dictionary that maps loss keys to more loss tensors

eval(sess, feed_dict, natoms)

Eval the loss function.

Parameters

sess

[**tf.Session**] TensorFlow session

feed_dict

[**dict**[**tf.placeholder**, **tf.Tensor**]] A dictionary that maps graph elements to values

natoms

[**tf.Tensor**] number of atoms

Returns

`dict`

A dictionary that maps keys to values. It should contain key `natoms`

```
class deepmd.loss.EnerSpinLoss(starter_learning_rate: float, start_pref_e: float = 0.02, limit_pref_e:
    float = 1.0, start_pref_fr: float = 1000, limit_pref_fr: float = 1.0,
    start_pref_fm: float = 10000, limit_pref_fm: float = 10.0,
    start_pref_v: float = 0.0, limit_pref_v: float = 0.0, start_pref_ae: float
    = 0.0, limit_pref_ae: float = 0.0, start_pref_pf: float = 0.0,
    limit_pref_pf: float = 0.0, relative_f: Optional[float] = None,
    enable_atom_ener_coeff: bool = False, use_spin: Optional[list] =
    None)
```

Bases: `Loss`

Methods

| | |
|--|--------------------------------|
| <code>build(learning_rate, natoms, model_dict, ...)</code> | Build the loss function graph. |
| <code>eval(sess, feed_dict, natoms)</code> | Eval the loss function. |

| | |
|--------------------------------|--|
| <code>print_header</code> | |
| <code>print_on_training</code> | |

build(learning_rate, natoms, model_dict, label_dict, suffix)

Build the loss function graph.

Parameters

`learning_rate`

`[tf.Tensor]` learning rate

`natoms`

`[tf.Tensor]` number of atoms

`model_dict`

`[dict[str, tf.Tensor]]` A dictionary that maps model keys to tensors

`label_dict`

`[dict[str, tf.Tensor]]` A dictionary that maps label keys to tensors

`suffix`

`[str]` suffix

Returns

`tf.Tensor`

the total squared loss

`dict[str, tf.Tensor]`

A dictionary that maps loss keys to more loss tensors

eval(sess, feed_dict, natoms)

Eval the loss function.

Parameters

`sess`

`[tf.Session]` TensorFlow session

```

    feed_dict
        [dict[tf.placeholder, tf.Tensor]] A dictionary that maps graph elements to values
    natoms
        [tf.Tensor] number of atoms
Returns
    dict
        A dictionary that maps keys to values. It should contain key natoms
print_header()

print_on_training(tb_writer, cur_batch, sess, natoms, feed_dict_test, feed_dict_batch)

class deepmd.loss.EnerStdLoss(starter_learning_rate: float, start_pref_e: float = 0.02, limit_pref_e:
    float = 1.0, start_pref_f: float = 1000, limit_pref_f: float = 1.0,
    start_pref_v: float = 0.0, limit_pref_v: float = 0.0, start_pref_ae: float
    = 0.0, limit_pref_ae: float = 0.0, start_pref_pf: float = 0.0,
    limit_pref_pf: float = 0.0, relative_f: Optional[float] = None,
    enable_atom_ener_coeff: bool = False, start_pref_gf: float = 0.0,
    limit_pref_gf: float = 0.0, numb_generalized_coord: int = 0, **kwargs)

```

Bases: *Loss*

Standard loss function for DP models.

Parameters

```

    starter_learning_rate
        [float] The learning rate at the start of the training.
    start_pref_e
        [float] The prefactor of energy loss at the start of the training.
    limit_pref_e
        [float] The prefactor of energy loss at the end of the training.
    start_pref_f
        [float] The prefactor of force loss at the start of the training.
    limit_pref_f
        [float] The prefactor of force loss at the end of the training.
    start_pref_v
        [float] The prefactor of virial loss at the start of the training.
    limit_pref_v
        [float] The prefactor of virial loss at the end of the training.
    start_pref_ae
        [float] The prefactor of atomic energy loss at the start of the training.
    limit_pref_ae
        [float] The prefactor of atomic energy loss at the end of the training.
    start_pref_pf
        [float] The prefactor of atomic prefactor force loss at the start of the training.
    limit_pref_pf
        [float] The prefactor of atomic prefactor force loss at the end of the training.

```


relative_f
 [float] If provided, relative force error will be used in the loss. The difference of force will be normalized by the magnitude of the force in the label with a shift given by relative_f

enable_atom_ener_coeff
 [bool] if true, the energy will be computed as $\sum_i c_i E_i$

start_pref_gf
 [float] The prefactor of generalized force loss at the start of the training.

limit_pref_gf
 [float] The prefactor of generalized force loss at the end of the training.

numb_generalized_coord
 [int] The dimension of generalized coordinates.

**kwargs
 Other keyword arguments.

Methods

| | |
|---|--------------------------------|
| <i>build</i> (learning_rate, natoms, model_dict, ...) | Build the loss function graph. |
| <i>eval</i> (sess, feed_dict, natoms) | Eval the loss function. |

build(learning_rate, natoms, model_dict, label_dict, suffix)

Build the loss function graph.

Parameters

learning_rate
 [tf.Tensor] learning rate

natoms
 [tf.Tensor] number of atoms

model_dict
 [dict[str, tf.Tensor]] A dictionary that maps model keys to tensors

label_dict
 [dict[str, tf.Tensor]] A dictionary that maps label keys to tensors

suffix
 [str] suffix

Returns

tf.Tensor
 the total squared loss

dict[str, tf.Tensor]
 A dictionary that maps loss keys to more loss tensors

eval(sess, feed_dict, natoms)

Eval the loss function.

Parameters

sess
 [tf.Session] TensorFlow session

`feed_dict`
 [dict[tf.placeholder, tf.Tensor]] A dictionary that maps graph elements to values

`natoms`
 [tf.Tensor] number of atoms

Returns

`dict`
 A dictionary that maps keys to values. It should contain key `natoms`

`class deepmd.loss.TensorLoss(jdata, **kwargs)`

Bases: *Loss*

Loss function for tensorial properties.

Methods

| | |
|---|--------------------------------|
| <code>build</code> (learning_rate, natoms, model_dict, ...) | Build the loss function graph. |
| <code>eval</code> (sess, feed_dict, natoms) | Eval the loss function. |

`build`(learning_rate, natoms, model_dict, label_dict, suffix)

Build the loss function graph.

Parameters

`learning_rate`
 [tf.Tensor] learning rate

`natoms`
 [tf.Tensor] number of atoms

`model_dict`
 [dict[str, tf.Tensor]] A dictionary that maps model keys to tensors

`label_dict`
 [dict[str, tf.Tensor]] A dictionary that maps label keys to tensors

`suffix`
 [str] suffix

Returns

`tf.Tensor`
 the total squared loss

`dict[str, tf.Tensor]`
 A dictionary that maps loss keys to more loss tensors

`eval`(sess, feed_dict, natoms)

Eval the loss function.

Parameters

`sess`
 [tf.Session] TensorFlow session

`feed_dict`
 [dict[tf.placeholder, tf.Tensor]] A dictionary that maps graph elements to values

natoms
 [`tf.Tensor`] number of atoms

Returns

`dict`
 A dictionary that maps keys to values. It should contain key `natoms`

Submodules

deepmd.loss.dos module

```
class deepmd.loss.dos.DOSLoss(starter_learning_rate: float, numb_dos: int = 500, start_pref_dos: float
                               = 1.0, limit_pref_dos: float = 1.0, start_pref_cdf: float = 1000,
                               limit_pref_cdf: float = 1.0, start_pref_adof: float = 0.0,
                               limit_pref_adof: float = 0.0, start_pref_acdf: float = 0.0,
                               limit_pref_acdf: float = 0.0, protect_value: float = 1e-08, log_fit: bool
                               = False, **kwargs)
```

Bases: `Loss`

Loss function for DeepDOS models.

Methods

| | |
|---|--------------------------------|
| <code>build</code> (learning_rate, natoms, model_dict, ...) | Build the loss function graph. |
| <code>eval</code> (sess, feed_dict, natoms) | Eval the loss function. |

`build`(learning_rate, natoms, model_dict, label_dict, suffix)

Build the loss function graph.

Parameters

learning_rate
 [`tf.Tensor`] learning rate

natoms
 [`tf.Tensor`] number of atoms

model_dict
 [`dict[str, tf.Tensor]`] A dictionary that maps model keys to tensors

label_dict
 [`dict[str, tf.Tensor]`] A dictionary that maps label keys to tensors

suffix
 [`str`] suffix

Returns

`tf.Tensor`
 the total squared loss

`dict[str, tf.Tensor]`
 A dictionary that maps loss keys to more loss tensors

`eval(sess, feed_dict, natoms)`

Eval the loss function.

Parameters

`sess`

[`tf.Session`] TensorFlow session

`feed_dict`

[`dict`[`tf.placeholder`, `tf.Tensor`]] A dictionary that maps graph elements to values

`natoms`

[`tf.Tensor`] number of atoms

Returns

`dict`

A dictionary that maps keys to values. It should contain key `natoms`

deepmd.loss.ener module

```
class deepmd.loss.ener.EnerDipoleLoss(starter_learning_rate: float, start_pref_e: float = 0.1,
                                      limit_pref_e: float = 1.0, start_pref_ed: float = 1.0,
                                      limit_pref_ed: float = 1.0)
```

Bases: *Loss*

Methods

| | |
|---|--------------------------------|
| <i>build</i> (learning_rate, natoms, model_dict, ...) | Build the loss function graph. |
| <i>eval</i> (sess, feed_dict, natoms) | Eval the loss function. |

`build(learning_rate, natoms, model_dict, label_dict, suffix)`

Build the loss function graph.

Parameters

`learning_rate`

[`tf.Tensor`] learning rate

`natoms`

[`tf.Tensor`] number of atoms

`model_dict`

[`dict`[`str`, `tf.Tensor`]] A dictionary that maps model keys to tensors

`label_dict`

[`dict`[`str`, `tf.Tensor`]] A dictionary that maps label keys to tensors

`suffix`

[`str`] suffix

Returns

`tf.Tensor`

the total squared loss

`dict[str, tf.Tensor]`

A dictionary that maps loss keys to more loss tensors

`eval(sess, feed_dict, natoms)`

Eval the loss function.

Parameters

`sess`

`[tf.Session]` TensorFlow session

`feed_dict`

`[dict[tf.placeholder, tf.Tensor]]` A dictionary that maps graph elements to values

`natoms`

`[tf.Tensor]` number of atoms

Returns

`dict`

A dictionary that maps keys to values. It should contain key `natoms`

```
class deepmd.loss.ener.EnerSpinLoss(starter_learning_rate: float, start_pref_e: float = 0.02,
                                     limit_pref_e: float = 1.0, start_pref_fr: float = 1000,
                                     limit_pref_fr: float = 1.0, start_pref_fm: float = 10000,
                                     limit_pref_fm: float = 10.0, start_pref_v: float = 0.0,
                                     limit_pref_v: float = 0.0, start_pref_ae: float = 0.0,
                                     limit_pref_ae: float = 0.0, start_pref_pf: float = 0.0,
                                     limit_pref_pf: float = 0.0, relative_f: Optional[float] = None,
                                     enable_atom_ener_coeff: bool = False, use_spin: Optional[list]
                                     = None)
```

Bases: *Loss*

Methods

| | |
|--|--------------------------------|
| <code>build(learning_rate, natoms, model_dict, ...)</code> | Build the loss function graph. |
| <code>eval(sess, feed_dict, natoms)</code> | Eval the loss function. |

| | |
|--------------------------------|--|
| <code>print_header</code> | |
| <code>print_on_training</code> | |

`build(learning_rate, natoms, model_dict, label_dict, suffix)`

Build the loss function graph.

Parameters

`learning_rate`

`[tf.Tensor]` learning rate

`natoms`

`[tf.Tensor]` number of atoms

`model_dict`

`[dict[str, tf.Tensor]]` A dictionary that maps model keys to tensors

```

    label_dict
        [dict[str, tf.Tensor]] A dictionary that maps label keys to tensors
    suffix
        [str] suffix
Returns
    tf.Tensor
        the total squared loss
    dict[str, tf.Tensor]
        A dictionary that maps loss keys to more loss tensors
eval(sess, feed_dict, natoms)
    Eval the loss function.
Parameters
    sess
        [tf.Session] TensorFlow session
    feed_dict
        [dict[tf.placeholder, tf.Tensor]] A dictionary that maps graph elements to values
    natoms
        [tf.Tensor] number of atoms
Returns
    dict
        A dictionary that maps keys to values. It should contain key natoms
print_header()
print_on_training(tb_writer, cur_batch, sess, natoms, feed_dict_test, feed_dict_batch)
class deepmd.loss.ener.EnerStdLoss(starter_learning_rate: float, start_pref_e: float = 0.02,
                                   limit_pref_e: float = 1.0, start_pref_f: float = 1000, limit_pref_f:
                                   float = 1.0, start_pref_v: float = 0.0, limit_pref_v: float = 0.0,
                                   start_pref_ae: float = 0.0, limit_pref_ae: float = 0.0,
                                   start_pref_pf: float = 0.0, limit_pref_pf: float = 0.0, relative_f:
                                   Optional[float] = None, enable_atom_ener_coeff: bool = False,
                                   start_pref_gf: float = 0.0, limit_pref_gf: float = 0.0,
                                   numb_generalized_coord: int = 0, **kwargs)
Bases: Loss
Standard loss function for DP models.
Parameters
    starter_learning_rate
        [float] The learning rate at the start of the training.
    start_pref_e
        [float] The prefactor of energy loss at the start of the training.
    limit_pref_e
        [float] The prefactor of energy loss at the end of the training.
    start_pref_f
        [float] The prefactor of force loss at the start of the training.

```

`limit_pref_f`
`[float]` The prefactor of force loss at the end of the training.

`start_pref_v`
`[float]` The prefactor of virial loss at the start of the training.

`limit_pref_v`
`[float]` The prefactor of virial loss at the end of the training.

`start_pref_ae`
`[float]` The prefactor of atomic energy loss at the start of the training.

`limit_pref_ae`
`[float]` The prefactor of atomic energy loss at the end of the training.

`start_pref_pf`
`[float]` The prefactor of atomic prefactor force loss at the start of the training.

`limit_pref_pf`
`[float]` The prefactor of atomic prefactor force loss at the end of the training.

`relative_f`
`[float]` If provided, relative force error will be used in the loss. The difference of force will be normalized by the magnitude of the force in the label with a shift given by `relative_f`

`enable_atom_ener_coeff`
`[bool]` if true, the energy will be computed as $\sum_i c_i E_i$

`start_pref_gf`
`[float]` The prefactor of generalized force loss at the start of the training.

`limit_pref_gf`
`[float]` The prefactor of generalized force loss at the end of the training.

`numb_generalized_coord`
`[int]` The dimension of generalized coordinates.

`**kwargs`
 Other keyword arguments.

Methods

| | |
|--|--------------------------------|
| <code>build(learning_rate, natoms, model_dict, ...)</code> | Build the loss function graph. |
| <code>eval(sess, feed_dict, natoms)</code> | Eval the loss function. |

build(learning_rate, natoms, model_dict, label_dict, suffix)

Build the loss function graph.

Parameters

learning_rate

`[tf.Tensor]` learning rate

natoms

`[tf.Tensor]` number of atoms

model_dict

`[dict[str, tf.Tensor]]` A dictionary that maps model keys to tensors

`label_dict`
[`dict[str, tf.Tensor]`] A dictionary that maps label keys to tensors

`suffix`
[`str`] suffix

Returns

`tf.Tensor`
the total squared loss

`dict[str, tf.Tensor]`
A dictionary that maps loss keys to more loss tensors

`eval(sess, feed_dict, natoms)`
Eval the loss function.

Parameters

`sess`
[`tf.Session`] TensorFlow session

`feed_dict`
[`dict[tf.placeholder, tf.Tensor]`] A dictionary that maps graph elements to values

`natoms`
[`tf.Tensor`] number of atoms

Returns

`dict`
A dictionary that maps keys to values. It should contain key `natoms`

deepmd.loss.loss module

`class deepmd.loss.loss.Loss`

Bases: `object`

The abstract class for the loss function.

Methods

| | |
|--|--------------------------------|
| <code>build(learning_rate, natoms, model_dict, ...)</code> | Build the loss function graph. |
| <code>eval(sess, feed_dict, natoms)</code> | Eval the loss function. |

abstract `build(learning_rate: Tensor, natoms: Tensor, model_dict: Dict[str, Tensor], label_dict: Dict[str, Tensor], suffix: str) → Tuple[Tensor, Dict[str, Tensor]]`

Build the loss function graph.

Parameters

`learning_rate`
[`tf.Tensor`] learning rate

`natoms`
[`tf.Tensor`] number of atoms

`model_dict`
`[dict[str, tf.Tensor]]` A dictionary that maps model keys to tensors

`label_dict`
`[dict[str, tf.Tensor]]` A dictionary that maps label keys to tensors

`suffix`
`[str]` suffix

Returns

`tf.Tensor`
 the total squared loss

`dict[str, tf.Tensor]`
 A dictionary that maps loss keys to more loss tensors

abstract eval(sess: Session, feed_dict: Dict[placeholder, Tensor], natoms: Tensor) → dict
 Eval the loss function.

Parameters

`sess`
`[tf.Session]` TensorFlow session

`feed_dict`
`[dict[tf.placeholder, tf.Tensor]]` A dictionary that maps graph elements to values

`natoms`
`[tf.Tensor]` number of atoms

Returns

`dict`
 A dictionary that maps keys to values. It should contain key natoms

deepmd.loss.tensor module

class deepmd.loss.tensor.TensorLoss(jdata, **kwarg)

Bases: *Loss*

Loss function for tensorial properties.

Methods

| | |
|---|--------------------------------|
| <i>build</i> (learning_rate, natoms, model_dict, ...) | Build the loss function graph. |
| <i>eval</i> (sess, feed_dict, natoms) | Eval the loss function. |

build(learning_rate, natoms, model_dict, label_dict, suffix)

Build the loss function graph.

Parameters

`learning_rate`
`[tf.Tensor]` learning rate

natoms
 [`tf.Tensor`] number of atoms

model_dict
 [`dict[str, tf.Tensor]`] A dictionary that maps model keys to tensors

label_dict
 [`dict[str, tf.Tensor]`] A dictionary that maps label keys to tensors

suffix
 [`str`] suffix

Returns

`tf.Tensor`
 the total squared loss

`dict[str, tf.Tensor]`
 A dictionary that maps loss keys to more loss tensors

`eval`(sess, feed_dict, natoms)
 Eval the loss function.

Parameters

 sess
 [`tf.Session`] TensorFlow session

 feed_dict
 [`dict[tf.placeholder, tf.Tensor]`] A dictionary that maps graph elements to values

 natoms
 [`tf.Tensor`] number of atoms

Returns

`dict`
 A dictionary that maps keys to values. It should contain key natoms

deepmd.model package

`class deepmd.model.DOSModel(*args, **kwargs)`
 Bases: *StandardModel*

DOS model.

Parameters

 descriptor
 Descriptor

 fitting_net
 Fitting net

 type_embedding
 Type embedding net

 type_map
 Mapping atom type to the name (str) of the type. For example `type_map[1]` gives the name of the type 1.

`data_stat_nbatch`
Number of frames used for data statistic

`data_stat_protect`
Protect parameter for atomic energy regression

Methods

| | |
|--|--|
| <code>build(coord_, atype_, natoms, box, mesh, ...)</code> | Build the model. |
| <code>build_descrpt(coord_, atype_, natoms, box, ...)</code> | Build the descriptor part of the model. |
| <code>change_energy_bias(data, frozen_model, ...)</code> | Change the energy bias according to the input data and the pretrained model. |
| <code>data_stat(data)</code> | Data statistics. |
| <code>enable_compression([suffix])</code> | Enable compression. |
| <code>enable_mixed_precision(mixed_prec)</code> | Enable mixed precision for the model. |
| <code>get_feed_dict(coord_, atype_, natoms, box, ...)</code> | Generate the feed_dict for current descriptor. |
| <code>get_fitting()</code> | Get the fitting(s). |
| <code>get_loss(loss, lr)</code> | Get the loss function(s). |
| <code>get_ntypes()</code> | Get the number of types. |
| <code>get_numb_aparam()</code> | Get the number of atomic parameters. |
| <code>get_numb_dos()</code> | Get the number of gridpoints in energy space. |
| <code>get_numb_fparam()</code> | Get the number of frame parameters. |
| <code>get_rcut()</code> | Get cutoff radius of the model. |
| <code>get_type_map()</code> | Get the type map. |
| <code>init_variables(graph, graph_def[, ...])</code> | Init the embedding net variables with the given frozen model. |

`build(coord_, atype_, natoms, box, mesh, input_dict, frz_model=None, ckpt_meta: Optional[str] = None, suffix="", reuse=None)`

Build the model.

Parameters

`coord_`
[`tf.Tensor`] The coordinates of atoms

`atype_`
[`tf.Tensor`] The atom types of atoms

`natoms`
[`tf.Tensor`] The number of atoms

`box`
[`tf.Tensor`] The box vectors

`mesh`
[`tf.Tensor`] The mesh vectors

`input_dict`
[`dict`] The input dict

`frz_model`
[`str`, `optional`] The path to the frozen model

`ckpt_meta`
[`str`, `optional`] The path to the checkpoint and meta file

```
    suffix
        [str, optional] The suffix of the scope

    reuse
        [bool or tf.AUTO_REUSE, optional] Whether to reuse the variables

Returns
    dict
        The output dict

data_stat(data)
    Data statistics.

get_ntypes()
    Get the number of types.

get_numb_apharam() → int
    Get the number of atomic parameters.

get_numb_dos()
    Get the number of gridpoints in energy space.

get_numb_fparam() → int
    Get the number of frame parameters.

get_rcut()
    Get cutoff radius of the model.

get_type_map()
    Get the type map.

init_variables(graph: Graph, graph_def: GraphDef, model_type: str = 'original_model', suffix: str
              = '') → None
    Init the embedding net variables with the given frozen model.

Parameters
    graph
        [tf.Graph] The input frozen model graph
    graph_def
        [tf.GraphDef] The input frozen model graph_def
    model_type
        [str] the type of the model
    suffix
        [str] suffix to name scope

model_type = 'dos'

class deepmd.model.DipoleModel(*args, **kwargs)
    Bases: TensorModel
```

Methods

| | |
|--|--|
| <code>build(coord_, atype_, natoms, box, mesh, ...)</code> | Build the model. |
| <code>build_descrpt(coord_, atype_, natoms, box, ...)</code> | Build the descriptor part of the model. |
| <code>change_energy_bias(data, frozen_model, ...)</code> | Change the energy bias according to the input data and the pretrained model. |
| <code>data_stat(data)</code> | Data statistics. |
| <code>enable_compression([suffix])</code> | Enable compression. |
| <code>enable_mixed_precision(mixed_prec)</code> | Enable mixed precision for the model. |
| <code>get_feed_dict(coord_, atype_, natoms, box, ...)</code> | Generate the feed_dict for current descriptor. |
| <code>get_fitting()</code> | Get the fitting(s). |
| <code>get_loss(loss, lr)</code> | Get the loss function(s). |
| <code>get_ntypes()</code> | Get the number of types. |
| <code>get_num_aparam()</code> | Get the number of atomic parameters. |
| <code>get_num_dos()</code> | Get the number of gridpoints in energy space. |
| <code>get_num_fparam()</code> | Get the number of frame parameters. |
| <code>get_rcut()</code> | Get cutoff radius of the model. |
| <code>get_type_map()</code> | Get the type map. |
| <code>init_variables(graph, graph_def[, ...])</code> | Init the embedding net variables with the given frozen model. |

| | |
|---------------------------|--|
| <code>get_out_size</code> | |
| <code>get_sel_type</code> | |

```
class deepmd.model.EnerModel(*args, **kwargs)
```

Bases: *StandardModel*

Energy model.

Parameters

descriptor
Descriptor

fitting_net
Fitting net

type_embedding
Type embedding net

type_map
Mapping atom type to the name (str) of the type. For example type_map[1] gives the name of the type 1.

data_stat_nbatch
Number of frames used for data statistic

data_stat_protect
Protect parameter for atomic energy regression

use_srtab
The table for the short-range pairwise interaction added on top of DP. The table is a text data file with $(N_t + 1) * N_t / 2 + 1$ columns. The first column is the distance between atoms. The second to the last columns are energies for pairs of certain types. For example we have two atom types, 0 and 1. The columns from 2nd to 4th are for 0-0, 0-1 and 1-1 correspondingly.

`smin_alpha`
The short-range tabulated interaction will be swithed according to the distance of the nearest neighbor. This distance is calculated by `softmin`. This parameter is the decaying parameter in the `softmin`. It is only required when `use_srtab` is provided.

`sw_rmin`
The lower boundary of the interpolation between short-range tabulated interaction and DP. It is only required when `use_srtab` is provided.

`sw_rmin`
The upper boundary of the interpolation between short-range tabulated interaction and DP. It is only required when `use_srtab` is provided.

`srtab_add_bias`
[bool] Whether add energy bias from the statistics of the data to short-range tabulated atomic energy. It only takes effect when `use_srtab` is provided.

`spin`
`spin`

`data_stat_nsample`
The number of training samples in a system to compute and change the energy bias.

Methods

| | |
|--|--|
| <code>build(coord_, atype_, natoms, box, mesh, ...)</code> | Build the model. |
| <code>build_descrpt(coord_, atype_, natoms, box, ...)</code> | Build the descriptor part of the model. |
| <code>change_energy_bias(data, frozen_model, ...)</code> | Change the energy bias according to the input data and the pretrained model. |
| <code>data_stat(data)</code> | Data staticis. |
| <code>enable_compression([suffix])</code> | Enable compression. |
| <code>enable_mixed_precision(mixed_prec)</code> | Enable mixed precision for the model. |
| <code>get_feed_dict(coord_, atype_, natoms, box, ...)</code> | Generate the <code>feed_dict</code> for current descriptor. |
| <code>get_fitting()</code> | Get the fitting(s). |
| <code>get_loss(loss, lr)</code> | Get the loss function(s). |
| <code>get_ntypes()</code> | Get the number of types. |
| <code>get_numb_aparam()</code> | Get the number of atomic parameters. |
| <code>get_numb_dos()</code> | Get the number of gridpoints in energy space. |
| <code>get_numb_fparam()</code> | Get the number of frame parameters. |
| <code>get_rcut()</code> | Get cutoff radius of the model. |
| <code>get_type_map()</code> | Get the type map. |
| <code>init_variables(graph, graph_def[, ...])</code> | Init the embedding net variables with the given frozen model. |

| | |
|-------------------------------|--|
| <code>natoms_match</code> | |
| <code>natoms_not_match</code> | |

`build(coord_, atype_, natoms, box, mesh, input_dict, frz_model=None, ckpt_meta: Optional[str] = None, suffix="", reuse=None)`

Build the model.

Parameters

`coord_`
`[tf.Tensor]` The coordinates of atoms
`atype_`
`[tf.Tensor]` The atom types of atoms
`natoms`
`[tf.Tensor]` The number of atoms
`box`
`[tf.Tensor]` The box vectors
`mesh`
`[tf.Tensor]` The mesh vectors
`input_dict`
`[dict]` The input dict
`frz_model`
`[str, optional]` The path to the frozen model
`ckpt_meta`
`[str, optional]` The path to the checkpoint and meta file
`suffix`
`[str, optional]` The suffix of the scope
`reuse`
`[bool or tf.AUTO_REUSE, optional]` Whether to reuse the variables

Returns

`dict`
 The output dict

change_energy_bias(data: `DeepmdDataSystem`, frozen_model: `str`, origin_type_map: `list`,
 full_type_map: `str`, bias_shift: `str` = 'delta') → `None`

Change the energy bias according to the input data and the pretrained model.

Parameters

`data`
`[DeepmdDataSystem]` The training data.
`frozen_model`
`[str]` The path file of frozen model.
`origin_type_map`
`[list]` The original type_map in dataset, they are targets to change the energy bias.
`full_type_map`
`[str]` The full type_map in pretrained model
`bias_shift`
`[str]` The mode for changing energy bias : ['delta', 'statistic'] 'delta' : perform
 predictions on energies of target dataset,
 and do least square on the errors to obtain the target shift as bias.
 'statistic' : directly use the statistic energy bias in the target dataset.

data_stat(data)
 Data statistics.

```
get_ntypes()
    Get the number of types.

get_numb_aparam() → int
    Get the number of atomic parameters.

get_numb_fparam() → int
    Get the number of frame parameters.

get_rcut()
    Get cutoff radius of the model.

get_type_map()
    Get the type map.

init_variables(graph: Graph, graph_def: GraphDef, model_type: str = 'original_model', suffix: str
               = '') → None
    Init the embedding net variables with the given frozen model.

    Parameters
        graph
            [tf.Graph] The input frozen model graph
        graph_def
            [tf.GraphDef] The input frozen model graph_def
        model_type
            [str] the type of the model
        suffix
            [str] suffix to name scope

model_type = 'ener'

natoms_match(force, natoms)

natoms_not_match(force, natoms, atype)

class deepmd.model.GlobalPolarModel(*args, **kwargs)
    Bases: TensorModel
```


Methods

| | |
|--|--|
| <code>build(coord_, atype_, natoms, box, mesh, ...)</code> | Build the model. |
| <code>build_descrpt(coord_, atype_, natoms, box, ...)</code> | Build the descriptor part of the model. |
| <code>change_energy_bias(data, frozen_model, ...)</code> | Change the energy bias according to the input data and the pretrained model. |
| <code>data_stat(data)</code> | Data statistics. |
| <code>enable_compression([suffix])</code> | Enable compression. |
| <code>enable_mixed_precision(mixed_prec)</code> | Enable mixed precision for the model. |
| <code>get_feed_dict(coord_, atype_, natoms, box, ...)</code> | Generate the feed_dict for current descriptor. |
| <code>get_fitting()</code> | Get the fitting(s). |
| <code>get_loss(loss, lr)</code> | Get the loss function(s). |
| <code>get_ntypes()</code> | Get the number of types. |
| <code>get_num_b_aram()</code> | Get the number of atomic parameters. |
| <code>get_num_b_dos()</code> | Get the number of gridpoints in energy space. |
| <code>get_num_b_fparam()</code> | Get the number of frame parameters. |
| <code>get_rcut()</code> | Get cutoff radius of the model. |
| <code>get_type_map()</code> | Get the type map. |
| <code>init_variables(graph, graph_def[, ...])</code> | Init the embedding net variables with the given frozen model. |

| | |
|---------------------------|--|
| <code>get_out_size</code> | |
| <code>get_sel_type</code> | |

```
class deepmd.model.MultiModel(*args, **kwargs)
```

Bases: *Model*

Multi-task model.

Parameters

`descriptor`
Descriptor

`fitting_net_dict`
Dictionary of fitting nets

`fitting_type_dict`
deprecated argument

`type_embedding`
Type embedding net

`type_map`
Mapping atom type to the name (str) of the type. For example `type_map[1]` gives the name of the type 1.

`data_stat_nbatch`
Number of frames used for data statistic

`data_stat_protect`
Protect parameter for atomic energy regression

`use_srtab`
The table for the short-range pairwise interaction added on top of DP. The table is a text data file with $(N_t + 1) * N_t / 2 + 1$ columns. The first column is the distance

between atoms. The second to the last columns are energies for pairs of certain types. For example we have two atom types, 0 and 1. The columns from 2nd to 4th are for 0-0, 0-1 and 1-1 correspondingly.

`smin_alpha`

The short-range tabulated interaction will be swithed according to the distance of the nearest neighbor. This distance is calculated by `softmin`. This parameter is the decaying parameter in the `softmin`. It is only required when `use_srtab` is provided.

`sw_rmin`

The lower boundary of the interpolation between short-range tabulated interaction and DP. It is only required when `use_srtab` is provided.

`sw_rmin`

The upper boundary of the interpolation between short-range tabulated interaction and DP. It is only required when `use_srtab` is provided.

Methods

| | |
|--|--|
| <code>build(coord_, atype_, natoms, box, mesh, ...)</code> | Build the model. |
| <code>build_descrpt(coord_, atype_, natoms, box, ...)</code> | Build the descriptor part of the model. |
| <code>change_energy_bias(data, frozen_model, ...)</code> | Change the energy bias according to the input data and the pretrained model. |
| <code>data_stat(data)</code> | Data statistics. |
| <code>enable_compression([suffix])</code> | Enable compression. |
| <code>enable_mixed_precision(mixed_prec)</code> | Enable mixed precision for the model. |
| <code>get_feed_dict(coord_, atype_, natoms, box, ...)</code> | Generate the <code>feed_dict</code> for current descriptor. |
| <code>get_fitting()</code> | Get the fitting(s). |
| <code>get_loss(loss, lr)</code> | Get the loss function(s). |
| <code>get_ntypes()</code> | Get the number of types. |
| <code>get_numb_aparam()</code> | Get the number of atomic parameters. |
| <code>get_numb_dos()</code> | Get the number of gridpoints in energy space. |
| <code>get_numb_fparam()</code> | Get the number of frame parameters. |
| <code>get_rcut()</code> | Get cutoff radius of the model. |
| <code>get_type_map()</code> | Get the type map. |
| <code>init_variables(graph, graph_def[, ...])</code> | Init the embedding net variables with the given frozen model. |

`build(coord_, atype_, natoms, box, mesh, input_dict, frz_model=None, ckpt_meta: Optional[str] = None, suffix='', reuse=None)`

Build the model.

Parameters

`coord_`
[`tf.Tensor`] The coordinates of atoms

`atype_`
[`tf.Tensor`] The atom types of atoms

`natoms`
[`tf.Tensor`] The number of atoms

`box`
[`tf.Tensor`] The box vectors

`mesh`
`[tf.Tensor]` The mesh vectors

`input_dict`
`[dict]` The input dict

`frz_model`
`[str, optional]` The path to the frozen model

`ckpt_meta`
`[str, optional]` The path to the checkpoint and meta file

`suffix`
`[str, optional]` The suffix of the scope

`reuse`
`[bool or tf.AUTO_REUSE, optional]` Whether to reuse the variables

Returns
`dict`
 The output dict

`data_stat(data)`
 Data staticis.

`enable_mixed_precision(mixed_prec: dict)`
 Enable mixed precision for the model.

Parameters
`mixed_prec`
`[dict]` The mixed precision config

`get_fitting() → dict`
 Get the fitting(s).

`get_loss(loss: dict, lr: dict) → Dict[str, Loss]`
 Get the loss function(s).

`get_ntypes()`
 Get the number of types.

`get_numb_aparam() → dict`
 Get the number of atomic parameters.

`get_numb_dos() → dict`
 Get the number of gridpoints in energy space.

`get_numb_fparam() → dict`
 Get the number of frame parameters.

`get_rcut()`
 Get cutoff radius of the model.

`get_type_map()`
 Get the type map.

`init_variables(graph: Graph, graph_def: GraphDef, model_type: str = 'original_model', suffix: str = '') → None`
 Init the embedding net variables with the given frozen model.

Parameters

graph
 [`tf.Graph`] The input frozen model graph

graph_def
 [`tf.GraphDef`] The input frozen model graph_def

model_type
 [`str`] the type of the model

suffix
 [`str`] suffix to name scope

```
model_type = 'multi_task'
```

```
class deepmd.model.PolarModel(*args, **kwargs)
```

Bases: *TensorModel*

Methods

| | |
|---|--|
| <code>build(coord_, atype_, natoms, box, mesh, ...)</code> | Build the model. |
| <code>build_descript(coord_, atype_, natoms, box, ...)</code> | Build the descriptor part of the model. |
| <code>change_energy_bias(data, frozen_model, ...)</code> | Change the energy bias according to the input data and the pretrained model. |
| <code>data_stat(data)</code> | Data statistics. |
| <code>enable_compression([suffix])</code> | Enable compression. |
| <code>enable_mixed_precision(mixed_prec)</code> | Enable mixed precision for the model. |
| <code>get_feed_dict(coord_, atype_, natoms, box, ...)</code> | Generate the feed_dict for current descriptor. |
| <code>get_fitting()</code> | Get the fitting(s). |
| <code>get_loss(loss, lr)</code> | Get the loss function(s). |
| <code>get_ntypes()</code> | Get the number of types. |
| <code>get_numb_aparam()</code> | Get the number of atomic parameters. |
| <code>get_numb_dos()</code> | Get the number of gridpoints in energy space. |
| <code>get_numb_fparam()</code> | Get the number of frame parameters. |
| <code>get_rcut()</code> | Get cutoff radius of the model. |
| <code>get_type_map()</code> | Get the type map. |
| <code>init_variables(graph, graph_def[, ...])</code> | Init the embedding net variables with the given frozen model. |

| | |
|---------------------------|--|
| <code>get_out_size</code> | |
| <code>get_sel_type</code> | |

```
class deepmd.model.WFCModel(*args, **kwargs)
```

Bases: *TensorModel*

Methods

| | |
|--|--|
| <code>build(coord_, atype_, natoms, box, mesh, ...)</code> | Build the model. |
| <code>build_descrpt(coord_, atype_, natoms, box, ...)</code> | Build the descriptor part of the model. |
| <code>change_energy_bias(data, frozen_model, ...)</code> | Change the energy bias according to the input data and the pretrained model. |
| <code>data_stat(data)</code> | Data statistics. |
| <code>enable_compression([suffix])</code> | Enable compression. |
| <code>enable_mixed_precision(mixed_prec)</code> | Enable mixed precision for the model. |
| <code>get_feed_dict(coord_, atype_, natoms, box, ...)</code> | Generate the feed_dict for current descriptor. |
| <code>get_fitting()</code> | Get the fitting(s). |
| <code>get_loss(loss, lr)</code> | Get the loss function(s). |
| <code>get_ntypes()</code> | Get the number of types. |
| <code>get_num_aparam()</code> | Get the number of atomic parameters. |
| <code>get_num_dos()</code> | Get the number of gridpoints in energy space. |
| <code>get_num_fparam()</code> | Get the number of frame parameters. |
| <code>get_rcut()</code> | Get cutoff radius of the model. |
| <code>get_type_map()</code> | Get the type map. |
| <code>init_variables(graph, graph_def[, ...])</code> | Init the embedding net variables with the given frozen model. |

| | |
|---------------------------|--|
| <code>get_out_size</code> | |
| <code>get_sel_type</code> | |

Submodules

deepmd.model.dos module

`class deepmd.model.dos.DOSModel(*args, **kwargs)`

Bases: *StandardModel*

DOS model.

Parameters

descriptor

Descriptor

fitting_net

Fitting net

type_embedding

Type embedding net

type_map

Mapping atom type to the name (str) of the type. For example `type_map[1]` gives the name of the type 1.

data_stat_nbatch

Number of frames used for data statistic

data_stat_protect

Protect parameter for atomic energy regression

Methods

| | |
|---|--|
| <i>build</i> (coord_, atype_, natoms, box, mesh, ...) | Build the model. |
| <i>build_descrpt</i> (coord_, atype_, natoms, box, ...) | Build the descriptor part of the model. |
| <i>change_energy_bias</i> (data, frozen_model, ...) | Change the energy bias according to the input data and the pretrained model. |
| <i>data_stat</i> (data) | Data statistics. |
| <i>enable_compression</i> ([suffix]) | Enable compression. |
| <i>enable_mixed_precision</i> (mixed_prec) | Enable mixed precision for the model. |
| <i>get_feed_dict</i> (coord_, atype_, natoms, box, ...) | Generate the feed_dict for current descriptor. |
| <i>get_fitting</i> () | Get the fitting(s). |
| <i>get_loss</i> (loss, lr) | Get the loss function(s). |
| <i>get_ntypes</i> () | Get the number of types. |
| <i>get_numb_aparam</i> () | Get the number of atomic parameters. |
| <i>get_numb_dos</i> () | Get the number of gridpoints in energy space. |
| <i>get_numb_fparam</i> () | Get the number of frame parameters. |
| <i>get_rcut</i> () | Get cutoff radius of the model. |
| <i>get_type_map</i> () | Get the type map. |
| <i>init_variables</i> (graph, graph_def[, ...]) | Init the embedding net variables with the given frozen model. |

build(coord_, atype_, natoms, box, mesh, input_dict, frz_model=None, ckpt_meta: Optional[str] = None, suffix="", reuse=None)

Build the model.

Parameters

coord_
[[tf.Tensor](#)] The coordinates of atoms

atype_
[[tf.Tensor](#)] The atom types of atoms

natoms
[[tf.Tensor](#)] The number of atoms

box
[[tf.Tensor](#)] The box vectors

mesh
[[tf.Tensor](#)] The mesh vectors

input_dict
[dict] The input dict

frz_model
[str, optional] The path to the frozen model

ckpt_meta
[str, optional] The path to the checkpoint and meta file

suffix
[str, optional] The suffix of the scope

reuse
[bool or [tf.AUTO_REUSE](#), optional] Whether to reuse the variables

Returns

```

        dict
            The output dict
    data_stat(data)
        Data staticis.
    get_ntypes()
        Get the number of types.
    get_numb_aparam() → int
        Get the number of atomic parameters.
    get_numb_dos()
        Get the number of gridpoints in energy space.
    get_numb_fparam() → int
        Get the number of frame parameters.
    get_rcut()
        Get cutoff radius of the model.
    get_type_map()
        Get the type map.
    init_variables(graph: Graph, graph_def: GraphDef, model_type: str = 'original_model', suffix: str
                  = '') → None
        Init the embedding net variables with the given frozen model.

    Parameters
        graph
            [tf.Graph] The input frozen model graph
        graph_def
            [tf.GraphDef] The input frozen model graph_def
        model_type
            [str] the type of the model
        suffix
            [str] suffix to name scope
    model_type = 'dos'

```

deepmd.model.ener module

```

class deepmd.model.ener.EnerModel(*args, **kwargs)
    Bases: StandardModel
    Energy model.

    Parameters
        descriptor
            Descriptor
        fitting_net
            Fitting net

```

`type_embedding`
Type embedding net

`type_map`
Mapping atom type to the name (str) of the type. For example `type_map[1]` gives the name of the type 1.

`data_stat_nbatch`
Number of frames used for data statistic

`data_stat_protect`
Protect parameter for atomic energy regression

`use_srtab`
The table for the short-range pairwise interaction added on top of DP. The table is a text data file with $(N_t + 1) * N_t / 2 + 1$ columns. The first column is the distance between atoms. The second to the last columns are energies for pairs of certain types. For example we have two atom types, 0 and 1. The columns from 2nd to 4th are for 0-0, 0-1 and 1-1 correspondingly.

`smin_alpha`
The short-range tabulated interaction will be swithed according to the distance of the nearest neighbor. This distance is calculated by softmin. This parameter is the decaying parameter in the softmin. It is only required when `use_srtab` is provided.

`sw_rmin`
The lower boundary of the interpolation between short-range tabulated interaction and DP. It is only required when `use_srtab` is provided.

`sw_rmin`
The upper boundary of the interpolation between short-range tabulated interaction and DP. It is only required when `use_srtab` is provided.

`srtab_add_bias`
[bool] Whether add energy bias from the statistics of the data to short-range tabulated atomic energy. It only takes effect when `use_srtab` is provided.

`spin`
spin

`data_stat_nsamples`
The number of training samples in a system to compute and change the energy bias.

Methods

| | |
|--|--|
| <code>build(coord_, atype_, natoms, box, mesh, ...)</code> | Build the model. |
| <code>build_descrpt(coord_, atype_, natoms, box, ...)</code> | Build the descriptor part of the model. |
| <code>change_energy_bias(data, frozen_model, ...)</code> | Change the energy bias according to the input data and the pretrained model. |
| <code>data_stat(data)</code> | Data statistics. |
| <code>enable_compression([suffix])</code> | Enable compression. |
| <code>enable_mixed_precision(mixed_prec)</code> | Enable mixed precision for the model. |
| <code>get_feed_dict(coord_, atype_, natoms, box, ...)</code> | Generate the feed_dict for current descriptor. |
| <code>get_fitting()</code> | Get the fitting(s). |
| <code>get_loss(loss, lr)</code> | Get the loss function(s). |
| <code>get_ntypes()</code> | Get the number of types. |
| <code>get_numb_aparam()</code> | Get the number of atomic parameters. |
| <code>get_numb_dos()</code> | Get the number of gridpoints in energy space. |
| <code>get_numb_fparam()</code> | Get the number of frame parameters. |
| <code>get_rcut()</code> | Get cutoff radius of the model. |
| <code>get_type_map()</code> | Get the type map. |
| <code>init_variables(graph, graph_def[, ...])</code> | Init the embedding net variables with the given frozen model. |

| | |
|------------------|--|
| natoms_match | |
| natoms_not_match | |

build(coord_, atype_, natoms, box, mesh, input_dict, frz_model=None, ckpt_meta: [Optional\[str\]](#) = None, suffix='', reuse=None)

Build the model.

Parameters

coord_
[[tf.Tensor](#)] The coordinates of atoms

atype_
[[tf.Tensor](#)] The atom types of atoms

natoms
[[tf.Tensor](#)] The number of atoms

box
[[tf.Tensor](#)] The box vectors

mesh
[[tf.Tensor](#)] The mesh vectors

input_dict
[[dict](#)] The input dict

frz_model
[[str](#), [optional](#)] The path to the frozen model

ckpt_meta
[[str](#), [optional](#)] The path to the checkpoint and meta file

suffix
[[str](#), [optional](#)] The suffix of the scope

reuse
[`bool` or `tf.AUTO_REUSE`, optional] Whether to reuse the variables

Returns

`dict`
The output dict

change_energy_bias(data: `DeepmdDataSystem`, frozen_model: `str`, origin_type_map: `list`,
full_type_map: `str`, bias_shift: `str` = 'delta') → `None`

Change the energy bias according to the input data and the pretrained model.

Parameters

data
[`DeepmdDataSystem`] The training data.

frozen_model
[`str`] The path file of frozen model.

origin_type_map
[`list`] The original type_map in dataset, they are targets to change the energy bias.

full_type_map
[`str`] The full type_map in pretrained model

bias_shift
[`str`] The mode for changing energy bias : ['delta', 'statistic'] 'delta' : perform predictions on energies of target dataset, and do least square on the errors to obtain the target shift as bias.
'statistic' : directly use the statistic energy bias in the target dataset.

data_stat(data)
Data statistics.

get_ntypes()
Get the number of types.

get_numb_aparam() → `int`
Get the number of atomic parameters.

get_numb_fparam() → `int`
Get the number of frame parameters.

get_rcut()
Get cutoff radius of the model.

get_type_map()
Get the type map.

init_variables(graph: `Graph`, graph_def: `GraphDef`, model_type: `str` = 'original_model', suffix: `str` = '') → `None`

Init the embedding net variables with the given frozen model.

Parameters

graph
[`tf.Graph`] The input frozen model graph

graph_def
[`tf.GraphDef`] The input frozen model graph_def

```

    model_type
        [str] the type of the model
    suffix
        [str] suffix to name scope
model_type = 'ener'

natoms_match(force, natoms)

natoms_not_match(force, natoms, atype)

```

deepmd.model.model module

```
class deepmd.model.model.Model(*args, **kwargs)
```

Bases: [ABC](#)

Abstract base model.

Parameters

```

    type_embedding
        Type embedding net
    type_map
        Mapping atom type to the name (str) of the type. For example type_map[1] gives
        the name of the type 1.
    data_stat_nbatch
        Number of frames used for data statistic
    data_bias_nsample
        The number of training samples in a system to compute and change the energy bias.
    data_stat_protect
        Protect parameter for atomic energy regression
    use_srtab
        The table for the short-range pairwise interaction added on top of DP. The table is
        a text data file with  $(N_t + 1) * N_t / 2 + 1$  columes. The first colum is the distance
        between atoms. The second to the last columes are energies for pairs of certain types.
        For example we have two atom types, 0 and 1. The columes from 2nd to 4th are for
        0-0, 0-1 and 1-1 correspondingly.
    smin_alpha
        The short-range tabulated interaction will be swithed according to the distance of
        the nearest neighbor. This distance is calculated by softmin. This parameter is the
        decaying parameter in the softmin. It is only required when use_srtab is provided.
    sw_rmin
        The lower boundary of the interpolation between short-range tabulated interaction
        and DP. It is only required when use_srtab is provided.
    sw_rmin
        The upper boundary of the interpolation between short-range tabulated interaction
        and DP. It is only required when use_srtab is provided.
    srtab_add_bias
        [bool] Whether add energy bias from the statistics of the data to short-range tabu-
        lated atomic energy. It only takes effect when use_srtab is provided.

```

spin
 spin
 compress
 Compression information for internal use

Methods

| | |
|---|--|
| <i>build</i> (coord_, atype_, natoms, box, mesh, ...) | Build the model. |
| <i>build_descrpt</i> (coord_, atype_, natoms, box, ...) | Build the descriptor part of the model. |
| <i>change_energy_bias</i> (data, frozen_model, ...) | Change the energy bias according to the input data and the pretrained model. |
| <i>data_stat</i> (data) | Data statistics. |
| <i>enable_compression</i> ([suffix]) | Enable compression. |
| <i>enable_mixed_precision</i> (mixed_prec) | Enable mixed precision for the model. |
| <i>get_feed_dict</i> (coord_, atype_, natoms, box, ...) | Generate the feed_dict for current descriptor. |
| <i>get_fitting</i> () | Get the fitting(s). |
| <i>get_loss</i> (loss, lr) | Get the loss function(s). |
| <i>get_ntypes</i> () | Get the number of types. |
| <i>get_numb_aparam</i> () | Get the number of atomic parameters. |
| <i>get_numb_dos</i> () | Get the number of gridpoints in energy space. |
| <i>get_numb_fparam</i> () | Get the number of frame parameters. |
| <i>get_rcut</i> () | Get cutoff radius of the model. |
| <i>get_type_map</i> () | Get the type map. |
| <i>init_variables</i> (graph, graph_def[, ...]) | Init the embedding net variables with the given frozen model. |

abstract `build`(coord_: Tensor, atype_: Tensor, natoms: Tensor, box: Tensor, mesh: Tensor, input_dict: dict, frz_model: Optional[str] = None, ckpt_meta: Optional[str] = None, suffix: str = "", reuse: Optional[Union[bool, Enum]] = None)

Build the model.

Parameters

coord_
 [tf.Tensor] The coordinates of atoms

atype_
 [tf.Tensor] The atom types of atoms

natoms
 [tf.Tensor] The number of atoms

box
 [tf.Tensor] The box vectors

mesh
 [tf.Tensor] The mesh vectors

input_dict
 [dict] The input dict

frz_model
 [str, optional] The path to the frozen model

ckpt_meta
 [str, optional] The path to the checkpoint and meta file
 suffix
 [str, optional] The suffix of the scope
 reuse
 [bool or tf.AUTO_REUSE, optional] Whether to reuse the variables

Returns

dict
 The output dict

build_descrpt(coord_: Tensor, atype_: Tensor, natoms: Tensor, box: Tensor, mesh: Tensor,
 input_dict: dict, frz_model: Optional[str] = None, ckpt_meta: Optional[str] = None,
 suffix: str = "", reuse: Optional[Union[bool, Enum]] = None)

Build the descriptor part of the model.

Parameters

coord_
 [tf.Tensor] The coordinates of atoms
 atype_
 [tf.Tensor] The atom types of atoms
 natoms
 [tf.Tensor] The number of atoms
 box
 [tf.Tensor] The box vectors
 mesh
 [tf.Tensor] The mesh vectors
 input_dict
 [dict] The input dict
 frz_model
 [str, optional] The path to the frozen model
 ckpt_meta
 [str, optional] The path to the checkpoint and meta file
 suffix
 [str, optional] The suffix of the scope
 reuse
 [bool or tf.AUTO_REUSE, optional] Whether to reuse the variables

Returns

tf.Tensor
 The descriptor tensor

change_energy_bias(data: DeepmdDataSystem, frozen_model: str, origin_type_map: list,
 full_type_map: str, bias_shift: str = 'delta') → None

Change the energy bias according to the input data and the pretrained model.

Parameters

data
 [DeepmdDataSystem] The training data.

`frozen_model`
 [`str`] The path file of frozen model.

`origin_type_map`
 [`list`] The original type_map in dataset, they are targets to change the energy bias.

`full_type_map`
 [`str`] The full type_map in pretrained model

`bias_shift`
 [`str`] The mode for changing energy bias : ['delta', 'statistic'] 'delta' : perform predictions on energies of target dataset,
 and do least square on the errors to obtain the target shift as bias.
 'statistic' : directly use the statistic energy bias in the target dataset.

abstract data_stat(data: `dict`)
 Data statistics.

enable_compression(suffix: `str` = "")
 Enable compression.

Parameters

suffix
 [`str`] suffix to name scope

enable_mixed_precision(mixed_prec: `dict`)
 Enable mixed precision for the model.

Parameters

mixed_prec
 [`dict`] The mixed precision config

get_feed_dict(coord_: `Tensor`, atype_: `Tensor`, natoms: `Tensor`, box: `Tensor`, mesh: `Tensor`,
 **kwargs) → `Dict[str, Tensor]`

Generate the feed_dict for current descriptor.

Parameters

coord_
 [`tf.Tensor`] The coordinate of atoms

atype_
 [`tf.Tensor`] The type of atoms

natoms
 [`tf.Tensor`] The number of atoms. This tensor has the length of Ntypes + 2
 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this
 processor natoms[i]: 2 ≤ i < Ntypes+2, number of type i atoms

box
 [`tf.Tensor`] The box. Can be generated by `deepmd.model.make_stat_input`

mesh
 [`tf.Tensor`] For historical reasons, only the length of the Tensor matters. if size of
 mesh == 6, pbc is assumed. if size of mesh == 0, no-pbc is assumed.

**kwargs
 [`dict`] The additional arguments

Returns

`feed_dict`

`[dict[str, tf.Tensor]]` The output `feed_dict` of current descriptor

abstract `get_fitting()` \rightarrow `Union[str, dict]`

Get the fitting(s).

abstract `get_loss(loss: dict, lr) \rightarrow Union[Loss, dict]`

Get the loss function(s).

abstract `get_ntypes()` \rightarrow `int`

Get the number of types.

`get_numb_aparam()` \rightarrow `Union[int, dict]`

Get the number of atomic parameters.

`get_numb_dos()` \rightarrow `Union[int, dict]`

Get the number of gridpoints in energy space.

`get_numb_fparam()` \rightarrow `Union[int, dict]`

Get the number of frame parameters.

abstract `get_rcut()` \rightarrow `float`

Get cutoff radius of the model.

`get_type_map()` \rightarrow `list`

Get the type map.

init_variables(graph: Graph, graph_def: GraphDef, model_type: str = 'original_model', suffix: str = '') \rightarrow `None`

Init the embedding net variables with the given frozen model.

Parameters

`graph`

`[tf.Graph]` The input frozen model graph

`graph_def`

`[tf.GraphDef]` The input frozen model graph_def

`model_type`

`[str]` the type of the model

`suffix`

`[str]` suffix to name scope

class `deepmd.model.model.StandardModel(*args, **kwargs)`

Bases: `Model`

Standard model, which must contain a descriptor and a fitting.

Parameters

`descriptor`

`[Union[dict, Descriptor]]` The descriptor

`fitting_net`

`[Union[dict, Fitting]]` The fitting network

`type_embedding`

`[dict, optional]` The type embedding

`type_map`
`[list of dict, optional]` The type map

Methods

| | |
|--|--|
| <code>build(coord_, atype_, natoms, box, mesh, ...)</code> | Build the model. |
| <code>build_descrpt(coord_, atype_, natoms, box, ...)</code> | Build the descriptor part of the model. |
| <code>change_energy_bias(data, frozen_model, ...)</code> | Change the energy bias according to the input data and the pretrained model. |
| <code>data_stat(data)</code> | Data statistics. |
| <code>enable_compression([suffix])</code> | Enable compression. |
| <code>enable_mixed_precision(mixed_prec)</code> | Enable mixed precision for the model. |
| <code>get_feed_dict(coord_, atype_, natoms, box, ...)</code> | Generate the feed_dict for current descriptor. |
| <code>get_fitting()</code> | Get the fitting(s). |
| <code>get_loss(loss, lr)</code> | Get the loss function(s). |
| <code>get_ntypes()</code> | Get the number of types. |
| <code>get_numb_aparam()</code> | Get the number of atomic parameters. |
| <code>get_numb_dos()</code> | Get the number of gridpoints in energy space. |
| <code>get_numb_fparam()</code> | Get the number of frame parameters. |
| <code>get_rcut()</code> | Get cutoff radius of the model. |
| <code>get_type_map()</code> | Get the type map. |
| <code>init_variables(graph, graph_def[, ...])</code> | Init the embedding net variables with the given frozen model. |

`enable_compression(suffix: str = "")`

Enable compression.

Parameters

`suffix`

`[str]` suffix to name scope

`enable_mixed_precision(mixed_prec: dict)`

Enable mixed precision for the model.

Parameters

`mixed_prec`

`[dict]` The mixed precision config

`get_fitting() → Union[Fitting, dict]`

Get the fitting(s).

`get_loss(loss: dict, lr) → Union[Loss, dict]`

Get the loss function(s).

`get_ntypes() → int`

Get the number of types.

`get_rcut() → float`

Get cutoff radius of the model.

deepmd.model.model_stat module

`deepmd.model.model_stat.make_stat_input(data, nbatches, merge_sys=True)`

Pack data for statistics.

Parameters

`data`
The data

`nbatches`
[`int`] The number of batches

`merge_sys`
[`bool` (`True`)] Merge system data

Returns

`all_stat`:
A dictionary of list of list storing data for stat. if `merge_sys == False` data can be accessed by

`all_stat[key][sys_idx][batch_idx][frame_idx]`

else `merge_sys == True` can be accessed by

`all_stat[key][batch_idx][frame_idx]`

`deepmd.model.model_stat.merge_sys_stat(all_stat)`

deepmd.model.multi module

`class deepmd.model.multi.MultiModel(*args, **kwargs)`

Bases: *Model*

Multi-task model.

Parameters

`descriptor`
Descriptor

`fitting_net_dict`
Dictionary of fitting nets

`fitting_type_dict`
deprecated argument

`type_embedding`
Type embedding net

`type_map`
Mapping atom type to the name (str) of the type. For example `type_map[1]` gives the name of the type 1.

`data_stat_nbatch`
Number of frames used for data statistic

`data_stat_protect`
Protect parameter for atomic energy regression

use_srtab

The table for the short-range pairwise interaction added on top of DP. The table is a text data file with $(N_t + 1) * N_t / 2 + 1$ columns. The first column is the distance between atoms. The second to the last columns are energies for pairs of certain types. For example we have two atom types, 0 and 1. The columns from 2nd to 4th are for 0-0, 0-1 and 1-1 correspondingly.

smin_alpha

The short-range tabulated interaction will be swithed according to the distance of the nearest neighbor. This distance is calculated by softmin. This parameter is the decaying parameter in the softmin. It is only required when use_srtab is provided.

sw_rmin

The lower boundary of the interpolation between short-range tabulated interaction and DP. It is only required when use_srtab is provided.

sw_rmin

The upper boundary of the interpolation between short-range tabulated interaction and DP. It is only required when use_srtab is provided.

Methods

| | |
|---|--|
| <i>build</i> (coord_, atype_, natoms, box, mesh, ...) | Build the model. |
| <i>build_descrpt</i> (coord_, atype_, natoms, box, ...) | Build the descriptor part of the model. |
| <i>change_energy_bias</i> (data, frozen_model, ...) | Change the energy bias according to the input data and the pretrained model. |
| <i>data_stat</i> (data) | Data statistics. |
| <i>enable_compression</i> ([suffix]) | Enable compression. |
| <i>enable_mixed_precision</i> (mixed_prec) | Enable mixed precision for the model. |
| <i>get_feed_dict</i> (coord_, atype_, natoms, box, ...) | Generate the feed_dict for current descriptor. |
| <i>get_fitting</i> () | Get the fitting(s). |
| <i>get_loss</i> (loss, lr) | Get the loss function(s). |
| <i>get_ntypes</i> () | Get the number of types. |
| <i>get_numb_aparam</i> () | Get the number of atomic parameters. |
| <i>get_numb_dos</i> () | Get the number of gridpoints in energy space. |
| <i>get_numb_fparam</i> () | Get the number of frame parameters. |
| <i>get_rcut</i> () | Get cutoff radius of the model. |
| <i>get_type_map</i> () | Get the type map. |
| <i>init_variables</i> (graph, graph_def[, ...]) | Init the embedding net variables with the given frozen model. |

build(coord_, atype_, natoms, box, mesh, input_dict, frz_model=None, ckpt_meta: Optional[str] = None, suffix="", reuse=None)

Build the model.

Parameters

coord_
[[tf.Tensor](#)] The coordinates of atoms

atype_
[[tf.Tensor](#)] The atom types of atoms

natoms
[[tf.Tensor](#)] The number of atoms

`box`
`[tf.Tensor]` The box vectors

`mesh`
`[tf.Tensor]` The mesh vectors

`input_dict`
`[dict]` The input dict

`frz_model`
`[str, optional]` The path to the frozen model

`ckpt_meta`
`[str, optional]` The path to the checkpoint and meta file

`suffix`
`[str, optional]` The suffix of the scope

`reuse`
`[bool or tf.AUTO_REUSE, optional]` Whether to reuse the variables

Returns
`dict`
 The output dict

`data_stat(data)`
 Data statistics.

`enable_mixed_precision(mixed_prec: dict)`
 Enable mixed precision for the model.

Parameters
`mixed_prec`
`[dict]` The mixed precision config

`get_fitting() → dict`
 Get the fitting(s).

`get_loss(loss: dict, lr: dict) → Dict[str, Loss]`
 Get the loss function(s).

`get_ntypes()`
 Get the number of types.

`get_numb_aparam() → dict`
 Get the number of atomic parameters.

`get_numb_dos() → dict`
 Get the number of gridpoints in energy space.

`get_numb_fparam() → dict`
 Get the number of frame parameters.

`get_rcut()`
 Get cutoff radius of the model.

`get_type_map()`
 Get the type map.

```
init_variables(graph: Graph, graph_def: GraphDef, model_type: str = 'original_model', suffix: str = '') → None
```

Init the embedding net variables with the given frozen model.

Parameters

`graph`
[`tf.Graph`] The input frozen model graph

`graph_def`
[`tf.GraphDef`] The input frozen model graph_def

`model_type`
[`str`] the type of the model

`suffix`
[`str`] suffix to name scope

```
model_type = 'multi_task'
```

deepmd.model.pairwise_dprc module

```
class deepmd.model.pairwise_dprc.PairwiseDPRC(*args, **kwargs)
```

Bases: *Model*

Pairwise Deep Potential - Range Correction.

Methods

| | |
|--|--|
| <code>build(coord_, atype_, natoms, box_, mesh, ...)</code> | Build the model. |
| <code>build_descrpt(coord_, atype_, natoms, box, ...)</code> | Build the descriptor part of the model. |
| <code>change_energy_bias(data, frozen_model, ...)</code> | Change the energy bias according to the input data and the pretrained model. |
| <code>data_stat(data)</code> | Data statistics. |
| <code>enable_compression([suffix])</code> | Enable compression. |
| <code>enable_mixed_precision(mixed_prec)</code> | Enable mixed precision for the model. |
| <code>get_feed_dict(coord_, atype_, natoms, box, ...)</code> | Generate the feed_dict for current descriptor. |
| <code>get_fitting()</code> | Get the fitting(s). |
| <code>get_loss(loss, lr)</code> | Get the loss function(s). |
| <code>get_ntypes()</code> | Get the number of types. |
| <code>get_num_apham()</code> | Get the number of atomic parameters. |
| <code>get_num_dos()</code> | Get the number of gridpoints in energy space. |
| <code>get_num_fparam()</code> | Get the number of frame parameters. |
| <code>get_rcut()</code> | Get cutoff radius of the model. |
| <code>get_type_map()</code> | Get the type map. |
| <code>init_variables(graph, graph_def[, ...])</code> | Init the embedding net variables with the given frozen model. |

```
build(coord_: Tensor, atype_: Tensor, natoms: Tensor, box_: Tensor, mesh: Tensor, input_dict: dict, frz_model=None, ckpt_meta: Optional[str] = None, suffix: str = "", reuse: Optional[bool] = None)
```

Build the model.

Parameters

```

coord_
    [tf.Tensor] The coordinates of atoms

atype_
    [tf.Tensor] The atom types of atoms

natoms
    [tf.Tensor] The number of atoms

box
    [tf.Tensor] The box vectors

mesh
    [tf.Tensor] The mesh vectors

input_dict
    [dict] The input dict

frz_model
    [str, optional] The path to the frozen model

ckpt_meta
    [str, optional] The path to the checkpoint and meta file

suffix
    [str, optional] The suffix of the scope

reuse
    [bool or tf.AUTO_REUSE, optional] Whether to reuse the variables

Returns
    dict
        The output dict

data_stat(data)
    Data statistics.

enable_compression(suffix: str = "") → None
    Enable compression.

Parameters
    suffix
        [str] suffix to name scope

get_feed_dict(coord_: Tensor, atype_: Tensor, natoms: Tensor, box: Tensor, mesh: Tensor,
               **kwargs) → Dict[str, Tensor]
    Generate the feed_dict for current descriptor.

Parameters
    coord_
        [tf.Tensor] The coordinate of atoms

    atype_
        [tf.Tensor] The type of atoms

    natoms
        [tf.Tensor] The number of atoms. This tensor has the length of Ntypes + 2
        natoms[0]: number of local atoms natoms[1]: total number of atoms held by this
        processor natoms[i]: 2 ≤ i < Ntypes+2, number of type i atoms

```

`box`
[`tf.Tensor`] The box. Can be generated by `deepmd.model.make_stat_input`

`mesh`
[`tf.Tensor`] For historical reasons, only the length of the Tensor matters. if size of `mesh == 6`, pbc is assumed. if size of `mesh == 0`, no-pbc is assumed.

`aparam`
[`tf.Tensor`] The parameters of the descriptor

`**kwargs`
[`dict`] The keyword arguments

Returns

`feed_dict`
[`dict[str, tf.Tensor]`] The output `feed_dict` of current descriptor

`get_fitting()` → `Union[str, dict]`
Get the fitting(s).

`get_loss(loss: dict, lr) → Union[Loss, dict]`
Get the loss function(s).

`get_ntypes()` → `int`
Get the number of types.

`get_rcut()`
Get cutoff radius of the model.

`init_variables(graph: Graph, graph_def: GraphDef, model_type: str = 'original_model', suffix: str = '')` → `None`
Init the embedding net variables with the given frozen model.

Parameters

`graph`
[`tf.Graph`] The input frozen model graph

`graph_def`
[`tf.GraphDef`] The input frozen model graph_def

`model_type`
[`str`] the type of the model

`suffix`
[`str`] suffix to name scope

`model_type = 'ener'`

`deepmd.model.pairwise_dprc.gather_placeholder(params: Tensor, indices: Tensor, placeholder: float = 0.0, **kwargs) → Tensor`
Call `tf.gather` but allow indices to contain placeholders (-1).

deepmd.model.tensor module

```
class deepmd.model.tensor.DipoleModel(*args, **kwargs)
```

Bases: *TensorModel*

Methods

| | |
|--|--|
| <code>build(coord_, atype_, natoms, box, mesh, ...)</code> | Build the model. |
| <code>build_descrpt(coord_, atype_, natoms, box, ...)</code> | Build the descriptor part of the model. |
| <code>change_energy_bias(data, frozen_model, ...)</code> | Change the energy bias according to the input data and the pretrained model. |
| <code>data_stat(data)</code> | Data statistics. |
| <code>enable_compression([suffix])</code> | Enable compression. |
| <code>enable_mixed_precision(mixed_prec)</code> | Enable mixed precision for the model. |
| <code>get_feed_dict(coord_, atype_, natoms, box, ...)</code> | Generate the feed_dict for current descriptor. |
| <code>get_fitting()</code> | Get the fitting(s). |
| <code>get_loss(loss, lr)</code> | Get the loss function(s). |
| <code>get_ntypes()</code> | Get the number of types. |
| <code>get_numb_aparam()</code> | Get the number of atomic parameters. |
| <code>get_numb_dos()</code> | Get the number of gridpoints in energy space. |
| <code>get_numb_fparam()</code> | Get the number of frame parameters. |
| <code>get_rcut()</code> | Get cutoff radius of the model. |
| <code>get_type_map()</code> | Get the type map. |
| <code>init_variables(graph, graph_def[, ...])</code> | Init the embedding net variables with the given frozen model. |

| | |
|---------------------------|--|
| <code>get_out_size</code> | |
| <code>get_sel_type</code> | |

```
class deepmd.model.tensor.GlobalPolarModel(*args, **kwargs)
```

Bases: *TensorModel*

Methods

| | |
|--|--|
| <code>build(coord_, atype_, natoms, box, mesh, ...)</code> | Build the model. |
| <code>build_descrpt(coord_, atype_, natoms, box, ...)</code> | Build the descriptor part of the model. |
| <code>change_energy_bias(data, frozen_model, ...)</code> | Change the energy bias according to the input data and the pretrained model. |
| <code>data_stat(data)</code> | Data statistics. |
| <code>enable_compression([suffix])</code> | Enable compression. |
| <code>enable_mixed_precision(mixed_prec)</code> | Enable mixed precision for the model. |
| <code>get_feed_dict(coord_, atype_, natoms, box, ...)</code> | Generate the feed_dict for current descriptor. |
| <code>get_fitting()</code> | Get the fitting(s). |
| <code>get_loss(loss, lr)</code> | Get the loss function(s). |
| <code>get_ntypes()</code> | Get the number of types. |
| <code>get_num_aparam()</code> | Get the number of atomic parameters. |
| <code>get_num_dos()</code> | Get the number of gridpoints in energy space. |
| <code>get_num_fparam()</code> | Get the number of frame parameters. |
| <code>get_rcut()</code> | Get cutoff radius of the model. |
| <code>get_type_map()</code> | Get the type map. |
| <code>init_variables(graph, graph_def[, ...])</code> | Init the embedding net variables with the given frozen model. |

| | |
|---------------------------|--|
| <code>get_out_size</code> | |
| <code>get_sel_type</code> | |

```
class deepmd.model.tensor.PolarModel(*args, **kwargs)
```

Bases: *TensorModel*

Methods

| | |
|--|--|
| <code>build(coord_, atype_, natoms, box, mesh, ...)</code> | Build the model. |
| <code>build_descrpt(coord_, atype_, natoms, box, ...)</code> | Build the descriptor part of the model. |
| <code>change_energy_bias(data, frozen_model, ...)</code> | Change the energy bias according to the input data and the pretrained model. |
| <code>data_stat(data)</code> | Data statistics. |
| <code>enable_compression([suffix])</code> | Enable compression. |
| <code>enable_mixed_precision(mixed_prec)</code> | Enable mixed precision for the model. |
| <code>get_feed_dict(coord_, atype_, natoms, box, ...)</code> | Generate the feed_dict for current descriptor. |
| <code>get_fitting()</code> | Get the fitting(s). |
| <code>get_loss(loss, lr)</code> | Get the loss function(s). |
| <code>get_ntypes()</code> | Get the number of types. |
| <code>get_num_aparam()</code> | Get the number of atomic parameters. |
| <code>get_num_dos()</code> | Get the number of gridpoints in energy space. |
| <code>get_num_fparam()</code> | Get the number of frame parameters. |
| <code>get_rcut()</code> | Get cutoff radius of the model. |
| <code>get_type_map()</code> | Get the type map. |
| <code>init_variables(graph, graph_def[, ...])</code> | Init the embedding net variables with the given frozen model. |

| | |
|--------------|--|
| get_out_size | |
| get_sel_type | |

```
class deepmd.model.tensor.TensorModel(*args, **kwargs)
```

Bases: *StandardModel*

Tensor model.

Parameters

| | |
|-------------------|--|
| tensor_name | Name of the tensor. |
| descriptor | Descriptor |
| fitting_net | Fitting net |
| type_embedding | Type embedding net |
| type_map | Mapping atom type to the name (str) of the type. For example type_map[1] gives the name of the type 1. |
| data_stat_nbatch | Number of frames used for data statistic |
| data_stat_protect | Protect parameter for atomic energy regression |

Methods

| | |
|---|--|
| <i>build</i> (coord_, atype_, natoms, box, mesh, ...) | Build the model. |
| <i>build_descrpt</i> (coord_, atype_, natoms, box, ...) | Build the descriptor part of the model. |
| <i>change_energy_bias</i> (data, frozen_model, ...) | Change the energy bias according to the input data and the pretrained model. |
| <i>data_stat</i> (data) | Data staticis. |
| <i>enable_compression</i> ([suffix]) | Enable compression. |
| <i>enable_mixed_precision</i> (mixed_prec) | Enable mixed precision for the model. |
| <i>get_feed_dict</i> (coord_, atype_, natoms, box, ...) | Generate the feed_dict for current descriptor. |
| <i>get_fitting</i> () | Get the fitting(s). |
| <i>get_loss</i> (loss, lr) | Get the loss function(s). |
| <i>get_ntypes</i> () | Get the number of types. |
| <i>get_num_aparam</i> () | Get the number of atomic parameters. |
| <i>get_num_dos</i> () | Get the number of gridpoints in energy space. |
| <i>get_num_fparam</i> () | Get the number of frame parameters. |
| <i>get_rcut</i> () | Get cutoff radius of the model. |
| <i>get_type_map</i> () | Get the type map. |
| <i>init_variables</i> (graph, graph_def[, ...]) | Init the embedding net variables with the given frozen model. |

| | |
|--------------|--|
| get_out_size | |
| get_sel_type | |

build(coord_, atype_, natoms, box, mesh, input_dict, frz_model=None, ckpt_meta: Optional[str] = None, suffix="", reuse=None)

Build the model.

Parameters

coord_
[tf.Tensor] The coordinates of atoms

atype_
[tf.Tensor] The atom types of atoms

natoms
[tf.Tensor] The number of atoms

box
[tf.Tensor] The box vectors

mesh
[tf.Tensor] The mesh vectors

input_dict
[dict] The input dict

frz_model
[str, optional] The path to the frozen model

ckpt_meta
[str, optional] The path to the checkpoint and meta file

suffix
[str, optional] The suffix of the scope

reuse
[bool or tf.AUTO_REUSE, optional] Whether to reuse the variables

Returns

dict
The output dict

data_stat(data)

Data statistics.

get_ntypes()

Get the number of types.

get_out_size()

get_rcut()

Get cutoff radius of the model.

get_sel_type()

get_type_map()

Get the type map.

init_variables(graph: Graph, graph_def: GraphDef, model_type: str = 'original_model', suffix: str = '') → None

Init the embedding net variables with the given frozen model.

Parameters

```

graph
    [tf.Graph] The input frozen model graph

graph_def
    [tf.GraphDef] The input frozen model graph_def

model_type
    [str] the type of the model

suffix
    [str] suffix to name scope

class deepmd.model.tensor.WFCModel(*args,**kwargs)
    Bases: TensorModel

```

Methods

| | |
|--|--|
| <code>build(coord_, atype_, natoms, box, mesh, ...)</code> | Build the model. |
| <code>build_descrpt(coord_, atype_, natoms, box, ...)</code> | Build the descriptor part of the model. |
| <code>change_energy_bias(data, frozen_model, ...)</code> | Change the energy bias according to the input data and the pretrained model. |
| <code>data_stat(data)</code> | Data statistics. |
| <code>enable_compression([suffix])</code> | Enable compression. |
| <code>enable_mixed_precision(mixed_prec)</code> | Enable mixed precision for the model. |
| <code>get_feed_dict(coord_, atype_, natoms, box, ...)</code> | Generate the feed_dict for current descriptor. |
| <code>get_fitting()</code> | Get the fitting(s). |
| <code>get_loss(loss, lr)</code> | Get the loss function(s). |
| <code>get_ntypes()</code> | Get the number of types. |
| <code>get_numb_aparam()</code> | Get the number of atomic parameters. |
| <code>get_numb_dos()</code> | Get the number of gridpoints in energy space. |
| <code>get_numb_fparam()</code> | Get the number of frame parameters. |
| <code>get_rcut()</code> | Get cutoff radius of the model. |
| <code>get_type_map()</code> | Get the type map. |
| <code>init_variables(graph, graph_def[, ...])</code> | Init the embedding net variables with the given frozen model. |

| | |
|---------------------------|--|
| <code>get_out_size</code> | |
| <code>get_sel_type</code> | |

deepmd.nvnmd package

Subpackages

deepmd.nvnmd.data package

nvnmd.data =====.

Provides

1. hardware configuration
2. default input script

3. title and citation

Data

`jdata_sys`
action configuration

`jdata_config`
hardware configuration

`dscp`
descriptor configuration

`fitn`
fitting network configuration

`size`
ram capacity

`ctrl`
control flag, such as Time Division Multiplexing (TDM)

`nbit`
number of bits of fixed-point number

`jdata_config_16 (disable)`
difference with configure fitting size as 16

`jdata_config_32 (disable)`
difference with configure fitting size as 32

`jdata_config_64 (disable)`
difference with configure fitting size as 64

`jdata_config_128 (default)`
difference with configure fitting size as 128

`jdata_configs`
all configure of `jdata_config{nfit_node}`

`jdata_deepmd_input`
default input script for `nvnmmd` training

`NVNMD_WELCOME`
`nvnmmd` title when logging

`NVNMD_CITATION`
citation of `nvnmmd`

Submodules

`deepmd.nvnmd.data.data` module

`deepmd.nvnmd.descriptor` package

`nvnmmd.se_a` =====.

Provides

1. building descriptor with continuous embedding network
2. building descriptor with quantized embedding network

Submodules

deepmd.nvnmd.descriptor.se_a module

`deepmd.nvnmd.descriptor.se_a.build_davg_dstd()`

Get the davg and dstd from the dictionary `nvnmd_cfg`. The davg and dstd have been obtained by training CNN.

`deepmd.nvnmd.descriptor.se_a.build_op_descriptor()`

Replace `se_a.py/DescrptSeA/build`.

`deepmd.nvnmd.descriptor.se_a.check_switch_range(davg, dstd)`

Check the range of switch, let it in range $[-2, 14]$.

`deepmd.nvnmd.descriptor.se_a.descrpt2r4(inputs, natoms)`

Replace $r_{ji} \rightarrow r'_{ji}$ where $r_{ji} = (x_{ji}, y_{ji}, z_{ji})$ and $r'_{ji} = (s_{ji}, \frac{s_{ji}x_{ji}}{r_{ji}}, \frac{s_{ji}y_{ji}}{r_{ji}}, \frac{s_{ji}z_{ji}}{r_{ji}})$.

`deepmd.nvnmd.descriptor.se_a.filter_GR2D(xyz_scatter_1)`

Replace `se_a.py/_filter`.

`deepmd.nvnmd.descriptor.se_a.filter_lower_R42GR(type_i, type_input, inputs_i, is_exclude, activation_fn, bavg, stddev, trainable, suffix, seed, seed_shift, uniform_seed, filter_neuron, filter_precision, filter_resnet_dt, embedding_net_variables)`

Replace `se_a.py/DescrptSeA/_filter_lower`.

deepmd.nvnmd.descriptor.se_atten module

`deepmd.nvnmd.descriptor.se_atten.build_davg_dstd()`

Get the davg and dstd from the dictionary `nvnmd_cfg`. The davg and dstd have been obtained by training CNN.

`deepmd.nvnmd.descriptor.se_atten.build_op_descriptor()`

Replace `se_a.py/DescrptSeA/build`.

`deepmd.nvnmd.descriptor.se_atten.check_switch_range(davg, dstd)`

Check the range of switch, let it in range $[-2, 14]$.

`deepmd.nvnmd.descriptor.se_atten.descrpt2r4(inputs, atype)`

Replace $r_{ji} \rightarrow r'_{ji}$ where $r_{ji} = (x_{ji}, y_{ji}, z_{ji})$ and $r'_{ji} = (s_{ji}, \frac{s_{ji}x_{ji}}{r_{ji}}, \frac{s_{ji}y_{ji}}{r_{ji}}, \frac{s_{ji}z_{ji}}{r_{ji}})$.

`deepmd.nvnmd.descriptor.se_atten.filter_GR2D(xyz_scatter_1)`

Replace `se_a.py/_filter`.

`deepmd.nvnmd.descriptor.se_atten.filter_lower_R42GR(inputs_i, atype, nei_type_vec)`

Replace `se_a.py/DescrptSeA/_filter_lower`.

deepmd.nvnmd.entrpoints package

```
class deepmd.nvnmd.entrpoints.MapTable(config_file: str, weight_file: str, map_file: str)
```

Bases: `object`

Generate the mapping table describing the relationship of atomic distance, cutoff function, and embedding matrix.

three mapping table will be built:

$$r_{ji}^2 \rightarrow s_{ji}$$

$$r_{ji}^2 \rightarrow h_{ji}$$

$$r_{ji}^2 \rightarrow \mathcal{G}_{ji}$$

where s_{ji} is cut-off function, $h_{ji} = \frac{s(r_{ji})}{r_{ji}}$, and \mathcal{G}_{ji} is embedding matrix.

The mapping function can be define as:

$$y = f(x) = y_k + (x - x_k) * dy_k$$

$$y_k = f(x_k)$$

$$dy_k = \frac{f(x_{k+1}) - f(x_k)}{dx}$$

$$x_k \leq x < x_{k+1}$$

$$x_k = k * dx$$

where dx is interpolation interval.

Parameters

`config_file`

input file name an .npz file containing the configuration information of NVNMD model

`weight_file`

input file name an .npz file containing the weights of NVNMD model

`map_file`

output file name an .npz file containing the mapping tables of NVNMD model

References

DOI: 10.1038/s41524-022-00773-z

Methods

| | |
|---|--|
| <i>build_grad</i> (x, y, Nr, Nc) | : Build gradient of tensor y of x. |
| <i>build_map_coef</i> (cfgs, x, ys, grads, ...) | Build mapping table coefficient cfgs: cfg list cfg = x0, x1, dx. |
| <i>build_s2g</i> (s) | Build s->G s is switch function G is embedding net output. |
| <i>build_s2g_grad</i> () | Build gradient of G with respect to s. |
| <i>build_t2g</i> () | Build t->G t is chemical species of center atom and neighbor atom G is embedding net output of type. |
| <i>build_u2s</i> (r2) | Build tensor s, s=s(r2). |
| <i>build_u2s_grad</i> () | Build gradient of s with respect to u (r^2). |
| <i>cal_coef4</i> (cfgs, x, y, dy) | Build mapping table coefficient for one line coef4: $a x^3 + b x^2 + c x + d = y$: $d = y_0$ $c = y'_0$ $b = (3 y_1 - dx dy' - 2dx y'_0 - 3y_0) / dx^2$ $a = (dx y'_1 - 2 y_1 + dx y'_0 + 2 y_0) / dx^3$. |
| <i>mapping</i> (x, dic_map, cfgs) | Evaluate value by mapping table operation of tensorflow. |
| <i>mapping2</i> (x, dic_map, cfgs) | Evaluate value by mapping table of numpy. |
| <i>plot_lines</i> (x, dic1[, dic2]) | Plot lines to see accuracy. |
| <i>run_s2g</i> () | Build s-> graph and run it to get value of mapping table. |
| <i>run_t2g</i> () | Build t-> graph and run it to get value of mapping table. |
| <i>run_u2s</i> () | Build u->s graph and run it to get value of mapping table. |

| | |
|---------------------|--|
| build_davg_dstd | |
| build_embedding_net | |
| build_map | |

build_davg_dstd()

build_embedding_net(xx, wbs, activation_fn=<function tanh>)

build_grad(x, y, Nr, Nc)

: Build gradient of tensor y of x.

build_map()

build_map_coef(cfgs, x, ys, grads, grad_grads, Nr, Nc)

Build mapping table coefficient cfgs: cfg list cfg = x0, x1, dx.

coef4: $a x^3 + b x^2 + c x + d = y$: $d = y_0$ | $c = y'_0$ | $b = (3 y_1 - dx dy' - 2dx y'_0 - 3y_0) / dx^2$ | $a = (dx y'_1 - 2 y_1 + dx y'_0 + 2 y_0) / dx^3$

build_s2g(s)

Build s->G s is switch function G is embedding net output.

build_s2g_grad()

Build gradient of G with respect to s.

build_t2g()

Build t->G t is chemical species of center atom and neighbor atom G is embedding net output of type.

build_u2s(r2)

Build tensor s, $s=s(r2)$.

build_u2s_grad()

Build gradient of s with respect to u (r^2).

cal_coef4(cfgs, x, y, dy)

Build mapping table coefficient for one line coef4: $a x^3 + b x^2 + c x + d = y$; $d = y0 \mid c = y0' \mid b = (3 y1 - dx dy' - 2dx y0' - 3y0) / dx^2$ $a = (dx y1' - 2 y1 + dx y0' + 2 y0) / dx^3$.

mapping(x, dic_map, cfgs)

Evaluate value by mapping table operation of tensorflow.

mapping2(x, dic_map, cfgs)

Evaluate value by mapping table of numpy.

plot_lines(x, dic1, dic2=None)

Plot lines to see accuracy.

run_s2g()

Build s-> graph and run it to get value of mapping table.

run_t2g()

Build t-> graph and run it to get value of mapping table.

run_u2s()

Build u->s graph and run it to get value of mapping table.

class deepmd.nvnmd.entrypoints.Wrap(config_file: str, weight_file: str, map_file: str, model_file: str)

Bases: `object`

Generate the binary model file (model.pb).

the model file can be use to run the NVNMD with lammmps the pair style need set as:

```
pair_style nvnmd model.pb
pair_coeff * *
```

Parameters

config_file

input file name an .npz file containing the configuration information of NVNMD model

weight_file

input file name an .npz file containing the weights of NVNMD model

map_file

input file name an .npz file containing the mapping tables of NVNMD model

model_file

output file name an .pb file containing the model using in the NVNMD

References

DOI: 10.1038/s41524-022-00773-z

Methods

| | |
|--|---|
| <code>wrap_dscp()</code> | Wrap the configuration of descriptor. |
| <code>wrap_fitn()</code> | Wrap the weights of fitting net. |
| <code>wrap_head(nhs, nws)</code> | Wrap the head information. |
| <code>wrap_lut()</code> | Wrap the LUT. |
| <code>wrap_map()</code> | Wrap the mapping table of embedding network. |
| <code>wrap_weight(weight, NBIT_DISP, NBIT_WEIGHT)</code> | weight: weights of fittingNet NBIT_DISP: nbits of exponent of weight max value NBIT_WEIGHT: nbits of mantissa of weights. |

| | |
|-----------|--|
| wrap | |
| wrap_bias | |

wrap()

wrap_bias(bias, NBIT_DATA, NBIT_DATA_FL)

wrap_dscp()

Wrap the configuration of descriptor.

version 0: [NBIT_IDX_S2G-1:0] SHIFT_IDX_S2G

[NBIT_NEIB*NTYPE-1:0] SELs [NBIT_FIXD*M1*NTYPE*NTYPE-1:0] GSs [NBIT_FLTE-1:0] NEXPO_DIV_NI

version 1:

[NBIT_FLTE-1:0] NEXPO_DIV_NI

wrap_fitn()

Wrap the weights of fitting net.

w weight b bias

wrap_head(nhs, nws)

Wrap the head information.

version nheight nweight rcut

wrap_lut()

Wrap the LUT.

wrap_map()

Wrap the mapping table of embedding network.

wrap_weight(weight, NBIT_DISP, NBIT_WEIGHT)

weight: weights of fittingNet
NBIT_DISP: nbits of exponent of weight max value
NBIT_WEIGHT: nbits of mantissa of weights.

`deepmd.nvnmd.entrypoints.save_weight(sess, file_name: str = 'nvnmd/weight.npy')`

Save the dictionary of weight to a npy file.

Submodules

deepmd.nvnmd.entrypoints.freeze module

deepmd.nvnmd.entrypoints.freeze.filter_tensorVariableList(tensorVariableList) → dict

Get the name of variable for NVNMD.

```

train_attr/min_nbor_dist
descript_attr/t_avg:0
descript_attr/t_std:0
type_embed_net/matrix_{layer 1}:0
type_embed_net/bias_{layer 1}:0

version 0: | filter_type_{atom i}/matrix_{layer 1}_{atomj}:0

filter_type_{atom i}/bias_{layer 1}_{atomj}:0
layer_{layer 1}_type_{atom i}/matrix:0
layer_{layer 1}_type_{atom i}/bias:0
final_layer_type_{atom i}/matrix:0
final_layer_type_{atom i}/bias:0

version 1: | filter_type_all/matrix_{layer 1}:0

filter_type_all/bias_{layer 1}:0
filter_type_all/matrix_{layer 1}_two_side_ebd:0
filter_type_all/bias_{layer 1}_two_side_ebd:0
layer_{layer 1}/matrix:0
layer_{layer 1}/bias:0
final_layer/matrix:0
final_layer/bias:0

```

deepmd.nvnmd.entrypoints.freeze.save_weight(sess, file_name: str = 'nvnmd/weight.npy')

Save the dictionary of weight to a npy file.

deepmd.nvnmd.entrypoints.mapt module

class deepmd.nvnmd.entrypoints.mapt.MapTable(config_file: str, weight_file: str, map_file: str)

Bases: object

Generate the mapping table describing the relationship of atomic distance, cutoff function, and embedding matrix.

three mapping table will be built:

$$r_{ji}^2 \rightarrow s_{ji}$$

$$r_{ji}^2 \rightarrow h_{ji}$$

$$r_{ji}^2 \rightarrow \mathcal{G}_{ji}$$

where s_{ji} is cut-off function, $h_{ji} = \frac{s(r_{ji})}{r_{ji}}$, and \mathcal{G}_{ji} is embedding matrix.

The mapping function can be define as:

$$y = f(x) = y_k + (x - x_k) * dy_k$$

$$y_k = f(x_k)$$

$$dy_k = \frac{f(x_{k+1}) - f(x_k)}{dx}$$

$$x_k \leq x < x_{k+1}$$

$$x_k = k * dx$$

where dx is interpolation interval.

Parameters

- config_file
input file name an .npz file containing the configuration information of NVNMD model
- weight_file
input file name an .npz file containing the weights of NVNMD model
- map_file
output file name an .npz file containing the mapping tables of NVNMD model

References

DOI: 10.1038/s41524-022-00773-z

Methods

| | |
|---|---|
| <i>build_grad</i> (x, y, Nr, Nc) | : Build gradient of tensor y of x. |
| <i>build_map_coef</i> (cfgs, x, ys, grads, ...) | Build mapping table coefficient cfgs: cfg list cfg = x0, x1, dx. |
| <i>build_s2g</i> (s) | Build s->G s is switch function G is embedding net output. |
| <i>build_s2g_grad</i> () | Build gradient of G with respect to s. |
| <i>build_t2g</i> () | Build t->G t is chemical species of center atom and neighbor atom G is embedding net output of type. |
| <i>build_u2s</i> (r2) | Build tensor s, s=s(r2). |
| <i>build_u2s_grad</i> () | Build gradient of s with respect to u (r^2). |
| <i>cal_coef4</i> (cfgs, x, y, dy) | Build mapping table coefficient for one line coef4: $a x^3 + b x^2 + c x + d = y$: $d = y_0$ $c = y'_0$ $b = (3 y_1 - dx dy' - 2dx y'_0 - 3y_0) / dx^2$ $a = (dx y'_1 - 2 y_1 + dx y'_0 + 2 y_0) / dx^3$. |
| <i>mapping</i> (x, dic_map, cfgs) | Evaluate value by mapping table operation of tensorflow. |
| <i>mapping2</i> (x, dic_map, cfgs) | Evaluate value by mapping table of numpy. |
| <i>plot_lines</i> (x, dic1[, dic2]) | Plot lines to see accuracy. |
| <i>run_s2g</i> () | Build s-> graph and run it to get value of mapping table. |
| <i>run_t2g</i> () | Build t-> graph and run it to get value of mapping table. |
| <i>run_u2s</i> () | Build u->s graph and run it to get value of mapping table. |

| | |
|---------------------|--|
| build_davg_dstd | |
| build_embedding_net | |
| build_map | |

build_davg_dstd()

build_embedding_net(xx, wbs, activation_fn=<function tanh>)

build_grad(x, y, Nr, Nc)

: Build gradient of tensor y of x.

build_map()

build_map_coef(cfgs, x, ys, grads, grad_grads, Nr, Nc)

Build mapping table coefficient cfgs: cfg list cfg = x0, x1, dx.

coef4: $a x^3 + b x^2 + c x + d = y$: $d = y_0$ | $c = y'_0$ | $b = (3 y_1 - dx dy' - 2dx y'_0 - 3y_0) / dx^2$
 $a = (dx y'_1 - 2 y_1 + dx y'_0 + 2 y_0) / dx^3$

build_s2g(s)

Build s->G s is switch function G is embedding net output.

build_s2g_grad()

Build gradient of G with respect to s.

```

build_t2g()
    Build t->G t is chemical species of center atom and neighbor atom G is embedding net output of
    type.

build_u2s(r2)
    Build tensor s, s=s(r2).

build_u2s_grad()
    Build gradient of s with respect to u (r^2).

cal_coef4(cfgs, x, y, dy)
    Build mapping table coefficient for one line coef4:  $a x^3 + b x^2 + c x + d = y$ :  $d = y0 \mid c = y0' \mid$ 
 $b = (3 y1 - dx dy' - 2dx y0' - 3y0) / dx^2$   $a = (dx y1' - 2 y1 + dx y0' + 2 y0) / dx^3$ .

mapping(x, dic_map, cfgs)
    Evaluate value by mapping table operation of tensorflow.

mapping2(x, dic_map, cfgs)
    Evaluate value by mapping table of numpy.

plot_lines(x, dic1, dic2=None)
    Plot lines to see accuracy.

run_s2g()
    Build s-> graph and run it to get value of mapping table.

run_t2g()
    Build t-> graph and run it to get value of mapping table.

run_u2s()
    Build u->s graph and run it to get value of mapping table.

deepmd.nvnmd.entrypoints.mapt.mapt(*, nvnmd_config: Optional[str] = 'nvnmd/config.npy',
                                   nvnmd_weight: Optional[str] = 'nvnmd/weight.npy',
                                   nvnmd_map: Optional[str] = 'nvnmd/map.npy', **kwargs)

```

deepmd.nvnmd.entrypoints.train module

```

deepmd.nvnmd.entrypoints.train.normalized_input(fn, PATH_CNN, CONFIG_CNN)
    Normalize a input script file for continuous neural network.

deepmd.nvnmd.entrypoints.train.normalized_input_qnn(jdata, PATH_QNN, CONFIG_CNN,
                                                    WEIGHT_CNN, MAP_CNN)
    Normalize a input script file for quantize neural network.

deepmd.nvnmd.entrypoints.train.train_nvnmd(*, INPUT: str, restart: Optional[str], step: str,
                                           skip_neighbor_stat: bool = False, **kwargs)

```

deepmd.nvnmd.entrypoints.wrap module

```
class deepmd.nvnmd.entrypoints.wrap.Wrap(config_file: str, weight_file: str, map_file: str, model_file: str)
```

Bases: `object`

Generate the binary model file (model.pb).

the model file can be use to run the NVNMD with lammmps the pair style need set as:

```
pair_style nvnmd model.pb
pair_coeff * *
```

Parameters

`config_file`
input file name an .npy file containing the configuration information of NVNMD model

`weight_file`
input file name an .npy file containing the weights of NVNMD model

`map_file`
input file name an .npy file containing the mapping tables of NVNMD model

`model_file`
output file name an .pb file containing the model using in the NVNMD

References

DOI: 10.1038/s41524-022-00773-z

Methods

| | |
|--|---|
| <code>wrap_dscp()</code> | Wrap the configuration of descriptor. |
| <code>wrap_fitn()</code> | Wrap the weights of fitting net. |
| <code>wrap_head(nhs, nws)</code> | Wrap the head information. |
| <code>wrap_lut()</code> | Wrap the LUT. |
| <code>wrap_map()</code> | Wrap the mapping table of embedding network. |
| <code>wrap_weight(weight, NBIT_DISP, NBIT_WEIGHT)</code> | weight: weights of fittingNet NBIT_DISP: nbits of exponent of weight max value NBIT_WEIGHT: nbits of mantissa of weights. |

| | |
|-----------|--|
| wrap | |
| wrap_bias | |

`wrap()`

`wrap_bias(bias, NBIT_DATA, NBIT_DATA_FL)`

wrap_dscp()

Wrap the configuration of descriptor.

version 0: [NBIT_IDX_S2G-1:0] SHIFT_IDX_S2G

[NBIT_NEIB*NTYPE-1:0] SELs [NBIT_FIXD*M1*NTYPE*NTYPE-1:0] GSs [NBIT_FLTE-1:0]
NEXPO_DIV_NI

version 1:

[NBIT_FLTE-1:0] NEXPO_DIV_NI

wrap_fitn()

Wrap the weights of fitting net.

w weight b bias

wrap_head(nhs, nws)

Wrap the head information.

version nheight nweight rcut

wrap_lut()

Wrap the LUT.

wrap_map()

Wrap the mapping table of embedding network.

wrap_weight(weight, NBIT_DISP, NBIT_WEIGHT)

weight: weights of fittingNet NBIT_DISP: nbits of exponent of weight max value NBIT_WEIGHT:
nbits of mantissa of weights.

```
deepmd.nvnmd.entrypoints.wrap.wrap(*, nvnm_config: Optional[str] = 'nvnm/config.npy',
                                     nvnm_weight: Optional[str] = 'nvnm/weight.npy',
                                     nvnm_map: Optional[str] = 'nvnm/map.npy', nvnm_model:
                                     Optional[str] = 'nvnm/model.pb', **kwargs)
```

deepmd.nvnmd.fit package

nvnm.fit =====.

Provides

1. continuous fitting network
2. quantized fitting network

Submodules**deepmd.nvnmd.fit.ener module**

```
deepmd.nvnmd.fit.ener.one_layer_nvnm(inputs, outputs_size, activation_fn=<function tanh>,
                                       precision=tf.float64, stddev=1.0, bavg=0.0, name='linear',
                                       reuse=None, seed=None, use_timestep=False,
                                       trainable=True, useBN=False, uniform_seed=False,
                                       initial_variables=None, mixed_prec=None,
                                       final_layer=False)
```

Build one layer with continuous or quantized value. Its weight and bias can be initialed with random or constant value.

deepmd.nvnmd.utils package

class deepmd.nvnmd.utils.Encode

Bases: `object`

Encoding value as hex, bin, and dec format.

Methods

| | |
|---|--|
| <i>bin2hex</i> (data) | Convert binary string list to hex string list. |
| <i>bin2hex_str</i> (sbin) | Convert binary string to hex string. |
| <i>byte2hex</i> (bs, nbyte) | Convert byte into hex bs: low byte in the first hex: low byte in the right. |
| <i>check_dec</i> (idec, nbit[, signed, name]) | Check whether the data (idec) is in the range range is $[0, 2^{nbit} - 1]$ for unsigned range is $[-2^{nbit-1}, 2^{nbit-1} - 1]$ for signed. |
| <i>dec2bin</i> (idec[, nbit, signed, name]) | Convert dec array to binary string list. |
| <i>extend_bin</i> (slbin, nfull) | Extend the element of list (slbin) to the length (nfull). |
| <i>extend_hex</i> (slhex, nfull) | Extend the element of list (slhex) to the length (nfull). |
| <i>extend_list</i> (slbin, nfull) | Extend the list (slbin) to the length (nfull) the attached element of list is 0. |
| <i>flt2bin</i> (data, nbit_expo, nbit_frac) | Convert float into binary string list. |
| <i>hex2bin</i> (data) | Convert hex string list to binary string list. |
| <i>hex2bin_str</i> (shex) | Convert hex string to binary string. |
| <i>merge_bin</i> (slbin, nmerge) | Merge binary string list per nmerge value. |
| <i>qc</i> (v[, nbit]) | Quantize value using ceil. |
| <i>qf</i> (v[, nbit]) | Quantize value using floor. |
| <i>qr</i> (v[, nbit]) | Quantize value using round. |
| <i>reverse_bin</i> (slbin, nreverse) | Reverse binary string list per nreverse value. |
| <i>split_bin</i> (sbin, nbit) | Split sbin into many segment with the length nbit. |

| | |
|-----------------|--|
| find_max_expo | |
| flt2bin_one | |
| norm_expo | |
| split_expo_mant | |

bin2hex(data)

Convert binary string list to hex string list.

bin2hex_str(sbin)

Convert binary string to hex string.

byte2hex(bs, nbyte)

Convert byte into hex bs: low byte in the first hex: low byte in the right.

check_dec(idec, nbit, signed=False, name='')

Check whether the data (idec) is in the range range is $[0, 2^{nbit} - 1]$ for unsigned range is $[-2^{nbit-1}, 2^{nbit-1} - 1]$ for signed.

dec2bin(idec, nbit=10, signed=False, name='')

Convert dec array to binary string list.

extend_bin(slbin, nfull)

Extend the element of list (slbin) to the length (nfull).

such as, when

```
slbin = ['10010', '10100'],
nfull = 6
```

extent to

```
['010010', '010100']
```

extend_hex(slhex, nfull)

Extend the element of list (slhex) to the length (nfull).

extend_list(slbin, nfull)

Extend the list (slbin) to the length (nfull) the attached element of list is 0.

such as, when

```
slbin = ['10010', '10100'],
nfull = 4
```

extent it to

```
['10010', '10100', '00000', '00000']
```

find_max_expo(v, expo_min=-1000)

flt2bin(data, nbit_expo, nbit_frac)

Convert float into binary string list.

flt2bin_one(v, nbit_expo, nbit_frac)

hex2bin(data)

Convert hex string list to binary string list.

hex2bin_str(shex)

Convert hex string to binary string.

merge_bin(slbin, nmerge)

Merge binary string list per nmerge value.

norm_expo(v, nbit_frac=20, expo_min=-1000)

```

qc(v, nbit: int = 14)
    Quantize value using ceil.
qf(v, nbit: int = 14)
    Quantize value using floor.
qr(v, nbit: int = 14)
    Quantize value using round.
reverse_bin(sbin, nreverse)
    Reverse binary string list per nreverse value.
split_bin(sbin, nbit: int)
    Split sbins into many segments with the length nbit.
split_expo_mant(v, min=-1000)

```

```
class deepmd.nvnmd.utils.FioBin
```

Bases: `object`

Input and output for binary file.

Methods

| | |
|---|------------------------------------|
| <code>load([file_name, default_value])</code> | Load binary file into bytes value. |
| <code>save(file_name, data)</code> | Save hex string into binary file. |

```
load(file_name="", default_value="")
    Load binary file into bytes value.
```

```
save(file_name: str, data: List[str])
    Save hex string into binary file.
```

```
class deepmd.nvnmd.utils.FioDic
```

Bases: `object`

Input and output for dict class data the file can be .json or .npz file containing a dictionary.

Methods

| | |
|-------------------------------------|---|
| <code>update(jdata, jdata_o)</code> | Update key-value pair is key in <code>jdata_o.keys()</code> . |
|-------------------------------------|---|

| | |
|------|--|
| get | |
| load | |
| save | |

```
get(jdata, key, default_value)
```

```
load(file_name="", default_value={})
```

```
save(file_name="", dic={})
```

update(jdata, jdata_o)

Update key-value pair is key in jdata_o.keys().

Parameters

jdata
new jdata
jdata_o
origin jdata

class deepmd.nvnmd.utils.FioTxt

Bases: `object`

Input and output for .txt file with string.

Methods

| | |
|--|----------------------------------|
| <code>load</code> ([file_name, default_value]) | Load .txt file into string list. |
| <code>save</code> ([file_name, data]) | Save string list into .txt file. |

load(file_name="", default_value=[])

Load .txt file into string list.

save(file_name: `str` = "", data: `list` = [])

Save string list into .txt file.

deepmd.nvnmd.utils.**get_filter_weight**(weights: `int`, spe_j: `int`, layer_l: `int`)

Get weight and bias of embedding network.

Parameters

weights
[`dict`] weights
spe_j
[`int`] special order of neighbor atom j 0~n`type`-1
layer_l
layer order in embedding network 1~nlayer

deepmd.nvnmd.utils.**get_fitnet_weight**(weights: `dict`, spe_i: `int`, layer_l: `int`, nlayer: `int` = 10)

Get weight and bias of fitting network.

Parameters

weights
[`dict`] weights
spe_i
[`int`] special order of central atom i 0~n`type`-1
layer_l
[`int`] layer order in embedding network 0~nlayer-1
nlayer
[`int`] number of layers

```
deepmd.nvnmd.utils.map_nvnmd(x, map_y, map_dy, prec, nbit=None)
```

Mapping function implemented by numpy.

```
deepmd.nvnmd.utils.nvnmd_args()
```

```
deepmd.nvnmd.utils.one_layer(inputs, outputs_size, activation_fn=<function tanh>,
                             precision=tf.float64, stddev=1.0, bavg=0.0, name='linear', reuse=None,
                             seed=None, use_timestep=False, trainable=True, useBN=False,
                             uniform_seed=False, initial_variables=None, mixed_prec=None,
                             final_layer=False)
```

Build one layer with continuous or quantized value. Its weight and bias can be initialed with random or constant value.

Submodules

`deepmd.nvnmd.utils.argcheck` module

```
deepmd.nvnmd.utils.argcheck.nvnmd_args()
```

`deepmd.nvnmd.utils.config` module

```
class deepmd.nvnmd.utils.config.NvnmdConfig(jdata: dict)
```

Bases: `object`

Configuration for NVNMD record the message of model such as size, using nvnmd or not.

Parameters

jdata

a dictionary of input script

References

DOI: 10.1038/s41524-022-00773-z

Methods

| | |
|---|--|
| <code>disp_message()</code> | Display the log of NVNMD. |
| <code>get_deepmd_jdata()</code> | Generate input script with member element one by one. |
| <code>get_dp_init_weights()</code> | Build the weight dict for initialization of net. |
| <code>get_dscp_jdata()</code> | Generate model/descriptor in input script. |
| <code>get_fitn_jdata()</code> | Generate model/fitting_net in input script. |
| <code>get_learning_rate_jdata()</code> | Generate learning_rate in input script. |
| <code>get_loss_jdata()</code> | Generate loss in input script. |
| <code>get_model_jdata()</code> | Generate model in input script. |
| <code>get_nvnmd_jdata()</code> | Generate nvnmd in input script. |
| <code>get_s_range(davg, dstd)</code> | Get the range of switch function. |
| <code>get_training_jdata()</code> | Generate training in input script. |
| <code>init_config_by_version(version)</code> | Initialize version-dependent parameters. |
| <code>init_ctrl(jdata[, jdata_parent])</code> | Initialize members about control signal. |
| <code>init_dpjn(jdata[, jdata_parent])</code> | Initialize members about other deepmd input. |
| <code>init_dscp(jdata[, jdata_parent])</code> | Initialize members about descriptor. |
| <code>init_fitn(jdata[, jdata_parent])</code> | Initialize members about fitting network. |
| <code>init_from_config(jdata)</code> | Initialize member element one by one. |
| <code>init_from_deepmd_input(jdata)</code> | Initialize members with input script of deepmd. |
| <code>init_from_jdata([jdata])</code> | Initialize this class with jdata loaded from input script. |
| <code>init_nbit(jdata[, jdata_parent])</code> | Initialize members about quantification precision. |
| <code>init_net_size()</code> | Initialize net_size. |
| <code>init_size(jdata[, jdata_parent])</code> | Initialize members about ram capacity. |
| <code>init_train_mode([mod])</code> | Configure for taining cnn or qnn. |
| <code>init_value()</code> | Initialize member with dict. |
| <code>save([file_name])</code> | Save all configuration to file. |
| <code>set_ntype(ntype)</code> | Set the number of type. |
| <code>update_config()</code> | Update config from dict. |

disp_message()

Display the log of NVNMD.

get_deepmd_jdata()

Generate input script with member element one by one.

get_dp_init_weights()

Build the weight dict for initialization of net.

get_dscp_jdata()

Generate model/descriptor in input script.

get_fitn_jdata()

Generate model/fitting_net in input script.

get_learning_rate_jdata()

Generate learning_rate in input script.

get_loss_jdata()

Generate loss in input script.

`get_model_jdata()`
Generate model in input script.

`get_nvnmmd_jdata()`
Generate nvnmmd in input script.

`get_s_range(davg, dstd)`
Get the range of switch function.

`get_training_jdata()`
Generate training in input script.

`init_config_by_version(version)`
Initialize version-dependent parameters.

`init_ctrl(jdata: dict, jdata_parent: dict = {}) → dict`
Initialize members about control signal.

`init_dpin(jdata: dict, jdata_parent: dict = {}) → dict`
Initialize members about other deepmd input.

`init_dscp(jdata: dict, jdata_parent: dict = {}) → dict`
Initialize members about descriptor.

`init_fitn(jdata: dict, jdata_parent: dict = {}) → dict`
Initialize members about fitting network.

`init_from_config(jdata)`
Initialize member element one by one.

`init_from_deepmd_input(jdata)`
Initialize members with input script of deepmd.

`init_from_jdata(jdata: dict = {})`
Initialize this class with jdata loaded from input script.

`init_nbit(jdata: dict, jdata_parent: dict = {}) → dict`
Initialize members about quantification precision.

`init_net_size()`
Initialize net_size.

`init_size(jdata: dict, jdata_parent: dict = {}) → dict`
Initialize members about ram capacity.

`init_train_mode(mod='cnn')`
Configure for training cnn or qnn.

`init_value()`
Initialize member with dict.

`save(file_name=None)`
Save all configuration to file.

`set_ntype(ntype)`
Set the number of type.

`update_config()`
Update config from dict.

deepmd.nvnmd.utils.encode module

class deepmd.nvnmd.utils.encode.Encode

Bases: `object`

Encoding value as hex, bin, and dec format.

Methods

| | |
|---|--|
| <i>bin2hex</i> (data) | Convert binary string list to hex string list. |
| <i>bin2hex_str</i> (sbin) | Convert binary string to hex string. |
| <i>byte2hex</i> (bs, nbyte) | Convert byte into hex bs: low byte in the first hex: low byte in the right. |
| <i>check_dec</i> (idec, nbit[, signed, name]) | Check whether the data (idec) is in the range range is $[0, 2^{nbit} - 1]$ for unsigned range is $[-2^{nbit-1}, 2^{nbit-1} - 1]$ for signed. |
| <i>dec2bin</i> (idec[, nbit, signed, name]) | Convert dec array to binary string list. |
| <i>extend_bin</i> (slbin, nfull) | Extend the element of list (slbin) to the length (nfull). |
| <i>extend_hex</i> (slhex, nfull) | Extend the element of list (slhex) to the length (nfull). |
| <i>extend_list</i> (slbin, nfull) | Extend the list (slbin) to the length (nfull) the attached element of list is 0. |
| <i>flt2bin</i> (data, nbit_expo, nbit_frac) | Convert float into binary string list. |
| <i>hex2bin</i> (data) | Convert hex string list to binary string list. |
| <i>hex2bin_str</i> (shex) | Convert hex string to binary string. |
| <i>merge_bin</i> (slbin, nmerge) | Merge binary string list per nmerge value. |
| <i>qc</i> (v[, nbit]) | Quantize value using ceil. |
| <i>qf</i> (v[, nbit]) | Quantize value using floor. |
| <i>qr</i> (v[, nbit]) | Quantize value using round. |
| <i>reverse_bin</i> (slbin, nreverse) | Reverse binary string list per nreverse value. |
| <i>split_bin</i> (sbin, nbit) | Split sbin into many segment with the length nbit. |

| | |
|-----------------|--|
| find_max_expo | |
| flt2bin_one | |
| norm_expo | |
| split_expo_mant | |

bin2hex(data)

Convert binary string list to hex string list.

bin2hex_str(sbin)

Convert binary string to hex string.

byte2hex(bs, nbyte)

Convert byte into hex bs: low byte in the first hex: low byte in the right.

check_dec(idec, nbit, signed=False, name='')

Check whether the data (idec) is in the range range is $[0, 2^{nbit} - 1]$ for unsigned range is $[-2^{nbit-1}, 2^{nbit-1} - 1]$ for signed.

dec2bin(idec, nbit=10, signed=False, name='')
Convert dec array to binary string list.

extend_bin(slbin, nfull)
Extend the element of list (slbin) to the length (nfull).
such as, when

slbin = ['10010', '10100'],
nfull = 6

extent to
['010010', '010100']

extend_hex(slhex, nfull)
Extend the element of list (slhex) to the length (nfull).

extend_list(slbin, nfull)
Extend the list (slbin) to the length (nfull) the attached element of list is 0.
such as, when

slbin = ['10010', '10100'],
nfull = 4

extent it to
['10010', '10100', '00000', '00000']

find_max_expo(v, expo_min=-1000)

flt2bin(data, nbit_expo, nbit_frac)
Convert float into binary string list.

flt2bin_one(v, nbit_expo, nbit_frac)

hex2bin(data)
Convert hex string list to binary string list.

hex2bin_str(shex)
Convert hex string to binary string.

merge_bin(slbin, nmerge)
Merge binary string list per nmerge value.

norm_expo(v, nbit_frac=20, expo_min=-1000)

qc(v, nbit: int = 14)
Quantize value using ceil.

qf(v, nbit: int = 14)
Quantize value using floor.


```

qr(v, nbit: int = 14)
    Quantize value using round.

reverse_bin(sbin, nreverse)
    Reverse binary string list per nreverse value.

split_bin(sbin, nbit: int)
    Split sbin into many segment with the length nbit.

split_expo_mant(v, min=-1000)

```

deepmd.nvnmd.utils.fio module

```

class deepmd.nvnmd.utils.fio.Fio
    Bases: object
    Basic class for FIO.

```

Methods

| | |
|------------------|--|
| create_file_path | |
| exits | |
| get_file_list | |
| is_file | |
| is_path | |
| mkdir | |

```

create_file_path(file_name='')

exits(file_name='')

get_file_list(path) → list

is_file(file_name)

is_path(path)

mkdir(path_name='')

class deepmd.nvnmd.utils.fio.FioBin
    Bases: object
    Input and output for binary file.

```

Methods

| | |
|---|------------------------------------|
| <code>load([file_name, default_value])</code> | Load binary file into bytes value. |
| <code>save(file_name, data)</code> | Save hex string into binary file. |

`load(file_name="", default_value="")`
Load binary file into bytes value.

`save(file_name: str, data: List[str])`
Save hex string into binary file.

`class deepmd.nvnmd.utils.fio.FioDic`

Bases: `object`

Input and output for dict class data the file can be .json or .npz file containing a dictionary.

Methods

| | |
|-------------------------------------|---|
| <code>update(jdata, jdata_o)</code> | Update key-value pair is key in jdata_o.keys(). |
|-------------------------------------|---|

| | |
|------|--|
| get | |
| load | |
| save | |

`get(jdata, key, default_value)`

`load(file_name="", default_value={})`

`save(file_name="", dic={})`

`update(jdata, jdata_o)`

Update key-value pair is key in jdata_o.keys().

Parameters

jdata
new jdata
jdata_o
origin jdata

`class deepmd.nvnmd.utils.fio.FioJsonDic`

Bases: `object`

Input and output for .json file containing dictionary.

Methods

| | |
|---|----------------------------|
| <code>load([file_name, default_value])</code> | Load .json file into dict. |
| <code>save([file_name, dic])</code> | Save dict into .json file. |

`load(file_name="", default_value={})`

Load .json file into dict.

`save(file_name="", dic={})`

Save dict into .json file.

`class deepmd.nvnmd.utils.fio.FioNpyDic`

Bases: `object`

Input and output for .npz file containing dictionary.

Methods

| | |
|-------------------|--|
| <code>load</code> | |
| <code>save</code> | |

`load(file_name="", default_value={})`

`save(file_name="", dic={})`

`class deepmd.nvnmd.utils.fio.FioTxt`

Bases: `object`

Input and output for .txt file with string.

Methods

| | |
|---|----------------------------------|
| <code>load([file_name, default_value])</code> | Load .txt file into string list. |
| <code>save([file_name, data])</code> | Save string list into .txt file. |

`load(file_name="", default_value=[])`

Load .txt file into string list.

`save(file_name: str = "", data: list = [])`

Save string list into .txt file.

deepmd.nvnmd.utils.network module

`deepmd.nvnmd.utils.network.get_sess()`

`deepmd.nvnmd.utils.network.matmul2_qq(a, b, nbit)`

Quantized matmul operation for 2d tensor. a and b is input tensor, nbit represent quantification precision.

`deepmd.nvnmd.utils.network.matmul3_qq(a, b, nbit)`

Quantized matmul operation for 3d tensor. a and b is input tensor, nbit represent quantification precision.

`deepmd.nvnmd.utils.network.one_layer(inputs, outputs_size, activation_fn=<function tanh>, precision=tf.float64, stddev=1.0, bavg=0.0, name='linear', reuse=None, seed=None, use_timestep=False, trainable=True, useBN=False, uniform_seed=False, initial_variables=None, mixed_prec=None, final_layer=False)`

Build one layer with continuous or quantized value. Its weight and bias can be initialed with random or constant value.

`deepmd.nvnmd.utils.network.one_layer_t(shape, outputs_size, bavg, stddev, precision, trainable, initial_variables, seed, uniform_seed, name)`

`deepmd.nvnmd.utils.network.one_layer_wb(shape, outputs_size, bavg, stddev, precision, trainable, initial_variables, seed, uniform_seed, name)`

`deepmd.nvnmd.utils.network.qf(x, nbit)`

Quantize and floor tensor x with quantification precision nbit.

`deepmd.nvnmd.utils.network.qr(x, nbit)`

Quantize and round tensor x with quantification precision nbit.

`deepmd.nvnmd.utils.network.tanh4(x)`

deepmd.nvnmd.utils.op module

`deepmd.nvnmd.utils.op.map_nvnmd(x, map_y, map_dy, prec, nbit=None)`

Mapping function implemented by numpy.

`deepmd.nvnmd.utils.op.r2s(r, rmin, rmax)`

deepmd.nvnmd.utils.weight module

`deepmd.nvnmd.utils.weight.get_constant_initializer(weights, name)`

Get initial value by name and create a initializer.

`deepmd.nvnmd.utils.weight.get_filter_type_weight(weights: dict, layer_l: int)`

Get weight and bias of two_side_type_embedding network.

Parameters

weights

[dict] weights

layer_l

layer order in embedding network 1~nlayer

`deepmd.nvnmd.utils.weight.get_filter_weight(weights: int, spe_j: int, layer_l: int)`

Get weight and bias of embedding network.

Parameters

weights

[dict] weights

```

    spe_j
        [int] special order of neighbor atom j 0~ntype-1
    layer_l
        layer order in embedding network 1~nlayer
deepmd.nvnmd.utils.weight.get_fitnet_weight(weights: dict, spe_i: int, layer_l: int, nlayer: int = 10)
    Get weight and bias of fitting network.
    Parameters
    weights
        [dict] weights
    spe_i
        [int] special order of central atom i 0~ntype-1
    layer_l
        [int] layer order in embedding network 0~nlayer-1
    nlayer
        [int] number of layers
deepmd.nvnmd.utils.weight.get_normalize(weights: dict)
    Get normalize parameter (avg and std) of  $s_{ji}$ .
deepmd.nvnmd.utils.weight.get_type_embedding_weight(weights: dict, layer_l: int)
    Get weight and bias of type_embedding network.
    Parameters
    weights
        [dict] weights
    layer_l
        layer order in embedding network 1~nlayer
deepmd.nvnmd.utils.weight.get_type_weight(weights: dict, layer_l: int)
    Get weight and bias of fitting network.
    Parameters
    weights
        [dict] weights
    layer_l
        [int] layer order in embedding network 0~nlayer-1
deepmd.nvnmd.utils.weight.get_weight(weights, key)
    Get weight value according to key.

```

deepmd.op package

This module will house cust Tf OPs after CMake installation.

```
deepmd.op.import_ops()
```

Import all custom TF ops that are present in this submodule.

Notes

Initially this subdir is unpopulated. CMake will install all the op module python files and shared libs.

deepmd.train package

Submodules

deepmd.train.run_options module

Module taking care of important package constants.

```
class deepmd.train.run_options.RunOptions(init_model: Optional[str] = None, init_frz_model:
                                          Optional[str] = None, finetune: Optional[str] = None,
                                          restart: Optional[str] = None, log_path: Optional[str] =
                                          None, log_level: int = 0, mpi_log: str = 'master')
```

Bases: `object`

Class with info on how to run training (cluster, MPI and GPU config).

Attributes

```
gpus: Optional[List[int]]
    list of GPUs if any are present else None

is_chief: bool
    in distribured training it is true for tha main MPI process in serail it is always true

world_size: int
    total worker count

my_rank: int
    index of the MPI task

nodename: str
    name of the node

node_list_
    [List[str]] the list of nodes of the current mpirun

my_device: str
    deviice type - gpu or cpu
```

Methods

| | |
|---------------------------------------|--|
| <code>print_resource_summary()</code> | Print build and current running cluster configuration summary. |
|---------------------------------------|--|

`gpus: Optional[List[int]]`
`property is_chief`
 Whether my rank is 0.
`my_device: str`
`my_rank: int`
`odelist: List[int]`
`nodename: str`
`print_resource_summary()`
 Print build and current running cluster configuration summary.
`world_size: int`

deepmd.train.trainer module

`class deepmd.train.trainer.DPTrainer(jdata, run_opt, is_compress=False)`
 Bases: `object`

Methods

| | |
|--------------------------------|----------------------------|
| <code>save_compressed()</code> | Save the compressed graph. |
|--------------------------------|----------------------------|

| | |
|------------------------|--|
| build | |
| eval_single_list | |
| get_evaluation_results | |
| get_feed_dict | |
| get_global_step | |
| print_header | |
| print_on_training | |
| save_checkpoint | |
| train | |
| valid_on_the_fly | |

`build(data=None, stop_batch=0, origin_type_map=None, suffix='')`
`static eval_single_list(single_batch_list, loss, sess, get_feed_dict_func, prefix='')`
`get_evaluation_results(batch_list)`
`get_feed_dict(batch, is_training)`

```
get_global_step()

static print_header(fp, train_results, valid_results, multi_task_mode=False)

static print_on_training(fp, train_results, valid_results, cur_batch, cur_lr,
                        multi_task_mode=False, cur_lr_dict=None)

save_checkpoint(cur_batch: int)

save_compressed()
    Save the compressed graph.

train(train_data=None, valid_data=None)

valid_on_the_fly(fp, train_batches, valid_batches, print_header=False, fitting_key=None)

class deepmd.train.trainer.DatasetLoader(train_data: DeepmdDataSystem)
    Bases: object

    Generate an OP that loads the training data from the given DeepmdDataSystem.

    It can be used to load the training data in the training process, so there is no waiting time between
    training steps.

    Parameters
        train_data
            [DeepmdDataSystem] The training data.
```

Examples

```
>>> loader = DatasetLoader(train_data)
>>> data_op = loader.build()
>>> with tf.Session() as sess:
>>>     data_list = sess.run(data_op)
>>> data_dict = loader.get_data_dict(data_list)
```

Methods

| | |
|--|--|
| <code>build()</code> | Build the OP that loads the training data. |
| <code>get_data_dict(batch_list)</code> | Generate a dict of the loaded data. |

`build()` → `List[Tensor]`

Build the OP that loads the training data.

Returns

`List[tf.Tensor]`

Tensor of the loaded data.

`get_data_dict(batch_list: List[ndarray])` → `Dict[str, ndarray]`

Generate a dict of the loaded data.

Parameters

`batch_list`

`[List[np.ndarray]]` The loaded data.

Returns

`Dict[str, np.ndarray]`
The dict of the loaded data.

deepmd.utils package

```
class deepmd.utils.DeepmdData(sys_path: str, set_prefix: str = 'set', shuffle_test: bool = True,
                              type_map: Optional[List[str]] = None, optional_type_map: bool =
                              True, modifier=None, trn_all_set: bool = False)
```

Bases: `object`

Class for a data system.

It loads data from hard disk, and mantains the data as a `data_dict`

Parameters

`sys_path`
Path to the data system

`set_prefix`
Prefix for the directories of different sets

`shuffle_test`
If the test data are shuffled

`type_map`
Gives the name of different atom types

`optional_type_map`
If the `type_map.raw` in each system is optional

`modifier`
Data modifier that has the method `modify_data`

`trn_all_set`
Use all sets as training dataset. Otherwise, if the number of sets is more than 1, the last set is left for test.

Methods

| | |
|---|--|
| <code>add(key, ndof[, atomic, must, high_prec, ...])</code> | Add a data item that to be loaded. |
| <code>avg(key)</code> | Return the average value of an item. |
| <code>check_batch_size(batch_size)</code> | Check if the system can get a batch of data with <code>batch_size</code> frames. |
| <code>check_test_size(test_size)</code> | Check if the system can get a test dataset with <code>test_size</code> frames. |
| <code>get_atom_type()</code> | Get atom types. |
| <code>get_batch(batch_size)</code> | Get a batch of data with <code>batch_size</code> frames. |
| <code>get_data_dict()</code> | Get the <code>data_dict</code> . |
| <code>get_natoms()</code> | Get number of atoms. |
| <code>get_natoms_vec(ntypes)</code> | Get number of atoms and number of atoms in different types. |
| <code>get_ntypes()</code> | Number of atom types in the system. |
| <code>get_num_batch(batch_size, set_idx)</code> | Get the number of batches in a set. |
| <code>get_num_set()</code> | Get number of training sets. |
| <code>get_sys_num_batch(batch_size)</code> | Get the number of batches in the data system. |
| <code>get_test([ntests])</code> | Get the test data with <code>ntests</code> frames. |
| <code>get_type_map()</code> | Get the type map. |
| <code>reduce(key_out, key_in)</code> | Generate a new item from the reduction of another atom. |

| | |
|-----------------|--|
| reset_get_batch | |
|-----------------|--|

add(key: str, ndof: int, atomic: bool = False, must: bool = False, high_prec: bool = False, type_sel: Optional[List[int]] = None, repeat: int = 1, default: float = 0.0, dtype: Optional[dtype] = None)
Add a data item that to be loaded.

Parameters

key

The key of the item. The corresponding data is stored in `sys_path/set.*/key.npy`

ndof

The number of dof

atomic

The item is an atomic property. If False, the size of the data should be `nframes x ndof` If True, the size of data should be `nframes x natoms x ndof`

must

The data file `sys_path/set.*/key.npy` must exist. If `must` is False and the data file does not exist, the `data_dict[find_key]` is set to 0.0

high_prec

Load the data and store in float64, otherwise in float32

type_sel

Select certain type of atoms

repeat

The data will be repeated `repeat` times.

default

[float, default=0.] default value of data

`dtype`
`[np.dtype, optional]` the dtype of data, overwrites `high_prec` if provided

avg(key)
 Return the average value of an item.

check_batch_size(batch_size)
 Check if the system can get a batch of data with `batch_size` frames.

check_test_size(test_size)
 Check if the system can get a test dataset with `test_size` frames.

get_atom_type() → `List[int]`
 Get atom types.

get_batch(batch_size: int) → dict
 Get a batch of data with `batch_size` frames. The frames are randomly picked from the data system.

Parameters

`batch_size`
 size of the batch

get_data_dict() → `dict`
 Get the `data_dict`.

get_natoms()
 Get number of atoms.

get_natoms_vec(ntypes: int)
 Get number of atoms and number of atoms in different types.

Parameters

`ntypes`
 Number of types (may be larger than the actual number of types in the system).

Returns

natoms
`natoms[0]`: number of local atoms `natoms[1]`: total number of atoms held by this processor `natoms[i]`: $2 \leq i < Ntypes+2$, number of type `i` atoms

get_ntypes() → `int`
 Number of atom types in the system.

get_numb_batch(batch_size: int, set_idx: int) → int
 Get the number of batches in a set.

get_numb_set() → `int`
 Get number of training sets.

get_sys_numb_batch(batch_size: int) → int
 Get the number of batches in the data system.

get_test(ntests: int = -1) → dict
 Get the test data with `ntests` frames.

Parameters

`ntests`
 Size of the test data set. If `ntests` is -1, all test data will be get.

`get_type_map()` → `List[str]`

Get the type map.

`reduce(key_out: str, key_in: str)`

Generate a new item from the reduction of another atom.

Parameters

`key_out`

The name of the reduced item

`key_in`

The name of the data item to be reduced

`reset_get_batch()`

```
class deepmd.utils.DeepmdDataSystem(systems: List[str], batch_size: int, test_size: int, rcut: float,
                                     set_prefix: str = 'set', shuffle_test: bool = True, type_map:
                                     Optional[List[str]] = None, optional_type_map: bool = True,
                                     modifier=None, trn_all_set=False, sys_probs=None,
                                     auto_prob_style='prob_sys_size')
```

Bases: `object`

Class for manipulating many data systems.

It is implemented with the help of `DeepmdData`

Attributes

`default_mesh`

Mesh for each system.

Methods

| | |
|---|---|
| <code>add(key, ndof[, atomic, must, high_prec, ...])</code> | Add a data item that to be loaded. |
| <code>add_dict(adict)</code> | Add items to the data system by a dict. |
| <code>get_batch([sys_idx])</code> | Get a batch of data from the data systems. |
| <code>get_batch_mixed()</code> | Get a batch of data from the data systems in the mixed way. |
| <code>get_batch_size()</code> | Get the batch size. |
| <code>get_batch_standard([sys_idx])</code> | Get a batch of data from the data systems in the standard way. |
| <code>get_nbatchs()</code> | Get the total number of batches. |
| <code>get_nsystems()</code> | Get the number of data systems. |
| <code>get_ntypes()</code> | Get the number of types. |
| <code>get_sys(idx)</code> | Get a certain data system. |
| <code>get_sys_ntest([sys_idx])</code> | Get number of tests for the currently selected system, or one defined by <code>sys_idx</code> . |
| <code>get_test([sys_idx, n_test])</code> | Get test data from the the data systems. |
| <code>get_type_map()</code> | Get the type map. |
| <code>reduce(key_out, key_in)</code> | Generate a new item from the reduction of another atom. |

| | |
|----------------------|--|
| compute_energy_shift | |
| get_data_dict | |
| print_summary | |
| set_sys_probs | |

add(key: str, ndof: int, atomic: bool = False, must: bool = False, high_prec: bool = False, type_sel: Optional[List[int]] = None, repeat: int = 1, default: float = 0.0)

Add a data item that to be loaded.

Parameters

key

The key of the item. The corresponding data is stored in sys_path/set.*/key.npy

ndof

The number of dof

atomic

The item is an atomic property. If False, the size of the data should be nframes x ndof If True, the size of data should be nframes x natoms x ndof

must

The data file sys_path/set.*/key.npy must exist. If must is False and the data file does not exist, the data_dict[find_key] is set to 0.0

high_prec

Load the data and store in float64, otherwise in float32

type_sel

Select certain type of atoms

repeat

The data will be repeated repeat times.

default, default=0.

Default value of data

add_dict(adict: dict) → None

Add items to the data system by a dict. adict should have items like .. code-block:: python.

```
adict[key] = {
    "ndof": ndof, "atomic": atomic, "must": must, "high_prec": high_prec, "type_sel":
    type_sel, "repeat": repeat,
}
```

For the explanation of the keys see add

compute_energy_shift(rcond=None, key='energy')

property default_mesh: List[ndarray]

Mesh for each system.

get_batch(sys_idx: Optional[int] = None) → dict

Get a batch of data from the data systems.

Parameters

sys_idx

[int] The index of system from which the batch is get. If sys_idx is not None,

`sys_probs` and `auto_prob_style` are ignored. If `sys_idx` is `None`, automatically determine the system according to `sys_probs` or `auto_prob_style`, see the following. This option does not work for mixed systems.

Returns

`dict`

The batch data

`get_batch_mixed()` → `dict`

Get a batch of data from the data systems in the mixed way.

Returns

`dict`

The batch data

`get_batch_size()` → `int`

Get the batch size.

`get_batch_standard(sys_idx: Optional[int] = None)` → `dict`

Get a batch of data from the data systems in the standard way.

Parameters

`sys_idx`

[`int`] The index of system from which the batch is get. If `sys_idx` is not `None`, `sys_probs` and `auto_prob_style` are ignored. If `sys_idx` is `None`, automatically determine the system according to `sys_probs` or `auto_prob_style`, see the following.

Returns

`dict`

The batch data

`get_data_dict(ii: int = 0)` → `dict`

`get_nbatches()` → `int`

Get the total number of batches.

`get_nsystems()` → `int`

Get the number of data systems.

`get_ntypes()` → `int`

Get the number of types.

`get_sys(idx: int)` → `DeepmdData`

Get a certain data system.

`get_sys_ntest(sys_idx=None)`

Get number of tests for the currently selected system, or one defined by `sys_idx`.

`get_test(sys_idx: Optional[int] = None, n_test: int = -1)`

Get test data from the the data systems.

Parameters

`sys_idx`

The test dat of system with index `sys_idx` will be returned. If is `None`, the currently selected system will be returned.

```

    n_test
        Number of test data. If set to -1 all test data will be get.

get_type_map() → List[str]
    Get the type map.

print_summary(name)

reduce(key_out, key_in)
    Generate a new item from the reduction of another atom.

    Parameters
        key_out
            The name of the reduced item
        key_in
            The name of the data item to be reduced

set_sys_probs(sys_probs=None, auto_prob_style: str = 'prob_sys_size')

class deepmd.utils.LearningRateExp(start_lr: float, stop_lr: float = 5e-08, decay_steps: int = 5000,
                                   decay_rate: float = 0.95)

```

Bases: `object`

The exponentially decaying learning rate.

The learning rate at step t is given by

$$\alpha(t) = \alpha_0 \lambda^{t/\tau}$$

where α is the learning rate, α_0 is the starting learning rate, λ is the decay rate, and τ is the decay steps.

Parameters

start_lr
Starting learning rate α_0

stop_lr
Stop learning rate α_1

decay_steps
Learning rate decay every this number of steps τ

decay_rate
The decay rate λ . If stop_step is provided in build, then it will be determined automatically and overwritten.

Methods

| | |
|--|-------------------------------|
| <code>build(global_step[, stop_step])</code> | Build the learning rate. |
| <code>start_lr()</code> | Get the start lr. |
| <code>value(step)</code> | Get the lr at a certain step. |

`build(global_step: Tensor, stop_step: Optional[int] = None) → Tensor`

Build the learning rate.

Parameters

`global_step`

The tf Tensor providing the global training step

`stop_step`

The stop step. If provided, the `decay_rate` will be determined automatically and overwritten.

Returns

`learning_rate`

The learning rate

`start_lr()` → float

Get the start lr.

`value(step: int)` → float

Get the lr at a certain step.

`class deepmd.utils.PairTab(filename: str)`

Bases: `object`

Pairwise tabulated potential.

Parameters

`filename`

File name for the short-range tabulated potential. The table is a text data file with $(N_t + 1) * N_t / 2 + 1$ columns. The first column is the distance between atoms. The second to the last columns are energies for pairs of certain types. For example we have two atom types, 0 and 1. The columns from 2nd to 4th are for 0-0, 0-1 and 1-1 correspondingly.

Methods

| | |
|-------------------------------|---------------------------------------|
| <code>get()</code> | Get the serialized table. |
| <code>reinit(filename)</code> | Initialize the tabulated interaction. |

`get()` → `Tuple[array, array]`

Get the serialized table.

`reinit(filename: str)` → `None`

Initialize the tabulated interaction.

Parameters

`filename`

File name for the short-range tabulated potential. The table is a text data file with $(N_t + 1) * N_t / 2 + 1$ columns. The first column is the distance between atoms. The second to the last columns are energies for pairs of certain types. For example we have two atom types, 0 and 1. The columns from 2nd to 4th are for 0-0, 0-1 and 1-1 correspondingly.

`class deepmd.utils.Plugin`

Bases: `object`

A class to register and restore plugins.

Examples

```
>>> plugin = Plugin()
>>> @plugin.register("xx")
    def xxx():
        pass
>>> print(plugin.plugins['xx'])
```

Attributes

plugins
[Dict[str, object]] plugins

Methods

| | |
|------------------------------|------------------------|
| <code>get_plugin(key)</code> | Visit a plugin by key. |
| <code>register(key)</code> | Register a plugin. |

`get_plugin(key) → object`

Visit a plugin by key.

Parameters

key
[str] key of the plugin

Returns

object
the plugin

`register(key: str) → Callable[[object], object]`

Register a plugin.

Parameters

key
[str] key of the plugin

Returns

Callable[[object], object]
decorator

`class deepmd.utils.PluginVariant(*args, **kwargs)`

Bases: object

A class to remove type from input arguments.

Submodules

deepmd.utils.argcheck module

class deepmd.utils.argcheck.ArgsPlugin

Bases: `object`

Methods

| | |
|---|--|
| <code>get_all_argument([exclude_hybrid])</code> | Get all arguments. |
| <code>register(name[, alias])</code> | Register a descriptor argument plugin. |

`get_all_argument(exclude_hybrid: bool = False) → List[Argument]`

Get all arguments.

Parameters

`exclude_hybrid`
[bool] exclude hybrid descriptor to prevent circular calls

Returns

`List[Argument]`
all arguments

`register(name: str, alias: Optional[List[str]] = None) → Callable[[], List[Argument]]`

Register a descriptor argument plugin.

Parameters

`name`
[str] the name of a descriptor
`alias`
[List[str], optional] the list of aliases of this descriptor

Returns

`Callable[[], List[Argument]]`
the registered descriptor argument method

Examples

```
>>> some_plugin = ArgsPlugin()
>>> @some_plugin.register("some_descrpt")
def descrpt_some_descrpt_args():
    return []
```

`deepmd.utils.argcheck.descrpt_hybrid_args()`

`deepmd.utils.argcheck.descrpt_local_frame_args()`

`deepmd.utils.argcheck.descrpt_se_a_args()`

`deepmd.utils.argcheck.descrpt_se_a_mask_args()`

```
deepmd.utils.argcheck.descript_se_a_tpe_args()
deepmd.utils.argcheck.descript_se_atten_args()
deepmd.utils.argcheck.descript_se_atten_common_args()
deepmd.utils.argcheck.descript_se_atten_v2_args()
deepmd.utils.argcheck.descript_se_r_args()
deepmd.utils.argcheck.descript_se_t_args()
deepmd.utils.argcheck.descript_variant_type_args(exclude_hybrid: bool = False) → Variant
deepmd.utils.argcheck.fitting_dipole()
deepmd.utils.argcheck.fitting_dos()
deepmd.utils.argcheck.fitting_ener()
deepmd.utils.argcheck.fitting_polar()
deepmd.utils.argcheck.fitting_variant_type_args()
deepmd.utils.argcheck.gen_args(**kwargs) → List[Argument]
deepmd.utils.argcheck.gen_doc(*, make_anchor=True, make_link=True, **kwargs)
deepmd.utils.argcheck.gen_json(**kwargs)
deepmd.utils.argcheck.learning_rate_args()
deepmd.utils.argcheck.learning_rate_dict_args()
deepmd.utils.argcheck.learning_rate_exp()
deepmd.utils.argcheck.learning_rate_variant_type_args()
deepmd.utils.argcheck.limit_pref(item)
deepmd.utils.argcheck.list_to_doc(xx)
deepmd.utils.argcheck.loss_args()
deepmd.utils.argcheck.loss_dict_args()
deepmd.utils.argcheck.loss_dos()
deepmd.utils.argcheck.loss_ener()
deepmd.utils.argcheck.loss_ener_spin()
deepmd.utils.argcheck.loss_tensor()
deepmd.utils.argcheck.loss_variant_type_args()
deepmd.utils.argcheck.make_index(keys)
deepmd.utils.argcheck.make_link(content, ref_key)
deepmd.utils.argcheck.mixed_precision_args()
```

```
deepmd.utils.argcheck.model_args(exclude_hybrid=False)
deepmd.utils.argcheck.model_compression()
deepmd.utils.argcheck.model_compression_type_args()
deepmd.utils.argcheck.modifier_dipole_charge()
deepmd.utils.argcheck.modifier_variant_type_args()
deepmd.utils.argcheck.multi_model_args() → Argument
deepmd.utils.argcheck.normalize(data)
deepmd.utils.argcheck.normalize_data_dict(data_dict)
deepmd.utils.argcheck.normalize_fitting_net_dict(fitting_net_dict)
deepmd.utils.argcheck.normalize_fitting_weight(fitting_keys, data_keys, fitting_weight=None)
deepmd.utils.argcheck.normalize_learning_rate_dict(fitting_keys, learning_rate_dict)
deepmd.utils.argcheck.normalize_learning_rate_dict_with_single_learning_rate(fitting_keys,
                                                                                learning_rate)

deepmd.utils.argcheck.normalize_loss_dict(fitting_keys, loss_dict)
deepmd.utils.argcheck.normalize_multi_task(data)
deepmd.utils.argcheck.pairwise_dprc() → Argument
deepmd.utils.argcheck.spin_args()
deepmd.utils.argcheck.standard_model_args() → Argument
deepmd.utils.argcheck.start_pref(item, label=None, abbr=None)
deepmd.utils.argcheck.training_args()
deepmd.utils.argcheck.training_data_args()
deepmd.utils.argcheck.type_embedding_args()
deepmd.utils.argcheck.validation_data_args()
```

deepmd.utils.batch_size module

```
class deepmd.utils.batch_size.AutoBatchSize(initial_batch_size: int = 1024, factor: float = 2.0)
```

Bases: `object`

This class allows DeePMD-kit to automatically decide the maximum batch size that will not cause an OOM error.

Parameters

`initial_batch_size`

[`int`, default: 1024] initial batch size (number of total atoms) when DP_INFER_BATCH_SIZE is not set

`factor`

[`float`, default: 2.] increased factor

Notes

In some CPU environments, the program may be directly killed when OOM. In this case, by default the batch size will not be increased for CPUs. The environment variable `DP_INFER_BATCH_SIZE` can be set as the batch size.

In other cases, we assume all OOM error will raise `OutOfMemoryError`.

Attributes

`current_batch_size`
`[int]` current batch size (number of total atoms)

`maximum_working_batch_size`
`[int]` maximum working batch size

`minimal_not_working_batch_size`
`[int]` minimal not working batch size

Methods

| | |
|---|---|
| <code>execute(callable, start_index, natoms)</code> | Excuate a method with given batch size. |
| <code>execute_all(callable, total_size, natoms, ...)</code> | Excuate a method with all given data. |

execute(callable: `Callable`, start_index: `int`, natoms: `int`) → `Tuple[int, tuple]`

Excuate a method with given batch size.

Parameters

`callable`
`[Callable]` The method should accept the batch size and start_index as parameters, and returns executed batch size and data.

`start_index`
`[int]` start index

`natoms`
`[int]` natoms

Returns

`int`
 executed batch size * number of atoms

`tuple`
 result from callable, None if failing to execute

Raises

OutOfMemoryError
 OOM when batch size is 1

execute_all(callable: `Callable`, total_size: `int`, natoms: `int`, *args, **kwargs) → `Tuple[ndarray]`

Excuate a method with all given data.

Parameters

`callable`
`[Callable]` The method should accept *args and **kwargs as input and return the similiar array.

`total_size`
 [`int`] Total size

`natoms`
 [`int`] The number of atoms

`*args`
 Variable length argument list.

`**kwargs`
 If 2D np.ndarray, assume the first axis is batch; otherwise do nothing.

deepmd.utils.compat module

Module providing compatibility between 0.x.x and 1.x.x input versions.

`deepmd.utils.compat.convert_input_v0_v1(jdata: Dict[str, Any], warning: bool = True, dump: Optional[Union[str, Path]] = None) → Dict[str, Any]`

Convert input from v0 format to v1.

Parameters

`jdata`
 [Dict[str, Any]] loaded json/yaml file

`warning`
 [bool, optional] whether to show deprecation warning, by default True

`dump`
 [Optional[Union[str, Path]], optional] whether to dump converted file, by default None

Returns

Dict[str, Any]
 converted output

`deepmd.utils.compat.convert_input_v1_v2(jdata: Dict[str, Any], warning: bool = True, dump: Optional[Union[str, Path]] = None) → Dict[str, Any]`

`deepmd.utils.compat.deprecate_numb_test(jdata: Dict[str, Any], warning: bool = True, dump: Optional[Union[str, Path]] = None) → Dict[str, Any]`

Deprecate `numb_test` since v2.1. It has taken no effect since v2.0.

See #1243.

Parameters

`jdata`
 [Dict[str, Any]] loaded json/yaml file

`warning`
 [bool, optional] whether to show deprecation warning, by default True

`dump`
 [Optional[Union[str, Path]], optional] whether to dump converted file, by default None

Returns

Dict[str, Any]
 converted output

```
deepmd.utils.compat.remove_decay_rate(jdata: Dict[str, Any])
```

Convert decay_rate to stop_lr.

Parameters

jdata
[Dict[str, Any]] input data

```
deepmd.utils.compat.update_deepmd_input(jdata: Dict[str, Any], warning: bool = True, dump:
Optional[Union[str, Path]] = None) → Dict[str, Any]
```

deepmd.utils.convert module

```
deepmd.utils.convert.convert_012_to_21(input_model: str, output_model: str)
```

Convert DP 0.12 graph to 2.1 graph.

Parameters

input_model
[str] filename of the input graph

output_model
[str] filename of the output graph

```
deepmd.utils.convert.convert_10_to_21(input_model: str, output_model: str)
```

Convert DP 1.0 graph to 2.1 graph.

Parameters

input_model
[str] filename of the input graph

output_model
[str] filename of the output graph

```
deepmd.utils.convert.convert_12_to_21(input_model: str, output_model: str)
```

Convert DP 1.2 graph to 2.1 graph.

Parameters

input_model
[str] filename of the input graph

output_model
[str] filename of the output graph

```
deepmd.utils.convert.convert_13_to_21(input_model: str, output_model: str)
```

Convert DP 1.3 graph to 2.1 graph.

Parameters

input_model
[str] filename of the input graph

output_model
[str] filename of the output graph

```
deepmd.utils.convert.convert_20_to_21(input_model: str, output_model: str)
```

Convert DP 2.0 graph to 2.1 graph.

Parameters

input_model
 [str] filename of the input graph

output_model
 [str] filename of the output graph

`deepmd.utils.convert.convert_dp012_to_dp10(file: str)`

Convert DP 0.12 graph text to 1.0 graph text.

Parameters

file
 [str] filename of the graph text

`deepmd.utils.convert.convert_dp10_to_dp11(file: str)`

Convert DP 1.0 graph text to 1.1 graph text.

Parameters

file
 [str] filename of the graph text

`deepmd.utils.convert.convert_dp12_to_dp13(file: str)`

Convert DP 1.2 graph text to 1.3 graph text.

Parameters

file
 [str] filename of the graph text

`deepmd.utils.convert.convert_dp13_to_dp20(fname: str)`

Convert DP 1.3 graph text to 2.0 graph text.

Parameters

fname
 [str] filename of the graph text

`deepmd.utils.convert.convert_dp20_to_dp21(fname: str)`

`deepmd.utils.convert.convert_pb_to_pbtxt(pbfile: str, pbtxtfile: str)`

Convert DP graph to graph text.

Parameters

pbfile
 [str] filename of the input graph

pbtxtfile
 [str] filename of the output graph text

`deepmd.utils.convert.convert_pbtxt_to_pb(pbtxtfile: str, pbfile: str)`

Convert DP graph text to graph.

Parameters

pbtxtfile
 [str] filename of the input graph text

pbfile
 [str] filename of the output graph


```
deepmd.utils.convert.convert_to_21(input_model: str, output_model: str)
```

Convert DP graph to 2.1 graph.

Parameters

input_model
[str] filename of the input graph

output_model
[str] filename of the output graph

```
deepmd.utils.convert.detect_model_version(input_model: str)
```

Detect DP graph version.

Parameters

input_model
[str] filename of the input graph

deepmd.utils.data module

```
class deepmd.utils.data.DeepmdData(sys_path: str, set_prefix: str = 'set', shuffle_test: bool = True,
                                   type_map: Optional[List[str]] = None, optional_type_map: bool
                                   = True, modifier=None, trn_all_set: bool = False)
```

Bases: `object`

Class for a data system.

It loads data from hard disk, and maintains the data as a data_dict

Parameters

sys_path
Path to the data system

set_prefix
Prefix for the directories of different sets

shuffle_test
If the test data are shuffled

type_map
Gives the name of different atom types

optional_type_map
If the type_map.raw in each system is optional

modifier
Data modifier that has the method modify_data

trn_all_set
Use all sets as training dataset. Otherwise, if the number of sets is more than 1, the last set is left for test.

Methods

| | |
|---|--|
| <code>add(key, ndof[, atomic, must, high_prec, ...])</code> | Add a data item that to be loaded. |
| <code>avg(key)</code> | Return the average value of an item. |
| <code>check_batch_size(batch_size)</code> | Check if the system can get a batch of data with <code>batch_size</code> frames. |
| <code>check_test_size(test_size)</code> | Check if the system can get a test dataset with <code>test_size</code> frames. |
| <code>get_atom_type()</code> | Get atom types. |
| <code>get_batch(batch_size)</code> | Get a batch of data with <code>batch_size</code> frames. |
| <code>get_data_dict()</code> | Get the <code>data_dict</code> . |
| <code>get_natoms()</code> | Get number of atoms. |
| <code>get_natoms_vec(ntypes)</code> | Get number of atoms and number of atoms in different types. |
| <code>get_ntypes()</code> | Number of atom types in the system. |
| <code>get_num_batch(batch_size, set_idx)</code> | Get the number of batches in a set. |
| <code>get_num_set()</code> | Get number of training sets. |
| <code>get_sys_num_batch(batch_size)</code> | Get the number of batches in the data system. |
| <code>get_test([ntests])</code> | Get the test data with <code>ntests</code> frames. |
| <code>get_type_map()</code> | Get the type map. |
| <code>reduce(key_out, key_in)</code> | Generate a new item from the reduction of another atom. |

| | |
|-----------------|--|
| reset_get_batch | |
|-----------------|--|

add(key: str, ndof: int, atomic: bool = False, must: bool = False, high_prec: bool = False, type_sel: Optional[List[int]] = None, repeat: int = 1, default: float = 0.0, dtype: Optional[dtype] = None)
 Add a data item that to be loaded.

Parameters

- key**
The key of the item. The corresponding data is stored in `sys_path/set.*/key.npy`
- ndof**
The number of dof
- atomic**
The item is an atomic property. If False, the size of the data should be `nframes x ndof` If True, the size of data should be `nframes x natoms x ndof`
- must**
The data file `sys_path/set.*/key.npy` must exist. If `must` is False and the data file does not exist, the `data_dict[find_key]` is set to 0.0
- high_prec**
Load the data and store in float64, otherwise in float32
- type_sel**
Select certain type of atoms
- repeat**
The data will be repeated `repeat` times.
- default**
[float, default=0.] default value of data

`dtype`
`[np.dtype, optional]` the dtype of data, overwrites `high_prec` if provided

avg(key)
 Return the average value of an item.

check_batch_size(batch_size)
 Check if the system can get a batch of data with `batch_size` frames.

check_test_size(test_size)
 Check if the system can get a test dataset with `test_size` frames.

get_atom_type() → `List[int]`
 Get atom types.

get_batch(batch_size: int) → `dict`
 Get a batch of data with `batch_size` frames. The frames are randomly picked from the data system.

Parameters

`batch_size`
 size of the batch

get_data_dict() → `dict`
 Get the `data_dict`.

get_natoms()
 Get number of atoms.

get_natoms_vec(ntypes: int)
 Get number of atoms and number of atoms in different types.

Parameters

`ntypes`
 Number of types (may be larger than the actual number of types in the system).

Returns

natoms
`natoms[0]`: number of local atoms `natoms[1]`: total number of atoms held by this processor `natoms[i]`: $2 \leq i < Ntypes+2$, number of type `i` atoms

get_ntypes() → `int`
 Number of atom types in the system.

get_numb_batch(batch_size: int, set_idx: int) → `int`
 Get the number of batches in a set.

get_numb_set() → `int`
 Get number of training sets.

get_sys_numb_batch(batch_size: int) → `int`
 Get the number of batches in the data system.

get_test(ntests: int = -1) → `dict`
 Get the test data with `ntests` frames.

Parameters

`ntests`
 Size of the test data set. If `ntests` is -1, all test data will be get.

`get_type_map()` → `List[str]`

Get the type map.

`reduce(key_out: str, key_in: str)`

Generate a new item from the reduction of another atom.

Parameters

`key_out`

The name of the reduced item

`key_in`

The name of the data item to be reduced

`reset_get_batch()`

`deepmd.utils.data_system` module

```
class deepmd.utils.data_system.DeepmdDataSystem(systems: List[str], batch_size: int, test_size: int,
rcut: float, set_prefix: str = 'set', shuffle_test:
bool = True, type_map: Optional[List[str]] =
None, optional_type_map: bool = True,
modifier=None, trn_all_set=False,
sys_probs=None,
auto_prob_style='prob_sys_size')
```

Bases: `object`

Class for manipulating many data systems.

It is implemented with the help of `DeepmdData`

Attributes

`default_mesh`

Mesh for each system.

Methods

| | |
|---|---|
| <code>add(key, ndof[, atomic, must, high_prec, ...])</code> | Add a data item that to be loaded. |
| <code>add_dict(adict)</code> | Add items to the data system by a dict. |
| <code>get_batch([sys_idx])</code> | Get a batch of data from the data systems. |
| <code>get_batch_mixed()</code> | Get a batch of data from the data systems in the mixed way. |
| <code>get_batch_size()</code> | Get the batch size. |
| <code>get_batch_standard([sys_idx])</code> | Get a batch of data from the data systems in the standard way. |
| <code>get_nbatches()</code> | Get the total number of batches. |
| <code>get_nsystems()</code> | Get the number of data systems. |
| <code>get_ntypes()</code> | Get the number of types. |
| <code>get_sys(idx)</code> | Get a certain data system. |
| <code>get_sys_ntest([sys_idx])</code> | Get number of tests for the currently selected system, or one defined by <code>sys_idx</code> . |
| <code>get_test([sys_idx, n_test])</code> | Get test data from the the data systems. |
| <code>get_type_map()</code> | Get the type map. |
| <code>reduce(key_out, key_in)</code> | Generate a new item from the reduction of another atom. |

| | |
|-----------------------------------|--|
| <code>compute_energy_shift</code> | |
| <code>get_data_dict</code> | |
| <code>print_summary</code> | |
| <code>set_sys_probs</code> | |

add(key: str, ndof: int, atomic: bool = False, must: bool = False, high_prec: bool = False, type_sel: Optional[List[int]] = None, repeat: int = 1, default: float = 0.0)

Add a data item that to be loaded.

Parameters

key

The key of the item. The corresponding data is stored in `sys_path/set.*/key.npy`

ndof

The number of dof

atomic

The item is an atomic property. If False, the size of the data should be `nframes x ndof` If True, the size of data should be `nframes x natoms x ndof`

must

The data file `sys_path/set.*/key.npy` must exist. If must is False and the data file does not exist, the `data_dict[find_key]` is set to 0.0

high_prec

Load the data and store in float64, otherwise in float32

type_sel

Select certain type of atoms

repeat

The data will be repeated repeat times.

default, default=0.
Default value of data

add_dict(adict: dict) → None

Add items to the data system by a dict. adict should have items like .. code-block:: python.

```
adict[key] = {
    "ndof": ndof, "atomic": atomic, "must": must, "high_prec": high_prec, "type_sel":
    type_sel, "repeat": repeat,
}
```

For the explanation of the keys see add

compute_energy_shift(rcond=None, key='energy')

property default_mesh: List[ndarray]

Mesh for each system.

get_batch(sys_idx: Optional[int] = None) → dict

Get a batch of data from the data systems.

Parameters

sys_idx
[int] The index of system from which the batch is get. If sys_idx is not None, sys_probs and auto_prob_style are ignored If sys_idx is None, automatically determine the system according to sys_probs or auto_prob_style, see the following. This option does not work for mixed systems.

Returns

dict
The batch data

get_batch_mixed() → dict

Get a batch of data from the data systems in the mixed way.

Returns

dict
The batch data

get_batch_size() → int

Get the batch size.

get_batch_standard(sys_idx: Optional[int] = None) → dict

Get a batch of data from the data systems in the standard way.

Parameters

sys_idx
[int] The index of system from which the batch is get. If sys_idx is not None, sys_probs and auto_prob_style are ignored If sys_idx is None, automatically determine the system according to sys_probs or auto_prob_style, see the following.

Returns

dict
The batch data

get_data_dict(ii: int = 0) → dict

`get_nbatches()` → `int`
 Get the total number of batches.

`get_nsystems()` → `int`
 Get the number of data systems.

`get_ntypes()` → `int`
 Get the number of types.

`get_sys(idx: int)` → `DeepmdData`
 Get a certain data system.

`get_sys_ntest(sys_idx=None)`
 Get number of tests for the currently selected system, or one defined by `sys_idx`.

`get_test(sys_idx: Optional[int] = None, n_test: int = -1)`
 Get test data from the the data systems.

Parameters

`sys_idx`
 The test dat of system with index `sys_idx` will be returned. If is None, the currently selected system will be returned.

`n_test`
 Number of test data. If set to -1 all test data will be get.

`get_type_map()` → `List[str]`
 Get the type map.

`print_summary(name)`

`reduce(key_out, key_in)`
 Generate a new item from the reduction of another atom.

Parameters

`key_out`
 The name of the reduced item

`key_in`
 The name of the data item to be reduced

`set_sys_probs(sys_probs=None, auto_prob_style: str = 'prob_sys_size')`

deepmd.utils.errors module

`exception deepmd.utils.errors.GraphTooLargeError`

Bases: `Exception`

The graph is too large, exceeding protobuf's hard limit of 2GB.

`exception deepmd.utils.errors.GraphWithoutTensorError`

Bases: `Exception`

`exception deepmd.utils.errors.OutOfMemoryError`

Bases: `Exception`

This error is caused by out-of-memory (OOM).

deepmd.utils.finetune module

```
deepmd.utils.finetune.replace_model_params_with_pretrained_model(jdata: Dict[str, Any],  
                                                                  pretrained_model: str)
```

Replace the model params in input script according to pretrained model.

Parameters

jdata
[Dict[str, Any]] input script

pretrained_model
[str] filename of the pretrained model

deepmd.utils.graph module

```
deepmd.utils.graph.get_attention_layer_nodes_from_graph_def(graph_def: GraphDef, suffix: str =  
                                                            "") → Dict
```

Get the attention layer nodes with the given tf.GraphDef object.

Parameters

graph_def
The input tf.GraphDef object

suffix
[str, optional] The scope suffix

Returns

Dict
The attention layer nodes within the given tf.GraphDef object

```
deepmd.utils.graph.get_attention_layer_variables_from_graph_def(graph_def: GraphDef, suffix:  
                                                                str = "") → Dict
```

Get the attention layer variables with the given tf.GraphDef object.

Parameters

graph_def
[tf.GraphDef] The input tf.GraphDef object

suffix
[str, optional] The suffix of the scope

Returns

Dict
The attention layer variables within the given tf.GraphDef object

```
deepmd.utils.graph.get_embedding_net_nodes(model_file: str, suffix: str = "") → Dict
```

Get the embedding net nodes with the given frozen model(model_file).

Parameters

model_file
The input frozen model path

suffix
[str, optional] The suffix of the scope

Returns

Dict

The embedding net nodes with the given frozen model

`deepmd.utils.graph.get_embedding_net_nodes_from_graph_def`(graph_def: GraphDef, suffix: str = "")
→ **Dict**

Get the embedding net nodes with the given tf.GraphDef object.

Parameters

graph_def

The input tf.GraphDef object

suffix

[str, optional] The scope suffix

Returns

Dict

The embedding net nodes within the given tf.GraphDef object

`deepmd.utils.graph.get_embedding_net_variables`(model_file: str, suffix: str = "") → **Dict**

Get the embedding net variables with the given frozen model(model_file).

Parameters

model_file

The input frozen model path

suffix

[str, optional] The suffix of the scope

Returns

Dict

The embedding net variables within the given frozen model

`deepmd.utils.graph.get_embedding_net_variables_from_graph_def`(graph_def: GraphDef, suffix: str = "") → **Dict**

Get the embedding net variables with the given tf.GraphDef object.

Parameters

graph_def

The input tf.GraphDef object

suffix

[str, optional] The suffix of the scope

Returns

Dict

The embedding net variables within the given tf.GraphDef object

`deepmd.utils.graph.get_fitting_net_nodes`(model_file: str) → **Dict**

Get the fitting net nodes with the given frozen model(model_file).

Parameters

model_file

The input frozen model path

Returns

Dict

The fitting net nodes with the given frozen model

`deepmd.utils.graph.get_fitting_net_nodes_from_graph_def`(`graph_def`: `GraphDef`, `suffix`: `str` = "")
→ **Dict**

Get the fitting net nodes with the given `tf.GraphDef` object.

Parameters

`graph_def`

The input `tf.GraphDef` object

`suffix`

suffix of the scope

Returns

Dict

The fitting net nodes within the given `tf.GraphDef` object

`deepmd.utils.graph.get_fitting_net_variables`(`model_file`: `str`, `suffix`: `str` = "") → **Dict**

Get the fitting net variables with the given frozen model(`model_file`).

Parameters

`model_file`

The input frozen model path

`suffix`

suffix of the scope

Returns

Dict

The fitting net variables within the given frozen model

`deepmd.utils.graph.get_fitting_net_variables_from_graph_def`(`graph_def`: `GraphDef`, `suffix`: `str` = "") → **Dict**

Get the fitting net variables with the given `tf.GraphDef` object.

Parameters

`graph_def`

The input `tf.GraphDef` object

`suffix`

suffix of the scope

Returns

Dict

The fitting net variables within the given `tf.GraphDef` object

`deepmd.utils.graph.get_pattern_nodes_from_graph_def`(`graph_def`: `GraphDef`, `pattern`: `str`) → **Dict**

Get the pattern nodes with the given `tf.GraphDef` object.

Parameters

`graph_def`

The input `tf.GraphDef` object

`pattern`

The node pattern within the `graph_def`

Returns

Dict

The fitting net nodes within the given `tf.GraphDef` object

`deepmd.utils.graph.get_tensor_by_name(model_file: str, tensor_name: str) → Tensor`

Load tensor value from the frozen model(`model_file`).

Parameters

`model_file`

[`str`] The input frozen model path

`tensor_name`

[`str`] Indicates which tensor which will be loaded from the frozen model

Returns

`tf.Tensor`

The tensor which was loaded from the frozen model

Raises

`GraphWithoutTensorError`

Whether the `tensor_name` is within the frozen model

`deepmd.utils.graph.get_tensor_by_name_from_graph(graph: Graph, tensor_name: str) → Tensor`

Load tensor value from the given `tf.Graph` object.

Parameters

`graph`

[**`tf.Graph`**] The input TensorFlow graph

`tensor_name`

[`str`] Indicates which tensor which will be loaded from the frozen model

Returns

`tf.Tensor`

The tensor which was loaded from the frozen model

Raises

`GraphWithoutTensorError`

Whether the `tensor_name` is within the frozen model

`deepmd.utils.graph.get_tensor_by_type(node, data_type: dtype) → Tensor`

Get the tensor value within the given node according to the input `data_type`.

Parameters

`node`

The given tensorflow graph node

`data_type`

The data type of the node

Returns

`tf.Tensor`

The tensor value of the given node

```
deepmd.utils.graph.get_type_embedding_net_nodes_from_graph_def(graph_def: GraphDef, suffix:
                                                                str = '') → Dict
```

Get the type embedding net nodes with the given tf.GraphDef object.

Parameters

graph_def
The input tf.GraphDef object

suffix
[**str**, optional] The scope suffix

Returns

Dict
The type embedding net nodes within the given tf.GraphDef object

```
deepmd.utils.graph.get_type_embedding_net_variables_from_graph_def(graph_def: GraphDef,
                                                                    suffix: str = '') → Dict
```

Get the type embedding net variables with the given tf.GraphDef object.

Parameters

graph_def
[**tf.GraphDef**] The input tf.GraphDef object

suffix
[**str**, optional] The suffix of the scope

Returns

Dict
The embedding net variables within the given tf.GraphDef object

```
deepmd.utils.graph.load_graph_def(model_file: str) → Tuple[Graph, GraphDef]
```

Load graph as well as the graph_def from the frozen model(model_file).

Parameters

model_file
[**str**] The input frozen model path

Returns

tf.Graph
The graph loaded from the frozen model

tf.GraphDef
The graph_def loaded from the frozen model

deepmd.utils.learning_rate module

```
class deepmd.utils.learning_rate.LearningRateExp(start_lr: float, stop_lr: float = 5e-08,
                                                  decay_steps: int = 5000, decay_rate: float =
                                                  0.95)
```

Bases: **object**

The exponentially decaying learning rate.

The learning rate at step t is given by

$$\alpha(t) = \alpha_0 \lambda^{t/\tau}$$

where α is the learning rate, α_0 is the starting learning rate, λ is the decay rate, and τ is the decay steps.

Parameters

- `start_lr`
Starting learning rate α_0
- `stop_lr`
Stop learning rate α_1
- `decay_steps`
Learning rate decay every this number of steps τ
- `decay_rate`
The decay rate λ . If `stop_step` is provided in `build`, then it will be determined automatically and overwritten.

Methods

| | |
|--|-------------------------------|
| <code>build(global_step[, stop_step])</code> | Build the learning rate. |
| <code>start_lr()</code> | Get the start lr. |
| <code>value(step)</code> | Get the lr at a certain step. |

build(global_step: Tensor, stop_step: Optional[int] = None) → Tensor

Build the learning rate.

Parameters

- `global_step`
The tf Tensor providing the global training step
- `stop_step`
The stop step. If provided, the `decay_rate` will be determined automatically and overwritten.

Returns

- learning_rate**
The learning rate

start_lr() → float

Get the start lr.

value(step: int) → float

Get the lr at a certain step.

deepmd.utils.multi_init module

deepmd.utils.multi_init.replace_model_params_with_frz_multi_model(jdata: Dict[str, Any], pretrained_model: str)

Replace the model params in input script according to pretrained frozen multi-task united model.

Parameters

- `jdata`
[Dict[str, Any]] input script

pretrained_model
[[str](#)] filename of the pretrained frozen multi-task united model

deepmd.utils.neighbor_stat module

`class deepmd.utils.neighbor_stat.NeighborStat(ntypes: int, rcut: float, one_type: bool = False)`

Bases: [object](#)

Class for getting training data information.

It loads data from DeepmdData object, and measures the data info, including neareest nbor distance between atoms, max nbor size of atoms and the output data range of the environment matrix.

Parameters

ntypes

The num of atom types

rcut

The cut-off radius

one_type

[[bool](#), optional, default=False] Treat all types as a single type.

Methods

get_stat(data)

Get the data statistics of the training data, including nearest nbor distance between atoms, max nbor size of atoms.

`get_stat`(data: [DeepmdDataSystem](#)) → [Tuple](#)[[float](#), [List](#)[[int](#)]]

Get the data statistics of the training data, including nearest nbor distance between atoms, max nbor size of atoms.

Parameters

data

Class for manipulating many data systems. It is implemented with the help of DeepmdData.

Returns

min_nbor_dist

The nearest distance between neighbor atoms

max_nbor_size

A list with ntypes integers, denotes the actual achieved max sel

deepmd.utils.network module

```
deepmd.utils.network.embedding_net(xx, network_size, precision, activation_fn=<function tanh>,
                                   resnet_dt=False, name_suffix='', stddev=1.0, bavg=0.0,
                                   seed=None, trainable=True, uniform_seed=False,
                                   initial_variables=None, mixed_prec=None)
```

The embedding network.

The embedding network function \mathcal{N} is constructed by is the composition of multiple layers $\mathcal{L}^{(i)}$:

$$\mathcal{N} = \mathcal{L}^{(n)} \circ \mathcal{L}^{(n-1)} \circ \dots \circ \mathcal{L}^{(1)}$$

A layer \mathcal{L} is given by one of the following forms, depending on the number of nodes: [1]

$$y = \mathcal{L}(x; w, b) = \begin{cases} \phi(x^T w + b) + x, & N_2 = N_1 \\ \phi(x^T w + b) + (x, x), & N_2 = 2N_1 \\ \phi(x^T w + b), & \text{otherwise} \end{cases}$$

where $x \in \mathbb{R}^{N_1}$ is the input vector and $y \in \mathbb{R}^{N_2}$ is the output vector. $w \in \mathbb{R}^{N_1 \times N_2}$ and $b \in \mathbb{R}^{N_2}$ are weights and biases, respectively, both of which are trainable if trainable is True. ϕ is the activation function.

Parameters

`xx`

[**Tensor**] Input tensor x of shape [-1,1]

`network_size`

[**list of int**] Size of the embedding network. For example [16,32,64]

`precision`:

Precision of network weights. For example, tf.float64

`activation_fn`:

Activation function ϕ

`resnet_dt`

[**bool**] Using time-step in the ResNet construction

`name_suffix`

[**str**] The name suffix append to each variable.

`stddev`

[**float**] Standard deviation of initializing network parameters

`bavg`

[**float**] Mean of network initial bias

`seed`

[**int**] Random seed for initializing network parameters

`trainable`

[**bool**] If the network is trainable

`uniform_seed`

[**bool**] Only for the purpose of backward compatibility, retrieves the old behavior of using the random seed

`initial_variables`

[**dict**] The input dict which stores the embedding net variables

`mixed_prec`
The input dict which stores the mixed precision setting for the embedding net

References

[1]

```
deepmd.utils.network.embedding_net_rand_seed_shift(network_size)

deepmd.utils.network.one_layer(inputs, outputs_size, activation_fn=<function tanh>,
                                precision=tf.float64, stddev=1.0, bavg=0.0, name='linear', scope='',
                                reuse=None, seed=None, use_timestep=False, trainable=True,
                                useBN=False, uniform_seed=False, initial_variables=None,
                                mixed_prec=None, final_layer=False)

deepmd.utils.network.one_layer_rand_seed_shift()

deepmd.utils.network.variable_summaries(var: VariableV1, name: str)
    Attach a lot of summaries to a Tensor (for TensorBoard visualization).

    Parameters
    var
        [tf.Variable] [description]
    name
        [str] variable name
```

deepmd.utils.pair_tab module

```
class deepmd.utils.pair_tab.PairTab(filename: str)
    Bases: object
    Pairwise tabulated potential.

    Parameters
    filename
        File name for the short-range tabulated potential. The table is a text data file with
         $(N_t + 1) * N_t / 2 + 1$  columes. The first colum is the distance between atoms. The
        second to the last columes are energies for pairs of certain types. For example we
        have two atom types, 0 and 1. The columes from 2nd to 4th are for 0-0, 0-1 and 1-1
        correspondingly.
```

Methods

| | |
|-------------------------------|---------------------------------------|
| <code>get()</code> | Get the serialized table. |
| <code>reinit(filename)</code> | Initialize the tabulated interaction. |

`get()` → `Tuple[array, array]`
Get the serialized table.

`reinit(filename: str) → None`

Initialize the tabulated interaction.

Parameters

filename

File name for the short-range tabulated potential. The table is a text data file with $(N_t + 1) * N_t / 2 + 1$ columns. The first column is the distance between atoms. The second to the last columns are energies for pairs of certain types. For example we have two atom types, 0 and 1. The columns from 2nd to 4th are for 0-0, 0-1 and 1-1 correspondingly.

deepmd.utils.parallel_op module

```
class deepmd.utils.parallel_op.ParallelOp(builder: Callable[[...], Tuple[Dict[str, Tensor],
                                                                    Tuple[Tensor]]], nthreads: Optional[int] = None, config:
                                                                    Optional[ConfigProto] = None)
```

Bases: `object`

Run an op with data parallelism.

Parameters

builder

`[Callable[...], Tuple[Dict[str, tf.Tensor], Tuple[tf.Tensor]]]` returns two objects: a dict which stores placeholders by key, and a tuple with the final op(s)

nthreads

`[int, optional]` the number of threads

config

`[tf.ConfigProto, optional]` `tf.ConfigProto`

Examples

```
>>> from deepmd.env import tf
>>> from deepmd.utils.parallel_op import ParallelOp
>>> def builder():
...     x = tf.placeholder(tf.int32, [1])
...     return {"x": x}, (x + 1)
...
>>> p = ParallelOp(builder, nthreads=4)
>>> def feed():
...     for ii in range(10):
...         yield {"x": [ii]}
...
>>> print(*p.generate(tf.Session(), feed()))
[1] [2] [3] [4] [5] [6] [7] [8] [9] [10]
```

Methods

| | |
|------------------------------|----------------------|
| <i>generate</i> (sess, feed) | Returns a generator. |
|------------------------------|----------------------|

generate(sess: Session, feed: Generator[Dict[str, Any], None, None]) → Generator[Tuple, None, None]

Returns a generator.

Parameters

sess
[tf.Session] TensorFlow session

feed
[Generator[dict, None, None]] generator which yields feed_dict

Yields

Generator[Tuple, None, None]
generator which yields session returns

deepmd.utils.path module

class deepmd.utils.path.DPH5Path(path: str)

Bases: *DPPath*

The path class to data system (DeepmdData) for HDF5 files.

Parameters

path
[str] path

Notes

OS - HDF5 relationship:
directory - Group file - Dataset

Methods

| | |
|---------------------------|---|
| <i>glob</i> (pattern) | Search path using the glob pattern. |
| <i>is_dir</i> () | Check if self is directory. |
| <i>is_file</i> () | Check if self is file. |
| <i>load_numpy</i> () | Load NumPy array. |
| <i>load_txt</i> ([dtype]) | Load NumPy array from text. |
| <i>rglob</i> (pattern) | This is like calling <i>DPPath.glob()</i> with <i>**/</i> added in front of the given relative pattern. |

glob(pattern: str) → List[DPPath]

Search path using the glob pattern.

Parameters

```

    pattern
    [str] glob pattern

Returns
    List[DPPath]
    list of paths

is_dir() → bool
    Check if self is directory.

is_file() → bool
    Check if self is file.

load_numpy() → ndarray
    Load NumPy array.

Returns
    np.ndarray
    loaded NumPy array

load_txt(dtype: Optional[dtype] = None, **kwargs) → ndarray
    Load NumPy array from text.

Returns
    np.ndarray
    loaded NumPy array

rglob(pattern: str) → List[DPPath]
    This is like calling DPPath.glob() with **/ added in front of the given relative pattern.

Parameters
    pattern
    [str] glob pattern

Returns
    List[DPPath]
    list of paths

class deepmd.utils.path.DPOSPath(path: str)
    Bases: DPPath

    The OS path class to data system (DeepmdData) for real directories.

Parameters
    path
    [str] path

```

Methods

| | |
|---------------------------------|---|
| <code>glob(pattern)</code> | Search path using the glob pattern. |
| <code>is_dir()</code> | Check if self is directory. |
| <code>is_file()</code> | Check if self is file. |
| <code>load_numpy()</code> | Load NumPy array. |
| <code>load_txt(**kwargs)</code> | Load NumPy array from text. |
| <code>rglob(pattern)</code> | This is like calling <code>DPPath.glob()</code> with <code>**/</code> added in front of the given relative pattern. |

`glob(pattern: str) → List[DPPath]`

Search path using the glob pattern.

Parameters

pattern
[str] glob pattern

Returns

List[DPPath]
list of paths

`is_dir() → bool`

Check if self is directory.

`is_file() → bool`

Check if self is file.

`load_numpy() → ndarray`

Load NumPy array.

Returns

np.ndarray
loaded NumPy array

`load_txt(**kwargs) → ndarray`

Load NumPy array from text.

Returns

np.ndarray
loaded NumPy array

`rglob(pattern: str) → List[DPPath]`

This is like calling `DPPath.glob()` with `**/` added in front of the given relative pattern.

Parameters

pattern
[str] glob pattern

Returns

List[DPPath]
list of paths

```
class deepmd.utils.path.DPPath(path: str)
```

Bases: `ABC`

The path class to data system (DeepmdData).

Parameters

path
[`str`] path

Methods

| | |
|---------------------------------|---|
| <code>glob(pattern)</code> | Search path using the glob pattern. |
| <code>is_dir()</code> | Check if self is directory. |
| <code>is_file()</code> | Check if self is file. |
| <code>load_numpy()</code> | Load NumPy array. |
| <code>load_txt(**kwargs)</code> | Load NumPy array from text. |
| <code>rglob(pattern)</code> | This is like calling <code>DPPath.glob()</code> with <code>**/</code> added in front of the given relative pattern. |

```
abstract glob(pattern: str) → List[DPPath]
```

Search path using the glob pattern.

Parameters

pattern
[`str`] glob pattern

Returns

`List[DPPath]`
list of paths

```
abstract is_dir() → bool
```

Check if self is directory.

```
abstract is_file() → bool
```

Check if self is file.

```
abstract load_numpy() → ndarray
```

Load NumPy array.

Returns

`np.ndarray`
loaded NumPy array

```
abstract load_txt(**kwargs) → ndarray
```

Load NumPy array from text.

Returns

`np.ndarray`
loaded NumPy array

```
abstract rglob(pattern: str) → List[DPPath]
```

This is like calling `DPPath.glob()` with `**/` added in front of the given relative pattern.

Parameters

pattern
 [str] glob pattern

Returns

 List[DPPath]
 list of paths

deepmd.utils.plugin module

Base of plugin systems.

class deepmd.utils.plugin.Plugin

Bases: object

A class to register and restore plugins.

Examples

```
>>> plugin = Plugin()
>>> @plugin.register("xx")
def xxx():
    pass
>>> print(plugin.plugins['xx'])
```

Attributes

plugins
 [Dict[str, object]] plugins

Methods

| | |
|------------------------------|------------------------|
| <code>get_plugin(key)</code> | Visit a plugin by key. |
| <code>register(key)</code> | Register a plugin. |

get_plugin(key) → object

Visit a plugin by key.

Parameters

key
 [str] key of the plugin

Returns

object
 the plugin

register(key: str) → Callable[[object], object]

Register a plugin.

Parameters

key
 [str] key of the plugin

Returns

`Callable[[object], object]`
decorator

`class deepmd.utils.plugin.PluginVariant(*args, **kwargs)`

Bases: `object`

A class to remove type from input arguments.

`class deepmd.utils.plugin.VariantABCMeta(name, bases, namespace, **kwargs)`

Bases: `VariantMeta`, `ABCMeta`

Methods

| | |
|--|---|
| <code>__call__(*args, **kwargs)</code> | Remove type and keys that starts with under-line. |
| <code>mro()</code> | Return a type's method resolution order. |
| <code>register(subclass)</code> | Register a virtual subclass of an ABC. |

`class deepmd.utils.plugin.VariantMeta`

Bases: `object`

Methods

| | |
|--|---|
| <code>__call__(*args, **kwargs)</code> | Remove type and keys that starts with under-line. |
|--|---|

deepmd.utils.random module

`deepmd.utils.random.choice(a: ndarray, p: Optional[ndarray] = None)`

Generates a random sample from a given 1-D array.

Parameters

`a`
`[np.ndarray]` A random sample is generated from its elements.

`p`
`[np.ndarray]` The probabilities associated with each entry in `a`.

Returns

`np.ndarray`
arrays with results and their shapes

`deepmd.utils.random.random(size=None)`

Return random floats in the half-open interval `[0.0, 1.0)`.

Parameters

`size`
Output shape.

Returns

`np.ndarray`

Arrays with results and their shapes.

`deepmd.utils.random.seed(val: Optional[int] = None)`

Seed the generator.

Parameters

`val`

`[int]` Seed.

`deepmd.utils.random.shuffle(x: ndarray)`

Modify a sequence in-place by shuffling its contents.

Parameters

`x`

`[np.ndarray]` The array or list to be shuffled.

deepmd.utils.sess module

`deepmd.utils.sess.run_sess(sess: Session, *args, **kwargs)`

Run session with errors caught.

Parameters

`sess`

`[tf.Session]` TensorFlow Session

`*args`

Variable length argument list.

`**kwargs`

Arbitrary keyword arguments.

Returns

`Any`

the result of `sess.run()`

deepmd.utils.spin module

`class deepmd.utils.spin.Spin(use_spin: Optional[List[bool]] = None, spin_norm: Optional[List[float]] = None, virtual_len: Optional[List[float]] = None)`

Bases: `object`

Class for spin.

Parameters

`use_spin`

Whether to use atomic spin model for each atom type

`spin_norm`

The magnitude of atomic spin for each atom type with spin

`virtual_len`

The distance between virtual atom representing spin and its corresponding real atom for each atom type with spin

Methods

| | |
|-------------------------------------|---|
| <code>build([reuse, suffix])</code> | Build the computational graph for the spin. |
| <code>get_ntypes_spin()</code> | Returns the number of atom types which contain spin. |
| <code>get_spin_norm()</code> | Returns the list of magnitude of atomic spin for each atom type. |
| <code>get_use_spin()</code> | Returns the list of whether to use spin for each atom type. |
| <code>get_virtual_len()</code> | Returns the list of distance between real atom and virtual atom for each atom type. |

`build(reuse=None, suffix='')`

Build the computational graph for the spin.

Parameters

`reuse`

The weights in the networks should be reused when get the variable.

`suffix`

Name suffix to identify this descriptor

Returns

`embedded_types`

The computational graph for embedded types

`get_ntypes_spin() → int`

Returns the number of atom types which contain spin.

`get_spin_norm() → List[float]`

Returns the list of magnitude of atomic spin for each atom type.

`get_use_spin() → List[bool]`

Returns the list of whether to use spin for each atom type.

`get_virtual_len() → List[float]`

Returns the list of distance between real atom and virtual atom for each atom type.

deepmd.utils.tabulate module

```
class deepmd.utils.tabulate.DPTabulate(descrpt: ~deepmd.descriptor.descriptor.Descriptor, neuron:
    ~typing.List[int], graph:
    ~tensorflow.python.framework.ops.Graph, graph_def:
    ~tensorflow.core.framework.graph_pb2.GraphDef,
    type_one_side: bool = False, exclude_types:
    ~typing.List[~typing.List[int]] = [], activation_fn: ~typing.
    Callable[~tensorflow.python.framework.ops.Tensor],
    ~tensorflow.python.framework.ops.Tensor] = <function
    tanh>, suffix: str = '')
```

Bases: `object`

Class for tabulation.

Compress a model, which including tabulating the embedding-net. The table is composed of fifth-order polynomial coefficients and is assembled from two sub-tables. The first table takes the `stride(parameter)` as it's uniform stride, while the second table takes `10 * stride` as it's uniform stride. The range of the first table is automatically detected by deepmd-kit, while the second table ranges from the first table's upper boundary(`upper`) to the `extrapolate(parameter) * upper`.

Parameters

`descript`
Descriptor of the original model

`neuron`
Number of neurons in each hidden layers of the embedding net
mathcal{N}

`graph`
[`tf.Graph`] The graph of the original model

`graph_def`
[`tf.GraphDef`] The graph_def of the original model

`type_one_side`
Try to build `N_types` tables. Otherwise, building `N_types^2` tables

`exclude_types`
[`List[List[int]]`] The excluded pairs of types which have no interaction with each other. For example, `[[0, 1]]` means no interaction between type 0 and type 1.

`activation_function`
The activation function in the embedding net. Supported options are {“tanh”, “gelu”} in common.ACTIVATION_FN_DICT.

`suffix`
[`str`, optional] The suffix of the scope

Methods

| | |
|--|---|
| <code>build(min_nbor_dist, extrapolate, stride0, ...)</code> | Build the tables for model compression. |
|--|---|

`build(min_nbor_dist: float, extrapolate: float, stride0: float, stride1: float) → Tuple[Dict[str, int], Dict[str, int]]`

Build the tables for model compression.

Parameters

`min_nbor_dist`
The nearest distance between neighbor atoms

`extrapolate`
The scale of model extrapolation

`stride0`
The uniform stride of the first table

`stride1`
The uniform stride of the second table

Returns

lower
 [dict[str, int]] The lower boundary of environment matrix by net

upper
 [dict[str, int]] The upper boundary of environment matrix by net

deepmd.utils.type_embed module

```
class deepmd.utils.type_embed.TypeEmbedNet(neuron: List[int] = [], resnet_dt: bool = False,
      activation_function: Optional[str] = 'tanh', precision:
      str = 'default', trainable: bool = True, seed:
      Optional[int] = None, uniform_seed: bool = False,
      padding: bool = False, **kwargs)
```

Bases: `object`

Type embedding network.

Parameters

neuron
 [list[int]] Number of neurons in each hidden layers of the embedding net

resnet_dt
 Time-step dt in the resnet construction: $y = x + dt * \phi(Wx + b)$

activation_function
 The activation function in the embedding net. Supported options are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”, “gelu_tf”, “None”, “none”.

precision
 The precision of the embedding net parameters. Supported options are “default”, “float16”, “float32”, “float64”, “bfloat16”.

trainable
 If the weights of embedding net are trainable.

seed
 Random seed for initializing the network parameters.

uniform_seed
 Only for the purpose of backward compatibility, retrieves the old behavior of using the random seed

padding
 Concat the zero padding to the output, as the default embedding of empty type.

Methods

| | |
|--|--|
| <code>build(ntypes[, reuse, suffix])</code> | Build the computational graph for the descriptor. |
| <code>init_variables(graph, graph_def[, suffix, ...])</code> | Init the type embedding net variables with the given dict. |

`build(ntypes: int, reuse=None, suffix='')`

Build the computational graph for the descriptor.

Parameters

`ntypes`
Number of atom types.

`reuse`
The weights in the networks should be reused when get the variable.

`suffix`
Name suffix to identify this descriptor

Returns

`embedded_types`
The computational graph for embedded types

`init_variables`(`graph`: Graph, `graph_def`: GraphDef, `suffix`='', `model_type`='original_model') →
`None`

Init the type embedding net variables with the given dict.

Parameters

`graph`
[`tf.Graph`] The input frozen model graph

`graph_def`
[`tf.GraphDef`] The input frozen model graph_def

`suffix`
Name suffix to identify this descriptor

`model_type`
Indicator of whether this model is a compressed model

`deepmd.utils.type_embed.embed_atom_type`(`ntypes`: int, `natoms`: Tensor, `type_embedding`: Tensor)

Make the embedded type for the atoms in system. The atoms are assumed to be sorted according to the type, thus their types are described by a `tf.Tensor` `natoms`, see explanation below.

Parameters

`ntypes`:
Number of types.

`natoms`:
The number of atoms. This tensor has the length of `Ntypes + 2` `natoms[0]`: number of local atoms `natoms[1]`: total number of atoms held by this processor `natoms[i]`: $2 \leq i < Ntypes+2$, number of type `i` atoms

`type_embedding`:
The type embedding. It has the shape of [`ntypes`, `embedding_dim`]

Returns

`atom_embedding`
The embedded type of each atom. It has the shape of [`numb_atoms`, `embedding_dim`]

deepmd.utils.weight_avg module

`deepmd.utils.weight_avg.weighted_average(errors: List[Dict[str, Tuple[float, float]]]) → Dict`

Compute wighted average of prediction errors (MAE or RMSE) for model.

Parameters

errors

[List[Dict[str, Tuple[float, float]]]] List: the error of systems Dict: the error of quantities, name given by the key str: the name of the quantity, must starts with 'mae' or 'rmse' Tuple: (error, weight)

Returns

Dict

weighted averages

17.1.2 Submodules

17.1.3 deepmd.calculator module

ASE calculator interface module.

`class deepmd.calculator.DP(model: Union[str, Path], label: str = 'DP', type_dict: Optional[Dict[str, int]] = None, **kwargs)`

Bases: `Calculator`

Implementation of ASE deepmd calculator.

Implemented propertie are energy, forces and stress

Parameters

model

[Union[str, Path]] path to the model

label

[str, optional] calculator label, by default "DP"

type_dict

[Dict[str, int], optional] mapping of element types and their numbers, best left None and the calculator will infer this information from model, by default None

Examples

Compute potential energy

```
>>> from ase import Atoms
>>> from deepmd.calculator import DP
>>> water = Atoms('H2O',
>>>               positions=[(0.7601, 1.9270, 1),
>>>                           (1.9575, 1, 1),
>>>                           (1., 1., 1.)],
>>>               cell=[100, 100, 100],
>>>               calculator=DP(model="frozen_model.pb"))
>>> print(water.get_potential_energy())
>>> print(water.get_forces())
```

Run BFGS structure optimization

```
>>> from ase.optimize import BFGS
>>> dyn = BFGS(water)
>>> dyn.run(fmax=1e-6)
>>> print(water.get_positions())
```

Attributes

directory
label

Methods

| | |
|---|--|
| <code>band_structure()</code> | Create band-structure object for plotting. |
| <code>calculate([atoms, properties, system_changes])</code> | Run calculation with deepmd model. |
| <code>calculate_numerical_forces(atoms[, d])</code> | Calculate numerical forces using finite difference. |
| <code>calculate_numerical_stress(atoms[, d, voigt])</code> | Calculate numerical stress using finite difference. |
| <code>calculate_properties(atoms, properties)</code> | This method is experimental; currently for internal use. |
| <code>check_state(atoms[, tol])</code> | Check for any system changes since last calculation. |
| <code>get_magnetic_moments([atoms])</code> | Calculate magnetic moments projected onto atoms. |
| <code>get_property(name[, atoms, allow_calculation])</code> | Get the named property. |
| <code>get_stresses([atoms])</code> | the calculator should return intensive stresses, i.e., such that <code>stresses.sum(axis=0) == stress</code> |
| <code>read(label)</code> | Read atoms, parameters and calculated properties from output file. |
| <code>reset()</code> | Clear all information from old calculation. |
| <code>set(**kwargs)</code> | Set parameters like <code>set(key1=value1, key2=value2, ...)</code> . |
| <code>set_label(label)</code> | Set label and convert label to directory and prefix. |

| | |
|------------------------|--|
| calculation_required | |
| export_properties | |
| get_atoms | |
| get_charges | |
| get_default_parameters | |
| get_dipole_moment | |
| get_forces | |
| get_magnetic_moment | |
| get_potential_energies | |
| get_potential_energy | |
| get_stress | |
| read_atoms | |
| todict | |

```
calculate(atoms: Optional[Atoms] = None, properties: List[str] = ['energy', 'forces', 'virial'],
          system_changes: List[str] = ['positions', 'numbers', 'cell', 'pbc', 'initial_charges',
          'initial_magnoms'])
```

Run calculation with deepmd model.

Parameters

atoms

[Optional[Atoms], optional] atoms object to run the calculation on, by default None

properties

[List[str], optional] unused, only for function signature compatibility, by default ["energy", "forces", "stress"]

system_changes

[List[str], optional] unused, only for function signature compatibility, by default all_changes

```
implemented_properties: List[str] = ['energy', 'free_energy', 'forces', 'virial',
'stress']
```

Properties calculator can handle (energy, forces, ...)

```
name = 'DP'
```

17.1.4 deepmd.common module

Collection of functions and classes used throughout the whole package.

```
deepmd.common.add_data_requirement(key: str, ndof: int, atomic: bool = False, must: bool = False,
                                   high_prec: bool = False, type_sel: Optional[bool] = None, repeat:
                                   int = 1, default: float = 0.0, dtype: Optional[dtype] = None)
```

Specify data requirements for training.

Parameters

key

[str] type of data stored in corresponding *.npz file e.g. forces or energy

ndof

[int] number of the degrees of freedom, this is tied to atomic parameter e.g. forces have atomic=True and ndof=3

atomic
 [bool, optional] specifies whether the ndof keyword applies to per atom quantity or not, by default False

must
 [bool, optional] specifies if the *.npz data file must exist, by default False

high_prec
 [bool, optional] if true load data to np.float64 else np.float32, by default False

type_sel
 [bool, optional] select only certain type of atoms, by default None

repeat
 [int, optional] if specify repeat data repeat times, by default 1

default
 [float, optional, default=0.] default value of data

dtype
 [np.dtype, optional] the dtype of data, overwrites high_prec if provided

`deepmd.common.cast_precision(func: Callable) → Callable`

A decorator that casts and casts back the input and output tensor of a method.

The decorator should be used in a classmethod.

The decorator will do the following thing: (1) It casts input Tensors from GLOBAL_TF_FLOAT_PRECISION to precision defined by property precision. (2) It casts output Tensors from precision to GLOBAL_TF_FLOAT_PRECISION. (3) It checks inputs and outputs and only casts when input or output is a Tensor and its dtype matches GLOBAL_TF_FLOAT_PRECISION and precision, respectively. If it does not match (e.g. it is an integer), the decorator will do nothing on it.

Returns

Callable

a decorator that casts and casts back the input and output tensor of a method

Examples

```
>>> class A:
...     @property
...     def precision(self):
...         return tf.float32
...
...     @cast_precision
...     def f(x: tf.Tensor, y: tf.Tensor) -> tf.Tensor:
...         return x ** 2 + y
```

`deepmd.common.clear_session()`

Reset all state generated by DeePMD-kit.

`deepmd.common.expand_sys_str(root_dir: Union[str, Path]) → List[str]`

Recursively iterate over directories taking those that contain type.raw file.

Parameters

root_dir
 [Union[str, Path]] starting directory

Returns

`List[str]`
list of string pointing to system directories

`deepmd.common.gelu(x: Tensor) → Tensor`

Gaussian Error Linear Unit.

This is a smoother version of the RELU, implemented by custom operator.

Parameters

`x`
`[tf.Tensor]` float Tensor to perform activation

Returns

`tf.Tensor`
x with the GELU activation applied

References

Original paper <https://arxiv.org/abs/1606.08415>

`deepmd.common.gelu_tf(x: Tensor) → Tensor`

Gaussian Error Linear Unit.

This is a smoother version of the RELU, implemented by TF.

Parameters

`x`
`[tf.Tensor]` float Tensor to perform activation

Returns

`tf.Tensor`
x with the GELU activation applied

References

Original paper <https://arxiv.org/abs/1606.08415>

`deepmd.common.get_activation_func(activation_fn: Optional[_ACTIVATION]) → Optional[Callable[[Tensor], Tensor]]`

Get activation function callable based on string name.

Parameters

`activation_fn`
`[_ACTIVATION]` one of the defined activation functions

Returns

`Callable[[tf.Tensor], tf.Tensor]`
correspondingg TF callable

Raises

`RuntimeError`
if unknown activation function is specified

`deepmd.common.get_np_precision(precision: _PRECISION) → dtype`

Get numpy precision constant from string.

Parameters

precision
[_PRECISION] string name of numpy constant or default

Returns

np.dtype
numpy precision constant

Raises

RuntimeError
if string is invalid

`deepmd.common.get_precision(precision: _PRECISION) → Any`

Convert str to TF DType constant.

Parameters

precision
[_PRECISION] one of the allowed precisions

Returns

tf.python.framework.dtypes.DType
appropriate TF constant

Raises

RuntimeError
if supplied precision string does not have a corresponding TF constant

`deepmd.common.j_loader(filename: Union[str, Path]) → Dict[str, Any]`

Load yaml or json settings file.

Parameters

filename
[Union[str, Path]] path to file

Returns

Dict[str, Any]
loaded dictionary

Raises

TypeError
if the supplied file is of unsupported type

`deepmd.common.j_must_have(jdata: Dict[str, _DICT_VAL], key: str, deprecated_key: List[str] = []) → _DICT_VAL`

Assert that supplied dictionary contains specified key.

Returns

_DICT_VAL
value that was stored under supplied key

Raises

`RuntimeError`

if the key is not present

`deepmd.common.make_default_mesh(pbc: bool, mixed_type: bool) → ndarray`

Make mesh.

Only the size of mesh matters, not the values: * 6 for PBC, no mixed types * 0 for no PBC, no mixed types * 7 for PBC, mixed types * 1 for no PBC, mixed types

Parameters

`pbc`

[bool] if True, the mesh will be made for periodic boundary conditions

`mixed_type`

[bool] if True, the mesh will be made for mixed types

Returns

`np.ndarray`

mesh

`deepmd.common.safe_cast_tensor(input: Tensor, from_precision: DType, to_precision: DType) → Tensor`

Convert a Tensor from a precision to another precision.

If input is not a Tensor or without the specific precision, the method will not cast it.

Parameters

`input`

[tf.Tensor] input tensor

`from_precision`

[tf.DType] Tensor data type that is casted from

`to_precision`

[tf.DType] Tensor data type that casts to

Returns

`tf.Tensor`

casted Tensor

`deepmd.common.select_idx_map(atom_types: ndarray, select_types: ndarray) → ndarray`

Build map of indices for element supplied element types from all atoms list.

Parameters

`atom_types`

[np.ndarray] array specifying type for each atoms as integer

`select_types`

[np.ndarray] types of atoms you want to find indices for

Returns

`np.ndarray`

indices of types of atoms defined by select_types in atom_types array

Warning: select_types array will be sorted before finding indices in atom_types

17.1.5 deepmd.env module

Module that sets tensorflow working environment and exports important constants.

`deepmd.env.GLOBAL_ENER_FLOAT_PRECISION`

alias of `float64`

`deepmd.env.GLOBAL_NP_FLOAT_PRECISION`

alias of `float64`

`deepmd.env.global_cvt_2_ener_float(xx: Tensor) → Tensor`

Cast tensor to globally set energy precision.

Parameters

`xx`

`[tf.Tensor]` input tensor

Returns

`tf.Tensor`

output tensor cast to `GLOBAL_ENER_FLOAT_PRECISION`

`deepmd.env.global_cvt_2_tf_float(xx: Tensor) → Tensor`

Cast tensor to globally set TF precision.

Parameters

`xx`

`[tf.Tensor]` input tensor

Returns

`tf.Tensor`

output tensor cast to `GLOBAL_TF_FLOAT_PRECISION`

`deepmd.env.reset_default_tf_session_config(cpu_only: bool)`

Limit tensorflow session to CPU or not.

Parameters

`cpu_only`

`[bool]` If enabled, no GPU device is visible to the TensorFlow Session.

17.1.6 deepmd.lmp module

Register entry points for lammmps-wheel.

`deepmd.lmp.get_env(paths: List[Optional[str]]) → str`

Get the environment variable from given paths.

`deepmd.lmp.get_library_path(module: str) → List[str]`

Get library path from a module.

Parameters

`module`

`[str]` The module name.

Returns

```
list[str]
```

The library path.

```
deepmd.lmp.get_op_dir() → str
```

Get the directory of the deepmd-kit OP library.

18.1 op_module

Python wrappers around TensorFlow ops.

This file is MACHINE GENERATED! Do not edit.

`deepmd.env.op_module.AddFltNvnmd(x, w, name=None)`

TODO: add doc.

Parameters

- **x** – A Tensor. Must be one of the following types: float32, float64.
- **w** – A Tensor. Must have the same type as x.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as x.

`deepmd.env.op_module.CopyFltNvnmd(x, name=None)`

TODO: add doc.

Parameters

- **x** – A Tensor. Must be one of the following types: float32, float64.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (y1, y2).

y1: A Tensor. Has the same type as x. y2: A Tensor. Has the same type as x.

`deepmd.env.op_module.Descript(coord, type, natoms, box, mesh, davg, dstd, rcut_a, rcut_r, sel_a, sel_r, axis_rule, name=None)`

TODO: add doc.

Parameters

- **coord** – A Tensor. Must be one of the following types: float32, float64.
- **type** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **box** – A Tensor. Must have the same type as coord.
- **mesh** – A Tensor of type int32.

- **davg** – A Tensor. Must have the same type as coord.
- **dstd** – A Tensor. Must have the same type as coord.
- **rcut_a** – A float.
- **rcut_r** – A float.
- **sel_a** – A list of ints.
- **sel_r** – A list of ints.
- **axis_rule** – A list of ints.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (descript, descript_deriv, rij, nlist, axis, rot_mat).

descript: A Tensor. Has the same type as coord. descript_deriv: A Tensor. Has the same type as coord. rij: A Tensor. Has the same type as coord. nlist: A Tensor of type int32. axis: A Tensor of type int32. rot_mat: A Tensor. Has the same type as coord.

```
deepmd.env.op_module.DescriptNorot(coord, type, natoms, box, mesh, davg, dstd, rcut_a, rcut_r,
                                   rcut_r_smth, sel_a, sel_r, name=None)
```

TODO: add doc.

Parameters

- **coord** – A Tensor. Must be one of the following types: float32, float64.
- **type** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **box** – A Tensor. Must have the same type as coord.
- **mesh** – A Tensor of type int32.
- **davg** – A Tensor. Must have the same type as coord.
- **dstd** – A Tensor. Must have the same type as coord.
- **rcut_a** – A float.
- **rcut_r** – A float.
- **rcut_r_smth** – A float.
- **sel_a** – A list of ints.
- **sel_r** – A list of ints.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (descript, descript_deriv, rij, nlist).

descript: A Tensor. Has the same type as coord. descript_deriv: A Tensor. Has the same type as coord. rij: A Tensor. Has the same type as coord. nlist: A Tensor of type int32.

```
deepmd.env.op_module.DescriptSeA(coord, type, natoms, box, mesh, davg, dstd, rcut_a, rcut_r,
                                  rcut_r_smth, sel_a, sel_r, name=None)
```

TODO: add doc.

Parameters

- **coord** – A Tensor. Must be one of the following types: float32, float64.
- **type** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **box** – A Tensor. Must have the same type as coord.
- **mesh** – A Tensor of type int32.
- **davg** – A Tensor. Must have the same type as coord.
- **dstd** – A Tensor. Must have the same type as coord.
- **rcut_a** – A float.
- **rcut_r** – A float.
- **rcut_r_smth** – A float.
- **sel_a** – A list of ints.
- **sel_r** – A list of ints.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (descript, descript_deriv, rij, nlist).

descript: A Tensor. Has the same type as coord. descript_deriv: A Tensor. Has the same type as coord. rij: A Tensor. Has the same type as coord. nlist: A Tensor of type int32.

```
deepmd.env.op_module.DescriptSeAEf(coord, type, natoms, box, mesh, ef, davg, dstd, rcut_a, rcut_r,
                                   rcut_r_smth, sel_a, sel_r, name=None)
```

TODO: add doc.

Parameters

- **coord** – A Tensor. Must be one of the following types: float32, float64.
- **type** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **box** – A Tensor. Must have the same type as coord.
- **mesh** – A Tensor of type int32.
- **ef** – A Tensor. Must have the same type as coord.
- **davg** – A Tensor. Must have the same type as coord.
- **dstd** – A Tensor. Must have the same type as coord.
- **rcut_a** – A float.
- **rcut_r** – A float.
- **rcut_r_smth** – A float.
- **sel_a** – A list of ints.
- **sel_r** – A list of ints.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (descript, descript_deriv, rij, nlist).

descript: A Tensor. Has the same type as coord. descript_deriv: A Tensor. Has the same type as coord. rij: A Tensor. Has the same type as coord. nlist: A Tensor of type int32.

```
deepmd.env.op_module.DescriptSeAEfPara(coord, type, natoms, box, mesh, ef, davg, dstd, rcut_a, rcut_r,
                                         rcut_r_smth, sel_a, sel_r, name=None)
```

TODO: add doc.

Parameters

- **coord** – A Tensor. Must be one of the following types: float32, float64.
- **type** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **box** – A Tensor. Must have the same type as coord.
- **mesh** – A Tensor of type int32.
- **ef** – A Tensor. Must have the same type as coord.
- **davg** – A Tensor. Must have the same type as coord.
- **dstd** – A Tensor. Must have the same type as coord.
- **rcut_a** – A float.
- **rcut_r** – A float.
- **rcut_r_smth** – A float.
- **sel_a** – A list of ints.
- **sel_r** – A list of ints.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (descript, descript_deriv, rij, nlist).

descript: A Tensor. Has the same type as coord. descript_deriv: A Tensor. Has the same type as coord. rij: A Tensor. Has the same type as coord. nlist: A Tensor of type int32.

```
deepmd.env.op_module.DescriptSeAEfVert(coord, type, natoms, box, mesh, ef, davg, dstd, rcut_a, rcut_r,
                                         rcut_r_smth, sel_a, sel_r, name=None)
```

TODO: add doc.

Parameters

- **coord** – A Tensor. Must be one of the following types: float32, float64.
- **type** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **box** – A Tensor. Must have the same type as coord.
- **mesh** – A Tensor of type int32.
- **ef** – A Tensor. Must have the same type as coord.
- **davg** – A Tensor. Must have the same type as coord.
- **dstd** – A Tensor. Must have the same type as coord.

- **rcut_a** – A float.
- **rcut_r** – A float.
- **rcut_r_smth** – A float.
- **sel_a** – A list of ints.
- **sel_r** – A list of ints.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (descript, descript_deriv, rij, nlist).

descript: A Tensor. Has the same type as coord. descript_deriv: A Tensor. Has the same type as coord. rij: A Tensor. Has the same type as coord. nlist: A Tensor of type int32.

`deepmd.env.op_module.DescriptSeAMask(coord, type, mask, box, natoms, mesh, name=None)`

TODO: add doc.

Parameters

- **coord** – A Tensor. Must be one of the following types: float32, float64.
- **type** – A Tensor of type int32.
- **mask** – A Tensor of type int32.
- **box** – A Tensor. Must have the same type as coord.
- **natoms** – A Tensor of type int32.
- **mesh** – A Tensor of type int32.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (descript, descript_deriv, rij, nlist).

descript: A Tensor. Has the same type as coord. descript_deriv: A Tensor. Has the same type as coord. rij: A Tensor. Has the same type as coord. nlist: A Tensor of type int32.

`deepmd.env.op_module.DescriptSeR(coord, type, natoms, box, mesh, davg, dstd, rcut, rcut_smth, sel, name=None)`

TODO: add doc.

Parameters

- **coord** – A Tensor. Must be one of the following types: float32, float64.
- **type** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **box** – A Tensor. Must have the same type as coord.
- **mesh** – A Tensor of type int32.
- **davg** – A Tensor. Must have the same type as coord.
- **dstd** – A Tensor. Must have the same type as coord.
- **rcut** – A float.
- **rcut_smth** – A float.

- **sel** – A list of ints.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (descript, descript_deriv, rij, nlist).

descript: A Tensor. Has the same type as coord. descript_deriv: A Tensor. Has the same type as coord. rij: A Tensor. Has the same type as coord. nlist: A Tensor of type int32.

`deepmd.env.op_module.DotmulFltNvnmd(x, w, name=None)`

TODO: add doc.

Parameters

- **x** – A Tensor. Must be one of the following types: float32, float64.
- **w** – A Tensor. Must have the same type as x.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as x.

`deepmd.env.op_module.DprcPairwiseIdx(idxs, natoms, name=None)`

TODO: add doc.

Parameters

- **idxs** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (forward_qm_map, backward_qm_map, forward_qmmm_map, backward_qmmm_map, natoms_qm, natoms_qmmm, qmmm_frame_idx).

forward_qm_map: A Tensor of type int32. backward_qm_map: A Tensor of type int32. forward_qmmm_map: A Tensor of type int32. backward_qmmm_map: A Tensor of type int32. natoms_qm: A Tensor of type int32. natoms_qmmm: A Tensor of type int32. qmmm_frame_idx: A Tensor of type int32.

`deepmd.env.op_module.EwaldRecp(coord, charge, natoms, box, ewald_beta, ewald_h, name=None)`

TODO: add doc.

Parameters

- **coord** – A Tensor. Must be one of the following types: float32, float64.
- **charge** – A Tensor. Must have the same type as coord.
- **natoms** – A Tensor of type int32.
- **box** – A Tensor. Must have the same type as coord.
- **ewald_beta** – A float.
- **ewald_h** – A float.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (energy, force, virial).

energy: A Tensor. Has the same type as coord. force: A Tensor. Has the same type as coord. virial: A Tensor. Has the same type as coord.

`deepmd.env.op_module.FltNvnmd(x, name=None)`

TODO: add doc.

Parameters

- **x** – A Tensor. Must be one of the following types: float32, float64.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as x.

`deepmd.env.op_module.Gelu(x, name=None)`

TODO: add doc.

Parameters

- **x** – A Tensor. Must be one of the following types: float32, float64.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as x.

`deepmd.env.op_module.GeluCustom(x, name=None)`

TODO: add doc.

Parameters

- **x** – A Tensor. Must be one of the following types: float32, float64.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as x.

`deepmd.env.op_module.GeluGrad(dy, x, name=None)`

TODO: add doc.

Parameters

- **dy** – A Tensor. Must be one of the following types: float32, float64.
- **x** – A Tensor. Must have the same type as dy.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as dy.

`deepmd.env.op_module.GeluGradCustom(dy, x, name=None)`

TODO: add doc.

Parameters

- **dy** – A Tensor. Must be one of the following types: float32, float64.
- **x** – A Tensor. Must have the same type as dy.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as dy.

`deepmd.env.op_module.GeluGradGrad(dy, dy_, x, name=None)`

TODO: add doc.

Parameters

- **dy** – A Tensor. Must be one of the following types: float32, float64.
- **dy** – A Tensor. Must have the same type as dy.
- **x** – A Tensor. Must have the same type as dy.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as dy.

`deepmd.env.op_module.GeluGradGradCustom(dy, dy_, x, name=None)`

TODO: add doc.

Parameters

- **dy** – A Tensor. Must be one of the following types: float32, float64.
- **dy** – A Tensor. Must have the same type as dy.
- **x** – A Tensor. Must have the same type as dy.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as dy.

`deepmd.env.op_module.MapAparam(aparam, nlist, natoms, n_a_sel, n_r_sel, name=None)`

TODO: add doc.

Parameters

- **aparam** – A Tensor. Must be one of the following types: float32, float64.
- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **n_a_sel** – An int.
- **n_r_sel** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as aparam.

`deepmd.env.op_module.MapFltNvnmd(x, table, table_grad, table_info, name=None)`

TODO: add doc.

Parameters

- **x** – A Tensor. Must be one of the following types: float32, float64.
- **table** – A Tensor. Must have the same type as x.
- **table_grad** – A Tensor. Must have the same type as x.
- **table_info** – A Tensor. Must have the same type as x.

- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as x.

`deepmd.env.op_module.MatmulFitnetNvnmd(x, w, nbitx, nbitw, normw, name=None)`

TODO: add doc.

Parameters

- **x** – A Tensor. Must be one of the following types: float32, float64.
- **w** – A Tensor. Must have the same type as x.
- **nbitx** – An int.
- **nbitw** – An int.
- **normw** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as x.

`deepmd.env.op_module.MatmulFlt2fixNvnmd(x, w, nbit, name=None)`

TODO: add doc.

Parameters

- **x** – A Tensor. Must be one of the following types: float32, float64.
- **w** – A Tensor. Must have the same type as x.
- **nbit** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as x.

`deepmd.env.op_module.MatmulFltNvnmd(x, w, normx, normw, name=None)`

TODO: add doc.

Parameters

- **x** – A Tensor. Must be one of the following types: float32, float64.
- **w** – A Tensor. Must have the same type as x.
- **normx** – An int.
- **normw** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as x.

`deepmd.env.op_module.MulFltNvnmd(x, w, name=None)`

TODO: add doc.

Parameters

- **x** – A Tensor. Must be one of the following types: float32, float64.
- **w** – A Tensor. Must have the same type as x.

- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as x.

`deepmd.env.op_module.NeighborStat(coord, type, natoms, box, mesh, rcut, name=None)`

TODO: add doc.

Parameters

- **coord** – A Tensor. Must be one of the following types: float32, float64.
- **type** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **box** – A Tensor. Must have the same type as coord.
- **mesh** – A Tensor of type int32.
- **rcut** – A float.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (max_nbor_size, min_nbor_dist).

max_nbor_size: A Tensor of type int32. min_nbor_dist: A Tensor. Has the same type as coord.

`deepmd.env.op_module.PairTab(table_info, table_data, type, rij, nlist, natoms, scale, sel_a, sel_r, name=None)`

TODO: add doc.

Parameters

- **table_info** – A Tensor of type float64.
- **table_data** – A Tensor of type float64.
- **type** – A Tensor of type int32.
- **rij** – A Tensor. Must be one of the following types: float32, float64.
- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **scale** – A Tensor. Must have the same type as rij.
- **sel_a** – A list of ints.
- **sel_r** – A list of ints.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (atom_energy, force, atom_virial).

atom_energy: A Tensor. Has the same type as rij. force: A Tensor. Has the same type as rij. atom_virial: A Tensor. Has the same type as rij.

`deepmd.env.op_module.ParallelProdForceSeA(net_deriv, in_deriv, nlist, natoms, n_a_sel, n_r_sel, parallel=False, start_frac=0, end_frac=1, name=None)`

TODO: add doc.

Parameters

- **net_deriv** – A Tensor. Must be one of the following types: float32, float64.
- **in_deriv** – A Tensor. Must have the same type as net_deriv.
- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **n_a_sel** – An int.
- **n_r_sel** – An int.
- **parallel** – An optional bool. Defaults to False.
- **start_frac** – An optional float. Defaults to 0.
- **end_frac** – An optional float. Defaults to 1.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as net_deriv.

`deepmd.env.op_module.ProdEnvMatA(coord, type, natoms, box, mesh, davg, dstd, rcut_a, rcut_r, rcut_r_smth, sel_a, sel_r, name=None)`

Compute the environment matrix for descriptor se_e2_a.

Each row of the environment matrix \mathcal{R}^i can be constructed as follows

$$(\mathcal{R}^i)_j = \begin{bmatrix} \frac{s(r_{ji})}{s(r_{ji})x_{ji}} \\ \frac{r_{ji}}{s(r_{ji})y_{ji}} \\ \frac{r_{ji}}{s(r_{ji})z_{ji}} \\ \frac{r_{ji}}{r_{ji}} \end{bmatrix}$$

In the above equation, $\mathbf{R}_{ji} = \mathbf{R}_j - \mathbf{R}_i = (x_{ji}, y_{ji}, z_{ji})$ is the relative coordinate and $r_{ji} = \|\mathbf{R}_{ji}\|$ is its norm. The switching function $s(r)$ is defined as:

$$s(r) = \begin{cases} \frac{1}{r}, & r < r_s \\ \frac{1}{r} \left\{ \left(\frac{r-r_s}{r_c-r_s} \right)^3 \left(-6 \left(\frac{r-r_s}{r_c-r_s} \right)^2 + 15 \frac{r-r_s}{r_c-r_s} - 10 \right) + 1 \right\}, & r_s \leq r < r_c \\ 0, & r \geq r_c \end{cases}$$

Note that the environment matrix is normalized by davg and dstd.

Parameters

- **coord** – A Tensor. Must be one of the following types: float32, float64. The coordinates of atoms.
- **type** – A Tensor of type int32. The types of atoms.
- **natoms** – A Tensor of type int32. The number of atoms. This tensor has the length of Ntypes + 2. natoms[0]: number of local atoms. natoms[1]: total number of atoms held by this processor. natoms[i]: 2 ≤ i < Ntypes+2, number of type i atoms.
- **box** – A Tensor. Must have the same type as coord. The box of frames.

- **mesh** – A Tensor of type int32. For historical reasons, only the length of the Tensor matters. If size of mesh == 6, pbc is assumed. If size of mesh == 0, no-pbc is assumed.
- **davg** – A Tensor. Must have the same type as coord. Average value of the environment matrix for normalization.
- **dstd** – A Tensor. Must have the same type as coord. Standard deviation of the environment matrix for normalization.
- **rcut_a** – A float. This argument is not used.
- **rcut_r** – A float. The cutoff radius for the environment matrix.
- **rcut_r_smth** – A float. From where the environment matrix should be smoothed.
- **sel_a** – A list of ints. sel_a[i] specifies the maximum number of type i atoms in the cut-off radius.
- **sel_r** – A list of ints. This argument is not used.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (descript, descript_deriv, rij, nlist).

descript: A Tensor. Has the same type as coord. The environment matrix. descript_deriv: A Tensor. Has the same type as coord. The derivative of the environment matrix. rij: A Tensor. Has the same type as coord. The distance between the atoms. nlist: A Tensor of type int32. The neighbor list of each atom.

```
deepmd.env.op_module.ProdEnvMatAMix(coord, type, natoms, box, mesh, davg, dstd, rcut_a, rcut_r,
                                     rcut_r_smth, sel_a, sel_r, name=None)
```

Compute the environment matrix mixing the atom types.

The sorting of neighbor atoms depends not on atom types, but on the distance and index. The atoms in nlist matrix will gather forward and thus save space for gaps of types in ProdEnvMatA, resulting in optimized and relative small sel_a.

The additional outputs are listed as following:

Parameters

- **coord** – A Tensor. Must be one of the following types: float32, float64.
- **type** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **box** – A Tensor. Must have the same type as coord.
- **mesh** – A Tensor of type int32.
- **davg** – A Tensor. Must have the same type as coord.
- **dstd** – A Tensor. Must have the same type as coord.
- **rcut_a** – A float.
- **rcut_r** – A float.
- **rcut_r_smth** – A float.
- **sel_a** – A list of ints.
- **sel_r** – A list of ints.

- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (descript, descript_deriv, rij, nlist, ntype, nmask).

descript: A Tensor. Has the same type as coord. descript_deriv: A Tensor. Has the same type as coord. rij: A Tensor. Has the same type as coord. nlist: A Tensor of type int32. ntype: A Tensor of type int32. The corresponding atom types in nlist. nmask: A Tensor of type bool. The atom mask in nlist.

```
deepmd.env.op_module.ProdEnvMatAMixNvnmdQuantize(coord, type, natoms, box, mesh, davg, dstd,
                                                    rcut_a, rcut_r, rcut_r_smth, sel_a, sel_r,
                                                    name=None)
```

TODO: add doc.

Parameters

- **coord** – A Tensor. Must be one of the following types: float32, float64.
- **type** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **box** – A Tensor. Must have the same type as coord.
- **mesh** – A Tensor of type int32.
- **davg** – A Tensor. Must have the same type as coord.
- **dstd** – A Tensor. Must have the same type as coord.
- **rcut_a** – A float.
- **rcut_r** – A float.
- **rcut_r_smth** – A float.
- **sel_a** – A list of ints.
- **sel_r** – A list of ints.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (descript, descript_deriv, rij, nlist, ntype, nmask).

descript: A Tensor. Has the same type as coord. descript_deriv: A Tensor. Has the same type as coord. rij: A Tensor. Has the same type as coord. nlist: A Tensor of type int32. ntype: A Tensor of type int32. nmask: A Tensor of type bool.

```
deepmd.env.op_module.ProdEnvMatANvnmdQuantize(coord, type, natoms, box, mesh, davg, dstd, rcut_a,
                                                rcut_r, rcut_r_smth, sel_a, sel_r, name=None)
```

TODO: add doc.

Parameters

- **coord** – A Tensor. Must be one of the following types: float32, float64.
- **type** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **box** – A Tensor. Must have the same type as coord.
- **mesh** – A Tensor of type int32.

- **davg** – A Tensor. Must have the same type as coord.
- **dstd** – A Tensor. Must have the same type as coord.
- **rcut_a** – A float.
- **rcut_r** – A float.
- **rcut_r_smth** – A float.
- **sel_a** – A list of ints.
- **sel_r** – A list of ints.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (descrpt, descrpt_deriv, rij, nlist).

descrpt: A Tensor. Has the same type as coord. descrpt_deriv: A Tensor. Has the same type as coord. rij: A Tensor. Has the same type as coord. nlist: A Tensor of type int32.

```
deepmd.env.op_module.ProdEnvMatR(coord, type, natoms, box, mesh, davg, dstd, rcut, rcut_smth, sel,
                                  name=None)
```

TODO: add doc.

Parameters

- **coord** – A Tensor. Must be one of the following types: float32, float64.
- **type** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **box** – A Tensor. Must have the same type as coord.
- **mesh** – A Tensor of type int32.
- **davg** – A Tensor. Must have the same type as coord.
- **dstd** – A Tensor. Must have the same type as coord.
- **rcut** – A float.
- **rcut_smth** – A float.
- **sel** – A list of ints.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (descrpt, descrpt_deriv, rij, nlist).

descrpt: A Tensor. Has the same type as coord. descrpt_deriv: A Tensor. Has the same type as coord. rij: A Tensor. Has the same type as coord. nlist: A Tensor of type int32.

```
deepmd.env.op_module.ProdForce(net_deriv, in_deriv, nlist, axis, natoms, n_a_sel, n_r_sel, name=None)
```

TODO: add doc.

Parameters

- **net_deriv** – A Tensor. Must be one of the following types: float32, float64.
- **in_deriv** – A Tensor. Must have the same type as net_deriv.
- **nlist** – A Tensor of type int32.

- **axis** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **n_a_sel** – An int.
- **n_r_sel** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as `net_deriv`.

```
deepmd.env.op_module.ProdForceNorot(net_deriv, in_deriv, nlist, natoms, n_a_sel, n_r_sel,
                                     name=None)
```

TODO: add doc.

Parameters

- **net_deriv** – A Tensor. Must be one of the following types: float32, float64.
- **in_deriv** – A Tensor. Must have the same type as `net_deriv`.
- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **n_a_sel** – An int.
- **n_r_sel** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as `net_deriv`.

```
deepmd.env.op_module.ProdForceSeA(net_deriv, in_deriv, nlist, natoms, n_a_sel, n_r_sel, name=None)
```

TODO: add doc.

Parameters

- **net_deriv** – A Tensor. Must be one of the following types: float32, float64.
- **in_deriv** – A Tensor. Must have the same type as `net_deriv`.
- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **n_a_sel** – An int.
- **n_r_sel** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as `net_deriv`.

```
deepmd.env.op_module.ProdForceSeAMask(net_deriv, in_deriv, mask, nlist, total_atom_num,
                                       name=None)
```

TODO: add doc.

Parameters

- **net_deriv** – A Tensor. Must be one of the following types: float32, float64.
- **in_deriv** – A Tensor. Must have the same type as `net_deriv`.

- **mask** – A Tensor of type int32.
- **nlist** – A Tensor of type int32.
- **total_atom_num** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as `net_deriv`.

```
deepmd.env.op_module.ProdForceSeR(net_deriv, in_deriv, nlist, natoms, name=None)
```

TODO: add doc.

Parameters

- **net_deriv** – A Tensor. Must be one of the following types: float32, float64.
- **in_deriv** – A Tensor. Must have the same type as `net_deriv`.
- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as `net_deriv`.

```
deepmd.env.op_module.ProdVirial(net_deriv, in_deriv, rij, nlist, axis, natoms, n_a_sel, n_r_sel,
                                name=None)
```

TODO: add doc.

Parameters

- **net_deriv** – A Tensor. Must be one of the following types: float32, float64.
- **in_deriv** – A Tensor. Must have the same type as `net_deriv`.
- **rij** – A Tensor. Must have the same type as `net_deriv`.
- **nlist** – A Tensor of type int32.
- **axis** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **n_a_sel** – An int.
- **n_r_sel** – An int.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (`virial`, `atom_virial`).

`virial`: A Tensor. Has the same type as `net_deriv`. `atom_virial`: A Tensor. Has the same type as `net_deriv`.

```
deepmd.env.op_module.ProdVirialNorot(net_deriv, in_deriv, rij, nlist, natoms, n_a_sel, n_r_sel,
                                      name=None)
```

TODO: add doc.

Parameters

- **net_deriv** – A Tensor. Must be one of the following types: float32, float64.

- **in_deriv** – A Tensor. Must have the same type as net_deriv.
- **rij** – A Tensor. Must have the same type as net_deriv.
- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **n_a_sel** – An int.
- **n_r_sel** – An int.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (virial, atom_virial).

virial: A Tensor. Has the same type as net_deriv. atom_virial: A Tensor. Has the same type as net_deriv.

```
deepmd.env.op_module.ProdVirialSeA(net_deriv, in_deriv, rij, nlist, natoms, n_a_sel, n_r_sel,
                                   name=None)
```

TODO: add doc.

Parameters

- **net_deriv** – A Tensor. Must be one of the following types: float32, float64.
- **in_deriv** – A Tensor. Must have the same type as net_deriv.
- **rij** – A Tensor. Must have the same type as net_deriv.
- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **n_a_sel** – An int.
- **n_r_sel** – An int.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (virial, atom_virial).

virial: A Tensor. Has the same type as net_deriv. atom_virial: A Tensor. Has the same type as net_deriv.

```
deepmd.env.op_module.ProdVirialSeR(net_deriv, in_deriv, rij, nlist, natoms, name=None)
```

TODO: add doc.

Parameters

- **net_deriv** – A Tensor. Must be one of the following types: float32, float64.
- **in_deriv** – A Tensor. Must have the same type as net_deriv.
- **rij** – A Tensor. Must have the same type as net_deriv.
- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (virial, atom_virial).

virial: A Tensor. Has the same type as net_deriv. atom_virial: A Tensor. Has the same type as net_deriv.

`deepmd.env.op_module.QuantizeNvnmd(x, isround, nbit1, nbit2, nbit3, name=None)`

TODO: add doc.

Parameters

- **x** – A Tensor. Must be one of the following types: float32, float64.
- **isround** – An int.
- **nbit1** – An int.
- **nbit2** – An int.
- **nbit3** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as x.

`deepmd.env.op_module.SoftMinForce(du, sw_deriv, nlist, natoms, n_a_sel, n_r_sel, name=None)`

TODO: add doc.

Parameters

- **du** – A Tensor. Must be one of the following types: float32, float64.
- **sw_deriv** – A Tensor. Must have the same type as du.
- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **n_a_sel** – An int.
- **n_r_sel** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as du.

`deepmd.env.op_module.SoftMinSwitch(type, rij, nlist, natoms, sel_a, sel_r, alpha, rmin, rmax, name=None)`

TODO: add doc.

Parameters

- **type** – A Tensor of type int32.
- **rij** – A Tensor. Must be one of the following types: float32, float64.
- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **sel_a** – A list of ints.
- **sel_r** – A list of ints.
- **alpha** – A float.

- **rmin** – A float.
- **rmax** – A float.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (sw_value, sw_deriv).

sw_value: A Tensor. Has the same type as rij. sw_deriv: A Tensor. Has the same type as rij.

`deepmd.env.op_module.SoftMinVirial(du, sw_deriv, rij, nlist, natoms, n_a_sel, n_r_sel, name=None)`

TODO: add doc.

Parameters

- **du** – A Tensor. Must be one of the following types: float32, float64.
- **sw_deriv** – A Tensor. Must have the same type as du.
- **rij** – A Tensor. Must have the same type as du.
- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **n_a_sel** – An int.
- **n_r_sel** – An int.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (virial, atom_virial).

virial: A Tensor. Has the same type as du. atom_virial: A Tensor. Has the same type as du.

`deepmd.env.op_module.TabulateFusion(table, table_info, em_x, em, last_layer_size, name=None)`

TODO: add doc.

Parameters

- **table** – A Tensor. Must be one of the following types: float32, float64.
- **table_info** – A Tensor. Must have the same type as table.
- **em_x** – A Tensor. Must have the same type as table.
- **em** – A Tensor. Must have the same type as table.
- **last_layer_size** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as table.

`deepmd.env.op_module.TabulateFusionGrad(table, table_info, em_x, em, dy, descriptor, name=None)`

TODO: add doc.

Parameters

- **table** – A Tensor. Must be one of the following types: float32, float64.
- **table_info** – A Tensor. Must have the same type as table.

- **em_x** – A Tensor. Must have the same type as table.
- **em** – A Tensor. Must have the same type as table.
- **dy** – A Tensor. Must have the same type as table.
- **descriptor** – A Tensor. Must have the same type as table.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (dy_dem_x, dy_dem).

dy_dem_x: A Tensor. Has the same type as table. dy_dem: A Tensor. Has the same type as table.

```
deepmd.env.op_module.TabulateFusionGradGrad(table, table_info, em_x, em, dz_dy_dem_x,
                                             dz_dy_dem, descriptor, name=None)
```

TODO: add doc.

Parameters

- **table** – A Tensor. Must be one of the following types: float32, float64.
- **table_info** – A Tensor. Must have the same type as table.
- **em_x** – A Tensor. Must have the same type as table.
- **em** – A Tensor. Must have the same type as table.
- **dz_dy_dem_x** – A Tensor. Must have the same type as table.
- **dz_dy_dem** – A Tensor. Must have the same type as table.
- **descriptor** – A Tensor. Must have the same type as table.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as table.

```
deepmd.env.op_module.TabulateFusionSeA(table, table_info, em_x, em, last_layer_size, name=None)
```

TODO: add doc.

Parameters

- **table** – A Tensor. Must be one of the following types: float32, float64.
- **table_info** – A Tensor. Must have the same type as table.
- **em_x** – A Tensor. Must have the same type as table.
- **em** – A Tensor. Must have the same type as table.
- **last_layer_size** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as table.

```
deepmd.env.op_module.TabulateFusionSeAGrad(table, table_info, em_x, em, dy, descriptor,
                                             name=None)
```

TODO: add doc.

Parameters

- **table** – A Tensor. Must be one of the following types: float32, float64.
- **table_info** – A Tensor. Must have the same type as table.
- **em_x** – A Tensor. Must have the same type as table.
- **em** – A Tensor. Must have the same type as table.
- **dy** – A Tensor. Must have the same type as table.
- **descriptor** – A Tensor. Must have the same type as table.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (dy_dem_x, dy_dem).

dy_dem_x: A Tensor. Has the same type as table. dy_dem: A Tensor. Has the same type as table.

```
deepmd.env.op_module.TabulateFusionSeAGradGrad(table, table_info, em_x, em, dz_dy_dem_x,
                                                dz_dy_dem, descriptor, is_sorted=True,
                                                name=None)
```

TODO: add doc.

Parameters

- **table** – A Tensor. Must be one of the following types: float32, float64.
- **table_info** – A Tensor. Must have the same type as table.
- **em_x** – A Tensor. Must have the same type as table.
- **em** – A Tensor. Must have the same type as table.
- **dz_dy_dem_x** – A Tensor. Must have the same type as table.
- **dz_dy_dem** – A Tensor. Must have the same type as table.
- **descriptor** – A Tensor. Must have the same type as table.
- **is_sorted** – An optional bool. Defaults to True.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as table.

```
deepmd.env.op_module.TabulateFusionSeAtten(table, table_info, em_x, em, two_embed,
                                            last_layer_size, is_sorted=True, name=None)
```

TODO: add doc.

Parameters

- **table** – A Tensor. Must be one of the following types: float32, float64.
- **table_info** – A Tensor. Must have the same type as table.
- **em_x** – A Tensor. Must have the same type as table.
- **em** – A Tensor. Must have the same type as table.
- **two_embed** – A Tensor. Must have the same type as table.
- **last_layer_size** – An int.
- **is_sorted** – An optional bool. Defaults to True.

- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as table.

```
deepmd.env.op_module.TabulateFusionSeAttenGrad(table, table_info, em_x, em, two_embed, dy,  
                                                descriptor, is_sorted=True, name=None)
```

TODO: add doc.

Parameters

- **table** – A Tensor. Must be one of the following types: float32, float64.
- **table_info** – A Tensor. Must have the same type as table.
- **em_x** – A Tensor. Must have the same type as table.
- **em** – A Tensor. Must have the same type as table.
- **two_embed** – A Tensor. Must have the same type as table.
- **dy** – A Tensor. Must have the same type as table.
- **descriptor** – A Tensor. Must have the same type as table.
- **is_sorted** – An optional bool. Defaults to True.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (dy_dem_x, dy_dem, dy_dtwo).

dy_dem_x: A Tensor. Has the same type as table. dy_dem: A Tensor. Has the same type as table. dy_dtwo: A Tensor. Has the same type as table.

```
deepmd.env.op_module.TabulateFusionSeR(table, table_info, em, last_layer_size, name=None)
```

TODO: add doc.

Parameters

- **table** – A Tensor. Must be one of the following types: float32, float64.
- **table_info** – A Tensor. Must have the same type as table.
- **em** – A Tensor. Must have the same type as table.
- **last_layer_size** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as table.

```
deepmd.env.op_module.TabulateFusionSeRGrad(table, table_info, em, dy, descriptor, name=None)
```

TODO: add doc.

Parameters

- **table** – A Tensor. Must be one of the following types: float32, float64.
- **table_info** – A Tensor. Must have the same type as table.
- **em** – A Tensor. Must have the same type as table.
- **dy** – A Tensor. Must have the same type as table.
- **descriptor** – A Tensor. Must have the same type as table.

- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as table.

```
deepmd.env.op_module.TabulateFusionSeRGradGrad(table, table_info, em, dz_dy_dem, descriptor,
                                                name=None)
```

TODO: add doc.

Parameters

- **table** – A Tensor. Must be one of the following types: float32, float64.
- **table_info** – A Tensor. Must have the same type as table.
- **em** – A Tensor. Must have the same type as table.
- **dz_dy_dem** – A Tensor. Must have the same type as table.
- **descriptor** – A Tensor. Must have the same type as table.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as table.

```
deepmd.env.op_module.TabulateFusionSeT(table, table_info, em_x, em, last_layer_size, name=None)
```

TODO: add doc.

Parameters

- **table** – A Tensor. Must be one of the following types: float32, float64.
- **table_info** – A Tensor. Must have the same type as table.
- **em_x** – A Tensor. Must have the same type as table.
- **em** – A Tensor. Must have the same type as table.
- **last_layer_size** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as table.

```
deepmd.env.op_module.TabulateFusionSeTGrad(table, table_info, em_x, em, dy, descriptor,
                                             name=None)
```

TODO: add doc.

Parameters

- **table** – A Tensor. Must be one of the following types: float32, float64.
- **table_info** – A Tensor. Must have the same type as table.
- **em_x** – A Tensor. Must have the same type as table.
- **em** – A Tensor. Must have the same type as table.
- **dy** – A Tensor. Must have the same type as table.
- **descriptor** – A Tensor. Must have the same type as table.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (dy_dem_x, dy_dem).

dy_dem_x: A Tensor. Has the same type as table. dy_dem: A Tensor. Has the same type as table.

```
deepmd.env.op_module.TabulateFusionSeTGradGrad(table, table_info, em_x, em, dz_dy_dem_x,
                                                  dz_dy_dem, descriptor, name=None)
```

TODO: add doc.

Parameters

- **table** – A Tensor. Must be one of the following types: float32, float64.
- **table_info** – A Tensor. Must have the same type as table.
- **em_x** – A Tensor. Must have the same type as table.
- **em** – A Tensor. Must have the same type as table.
- **dz_dy_dem_x** – A Tensor. Must have the same type as table.
- **dz_dy_dem** – A Tensor. Must have the same type as table.
- **descriptor** – A Tensor. Must have the same type as table.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as table.

```
deepmd.env.op_module.Tanh4FltNvnmd(x, name=None)
```

TODO: add doc.

Parameters

- **x** – A Tensor. Must be one of the following types: float32, float64.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as x.

```
deepmd.env.op_module.UnaggregatedDy2Dx(z, w, dy_dx, dy2_dx, ybar, functype, name=None)
```

TODO: add doc.

Parameters

- **z** – A Tensor. Must be one of the following types: float32, float64.
- **w** – A Tensor. Must have the same type as z.
- **dy_dx** – A Tensor. Must have the same type as z.
- **dy2_dx** – A Tensor. Must have the same type as z.
- **ybar** – A Tensor. Must have the same type as z.
- **functype** – A Tensor of type int32.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as z.

`deepmd.env.op_module.UnaggregatedDy2DxS(y, dy, w, xbar, functype, name=None)`

TODO: add doc.

Parameters

- **y** – A Tensor. Must be one of the following types: float32, float64.
- **dy** – A Tensor. Must have the same type as y.
- **w** – A Tensor. Must have the same type as y.
- **xbar** – A Tensor. Must have the same type as y.
- **functype** – A Tensor of type int32.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as y.

`deepmd.env.op_module.UnaggregatedDyDx(z, w, dy_dx, ybar, functype, name=None)`

TODO: add doc.

Parameters

- **z** – A Tensor. Must be one of the following types: float32, float64.
- **w** – A Tensor. Must have the same type as z.
- **dy_dx** – A Tensor. Must have the same type as z.
- **ybar** – A Tensor. Must have the same type as z.
- **functype** – A Tensor of type int32.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as z.

`deepmd.env.op_module.UnaggregatedDyDxS(y, w, xbar, functype, name=None)`

TODO: add doc.

Parameters

- **y** – A Tensor. Must be one of the following types: float32, float64.
- **w** – A Tensor. Must have the same type as y.
- **xbar** – A Tensor. Must have the same type as y.
- **functype** – A Tensor of type int32.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as y.

`deepmd.env.op_module.add_flt_nvnmd(x, w, name=None)`

TODO: add doc.

Parameters

- **x** – A Tensor. Must be one of the following types: float32, float64.
- **w** – A Tensor. Must have the same type as x.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as x.

`deepmd.env.op_module.copy_flt_nvnmmd(x, name=None)`

TODO: add doc.

Parameters

- **x** – A Tensor. Must be one of the following types: float32, float64.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (y1, y2).

y1: A Tensor. Has the same type as x. y2: A Tensor. Has the same type as x.

`deepmd.env.op_module.descript(coord, type, natoms, box, mesh, davg, dstd, rcut_a, rcut_r, sel_a, sel_r, axis_rule, name=None)`

TODO: add doc.

Parameters

- **coord** – A Tensor. Must be one of the following types: float32, float64.
- **type** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **box** – A Tensor. Must have the same type as coord.
- **mesh** – A Tensor of type int32.
- **davg** – A Tensor. Must have the same type as coord.
- **dstd** – A Tensor. Must have the same type as coord.
- **rcut_a** – A float.
- **rcut_r** – A float.
- **sel_a** – A list of ints.
- **sel_r** – A list of ints.
- **axis_rule** – A list of ints.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (descript, descript_deriv, rij, nlist, axis, rot_mat).

descript: A Tensor. Has the same type as coord. descript_deriv: A Tensor. Has the same type as coord. rij: A Tensor. Has the same type as coord. nlist: A Tensor of type int32.

axis: A Tensor of type int32. rot_mat: A Tensor. Has the same type as coord.

`deepmd.env.op_module.descript_norot(coord, type, natoms, box, mesh, davg, dstd, rcut_a, rcut_r, rcut_r_smth, sel_a, sel_r, name=None)`

TODO: add doc.

Parameters

- **coord** – A Tensor. Must be one of the following types: float32, float64.
- **type** – A Tensor of type int32.

- **natoms** – A Tensor of type int32.
- **box** – A Tensor. Must have the same type as coord.
- **mesh** – A Tensor of type int32.
- **davg** – A Tensor. Must have the same type as coord.
- **dstd** – A Tensor. Must have the same type as coord.
- **rcut_a** – A float.
- **rcut_r** – A float.
- **rcut_r_smth** – A float.
- **sel_a** – A list of ints.
- **sel_r** – A list of ints.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (descript, descript_deriv, rij, nlist).

descript: A Tensor. Has the same type as coord. descript_deriv: A Tensor. Has the same type as coord. rij: A Tensor. Has the same type as coord. nlist: A Tensor of type int32.

```
deepmd.env.op_module.descript_se_a(coord, type, natoms, box, mesh, davg, dstd, rcut_a, rcut_r,
                                   rcut_r_smth, sel_a, sel_r, name=None)
```

TODO: add doc.

Parameters

- **coord** – A Tensor. Must be one of the following types: float32, float64.
- **type** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **box** – A Tensor. Must have the same type as coord.
- **mesh** – A Tensor of type int32.
- **davg** – A Tensor. Must have the same type as coord.
- **dstd** – A Tensor. Must have the same type as coord.
- **rcut_a** – A float.
- **rcut_r** – A float.
- **rcut_r_smth** – A float.
- **sel_a** – A list of ints.
- **sel_r** – A list of ints.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (descript, descript_deriv, rij, nlist).

descript: A Tensor. Has the same type as coord. descript_deriv: A Tensor. Has the same type as coord. rij: A Tensor. Has the same type as coord. nlist: A Tensor of type int32.

```
deepmd.env.op_module.descript_se_a_ef(coord, type, natoms, box, mesh, ef, davg, dstd, rcut_a, rcut_r,
                                       rcut_r_smth, sel_a, sel_r, name=None)
```

TODO: add doc.

Parameters

- **coord** – A Tensor. Must be one of the following types: float32, float64.
- **type** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **box** – A Tensor. Must have the same type as coord.
- **mesh** – A Tensor of type int32.
- **ef** – A Tensor. Must have the same type as coord.
- **davg** – A Tensor. Must have the same type as coord.
- **dstd** – A Tensor. Must have the same type as coord.
- **rcut_a** – A float.
- **rcut_r** – A float.
- **rcut_r_smth** – A float.
- **sel_a** – A list of ints.
- **sel_r** – A list of ints.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (descript, descript_deriv, rij, nlist).

descript: A Tensor. Has the same type as coord. descript_deriv: A Tensor. Has the same type as coord. rij: A Tensor. Has the same type as coord. nlist: A Tensor of type int32.

```
deepmd.env.op_module.descript_se_a_ef_para(coord, type, natoms, box, mesh, ef, davg, dstd, rcut_a,
                                           rcut_r, rcut_r_smth, sel_a, sel_r, name=None)
```

TODO: add doc.

Parameters

- **coord** – A Tensor. Must be one of the following types: float32, float64.
- **type** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **box** – A Tensor. Must have the same type as coord.
- **mesh** – A Tensor of type int32.
- **ef** – A Tensor. Must have the same type as coord.
- **davg** – A Tensor. Must have the same type as coord.
- **dstd** – A Tensor. Must have the same type as coord.
- **rcut_a** – A float.
- **rcut_r** – A float.
- **rcut_r_smth** – A float.

- **sel_a** – A list of ints.
- **sel_r** – A list of ints.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (descript, descript_deriv, rij, nlist).

descript: A Tensor. Has the same type as coord. descript_deriv: A Tensor. Has the same type as coord. rij: A Tensor. Has the same type as coord. nlist: A Tensor of type int32.

`deepmd.env.op_module.descript_se_a_ef_vert(coord, type, natoms, box, mesh, ef, davg, dstd, rcut_a, rcut_r, rcut_r_smth, sel_a, sel_r, name=None)`

TODO: add doc.

Parameters

- **coord** – A Tensor. Must be one of the following types: float32, float64.
- **type** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **box** – A Tensor. Must have the same type as coord.
- **mesh** – A Tensor of type int32.
- **ef** – A Tensor. Must have the same type as coord.
- **davg** – A Tensor. Must have the same type as coord.
- **dstd** – A Tensor. Must have the same type as coord.
- **rcut_a** – A float.
- **rcut_r** – A float.
- **rcut_r_smth** – A float.
- **sel_a** – A list of ints.
- **sel_r** – A list of ints.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (descript, descript_deriv, rij, nlist).

descript: A Tensor. Has the same type as coord. descript_deriv: A Tensor. Has the same type as coord. rij: A Tensor. Has the same type as coord. nlist: A Tensor of type int32.

`deepmd.env.op_module.descript_se_a_mask(coord, type, mask, box, natoms, mesh, name=None)`

TODO: add doc.

Parameters

- **coord** – A Tensor. Must be one of the following types: float32, float64.
- **type** – A Tensor of type int32.
- **mask** – A Tensor of type int32.
- **box** – A Tensor. Must have the same type as coord.
- **natoms** – A Tensor of type int32.

- **mesh** – A Tensor of type int32.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (descript, descript_deriv, rij, nlist).

descript: A Tensor. Has the same type as coord. descript_deriv: A Tensor. Has the same type as coord. rij: A Tensor. Has the same type as coord. nlist: A Tensor of type int32.

```
deepmd.env.op_module.descript_se_r(coord, type, natoms, box, mesh, davg, dstd, rcut, rcut_smth, sel,
                                   name=None)
```

TODO: add doc.

Parameters

- **coord** – A Tensor. Must be one of the following types: float32, float64.
- **type** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **box** – A Tensor. Must have the same type as coord.
- **mesh** – A Tensor of type int32.
- **davg** – A Tensor. Must have the same type as coord.
- **dstd** – A Tensor. Must have the same type as coord.
- **rcut** – A float.
- **rcut_smth** – A float.
- **sel** – A list of ints.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (descript, descript_deriv, rij, nlist).

descript: A Tensor. Has the same type as coord. descript_deriv: A Tensor. Has the same type as coord. rij: A Tensor. Has the same type as coord. nlist: A Tensor of type int32.

```
deepmd.env.op_module.dotmul_flt_nvnm(x, w, name=None)
```

TODO: add doc.

Parameters

- **x** – A Tensor. Must be one of the following types: float32, float64.
- **w** – A Tensor. Must have the same type as x.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as x.

```
deepmd.env.op_module.dprc_pairwise_idx(idxs, natoms, name=None)
```

TODO: add doc.

Parameters

- **idxs** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.

- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (forward_qm_map, backward_qm_map, forward_qmmm_map, backward_qmmm_map, natoms_qm, natoms_qmmm, qmmm_frame_idx).

forward_qm_map: A Tensor of type int32. backward_qm_map: A Tensor of type int32.
 forward_qmmm_map: A Tensor of type int32. backward_qmmm_map: A Tensor of type int32.
 natoms_qm: A Tensor of type int32. natoms_qmmm: A Tensor of type int32.
 qmmm_frame_idx: A Tensor of type int32.

`deepmd.env.op_module.ewald_recip(coord, charge, natoms, box, ewald_beta, ewald_h, name=None)`

TODO: add doc.

Parameters

- **coord** – A Tensor. Must be one of the following types: float32, float64.
- **charge** – A Tensor. Must have the same type as coord.
- **natoms** – A Tensor of type int32.
- **box** – A Tensor. Must have the same type as coord.
- **ewald_beta** – A float.
- **ewald_h** – A float.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (energy, force, virial).

energy: A Tensor. Has the same type as coord. force: A Tensor. Has the same type as coord.
 virial: A Tensor. Has the same type as coord.

`deepmd.env.op_module.flt_nvnmmd(x, name=None)`

TODO: add doc.

Parameters

- **x** – A Tensor. Must be one of the following types: float32, float64.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as x.

`deepmd.env.op_module.gelu(x, name=None)`

TODO: add doc.

Parameters

- **x** – A Tensor. Must be one of the following types: float32, float64.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as x.

`deepmd.env.op_module.gelu_custom(x, name=None)`

TODO: add doc.

Parameters

- **x** – A Tensor. Must be one of the following types: float32, float64.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as x.

`deepmd.env.op_module.gelu_grad(dy, x, name=None)`

TODO: add doc.

Parameters

- **dy** – A Tensor. Must be one of the following types: float32, float64.
- **x** – A Tensor. Must have the same type as dy.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as dy.

`deepmd.env.op_module.gelu_grad_custom(dy, x, name=None)`

TODO: add doc.

Parameters

- **dy** – A Tensor. Must be one of the following types: float32, float64.
- **x** – A Tensor. Must have the same type as dy.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as dy.

`deepmd.env.op_module.gelu_grad_grad(dy, dy_, x, name=None)`

TODO: add doc.

Parameters

- **dy** – A Tensor. Must be one of the following types: float32, float64.
- **dy_** – A Tensor. Must have the same type as dy.
- **x** – A Tensor. Must have the same type as dy.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as dy.

`deepmd.env.op_module.gelu_grad_grad_custom(dy, dy_, x, name=None)`

TODO: add doc.

Parameters

- **dy** – A Tensor. Must be one of the following types: float32, float64.
- **dy_** – A Tensor. Must have the same type as dy.
- **x** – A Tensor. Must have the same type as dy.

- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as dy.

`deepmd.env.op_module.map_aparam(aparam, nlist, natoms, n_a_sel, n_r_sel, name=None)`

TODO: add doc.

Parameters

- **aparam** – A Tensor. Must be one of the following types: float32, float64.
- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **n_a_sel** – An int.
- **n_r_sel** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as aparam.

`deepmd.env.op_module.map_flt_nvnmmd(x, table, table_grad, table_info, name=None)`

TODO: add doc.

Parameters

- **x** – A Tensor. Must be one of the following types: float32, float64.
- **table** – A Tensor. Must have the same type as x.
- **table_grad** – A Tensor. Must have the same type as x.
- **table_info** – A Tensor. Must have the same type as x.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as x.

`deepmd.env.op_module.matmul_fitnet_nvnmmd(x, w, nbitx, nbitw, normw, name=None)`

TODO: add doc.

Parameters

- **x** – A Tensor. Must be one of the following types: float32, float64.
- **w** – A Tensor. Must have the same type as x.
- **nbitx** – An int.
- **nbitw** – An int.
- **normw** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as x.

`deepmd.env.op_module.matmul_flt2fix_nvnmmd(x, w, nbit, name=None)`

TODO: add doc.

Parameters

- **x** – A Tensor. Must be one of the following types: float32, float64.
- **w** – A Tensor. Must have the same type as x.
- **nbit** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as x.

```
deepmd.env.op_module.matmul_flt_nvnmd(x, w, normx, normw, name=None)
```

TODO: add doc.

Parameters

- **x** – A Tensor. Must be one of the following types: float32, float64.
- **w** – A Tensor. Must have the same type as x.
- **normx** – An int.
- **normw** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as x.

```
deepmd.env.op_module.mul_flt_nvnmd(x, w, name=None)
```

TODO: add doc.

Parameters

- **x** – A Tensor. Must be one of the following types: float32, float64.
- **w** – A Tensor. Must have the same type as x.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as x.

```
deepmd.env.op_module.neighbor_stat(coord, type, natoms, box, mesh, rcut, name=None)
```

TODO: add doc.

Parameters

- **coord** – A Tensor. Must be one of the following types: float32, float64.
- **type** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **box** – A Tensor. Must have the same type as coord.
- **mesh** – A Tensor of type int32.
- **rcut** – A float.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (max_nbor_size, min_nbor_dist).

max_nbor_size: A Tensor of type int32. min_nbor_dist: A Tensor. Has the same type as coord.

```
deepmd.env.op_module.pair_tab(table_info, table_data, type, rij, nlist, natoms, scale, sel_a, sel_r,
                              name=None)
```

TODO: add doc.

Parameters

- **table_info** – A Tensor of type float64.
- **table_data** – A Tensor of type float64.
- **type** – A Tensor of type int32.
- **rij** – A Tensor. Must be one of the following types: float32, float64.
- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **scale** – A Tensor. Must have the same type as rij.
- **sel_a** – A list of ints.
- **sel_r** – A list of ints.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (atom_energy, force, atom_virial).

atom_energy: A Tensor. Has the same type as rij. force: A Tensor. Has the same type as rij. atom_virial: A Tensor. Has the same type as rij.

```
deepmd.env.op_module.parallel_prod_force_se_a(net_deriv, in_deriv, nlist, natoms, n_a_sel, n_r_sel,
                                              parallel=False, start_frac=0, end_frac=1,
                                              name=None)
```

TODO: add doc.

Parameters

- **net_deriv** – A Tensor. Must be one of the following types: float32, float64.
- **in_deriv** – A Tensor. Must have the same type as net_deriv.
- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **n_a_sel** – An int.
- **n_r_sel** – An int.
- **parallel** – An optional bool. Defaults to False.
- **start_frac** – An optional float. Defaults to 0.
- **end_frac** – An optional float. Defaults to 1.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as net_deriv.

```
deepmd.env.op_module.prod_env_mat_a(coord, type, natoms, box, mesh, davg, dstd, rcut_a, rcut_r,
                                     rcut_r_smth, sel_a, sel_r, name=None)
```

Compute the environment matrix for descriptor se_e2_a.

Each row of the environment matrix \mathcal{R}^i can be constructed as follows

$$(\mathcal{R}^i)_j = \begin{bmatrix} \frac{s(r_{ji})}{r_{ji}} \\ \frac{s(r_{ji})x_{ji}}{r_{ji}} \\ \frac{s(r_{ji})y_{ji}}{r_{ji}} \\ \frac{s(r_{ji})z_{ji}}{r_{ji}} \end{bmatrix}$$

In the above equation, $\mathbf{R}_{ji} = \mathbf{R}_j - \mathbf{R}_i = (x_{ji}, y_{ji}, z_{ji})$ is the relative coordinate and $r_{ji} = \|\mathbf{R}_{ji}\|$ is its norm. The switching function $s(r)$ is defined as:

$$s(r) = \begin{cases} \frac{1}{r}, & r < r_s \\ \frac{1}{r} \left\{ \left(\frac{r-r_s}{r_c-r_s} \right)^3 \left(-6 \left(\frac{r-r_s}{r_c-r_s} \right)^2 + 15 \frac{r-r_s}{r_c-r_s} - 10 \right) + 1 \right\}, & r_s \leq r < r_c \\ 0, & r \geq r_c \end{cases}$$

Note that the environment matrix is normalized by `davg` and `dstd`.

Parameters

- **coord** – A Tensor. Must be one of the following types: float32, float64. The coordinates of atoms.
- **type** – A Tensor of type int32. The types of atoms.
- **natoms** – A Tensor of type int32. The number of atoms. This tensor has the length of `Ntypes + 2`. `natoms[0]`: number of local atoms. `natoms[1]`: total number of atoms held by this processor. `natoms[i]`: $2 \leq i < \text{Ntypes} + 2$, number of type *i* atoms.
- **box** – A Tensor. Must have the same type as `coord`. The box of frames.
- **mesh** – A Tensor of type int32. For historical reasons, only the length of the Tensor matters. If size of `mesh` == 6, pbc is assumed. If size of `mesh` == 0, no-pbc is assumed.
- **davg** – A Tensor. Must have the same type as `coord`. Average value of the environment matrix for normalization.
- **dstd** – A Tensor. Must have the same type as `coord`. Standard deviation of the environment matrix for normalization.
- **rcut_a** – A float. This argument is not used.
- **rcut_r** – A float. The cutoff radius for the environment matrix.
- **rcut_r_smth** – A float. From where the environment matrix should be smoothed.
- **sel_a** – A list of ints. `sel_a[i]` specifies the maximum number of type *i* atoms in the cut-off radius.
- **sel_r** – A list of ints. This argument is not used.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (`descript`, `descript_deriv`, `rij`, `nlist`).

`descript`: A Tensor. Has the same type as `coord`. The environment matrix. `descript_deriv`: A Tensor. Has the same type as `coord`. The derivative of the environment matrix. `rij`: A Tensor. Has the same type as `coord`. The distance between the atoms. `nlist`: A Tensor of type int32. The neighbor list of each atom.

```
deepmd.env.op_module.prod_env_mat_a_mix(coord, type, natoms, box, mesh, davg, dstd, rcut_a, rcut_r,
                                         rcut_r_smth, sel_a, sel_r, name=None)
```

Compute the environment matrix mixing the atom types.

The sorting of neighbor atoms depends not on atom types, but on the distance and index. The atoms in nlist matrix will gather forward and thus save space for gaps of types in ProdEnvMatA, resulting in optimized and relative small sel_a.

The additional outputs are listed as following:

Parameters

- **coord** – A Tensor. Must be one of the following types: float32, float64.
- **type** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **box** – A Tensor. Must have the same type as coord.
- **mesh** – A Tensor of type int32.
- **davg** – A Tensor. Must have the same type as coord.
- **dstd** – A Tensor. Must have the same type as coord.
- **rcut_a** – A float.
- **rcut_r** – A float.
- **rcut_r_smth** – A float.
- **sel_a** – A list of ints.
- **sel_r** – A list of ints.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (descript, descript_deriv, rij, nlist, ntype, nmask).

descript: A Tensor. Has the same type as coord. descript_deriv: A Tensor. Has the same type as coord. rij: A Tensor. Has the same type as coord. nlist: A Tensor of type int32. ntype: A Tensor of type int32. The corresponding atom types in nlist. nmask: A Tensor of type bool. The atom mask in nlist.

```
deepmd.env.op_module.prod_env_mat_a_mix_nvnmnd_quantize(coord, type, natoms, box, mesh, davg,
                                                         dstd, rcut_a, rcut_r, rcut_r_smth, sel_a,
                                                         sel_r, name=None)
```

TODO: add doc.

Parameters

- **coord** – A Tensor. Must be one of the following types: float32, float64.
- **type** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **box** – A Tensor. Must have the same type as coord.
- **mesh** – A Tensor of type int32.
- **davg** – A Tensor. Must have the same type as coord.
- **dstd** – A Tensor. Must have the same type as coord.

- **rcut_a** – A float.
- **rcut_r** – A float.
- **rcut_r_smth** – A float.
- **sel_a** – A list of ints.
- **sel_r** – A list of ints.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (descrpt, descrpt_deriv, rij, nlist, ntype, nmask).

descrpt: A Tensor. Has the same type as coord. descrpt_deriv: A Tensor. Has the same type as coord. rij: A Tensor. Has the same type as coord. nlist: A Tensor of type int32. ntype: A Tensor of type int32. nmask: A Tensor of type bool.

```
deepmd.env.op_module.prod_env_mat_a_nvnmmd_quantize(coord, type, natoms, box, mesh, davg, dstd,
                                                    rcut_a, rcut_r, rcut_r_smth, sel_a, sel_r,
                                                    name=None)
```

TODO: add doc.

Parameters

- **coord** – A Tensor. Must be one of the following types: float32, float64.
- **type** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **box** – A Tensor. Must have the same type as coord.
- **mesh** – A Tensor of type int32.
- **davg** – A Tensor. Must have the same type as coord.
- **dstd** – A Tensor. Must have the same type as coord.
- **rcut_a** – A float.
- **rcut_r** – A float.
- **rcut_r_smth** – A float.
- **sel_a** – A list of ints.
- **sel_r** – A list of ints.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (descrpt, descrpt_deriv, rij, nlist).

descrpt: A Tensor. Has the same type as coord. descrpt_deriv: A Tensor. Has the same type as coord. rij: A Tensor. Has the same type as coord. nlist: A Tensor of type int32.

```
deepmd.env.op_module.prod_env_mat_r(coord, type, natoms, box, mesh, davg, dstd, rcut, rcut_smth, sel,
                                     name=None)
```

TODO: add doc.

Parameters

- **coord** – A Tensor. Must be one of the following types: float32, float64.

- **type** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **box** – A Tensor. Must have the same type as coord.
- **mesh** – A Tensor of type int32.
- **davg** – A Tensor. Must have the same type as coord.
- **dstd** – A Tensor. Must have the same type as coord.
- **rcut** – A float.
- **rcut_smth** – A float.
- **sel** – A list of ints.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (descrpt, descrpt_deriv, rij, nlist).

descrpt: A Tensor. Has the same type as coord. descrpt_deriv: A Tensor. Has the same type as coord. rij: A Tensor. Has the same type as coord. nlist: A Tensor of type int32.

```
deepmd.env.op_module.prod_force(net_deriv, in_deriv, nlist, axis, natoms, n_a_sel, n_r_sel,
                                name=None)
```

TODO: add doc.

Parameters

- **net_deriv** – A Tensor. Must be one of the following types: float32, float64.
- **in_deriv** – A Tensor. Must have the same type as net_deriv.
- **nlist** – A Tensor of type int32.
- **axis** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **n_a_sel** – An int.
- **n_r_sel** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as net_deriv.

```
deepmd.env.op_module.prod_force_norot(net_deriv, in_deriv, nlist, natoms, n_a_sel, n_r_sel,
                                       name=None)
```

TODO: add doc.

Parameters

- **net_deriv** – A Tensor. Must be one of the following types: float32, float64.
- **in_deriv** – A Tensor. Must have the same type as net_deriv.
- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **n_a_sel** – An int.
- **n_r_sel** – An int.

- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as `net_deriv`.

```
deepmd.env.op_module.prod_force_se_a(net_deriv, in_deriv, nlist, natoms, n_a_sel, n_r_sel,  
                                     name=None)
```

TODO: add doc.

Parameters

- **net_deriv** – A Tensor. Must be one of the following types: float32, float64.
- **in_deriv** – A Tensor. Must have the same type as `net_deriv`.
- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **n_a_sel** – An int.
- **n_r_sel** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as `net_deriv`.

```
deepmd.env.op_module.prod_force_se_a_mask(net_deriv, in_deriv, mask, nlist, total_atom_num,  
                                           name=None)
```

TODO: add doc.

Parameters

- **net_deriv** – A Tensor. Must be one of the following types: float32, float64.
- **in_deriv** – A Tensor. Must have the same type as `net_deriv`.
- **mask** – A Tensor of type int32.
- **nlist** – A Tensor of type int32.
- **total_atom_num** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as `net_deriv`.

```
deepmd.env.op_module.prod_force_se_r(net_deriv, in_deriv, nlist, natoms, name=None)
```

TODO: add doc.

Parameters

- **net_deriv** – A Tensor. Must be one of the following types: float32, float64.
- **in_deriv** – A Tensor. Must have the same type as `net_deriv`.
- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as `net_deriv`.

```
deepmd.env.op_module.prod_virial(net_deriv, in_deriv, rij, nlist, axis, natoms, n_a_sel, n_r_sel,
                                name=None)
```

TODO: add doc.

Parameters

- **net_deriv** – A Tensor. Must be one of the following types: float32, float64.
- **in_deriv** – A Tensor. Must have the same type as net_deriv.
- **rij** – A Tensor. Must have the same type as net_deriv.
- **nlist** – A Tensor of type int32.
- **axis** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **n_a_sel** – An int.
- **n_r_sel** – An int.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (virial, atom_virial).

virial: A Tensor. Has the same type as net_deriv. atom_virial: A Tensor. Has the same type as net_deriv.

```
deepmd.env.op_module.prod_virial_norot(net_deriv, in_deriv, rij, nlist, natoms, n_a_sel, n_r_sel,
                                       name=None)
```

TODO: add doc.

Parameters

- **net_deriv** – A Tensor. Must be one of the following types: float32, float64.
- **in_deriv** – A Tensor. Must have the same type as net_deriv.
- **rij** – A Tensor. Must have the same type as net_deriv.
- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **n_a_sel** – An int.
- **n_r_sel** – An int.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (virial, atom_virial).

virial: A Tensor. Has the same type as net_deriv. atom_virial: A Tensor. Has the same type as net_deriv.

```
deepmd.env.op_module.prod_virial_se_a(net_deriv, in_deriv, rij, nlist, natoms, n_a_sel, n_r_sel,
                                       name=None)
```

TODO: add doc.

Parameters

- **net_deriv** – A Tensor. Must be one of the following types: float32, float64.

- **in_deriv** – A Tensor. Must have the same type as `net_deriv`.
- **rij** – A Tensor. Must have the same type as `net_deriv`.
- **nlist** – A Tensor of type `int32`.
- **natoms** – A Tensor of type `int32`.
- **n_a_sel** – An int.
- **n_r_sel** – An int.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (`virial`, `atom_virial`).

`virial`: A Tensor. Has the same type as `net_deriv`. `atom_virial`: A Tensor. Has the same type as `net_deriv`.

`deepmd.env.op_module.prod_virial_se_r(net_deriv, in_deriv, rij, nlist, natoms, name=None)`

TODO: add doc.

Parameters

- **net_deriv** – A Tensor. Must be one of the following types: `float32`, `float64`.
- **in_deriv** – A Tensor. Must have the same type as `net_deriv`.
- **rij** – A Tensor. Must have the same type as `net_deriv`.
- **nlist** – A Tensor of type `int32`.
- **natoms** – A Tensor of type `int32`.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (`virial`, `atom_virial`).

`virial`: A Tensor. Has the same type as `net_deriv`. `atom_virial`: A Tensor. Has the same type as `net_deriv`.

`deepmd.env.op_module.quantize_nvnm(x, isround, nbit1, nbit2, nbit3, name=None)`

TODO: add doc.

Parameters

- **x** – A Tensor. Must be one of the following types: `float32`, `float64`.
- **isround** – An int.
- **nbit1** – An int.
- **nbit2** – An int.
- **nbit3** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as `x`.

`deepmd.env.op_module.soft_min_force(du, sw_deriv, nlist, natoms, n_a_sel, n_r_sel, name=None)`

TODO: add doc.

Parameters

- **du** – A Tensor. Must be one of the following types: float32, float64.
- **sw_deriv** – A Tensor. Must have the same type as du.
- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **n_a_sel** – An int.
- **n_r_sel** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as du.

`deepmd.env.op_module.soft_min_switch(type, rij, nlist, natoms, sel_a, sel_r, alpha, rmin, rmax, name=None)`

TODO: add doc.

Parameters

- **type** – A Tensor of type int32.
- **rij** – A Tensor. Must be one of the following types: float32, float64.
- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **sel_a** – A list of ints.
- **sel_r** – A list of ints.
- **alpha** – A float.
- **rmin** – A float.
- **rmax** – A float.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (sw_value, sw_deriv).

sw_value: A Tensor. Has the same type as rij. sw_deriv: A Tensor. Has the same type as rij.

`deepmd.env.op_module.soft_min_virial(du, sw_deriv, rij, nlist, natoms, n_a_sel, n_r_sel, name=None)`

TODO: add doc.

Parameters

- **du** – A Tensor. Must be one of the following types: float32, float64.
- **sw_deriv** – A Tensor. Must have the same type as du.
- **rij** – A Tensor. Must have the same type as du.
- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.

- **n_a_sel** – An int.
- **n_r_sel** – An int.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (virial, atom_virial).

virial: A Tensor. Has the same type as du. atom_virial: A Tensor. Has the same type as du.

`deepmd.env.op_module.tabulate_fusion(table, table_info, em_x, em, last_layer_size, name=None)`

TODO: add doc.

Parameters

- **table** – A Tensor. Must be one of the following types: float32, float64.
- **table_info** – A Tensor. Must have the same type as table.
- **em_x** – A Tensor. Must have the same type as table.
- **em** – A Tensor. Must have the same type as table.
- **last_layer_size** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as table.

`deepmd.env.op_module.tabulate_fusion_grad(table, table_info, em_x, em, dy, descriptor, name=None)`

TODO: add doc.

Parameters

- **table** – A Tensor. Must be one of the following types: float32, float64.
- **table_info** – A Tensor. Must have the same type as table.
- **em_x** – A Tensor. Must have the same type as table.
- **em** – A Tensor. Must have the same type as table.
- **dy** – A Tensor. Must have the same type as table.
- **descriptor** – A Tensor. Must have the same type as table.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (dy_dem_x, dy_dem).

dy_dem_x: A Tensor. Has the same type as table. dy_dem: A Tensor. Has the same type as table.

`deepmd.env.op_module.tabulate_fusion_grad_grad(table, table_info, em_x, em, dz_dy_dem_x, dz_dy_dem, descriptor, name=None)`

TODO: add doc.

Parameters

- **table** – A Tensor. Must be one of the following types: float32, float64.
- **table_info** – A Tensor. Must have the same type as table.

- **em_x** – A Tensor. Must have the same type as table.
- **em** – A Tensor. Must have the same type as table.
- **dz_dy_dem_x** – A Tensor. Must have the same type as table.
- **dz_dy_dem** – A Tensor. Must have the same type as table.
- **descriptor** – A Tensor. Must have the same type as table.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as table.

```
deepmd.env.op_module.tabulate_fusion_se_a(table, table_info, em_x, em, last_layer_size,
                                           name=None)
```

TODO: add doc.

Parameters

- **table** – A Tensor. Must be one of the following types: float32, float64.
- **table_info** – A Tensor. Must have the same type as table.
- **em_x** – A Tensor. Must have the same type as table.
- **em** – A Tensor. Must have the same type as table.
- **last_layer_size** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as table.

```
deepmd.env.op_module.tabulate_fusion_se_a_grad(table, table_info, em_x, em, dy, descriptor,
                                                name=None)
```

TODO: add doc.

Parameters

- **table** – A Tensor. Must be one of the following types: float32, float64.
- **table_info** – A Tensor. Must have the same type as table.
- **em_x** – A Tensor. Must have the same type as table.
- **em** – A Tensor. Must have the same type as table.
- **dy** – A Tensor. Must have the same type as table.
- **descriptor** – A Tensor. Must have the same type as table.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (dy_dem_x, dy_dem).

dy_dem_x: A Tensor. Has the same type as table. dy_dem: A Tensor. Has the same type as table.

```
deepmd.env.op_module.tabulate_fusion_se_a_grad_grad(table, table_info, em_x, em, dz_dy_dem_x,
                                                    dz_dy_dem, descriptor, is_sorted=True,
                                                    name=None)
```

TODO: add doc.

Parameters

- **table** – A Tensor. Must be one of the following types: float32, float64.
- **table_info** – A Tensor. Must have the same type as table.
- **em_x** – A Tensor. Must have the same type as table.
- **em** – A Tensor. Must have the same type as table.
- **dz_dy_dem_x** – A Tensor. Must have the same type as table.
- **dz_dy_dem** – A Tensor. Must have the same type as table.
- **descriptor** – A Tensor. Must have the same type as table.
- **is_sorted** – An optional bool. Defaults to True.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as table.

```
deepmd.env.op_module.tabulate_fusion_se_atten(table, table_info, em_x, em, two_embed,  
                                              last_layer_size, is_sorted=True, name=None)
```

TODO: add doc.

Parameters

- **table** – A Tensor. Must be one of the following types: float32, float64.
- **table_info** – A Tensor. Must have the same type as table.
- **em_x** – A Tensor. Must have the same type as table.
- **em** – A Tensor. Must have the same type as table.
- **two_embed** – A Tensor. Must have the same type as table.
- **last_layer_size** – An int.
- **is_sorted** – An optional bool. Defaults to True.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as table.

```
deepmd.env.op_module.tabulate_fusion_se_atten_grad(table, table_info, em_x, em, two_embed, dy,  
                                                  descriptor, is_sorted=True, name=None)
```

TODO: add doc.

Parameters

- **table** – A Tensor. Must be one of the following types: float32, float64.
- **table_info** – A Tensor. Must have the same type as table.
- **em_x** – A Tensor. Must have the same type as table.
- **em** – A Tensor. Must have the same type as table.
- **two_embed** – A Tensor. Must have the same type as table.
- **dy** – A Tensor. Must have the same type as table.
- **descriptor** – A Tensor. Must have the same type as table.
- **is_sorted** – An optional bool. Defaults to True.

- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (dy_dem_x, dy_dem, dy_dtwo).

dy_dem_x: A Tensor. Has the same type as table. dy_dem: A Tensor. Has the same type as table. dy_dtwo: A Tensor. Has the same type as table.

`deepmd.env.op_module.tabulate_fusion_se_r(table, table_info, em, last_layer_size, name=None)`

TODO: add doc.

Parameters

- **table** – A Tensor. Must be one of the following types: float32, float64.
- **table_info** – A Tensor. Must have the same type as table.
- **em** – A Tensor. Must have the same type as table.
- **last_layer_size** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as table.

`deepmd.env.op_module.tabulate_fusion_se_r_grad(table, table_info, em, dy, descriptor, name=None)`

TODO: add doc.

Parameters

- **table** – A Tensor. Must be one of the following types: float32, float64.
- **table_info** – A Tensor. Must have the same type as table.
- **em** – A Tensor. Must have the same type as table.
- **dy** – A Tensor. Must have the same type as table.
- **descriptor** – A Tensor. Must have the same type as table.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as table.

`deepmd.env.op_module.tabulate_fusion_se_r_grad_grad(table, table_info, em, dz_dy_dem, descriptor, name=None)`

TODO: add doc.

Parameters

- **table** – A Tensor. Must be one of the following types: float32, float64.
- **table_info** – A Tensor. Must have the same type as table.
- **em** – A Tensor. Must have the same type as table.
- **dz_dy_dem** – A Tensor. Must have the same type as table.
- **descriptor** – A Tensor. Must have the same type as table.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as table.

```
deepmd.env.op_module.tabulate_fusion_se_t(table, table_info, em_x, em, last_layer_size,
                                           name=None)
```

TODO: add doc.

Parameters

- **table** – A Tensor. Must be one of the following types: float32, float64.
- **table_info** – A Tensor. Must have the same type as table.
- **em_x** – A Tensor. Must have the same type as table.
- **em** – A Tensor. Must have the same type as table.
- **last_layer_size** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as table.

```
deepmd.env.op_module.tabulate_fusion_se_t_grad(table, table_info, em_x, em, dy, descriptor,
                                              name=None)
```

TODO: add doc.

Parameters

- **table** – A Tensor. Must be one of the following types: float32, float64.
- **table_info** – A Tensor. Must have the same type as table.
- **em_x** – A Tensor. Must have the same type as table.
- **em** – A Tensor. Must have the same type as table.
- **dy** – A Tensor. Must have the same type as table.
- **descriptor** – A Tensor. Must have the same type as table.
- **name** – A name for the operation (optional).

Returns

A tuple of Tensor objects (dy_dem_x, dy_dem).

dy_dem_x: A Tensor. Has the same type as table. dy_dem: A Tensor. Has the same type as table.

```
deepmd.env.op_module.tabulate_fusion_se_t_grad_grad(table, table_info, em_x, em, dz_dy_dem_x,
                                                    dz_dy_dem, descriptor, name=None)
```

TODO: add doc.

Parameters

- **table** – A Tensor. Must be one of the following types: float32, float64.
- **table_info** – A Tensor. Must have the same type as table.
- **em_x** – A Tensor. Must have the same type as table.
- **em** – A Tensor. Must have the same type as table.
- **dz_dy_dem_x** – A Tensor. Must have the same type as table.
- **dz_dy_dem** – A Tensor. Must have the same type as table.
- **descriptor** – A Tensor. Must have the same type as table.

- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as table.

`deepmd.env.op_module.tanh4_flt_nvnmmd(x, name=None)`

TODO: add doc.

Parameters

- **x** – A Tensor. Must be one of the following types: float32, float64.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as x.

`deepmd.env.op_module.unaggregated_dy2_dx(z, w, dy_dx, dy2_dx, ybar, functype, name=None)`

TODO: add doc.

Parameters

- **z** – A Tensor. Must be one of the following types: float32, float64.
- **w** – A Tensor. Must have the same type as z.
- **dy_dx** – A Tensor. Must have the same type as z.
- **dy2_dx** – A Tensor. Must have the same type as z.
- **ybar** – A Tensor. Must have the same type as z.
- **functype** – A Tensor of type int32.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as z.

`deepmd.env.op_module.unaggregated_dy2_dx_s(y, dy, w, xbar, functype, name=None)`

TODO: add doc.

Parameters

- **y** – A Tensor. Must be one of the following types: float32, float64.
- **dy** – A Tensor. Must have the same type as y.
- **w** – A Tensor. Must have the same type as y.
- **xbar** – A Tensor. Must have the same type as y.
- **functype** – A Tensor of type int32.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as y.

`deepmd.env.op_module.unaggregated_dy_dx(z, w, dy_dx, ybar, functype, name=None)`

TODO: add doc.

Parameters

- **z** – A Tensor. Must be one of the following types: float32, float64.
- **w** – A Tensor. Must have the same type as z.

- **dy_dx** – A Tensor. Must have the same type as z.
- **ybar** – A Tensor. Must have the same type as z.
- **functype** – A Tensor of type int32.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as z.

`deepmd.env.op_module.unaggregated_dy_dx_s(y, w, xbar, functype, name=None)`

TODO: add doc.

Parameters

- **y** – A Tensor. Must be one of the following types: float32, float64.
- **w** – A Tensor. Must have the same type as y.
- **xbar** – A Tensor. Must have the same type as y.
- **functype** – A Tensor of type int32.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as y.

18.2 op_grads_module

Python wrappers around TensorFlow ops.

This file is MACHINE GENERATED! Do not edit.

`deepmd.env.op_grads_module.ProdForceGrad(grad, net_deriv, in_deriv, nlist, axis, natoms, n_a_sel, n_r_sel, name=None)`

TODO: add doc.

Parameters

- **grad** – A Tensor. Must be one of the following types: float32, float64.
- **net_deriv** – A Tensor. Must have the same type as grad.
- **in_deriv** – A Tensor. Must have the same type as grad.
- **nlist** – A Tensor of type int32.
- **axis** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **n_a_sel** – An int.
- **n_r_sel** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as grad.


```
deepmd.env.op_grads_module.ProdForceSeAGrad(grad, net_deriv, in_deriv, nlist, natoms, n_a_sel,
                                             n_r_sel, name=None)
```

TODO: add doc.

Parameters

- **grad** – A Tensor. Must be one of the following types: float32, float64.
- **net_deriv** – A Tensor. Must have the same type as grad.
- **in_deriv** – A Tensor. Must have the same type as grad.
- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **n_a_sel** – An int.
- **n_r_sel** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as grad.

```
deepmd.env.op_grads_module.ProdForceSeAMaskGrad(grad, net_deriv, in_deriv, mask, nlist,
                                                  total_atom_num, name=None)
```

TODO: add doc.

Parameters

- **grad** – A Tensor. Must be one of the following types: float32, float64.
- **net_deriv** – A Tensor. Must have the same type as grad.
- **in_deriv** – A Tensor. Must have the same type as grad.
- **mask** – A Tensor of type int32.
- **nlist** – A Tensor of type int32.
- **total_atom_num** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as grad.

```
deepmd.env.op_grads_module.ProdForceSeRGrad(grad, net_deriv, in_deriv, nlist, natoms, name=None)
```

TODO: add doc.

Parameters

- **grad** – A Tensor. Must be one of the following types: float32, float64.
- **net_deriv** – A Tensor. Must have the same type as grad.
- **in_deriv** – A Tensor. Must have the same type as grad.
- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as grad.

```
deepmd.env.op_grads_module.ProdVirialGrad(grad, net_deriv, in_deriv, rij, nlist, axis, natoms, n_a_sel,
                                           n_r_sel, name=None)
```

TODO: add doc.

Parameters

- **grad** – A Tensor. Must be one of the following types: float32, float64.
- **net_deriv** – A Tensor. Must have the same type as grad.
- **in_deriv** – A Tensor. Must have the same type as grad.
- **rij** – A Tensor. Must have the same type as grad.
- **nlist** – A Tensor of type int32.
- **axis** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **n_a_sel** – An int.
- **n_r_sel** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as grad.

```
deepmd.env.op_grads_module.ProdVirialSeAGrad(grad, net_deriv, in_deriv, rij, nlist, natoms, n_a_sel,
                                              n_r_sel, name=None)
```

TODO: add doc.

Parameters

- **grad** – A Tensor. Must be one of the following types: float32, float64.
- **net_deriv** – A Tensor. Must have the same type as grad.
- **in_deriv** – A Tensor. Must have the same type as grad.
- **rij** – A Tensor. Must have the same type as grad.
- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **n_a_sel** – An int.
- **n_r_sel** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as grad.

```
deepmd.env.op_grads_module.ProdVirialSeRGrad(grad, net_deriv, in_deriv, rij, nlist, natoms,
                                              name=None)
```

TODO: add doc.

Parameters

- **grad** – A Tensor. Must be one of the following types: float32, float64.
- **net_deriv** – A Tensor. Must have the same type as grad.
- **in_deriv** – A Tensor. Must have the same type as grad.

- **rij** – A Tensor. Must have the same type as **grad**.
- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as **grad**.

```
deepmd.env.op_grads_module.SoftMinForceGrad(grad, du, sw_deriv, nlist, natoms, n_a_sel, n_r_sel,
                                             name=None)
```

TODO: add doc.

Parameters

- **grad** – A Tensor. Must be one of the following types: float32, float64.
- **du** – A Tensor. Must have the same type as **grad**.
- **sw_deriv** – A Tensor. Must have the same type as **grad**.
- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **n_a_sel** – An int.
- **n_r_sel** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as **grad**.

```
deepmd.env.op_grads_module.SoftMinVirialGrad(grad, du, sw_deriv, rij, nlist, natoms, n_a_sel, n_r_sel,
                                              name=None)
```

TODO: add doc.

Parameters

- **grad** – A Tensor. Must be one of the following types: float32, float64.
- **du** – A Tensor. Must have the same type as **grad**.
- **sw_deriv** – A Tensor. Must have the same type as **grad**.
- **rij** – A Tensor. Must have the same type as **grad**.
- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **n_a_sel** – An int.
- **n_r_sel** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as **grad**.

```
deepmd.env.op_grads_module.prod_force_grad(grad, net_deriv, in_deriv, nlist, axis, natoms, n_a_sel,
                                             n_r_sel, name=None)
```

TODO: add doc.

Parameters

- **grad** – A Tensor. Must be one of the following types: float32, float64.
- **net_deriv** – A Tensor. Must have the same type as grad.
- **in_deriv** – A Tensor. Must have the same type as grad.
- **nlist** – A Tensor of type int32.
- **axis** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **n_a_sel** – An int.
- **n_r_sel** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as grad.

```
deepmd.env.op_grads_module.prod_force_se_a_grad(grad, net_deriv, in_deriv, nlist, natoms, n_a_sel,  
                                                n_r_sel, name=None)
```

TODO: add doc.

Parameters

- **grad** – A Tensor. Must be one of the following types: float32, float64.
- **net_deriv** – A Tensor. Must have the same type as grad.
- **in_deriv** – A Tensor. Must have the same type as grad.
- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **n_a_sel** – An int.
- **n_r_sel** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as grad.

```
deepmd.env.op_grads_module.prod_force_se_a_mask_grad(grad, net_deriv, in_deriv, mask, nlist,  
                                                    total_atom_num, name=None)
```

TODO: add doc.

Parameters

- **grad** – A Tensor. Must be one of the following types: float32, float64.
- **net_deriv** – A Tensor. Must have the same type as grad.
- **in_deriv** – A Tensor. Must have the same type as grad.
- **mask** – A Tensor of type int32.
- **nlist** – A Tensor of type int32.
- **total_atom_num** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as grad.

```
deepmd.env.op_grads_module.prod_force_se_r_grad(grad, net_deriv, in_deriv, nlist, natoms,
                                                name=None)
```

TODO: add doc.

Parameters

- **grad** – A Tensor. Must be one of the following types: float32, float64.
- **net_deriv** – A Tensor. Must have the same type as grad.
- **in_deriv** – A Tensor. Must have the same type as grad.
- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as grad.

```
deepmd.env.op_grads_module.prod_virial_grad(grad, net_deriv, in_deriv, rij, nlist, axis, natoms,
                                             n_a_sel, n_r_sel, name=None)
```

TODO: add doc.

Parameters

- **grad** – A Tensor. Must be one of the following types: float32, float64.
- **net_deriv** – A Tensor. Must have the same type as grad.
- **in_deriv** – A Tensor. Must have the same type as grad.
- **rij** – A Tensor. Must have the same type as grad.
- **nlist** – A Tensor of type int32.
- **axis** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **n_a_sel** – An int.
- **n_r_sel** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as grad.

```
deepmd.env.op_grads_module.prod_virial_se_a_grad(grad, net_deriv, in_deriv, rij, nlist, natoms,
                                                  n_a_sel, n_r_sel, name=None)
```

TODO: add doc.

Parameters

- **grad** – A Tensor. Must be one of the following types: float32, float64.
- **net_deriv** – A Tensor. Must have the same type as grad.
- **in_deriv** – A Tensor. Must have the same type as grad.
- **rij** – A Tensor. Must have the same type as grad.

- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **n_a_sel** – An int.
- **n_r_sel** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as grad.

```
deepmd.env.op_grads_module.prod_virial_se_r_grad(grad, net_deriv, in_deriv, rij, nlist, natoms,  
                                                name=None)
```

TODO: add doc.

Parameters

- **grad** – A Tensor. Must be one of the following types: float32, float64.
- **net_deriv** – A Tensor. Must have the same type as grad.
- **in_deriv** – A Tensor. Must have the same type as grad.
- **rij** – A Tensor. Must have the same type as grad.
- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as grad.

```
deepmd.env.op_grads_module.soft_min_force_grad(grad, du, sw_deriv, nlist, natoms, n_a_sel, n_r_sel,  
                                                name=None)
```

TODO: add doc.

Parameters

- **grad** – A Tensor. Must be one of the following types: float32, float64.
- **du** – A Tensor. Must have the same type as grad.
- **sw_deriv** – A Tensor. Must have the same type as grad.
- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **n_a_sel** – An int.
- **n_r_sel** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as grad.

```
deepmd.env.op_grads_module.soft_min_virial_grad(grad, du, sw_deriv, rij, nlist, natoms, n_a_sel,  
                                                n_r_sel, name=None)
```

TODO: add doc.

Parameters

- **grad** – A Tensor. Must be one of the following types: float32, float64.
- **du** – A Tensor. Must have the same type as grad.
- **sw_deriv** – A Tensor. Must have the same type as grad.
- **rij** – A Tensor. Must have the same type as grad.
- **nlist** – A Tensor of type int32.
- **natoms** – A Tensor of type int32.
- **n_a_sel** – An int.
- **n_r_sel** – An int.
- **name** – A name for the operation (optional).

Returns

A Tensor. Has the same type as grad.

19.1 Class Hierarchy

- Namespace deepmd
 - Struct deepmd_exception
 - Struct NeighborListData
 - Struct tf_exception
 - Class AtomMap
 - Class DeepPot
 - Class DeepPotModelDevi
 - Class DeepTensor
 - Class DipoleChargeModifier

19.2 File Hierarchy

- dir_source
 - dir_source_api_cc
 - *dir_source_api_cc_include
 - file_source_api_cc_include_AtomMap.h
 - file_source_api_cc_include_common.h
 - file_source_api_cc_include_DataModifier.h
 - file_source_api_cc_include_DeepPot.h
 - file_source_api_cc_include_DeepTensor.h
 - file_source_api_cc_include_tf_private.h
 - file_source_api_cc_include_tf_public.h

19.3 Full API

19.3.1 Namespaces

Namespace deepmd

Contents

- Classes
- Functions
- Typedefs

Classes

- Struct deepmd_exception
- Struct NeighborListData
- Struct tf_exception
- Class AtomMap
- Class DeepPot
- Class DeepPotModelDevi
- Class DeepTensor
- Class DipoleChargeModifier

Functions

- Function deepmd::check_status
- Function deepmd::convert_pbtxt_to_pb
- Function deepmd::get_env_nthreads
- Function deepmd::load_op_library
- Function deepmd::model_compatible
- Function deepmd::name_prefix
- Function deepmd::print_summary
- Function deepmd::read_file_to_string
- Template Function deepmd::select_by_type
- Template Function deepmd::select_map(std::vector<VT>&, const std::vector<VT>&, const std::vector<int>&, const int&, const int&, const int&, const int&)
- Template Function deepmd::select_map(typename std::vector<VT>::iterator, const typename std::vector<VT>::const_iterator, const std::vector<int>&, const int&, const int&, const int&, const int&)

- Template Function `deepmd::select_map_inv(std::vector<VT>&, const std::vector<VT>&, const std::vector<int>&, const int&)`
- Template Function `deepmd::select_map_inv(typename std::vector<VT>::iterator, const typename std::vector<VT>::const_iterator, const std::vector<int>&, const int&)`
- Template Function `deepmd::select_real_atoms`
- Template Function `deepmd::select_real_atoms_coord`
- Function `deepmd::session_get_dtype`
- Template Function `deepmd::session_get_scalar`
- Template Function `deepmd::session_get_vector`
- Template Function `deepmd::session_input_tensors(std::vector<std::pair<std::string, tensorflow::Tensor>>&, const std::vector<VALUETYPE>&, const int&, const std::vector<int>&, const std::vector<VALUETYPE>&, const double&, const std::vector<VALUETYPE>&, const std::vector<VALUETYPE>&, const deepmd::AtomMap&, const std::string)`
- Template Function `deepmd::session_input_tensors(std::vector<std::pair<std::string, tensorflow::Tensor>>&, const std::vector<VALUETYPE>&, const int&, const std::vector<int>&, const std::vector<VALUETYPE>&, InputNlist&, const std::vector<VALUETYPE>&, const std::vector<VALUETYPE>&, const deepmd::AtomMap&, const int, const int, const std::string)`
- Template Function `deepmd::session_input_tensors_mixed_type`

Typedefs

- Typedef `deepmd::ENERGYTYPE`
- Typedef `deepmd::STRINGTYPE`

Namespace tensorflow

19.3.2 Classes and Structs

Struct `deepmd_exception`

- Defined in `file_source_api_cc_include_common.h`

Inheritance Relationships

Derived Type

- `public deepmd::tf_exception(Struct tf_exception)`

Struct Documentation

struct `deepmd_exception`

Subclassed by `deepmd::tf_exception`

Struct NeighborListData

- Defined in file `_source_api_cc_include_common.h`

Struct Documentation

struct `NeighborListData`

Public Functions

void `copy_from_nlist`(const `InputNlist` &inlist)

void `shuffle`(const std::vector<int> &fwd_map)

void `shuffle`(const deepmd::AtomMap &map)

void `shuffle_exclude_empty`(const std::vector<int> &fwd_map)

void `make_inlist`(`InputNlist` &inlist)

Public Members

std::vector<int> `ilist`

Array stores the core region atom's index.

std::vector<std::vector<int>> `jlist`

Array stores the core region atom's neighbor index.

std::vector<int> `numneigh`

Array stores the number of neighbors of core region atoms.

std::vector<int*> `firstneigh`

Array stores the the location of the first neighbor of core region atoms.

Struct `tf_exception`

- Defined in file `_source_api_cc_include_common.h`

Inheritance Relationships

Base Type

- `public deepmd_exception (Struct deepmd_exception)`

Struct Documentation

```
struct tf_exception : public deepmd_exception
    Throw exception if TensorFlow doesn't work.
```

Public Functions

```
inline tf_exception()
inline tf_exception(const std::string &msg)
```

Class `AtomMap`

- Defined in file `_source_api_cc_include_AtomMap.h`

Class Documentation

```
class AtomMap
```

Public Functions

```
AtomMap()

AtomMap(const std::vector<int>::const_iterator in_begin, const std::vector<int>::const_iterator
    in_end)

template<typename VALUETYPE>
void forward(typename std::vector<VALUETYPE>::iterator out, const typename
    std::vector<VALUETYPE>::const_iterator in, const int stride = 1, const int nframes =
    1, const int nall = 0) const

template<typename VALUETYPE>
void backward(typename std::vector<VALUETYPE>::iterator out, const typename
    std::vector<VALUETYPE>::const_iterator in, const int stride = 1, const int nframes
    = 1, const int nall = 0) const
```

```
inline const std::vector<int> &get_type() const  
inline const std::vector<int> &get_fwd_map() const  
inline const std::vector<int> &get_bkw_map() const
```

Class DeepPot

- Defined in file_source_api_cc_include_DeepPot.h

Class Documentation

class **DeepPot**

Deep Potential.

Public Functions

DeepPot()

DP constructor without initialization.

~DeepPot()

DeepPot(const std::string &model, const int &gpu_rank = 0, const std::string &file_content = "")

DP constructor with initialization.

Parameters

- **model** – [in] The name of the frozen model file.
- **gpu_rank** – [in] The GPU rank. Default is 0.
- **file_content** – [in] The content of the model file. If it is not empty, DP will read from the string instead of the file.

void **init**(const std::string &model, const int &gpu_rank = 0, const std::string &file_content = "")

Initialize the DP.

Parameters

- **model** – [in] The name of the frozen model file.
- **gpu_rank** – [in] The GPU rank. Default is 0.
- **file_content** – [in] The content of the model file. If it is not empty, DP will read from the string instead of the file.

void **print_summary**(const std::string &pre) const

Print the DP summary to the screen.

Parameters

- **pre** – [in] The prefix to each line.

template<typename **VALUETYPE**, typename **ENERGYVTYPE**>

```
void compute(ENERGYVTYPE &ener, std::vector<VALUETYPE> &force,
             std::vector<VALUETYPE> &virial, const std::vector<VALUETYPE> &coord, const
             std::vector<int> &atype, const std::vector<VALUETYPE> &box, const
             std::vector<VALUETYPE> &fparam = std::vector<VALUETYPE>(), const
             std::vector<VALUETYPE> &aparam = std::vector<VALUETYPE>())
```

Evaluate the energy, force and virial by using this DP.

Parameters

- **ener** – [out] The system energy.
- **force** – [out] The force on each atom.
- **virial** – [out] The virial.
- **coord** – [in] The coordinates of atoms. The array should be of size nframes x natoms x 3.
- **atype** – [in] The atom types. The list should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size nframes x 9.
- **fparam** – [in] The frame parameter. The array can be of size : nframes x dim_fparam. dim_fparam. Then all frames are assumed to be provided with the same fparam.
- **aparam** – [in] The atomic parameter The array can be of size : nframes x natoms x dim_aparam. natoms x dim_aparam. Then all frames are assumed to be provided with the same aparam.

```
template<typename VALUETYPE, typename ENERGYVTYPE>
void compute(ENERGYVTYPE &ener, std::vector<VALUETYPE> &force,
             std::vector<VALUETYPE> &virial, const std::vector<VALUETYPE> &coord, const
             std::vector<int> &atype, const std::vector<VALUETYPE> &box, const int nghost,
             const InputNlist &inlist, const int &ago, const std::vector<VALUETYPE> &fparam =
             std::vector<VALUETYPE>(), const std::vector<VALUETYPE> &aparam =
             std::vector<VALUETYPE>())
```

Evaluate the energy, force and virial by using this DP.

Parameters

- **ener** – [out] The system energy.
- **force** – [out] The force on each atom.
- **virial** – [out] The virial.
- **coord** – [in] The coordinates of atoms. The array should be of size nframes x natoms x 3.
- **atype** – [in] The atom types. The list should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size nframes x 9.
- **nghost** – [in] The number of ghost atoms.
- **inlist** – [in] The input neighbour list.
- **ago** – [in] Update the internal neighbour list if ago is 0.
- **fparam** – [in] The frame parameter. The array can be of size : nframes x dim_fparam. dim_fparam. Then all frames are assumed to be provided with the same fparam.

- **aparam** – [in] The atomic parameter The array can be of size : nframes x natoms x dim_aparam. natoms x dim_aparam. Then all frames are assumed to be provided with the same aparam.

```
template<typename VALUETYPE, typename ENERGYVTYPE>
void compute(ENERGYVTYPE &ener, std::vector<VALUETYPE> &force,
             std::vector<VALUETYPE> &virial, std::vector<VALUETYPE> &atom_energy,
             std::vector<VALUETYPE> &atom_virial, const std::vector<VALUETYPE> &coord,
             const std::vector<int> &atype, const std::vector<VALUETYPE> &box, const
             std::vector<VALUETYPE> &fparam = std::vector<VALUETYPE>(), const
             std::vector<VALUETYPE> &aparam = std::vector<VALUETYPE>())
```

Evaluate the energy, force, virial, atomic energy, and atomic virial by using this DP.

Parameters

- **ener** – [out] The system energy.
- **force** – [out] The force on each atom.
- **virial** – [out] The virial.
- **atom_energy** – [out] The atomic energy.
- **atom_virial** – [out] The atomic virial.
- **coord** – [in] The coordinates of atoms. The array should be of size nframes x natoms x 3.
- **atype** – [in] The atom types. The list should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size nframes x 9.
- **fparam** – [in] The frame parameter. The array can be of size : nframes x dim_fparam. dim_fparam. Then all frames are assumed to be provided with the same fparam.
- **aparam** – [in] The atomic parameter The array can be of size : nframes x natoms x dim_aparam. natoms x dim_aparam. Then all frames are assumed to be provided with the same aparam.

```
template<typename VALUETYPE, typename ENERGYVTYPE>
void compute(ENERGYVTYPE &ener, std::vector<VALUETYPE> &force,
             std::vector<VALUETYPE> &virial, std::vector<VALUETYPE> &atom_energy,
             std::vector<VALUETYPE> &atom_virial, const std::vector<VALUETYPE> &coord,
             const std::vector<int> &atype, const std::vector<VALUETYPE> &box, const int
             nghost, const InputNlist &imp_list, const int &ago, const std::vector<VALUETYPE>
             &fparam = std::vector<VALUETYPE>(), const std::vector<VALUETYPE>
             &aparam = std::vector<VALUETYPE>())
```

Evaluate the energy, force, virial, atomic energy, and atomic virial by using this DP.

Parameters

- **ener** – [out] The system energy.
- **force** – [out] The force on each atom.
- **virial** – [out] The virial.
- **atom_energy** – [out] The atomic energy.
- **atom_virial** – [out] The atomic virial.

- **coord** – [in] The coordinates of atoms. The array should be of size nframes x natoms x 3.
- **atype** – [in] The atom types. The list should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size nframes x 9.
- **nghost** – [in] The number of ghost atoms.
- **lmp_list** – [in] The input neighbour list.
- **ago** – [in] Update the internal neighbour list if ago is 0.
- **fparam** – [in] The frame parameter. The array can be of size : nframes x dim_fparam. dim_fparam. Then all frames are assumed to be provided with the same fparam.
- **aparam** – [in] The atomic parameter The array can be of size : nframes x natoms x dim_aparam. natoms x dim_aparam. Then all frames are assumed to be provided with the same aparam.

```
template<typename VALUETYPE, typename ENERGYVTYPE>
void compute_mixed_type(ENERGYVTYPE &ener, std::vector<VALUETYPE> &force,
                        std::vector<VALUETYPE> &virial, const int &nframes, const
                        std::vector<VALUETYPE> &coord, const std::vector<int> &atype,
                        const std::vector<VALUETYPE> &box, const
                        std::vector<VALUETYPE> &fparam = std::vector<VALUETYPE>(),
                        const std::vector<VALUETYPE> &aparam =
                        std::vector<VALUETYPE>())
```

Evaluate the energy, force, and virial with the mixed type by using this DP.

Parameters

- **ener** – [out] The system energy.
- **force** – [out] The force on each atom.
- **virial** – [out] The virial.
- **nframes** – [in] The number of frames.
- **coord** – [in] The coordinates of atoms. The array should be of size nframes x natoms x 3.
- **atype** – [in] The atom types. The array should be of size nframes x natoms.
- **box** – [in] The cell of the region. The array should be of size nframes x 9.
- **fparam** – [in] The frame parameter. The array can be of size : nframes x dim_fparam. dim_fparam. Then all frames are assumed to be provided with the same fparam.
- **aparam** – [in] The atomic parameter The array can be of size : nframes x natoms x dim_aparam. natoms x dim_aparam. Then all frames are assumed to be provided with the same aparam.

```
template<typename VALUETYPE, typename ENERGYVTYPE>
```

```
void compute_mixed_type(ENERGYVTYPE &ener, std::vector<VALUETYPE> &force,
    std::vector<VALUETYPE> &virial, std::vector<VALUETYPE>
    &atom_energy, std::vector<VALUETYPE> &atom_virial, const int
    &nframes, const std::vector<VALUETYPE> &coord, const
    std::vector<int> &atype, const std::vector<VALUETYPE> &box, const
    std::vector<VALUETYPE> &fparam = std::vector<VALUETYPE>(),
    const std::vector<VALUETYPE> &aparam =
    std::vector<VALUETYPE>())
```

Evaluate the energy, force, and virial with the mixed type by using this DP.

Parameters

- **ener** – [out] The system energy.
- **force** – [out] The force on each atom.
- **virial** – [out] The virial.
- **atom_energy** – [out] The atomic energy.
- **atom_virial** – [out] The atomic virial.
- **nframes** – [in] The number of frames.
- **coord** – [in] The coordinates of atoms. The array should be of size nframes x natoms x 3.
- **atype** – [in] The atom types. The array should be of size nframes x natoms.
- **box** – [in] The cell of the region. The array should be of size nframes x 9.
- **fparam** – [in] The frame parameter. The array can be of size : nframes x dim_fparam. dim_fparam. Then all frames are assumed to be provided with the same fparam.
- **aparam** – [in] The atomic parameter The array can be of size : nframes x natoms x dim_aparam. natoms x dim_aparam. Then all frames are assumed to be provided with the same aparam.

```
inline double cutoff() const
```

Get the cutoff radius.

Returns

The cutoff radius.

```
inline int numb_types() const
```

Get the number of types.

Returns

The number of types.

```
inline int numb_types_spin() const
```

Get the number of types with spin.

Returns

The number of types with spin.

```
inline int dim_fparam() const
```

Get the dimension of the frame parameter.

Returns

The dimension of the frame parameter.

```
inline int dim_aparam() const
    Get the dimension of the atomic parameter.

    Returns
        The dimension of the atomic parameter.

void get_type_map(std::string &type_map)
    Get the type map (element name of the atom types) of this model.

    Parameters
        type_map – [out] The type map of this model.
```

Class DeepPotModelDevi

- Defined in file_source_api_cc_include_DeepPot.h

Class Documentation

```
class DeepPotModelDevi
```

Public Functions

```
DeepPotModelDevi()
```

DP model deviation constructor without initialization.

```
~DeepPotModelDevi()
```

```
DeepPotModelDevi(const std::vector<std::string> &models, const int &gpu_rank = 0, const
                  std::vector<std::string> &file_contents = std::vector<std::string>())
```

DP model deviation constructor with initialization.

Parameters

- **models** – [in] The names of the frozen model files.
- **gpu_rank** – [in] The GPU rank. Default is 0.
- **file_contents** – [in] The contents of the model files. If it is not empty, DP will read from the strings instead of the files.

```
void init(const std::vector<std::string> &models, const int &gpu_rank = 0, const
          std::vector<std::string> &file_contents = std::vector<std::string>())
```

Initialize the DP model deviation contrcutor.

Parameters

- **models** – [in] The names of the frozen model files.
- **gpu_rank** – [in] The GPU rank. Default is 0.
- **file_contents** – [in] The contents of the model files. If it is not empty, DP will read from the strings instead of the files.

```
template<typename VALUETYPE>
```

```
void compute(std::vector<ENERGYTYPE> &all_ener, std::vector<std::vector<VALUETYPE>>
    &all_force, std::vector<std::vector<VALUETYPE>> &all_virial, const
    std::vector<VALUETYPE> &coord, const std::vector<int> &atype, const
    std::vector<VALUETYPE> &box, const int nghost, const InputNlist &imp_list, const
    int &ago, const std::vector<VALUETYPE> &fparam = std::vector<VALUETYPE>(),
    const std::vector<VALUETYPE> &aparam = std::vector<VALUETYPE>())
```

Evaluate the energy, force and virial by using these DP models.

Parameters

- **all_ener** – [out] The system energies of all models.
- **all_force** – [out] The forces on each atom of all models.
- **all_virial** – [out] The virials of all models.
- **coord** – [in] The coordinates of atoms. The array should be of size nframes x natoms x 3.
- **atype** – [in] The atom types. The list should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size nframes x 9.
- **nghost** – [in] The number of ghost atoms.
- **imp_list** – [in] The input neighbour list.
- **ago** – [in] Update the internal neighbour list if ago is 0.
- **fparam** – [in] The frame parameter. The array can be of size : nframes x dim_fparam. dim_fparam. Then all frames are assumed to be provided with the same fparam.
- **aparam** – [in] The atomic parameter The array can be of size : nframes x natoms x dim_aparam. natoms x dim_aparam. Then all frames are assumed to be provided with the same aparam. dim_aparam. Then all frames and atoms are provided with the same aparam.

```
template<typename VALUETYPE>
void compute(std::vector<ENERGYTYPE> &all_ener, std::vector<std::vector<VALUETYPE>>
    &all_force, std::vector<std::vector<VALUETYPE>> &all_virial,
    std::vector<std::vector<VALUETYPE>> &all_atom_energy,
    std::vector<std::vector<VALUETYPE>> &all_atom_virial, const
    std::vector<VALUETYPE> &coord, const std::vector<int> &atype, const
    std::vector<VALUETYPE> &box, const int nghost, const InputNlist &imp_list, const
    int &ago, const std::vector<VALUETYPE> &fparam = std::vector<VALUETYPE>(),
    const std::vector<VALUETYPE> &aparam = std::vector<VALUETYPE>())
```

Evaluate the energy, force, virial, atomic energy, and atomic virial by using these DP models.

Parameters

- **all_ener** – [out] The system energies of all models.
- **all_force** – [out] The forces on each atom of all models.
- **all_virial** – [out] The virials of all models.
- **all_atom_energy** – [out] The atomic energies of all models.
- **all_atom_virial** – [out] The atomic virials of all models.
- **coord** – [in] The coordinates of atoms. The array should be of size nframes x natoms x 3.

- **atype** – [in] The atom types. The list should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size nframes x 9.
- **nghost** – [in] The number of ghost atoms.
- **lmp_list** – [in] The input neighbour list.
- **ago** – [in] Update the internal neighbour list if ago is 0.
- **fparam** – [in] The frame parameter. The array can be of size : nframes x dim_fparam. dim_fparam. Then all frames are assumed to be provided with the same fparam.
- **aparam** – [in] The atomic parameter The array can be of size : nframes x natoms x dim_aparam. natoms x dim_aparam. Then all frames are assumed to be provided with the same aparam. dim_aparam. Then all frames and atoms are provided with the same aparam.

inline double **cutoff**() const

Get the cutoff radius.

Returns

The cutoff radius.

inline int **numb_types**() const

Get the number of types.

Returns

The number of types.

inline int **numb_types_spin**() const

Get the number of types with spin.

Returns

The number of types with spin.

inline int **dim_fparam**() const

Get the dimension of the frame parameter.

Returns

The dimension of the frame parameter.

inline int **dim_aparam**() const

Get the dimension of the atomic parameter.

Returns

The dimension of the atomic parameter.

template<typename **VALUETYPE**>

void **compute_avg**(**VALUETYPE** &dener, const std::vector<**VALUETYPE**> &all_energy)

Compute the average energy.

Parameters

- **dener** – [out] The average energy.
- **all_energy** – [in] The energies of all models.

template<typename **VALUETYPE**>

```
void compute_avg(std::vector<VALUETYPE> &avg, const
                std::vector<std::vector<VALUETYPE>> &xx)
```

Compute the average of vectors.

Parameters

- **avg** – [out] The average of vectors.
- **xx** – [in] The vectors of all models.

```
template<typename VALUETYPE>
void compute_std(std::vector<VALUETYPE> &std, const std::vector<VALUETYPE> &avg, const
                std::vector<std::vector<VALUETYPE>> &xx, const int &stride)
```

Compute the standard deviation of vectors.

Parameters

- **std** – [out] The standard deviation of vectors.
- **avg** – [in] The average of vectors.
- **xx** – [in] The vectors of all models.
- **stride** – [in] The stride to compute the deviation.

```
template<typename VALUETYPE>
void compute_relative_std(std::vector<VALUETYPE> &std, const std::vector<VALUETYPE>
                        &avg, const VALUETYPE eps, const int &stride)
```

Compute the relative standard deviation of vectors.

Parameters

- **std** – [out] The standard deviation of vectors.
- **avg** – [in] The average of vectors.
- **eps** – [in] The level parameter for computing the deviation.
- **stride** – [in] The stride to compute the deviation.

```
template<typename VALUETYPE>
void compute_std_e(std::vector<VALUETYPE> &std, const std::vector<VALUETYPE> &avg,
                  const std::vector<std::vector<VALUETYPE>> &xx)
```

Compute the standard deviation of atomic energies.

Parameters

- **std** – [out] The standard deviation of atomic energies.
- **avg** – [in] The average of atomic energies.
- **xx** – [in] The vectors of all atomic energies.

```
template<typename VALUETYPE>
void compute_std_f(std::vector<VALUETYPE> &std, const std::vector<VALUETYPE> &avg,
                  const std::vector<std::vector<VALUETYPE>> &xx)
```

Compute the standard deviation of forces.

Parameters

- **std** – [out] The standard deviation of forces.
- **avg** – [in] The average of forces.
- **xx** – [in] The vectors of all forces.

```
template<typename VALUETYPE>
void compute_relative_std_f(std::vector<VALUETYPE> &std, const std::vector<VALUETYPE>
                           &avg, const VALUETYPE eps)
```

Compute the relative standard deviation of forces.

Parameters

- **std** – [out] The relative standard deviation of forces.
- **avg** – [in] The relative average of forces.
- **eps** – [in] The level parameter for computing the deviation.

Class DeepTensor

- Defined in file `_source_api_cc_include_DeepTensor.h`

Class Documentation

class **DeepTensor**

Deep Tensor.

Public Functions

DeepTensor()

Deep Tensor constructor without initialization.

~DeepTensor()

DeepTensor(const std::string &model, const int &gpu_rank = 0, const std::string &name_scope = "")

Deep Tensor constructor with initialization..

Parameters

- **model** – [in] The name of the frozen model file.
- **gpu_rank** – [in] The GPU rank. Default is 0.
- **name_scope** – [in] Name scopes of operations.

void **init**(const std::string &model, const int &gpu_rank = 0, const std::string &name_scope = "")

Initialize the Deep Tensor.

Parameters

- **model** – [in] The name of the frozen model file.
- **gpu_rank** – [in] The GPU rank. Default is 0.
- **name_scope** – [in] Name scopes of operations.

void **print_summary**(const std::string &pre) const

Print the DP summary to the screen.

Parameters

- **pre** – [in] The prefix to each line.

```
template<typename VALUETYPE>
```

```
void compute(std::vector<VALUETYPE> &value, const std::vector<VALUETYPE> &coord, const
            std::vector<int> &atype, const std::vector<VALUETYPE> &box)
```

Evaluate the value by using this model.

Parameters

- **value** – [out] The value to evaluate, usually would be the atomic tensor.
- **coord** – [in] The coordinates of atoms. The array should be of size natoms x 3.
- **atype** – [in] The atom types. The list should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size 9.

```
template<typename VALUETYPE>
void compute(std::vector<VALUETYPE> &value, const std::vector<VALUETYPE> &coord, const
            std::vector<int> &atype, const std::vector<VALUETYPE> &box, const int nghost,
            const InputNlist &inlist)
```

Evaluate the value by using this model.

Parameters

- **value** – [out] The value to evaluate, usually would be the atomic tensor.
- **coord** – [in] The coordinates of atoms. The array should be of size natoms x 3.
- **atype** – [in] The atom types. The list should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size 9.
- **nghost** – [in] The number of ghost atoms.
- **inlist** – [in] The input neighbour list.

```
template<typename VALUETYPE>
void compute(std::vector<VALUETYPE> &global_tensor, std::vector<VALUETYPE> &force,
            std::vector<VALUETYPE> &virial, const std::vector<VALUETYPE> &coord, const
            std::vector<int> &atype, const std::vector<VALUETYPE> &box)
```

Evaluate the global tensor and component-wise force and virial.

Parameters

- **global_tensor** – [out] The global tensor to evaluate.
- **force** – [out] The component-wise force of the global tensor, size odim x natoms x 3.
- **virial** – [out] The component-wise virial of the global tensor, size odim x 9.
- **coord** – [in] The coordinates of atoms. The array should be of size natoms x 3.
- **atype** – [in] The atom types. The list should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size 9.

```
template<typename VALUETYPE>
void compute(std::vector<VALUETYPE> &global_tensor, std::vector<VALUETYPE> &force,
            std::vector<VALUETYPE> &virial, const std::vector<VALUETYPE> &coord, const
            std::vector<int> &atype, const std::vector<VALUETYPE> &box, const int nghost,
            const InputNlist &inlist)
```

Evaluate the global tensor and component-wise force and virial.

Parameters

- **global_tensor** – [out] The global tensor to evaluate.

- **force** – [out] The component-wise force of the global tensor, size odim x natoms x 3.
- **virial** – [out] The component-wise virial of the global tensor, size odim x 9.
- **coord** – [in] The coordinates of atoms. The array should be of size natoms x 3.
- **atype** – [in] The atom types. The list should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size 9.
- **nghost** – [in] The number of ghost atoms.
- **inlist** – [in] The input neighbour list.

```
template<typename VALUETYPE>
void compute(std::vector<VALUETYPE> &global_tensor, std::vector<VALUETYPE> &force,
             std::vector<VALUETYPE> &virial, std::vector<VALUETYPE> &atom_tensor,
             std::vector<VALUETYPE> &atom_virial, const std::vector<VALUETYPE> &coord,
             const std::vector<int> &atype, const std::vector<VALUETYPE> &box)
```

Evaluate the global tensor and component-wise force and virial.

Parameters

- **global_tensor** – [out] The global tensor to evaluate.
- **force** – [out] The component-wise force of the global tensor, size odim x natoms x 3.
- **virial** – [out] The component-wise virial of the global tensor, size odim x 9.
- **atom_tensor** – [out] The atomic tensor value of the model, size natoms x odim.
- **atom_virial** – [out] The component-wise atomic virial of the global tensor, size odim x natoms x 9.
- **coord** – [in] The coordinates of atoms. The array should be of size natoms x 3.
- **atype** – [in] The atom types. The list should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size 9.

```
template<typename VALUETYPE>
void compute(std::vector<VALUETYPE> &global_tensor, std::vector<VALUETYPE> &force,
             std::vector<VALUETYPE> &virial, std::vector<VALUETYPE> &atom_tensor,
             std::vector<VALUETYPE> &atom_virial, const std::vector<VALUETYPE> &coord,
             const std::vector<int> &atype, const std::vector<VALUETYPE> &box, const int
             nghost, const InputNlist &inlist)
```

Evaluate the global tensor and component-wise force and virial.

Parameters

- **global_tensor** – [out] The global tensor to evaluate.
- **force** – [out] The component-wise force of the global tensor, size odim x natoms x 3.
- **virial** – [out] The component-wise virial of the global tensor, size odim x 9.
- **atom_tensor** – [out] The atomic tensor value of the model, size natoms x odim.
- **atom_virial** – [out] The component-wise atomic virial of the global tensor, size odim x natoms x 9.
- **coord** – [in] The coordinates of atoms. The array should be of size natoms x 3.

- **atype** – [in] The atom types. The list should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size 9.
- **nghost** – [in] The number of ghost atoms.
- **inlist** – [in] The input neighbour list.

inline double **cutoff()** const

Get the cutoff radius.

Returns

The cutoff radius.

inline int **numb_types()** const

Get the number of types.

Returns

The number of types.

inline int **output_dim()** const

Get the output dimension.

Returns

The output dimension.

inline const std::vector<int> &**sel_types()** const

Get the list of sel types.

Returns

The list of sel types.

Class **DipoleChargeModifier**

- Defined in file_source_api_cc_include_DataModifier.h

Class Documentation

class **DipoleChargeModifier**

Dipole charge modifier.

Public Functions

DipoleChargeModifier()

Dipole charge modifier without initialization.

DipoleChargeModifier(const std::string &model, const int &gpu_rank = 0, const std::string &name_scope = "")

Dipole charge modifier without initialization.

Parameters

- **model** – [in] The name of the frozen model file.
- **gpu_rank** – [in] The GPU rank. Default is 0.
- **name_scope** – [in] The name scope.

`~DipoleChargeModifier()`

void **init**(const std::string &model, const int &gpu_rank = 0, const std::string &name_scope = "")
Initialize the dipole charge modifier.

Parameters

- **model** – [in] The name of the frozen model file.
- **gpu_rank** – [in] The GPU rank. Default is 0.
- **name_scope** – [in] The name scope.

void **print_summary**(const std::string &pre) const
Print the DP summary to the screen.

Parameters

pre – [in] The prefix to each line.

template<typename VALUETYPE>

void **compute**(std::vector<VALUETYPE> &dfcorr_, std::vector<VALUETYPE> &dvcorr_, const
std::vector<VALUETYPE> &dcoord_, const std::vector<int> &dtype_, const
std::vector<VALUETYPE> &dbox, const std::vector<std::pair<int, int>> &pairs,
const std::vector<VALUETYPE> &delef_, const int nghost, const [InputNlist](#)
&imp_list)

Evaluate the force and virial correction by using this dipole charge modifier.

Parameters

- **dfcorr_** – [out] The force correction on each atom.
- **dvcorr_** – [out] The virial correction.
- **dcoord_** – [in] The coordinates of atoms. The array should be of size natoms x 3.
- **dtype_** – [in] The atom types. The list should contain natoms ints.
- **dbox** – [in] The cell of the region. The array should be of size 9.
- **pairs** – [in] The pairs of atoms. The list should contain npairs pairs of ints.
- **delef_** – [in] The electric field on each atom. The array should be of size natoms x 3.
- **nghost** – [in] The number of ghost atoms.
- **imp_list** – [in] The neighbor list.

inline double **cutoff**() const

Get cutoff radius.

Returns

double cutoff radius.

inline int **numb_types**() const

Get the number of atom types.

Returns

int number of atom types.

inline std::vector<int> **sel_types**() const

Get the list of sel types.

Returns
The list of sel types.

19.3.3 Functions

Function `deepmd::check_status`

- Defined in `file_source_api_cc_include_common.h`

Function Documentation

`void deepmd::check_status(const tensorflow::Status &status)`

Check TensorFlow status. Exit if not OK.

Parameters

status – [in] TensorFlow status.

Function `deepmd::convert_pbtxt_to_pb`

- Defined in `file_source_api_cc_include_common.h`

Function Documentation

`void deepmd::convert_pbtxt_to_pb(std::string fn_pb_txt, std::string fn_pb)`

Convert pbtxt to pb.

Parameters

- **fn_pb_txt** – [in] Filename of the pb txt file.
- **fn_pb** – [in] Filename of the pb file.

Function `deepmd::get_env_nthreads`

- Defined in `file_source_api_cc_include_common.h`

Function Documentation

`void deepmd::get_env_nthreads(int &num_intra_nthreads, int &num_inter_nthreads)`

Get the number of threads from the environment variable.

A warning will be thrown if environmental variables are not set.

Parameters

- **num_intra_nthreads** – [out] The number of intra threads. Read from `TF_INTRA_OP_PARALLELISM_THREADS`.
- **num_inter_nthreads** – [out] The number of inter threads. Read from `TF_INTER_OP_PARALLELISM_THREADS`.

Function `deepmd::load_op_library`

- Defined in `file_source_api_cc_include_common.h`

Function Documentation

`void deepmd::load_op_library()`

Dynamically load OP library. This should be called before loading graphs.

Function `deepmd::model_compatible`

- Defined in `file_source_api_cc_include_common.h`

Function Documentation

`bool deepmd::model_compatible(std::string &model_version)`

Check if the model version is supported.

Parameters

model_version – [in] The model version.

Returns

Whether the model is supported (true or false).

Function `deepmd::name_prefix`

- Defined in `file_source_api_cc_include_common.h`

Function Documentation

`std::string deepmd::name_prefix(const std::string &name_scope)`

Function `deepmd::print_summary`

- Defined in `file_source_api_cc_include_common.h`

Function Documentation

`void deepmd::print_summary(const std::string &pre)`

Print the summary of DeePMD-kit, including the version and the build information.

Parameters

pre – [in] The prefix to each line.

Function `deepmd::read_file_to_string`

- Defined in `file_source_api_cc_include_common.h`

Function Documentation

`void deepmd::read_file_to_string(std::string model, std::string &file_content)`

Read model file to a string.

Parameters

- **model** – [in] Path to the model.
- **file_content** – [out] Content of the model file.

Template Function `deepmd::select_by_type`

- Defined in `file_source_api_cc_include_common.h`

Function Documentation

`template<typename VALUETYPE>`

`void deepmd::select_by_type(std::vector<int> &fwd_map, std::vector<int> &bkw_map, int
 &nghost_real, const std::vector<VALUETYPE> &dcoord_, const
 std::vector<int> &dtype_, const int &nghost, const std::vector<int>
 &sel_type_)`

Get forward and backward map of selected atoms by atom types.

Parameters

- **fwd_map** – [out] The forward map with size `natoms`.
- **bkw_map** – [out] The backward map with size `nreal`.
- **nghost_real** – [out] The number of selected ghost atoms.
- **dcoord_** – [in] The coordinates of all atoms. Reserved for compatibility.
- **dtype_** – [in] The atom types of all atoms.
- **nghost** – [in] The number of ghost atoms.
- **sel_type_** – [in] The selected atom types.

Template Function `deepmd::select_map``(std::vector<VT>&, const std::vector<VT>&, const
std::vector<int>&, const int&, const int&, const int&, const int&)`

- Defined in `file_source_api_cc_include_common.h`

Function Documentation

```
template<typename VT>
void deepmd::select_map(std::vector<VT> &out, const std::vector<VT> &in, const std::vector<int>
                        &fwd_map, const int &stride, const int &nframes = 1, const int &nall1 = 0,
                        const int &nall2 = 0)
```

Apply the given map to a vector.

Parameters

- **out** – [out] The output vector.
- **in** – [in] The input vector.
- **fwd_map** – [in] The map.
- **stride** – [in] The stride of the input vector.
- **nframes** – [in] The number of frames.
- **nall1** – [in] The number of atoms in the input vector.
- **nall2** – [in] The number of atoms in the output vector.

Template Function `deepmd::select_map(typename std::vector<VT>::iterator, const typename std::vector<VT>::const_iterator, const std::vector<int>&, const int&, const int&, const int&, const int&)`

- Defined in file_source_api_cc_include_common.h

Function Documentation

```
template<typename VT>
void deepmd::select_map(typename std::vector<VT>::iterator out, const typename
                        std::vector<VT>::const_iterator in, const std::vector<int> &fwd_map, const
                        int &stride, const int &nframes = 1, const int &nall1 = 0, const int &nall2 = 0)
```

Apply the given map to a vector.

Parameters

- **out** – [out] The output vector.
- **in** – [in] The input vector.
- **fwd_map** – [in] The map.
- **stride** – [in] The stride of the input vector.
- **nframes** – [in] The number of frames.
- **nall1** – [in] The number of atoms in the input vector.
- **nall2** – [in] The number of atoms in the output vector.

Template Function `deepmd::select_map_inv(std::vector<VT>&, const std::vector<VT>&, const std::vector<int>&, const int&)`

- Defined in file `_source_api_cc_include_common.h`

Function Documentation

```
template<typename VT>
void deepmd::select_map_inv(std::vector<VT> &out, const std::vector<VT> &in, const
                           std::vector<int> &fwd_map, const int &stride)
```

Template Function `deepmd::select_map_inv(typename std::vector<VT>::iterator, const typename std::vector<VT>::const_iterator, const std::vector<int>&, const int&)`

- Defined in file `_source_api_cc_include_common.h`

Function Documentation

```
template<typename VT>
void deepmd::select_map_inv(typename std::vector<VT>::iterator out, const typename
                           std::vector<VT>::const_iterator in, const std::vector<int> &fwd_map,
                           const int &stride)
```

Template Function `deepmd::select_real_atoms`

- Defined in file `_source_api_cc_include_common.h`

Function Documentation

```
template<typename VALUETYPE>
void deepmd::select_real_atoms(std::vector<int> &fwd_map, std::vector<int> &bkw_map, int
                              &nghost_real, const std::vector<VALUETYPE> &dcoord_, const
                              std::vector<int> &dtype_, const int &nghost, const int &ntypes)
```

Template Function `deepmd::select_real_atoms_coord`

- Defined in file `_source_api_cc_include_common.h`

Function Documentation

```
template<typename VALUETYPE>
void deepmd::select_real_atoms_coord(std::vector<VALUETYPE> &dcoord, std::vector<int>
                                     &dtype, std::vector<VALUETYPE> &aparam, int
                                     &nghost_real, std::vector<int> &fwd_map, std::vector<int>
                                     &bkwd_map, int &nall_real, int &nloc_real, const
                                     std::vector<VALUETYPE> &dcoord_, const std::vector<int>
                                     &dtype_, const std::vector<VALUETYPE> &aparam_, const
                                     int &nghost, const int &ntypes, const int &nframes, const int
                                     &daparam, const int &nall)
```

Function deepmd::session_get_dtype

- Defined in file_source_api_cc_include_common.h

Function Documentation

```
int deepmd::session_get_dtype(tensorflow::Session *session, const std::string name, const std::string
                             scope = "")
```

Get the type of a tensor.

Parameters

- **session** – [in] TensorFlow session.
- **name** – [in] The name of the tensor.
- **scope** – [in] The scope of the tensor.

Returns

The type of the tensor as int.

Template Function deepmd::session_get_scalar

- Defined in file_source_api_cc_include_common.h

Function Documentation

```
template<typename VT>
VT deepmd::session_get_scalar(tensorflow::Session *session, const std::string name, const std::string
                              scope = "")
```

Get the value of a tensor.

Parameters

- **session** – [in] TensorFlow session.
- **name** – [in] The name of the tensor.
- **scope** – [in] The scope of the tensor.

Returns

The value of the tensor.

Template Function `deepmd::session_get_vector`

- Defined in file `_source_api_cc_include_common.h`

Function Documentation

```
template<typename VT>
void deepmd::session_get_vector(std::vector<VT> &o_vec, tensorflow::Session *session, const
                                std::string name_, const std::string scope = "")
```

Get the vector of a tensor.

Parameters

- **o_vec** – [out] The output vector.
- **session** – [in] TensorFlow session.
- **name** – [in] The name of the tensor.
- **scope** – [in] The scope of the tensor.

Template Function `deepmd::session_input_tensors`(`std::vector<std::pair<std::string, tensorflow::Tensor>>&`, `const std::vector<VALUETYPE>&`, `const int&`, `const std::vector<int>&`, `const std::vector<VALUETYPE>&`, `const double&`, `const std::vector<VALUETYPE>&`, `const std::vector<VALUETYPE>&`, `const deepmd::AtomMap&`, `const std::string`)

- Defined in file `_source_api_cc_include_common.h`

Function Documentation

```
template<typename MODELTYPE, typename VALUETYPE>
int deepmd::session_input_tensors(std::vector<std::pair<std::string, tensorflow::Tensor>>
                                   &input_tensors, const std::vector<VALUETYPE> &dcoord_, const
                                   int &ntypes, const std::vector<int> &dtype_, const
                                   std::vector<VALUETYPE> &dbox, const double &cell_size, const
                                   std::vector<VALUETYPE> &fparam_, const
                                   std::vector<VALUETYPE> &aparam_, const deepmd::AtomMap
                                   &atommap, const std::string scope = "")
```

Get input tensors.

Parameters

- **input_tensors** – [out] Input tensors.
- **dcoord_** – [in] Coordinates of atoms.
- **ntypes** – [in] Number of atom types.
- **dtype_** – [in] Atom types.
- **dbox** – [in] Box matrix.
- **cell_size** – [in] Cell size.
- **fparam_** – [in] Frame parameters.
- **aparam_** – [in] Atom parameters.

- **atommap** – [in] Atom map.
- **scope** – [in] The scope of the tensors.

Template Function `deepmd::session_input_tensors(std::vector<std::pair<std::string, tensorflow::Tensor>>&, const std::vector<VALUETYPE>&, const int&, const std::vector<int>&, const std::vector<VALUETYPE>&, InputNlist&, const std::vector<VALUETYPE>&, const std::vector<VALUETYPE>&, const deepmd::AtomMap&, const int, const int, const std::string)`

- Defined in `file_source_api_cc_include_common.h`

Function Documentation

```
template<typename MODELTYPE, typename VALUETYPE>
int deepmd::session_input_tensors(std::vector<std::pair<std::string, tensorflow::Tensor>>
                                &input_tensors, const std::vector<VALUETYPE> &dcoord_, const
                                int &ntypes, const std::vector<int> &dtype_, const
                                std::vector<VALUETYPE> &dbox, InputNlist &dlist, const
                                std::vector<VALUETYPE> &fparam_, const
                                std::vector<VALUETYPE> &aparam_, const deepmd::AtomMap
                                &atommap, const int nghost, const int ago, const std::string scope =
                                "")
```

Get input tensors.

Parameters

- **input_tensors** – [out] Input tensors.
- **dcoord_** – [in] Coordinates of atoms.
- **ntypes** – [in] Number of atom types.
- **dtype_** – [in] Atom types.
- **dlist** – [in] Neighbor list.
- **fparam_** – [in] Frame parameters.
- **aparam_** – [in] Atom parameters.
- **atommap** – [in] Atom map.
- **nghost** – [in] Number of ghost atoms.
- **ago** – [in] Update the internal neighbour list if ago is 0.
- **scope** – [in] The scope of the tensors.

Template Function `deepmd::session_input_tensors_mixed_type`

- Defined in file `_source_api_cc_include_common.h`

Function Documentation

```
template<typename MODELTYPE, typename VALUETYPE>
int deepmd::session_input_tensors_mixed_type(std::vector<std::pair<std::string,
    tensorflow::Tensor>> &input_tensors, const int
    &nframes, const std::vector<VALUETYPE>
    &dcoord_, const int &ntypes, const std::vector<int>
    &dtype_, const std::vector<VALUETYPE> &dbox,
    const double &cell_size, const
    std::vector<VALUETYPE> &fparam_, const
    std::vector<VALUETYPE> &aparam_, const
    deepmd::AtomMap &atommap, const std::string scope
    = "")
```

Get input tensors for mixed type.

Parameters

- **input_tensors** – [out] Input tensors.
- **nframes** – [in] Number of frames.
- **dcoord_** – [in] Coordinates of atoms.
- **ntypes** – [in] Number of atom types.
- **dtype_** – [in] Atom types.
- **dlist** – [in] Neighbor list.
- **fparam_** – [in] Frame parameters.
- **aparam_** – [in] Atom parameters.
- **atommap** – [in] Atom map.
- **nghost** – [in] Number of ghost atoms.
- **ago** – [in] Update the internal neighbour list if ago is 0.
- **scope** – [in] The scope of the tensors.

19.3.4 Typedefs

Typedef `deepmd::ENERGYTYPE`

- Defined in file `_source_api_cc_include_common.h`

Typedef Documentation

`typedef double deepmd::ENERGYTYPE`

Typedef `deepmd::STRINGTYPE`

- Defined in `file_source_api_cc_include_tf_private.h`

Typedef Documentation

`typedef std::string deepmd::STRINGTYPE`

20.1 Class Hierarchy

- Namespace deepmd
 - Namespace deepmd::hpp
 - * Struct deepmd_exception
 - * Struct InputNlist
 - * Class DeepPot
 - * Class DeepPotModelDevi
 - * Class DeepTensor
 - * Class DipoleChargeModifier
- Struct DP_DeepPot
- Struct DP_DeepPotModelDevi
- Struct DP_DeepTensor
- Struct DP_DipoleChargeModifier
- Struct DP_Nlist

20.2 File Hierarchy

- dir_source
 - dir_source_api_c
 - * dir_source_api_c_include
 - file_source_api_c_include_c_api.h
 - file_source_api_c_include_c_api_internal.h
 - file_source_api_c_include_deepmd.hpp

20.3 Full API

20.3.1 Namespaces

Namespace `deepmd`

Contents

- [Namespaces](#)

Namespaces

- [Namespace `deepmd::hpp`](#)

Namespace `deepmd::hpp`

Contents

- [Classes](#)
- [Functions](#)

Classes

- [Struct `deepmd_exception`](#)
- [Struct `InputNlist`](#)
- [Class `DeepPot`](#)
- [Class `DeepPotModelDevi`](#)
- [Class `DeepTensor`](#)
- [Class `DipoleChargeModifier`](#)

Functions

- [Function `deepmd::hpp::convert_nlist`](#)
- [Function `deepmd::hpp::convert_pbtxt_to_pb`](#)
- [Function `deepmd::hpp::read_file_to_string`](#)
- [Template Function `deepmd::hpp::select_by_type`](#)
- [Template Function `deepmd::hpp::select_map`](#)

Namespace `std`

20.3.2 Classes and Structs

Struct `deepmd_exception`

- Defined in `file_source_api_c_include_deepmd.hpp`

Inheritance Relationships

Base Type

- `public std::runtime_error`

Struct Documentation

```
struct deepmd_exception : public std::runtime_error
    General DeePMD-kit exception. Throw if anything doesn't work.
```

Public Functions

```
inline deepmd_exception()
inline deepmd_exception(const std::string &msg)
```

Struct `InputNlist`

- Defined in `file_source_api_c_include_deepmd.hpp`

Struct Documentation

```
struct InputNlist
    Neighbor list.
```

Public Functions

```
inline InputNlist()
inline InputNlist(int inum_, int *ilist_, int *numneigh_, int **firstneigh_)
```

Public Members

`DP_Nlist *nl`

C API neighbor list.

`int inum`

Number of core region atoms.

`int *ilist`

Array stores the core region atom's index.

`int *numneigh`

Array stores the core region atom's neighbor atom number.

`int **firstneigh`

Array stores the core region atom's neighbor index.

Struct DP_DeepPot

- Defined in file `source_api_c_include_c_api_internal.h`

Struct Documentation

`struct DP_DeepPot`

Public Functions

`DP_DeepPot()`

`DP_DeepPot(deepmd::DeepPot &dp)`

Public Members

`deepmd::DeepPot dp`

`std::string exception`

`int dfparam`

`int daparam`

Struct DP_DeepPotModelDevi

- Defined in file `_source_api_c_include_c_api_internal.h`

Struct Documentation

```
struct DP_DeepPotModelDevi
```

Public Functions

```
DP_DeepPotModelDevi()
```

```
DP_DeepPotModelDevi(deepmd::DeepPotModelDevi &dp)
```

Public Members

```
deepmd::DeepPotModelDevi dp
```

```
std::string exception
```

```
int dfparam
```

```
int daparam
```

Struct DP_DeepTensor

- Defined in file `_source_api_c_include_c_api_internal.h`

Struct Documentation

```
struct DP_DeepTensor
```

Public Functions

```
DP_DeepTensor()
```

```
DP_DeepTensor(deepmd::DeepTensor &dt)
```

Public Members

deepmd::DeepTensor dt

std::string exception

Struct DP_DipoleChargeModifier

- Defined in file_source_api_c_include_c_api_internal.h

Struct Documentation

struct DP_DipoleChargeModifier

Public Functions

DP_DipoleChargeModifier()

DP_DipoleChargeModifier(deepmd::DipoleChargeModifier &dcm)

Public Members

deepmd::DipoleChargeModifier dcm

std::string exception

Struct DP_Nlist

- Defined in file_source_api_c_include_c_api_internal.h

Struct Documentation

struct DP_Nlist

Public Functions

`DP_Nlist()`

`DP_Nlist(deepmd::InputNlist &nl)`

Public Members

`deepmd::InputNlist nl`

`std::string exception`

Class DeepPot

- Defined in file `_source_api_c_include_deepmd.hpp`

Class Documentation

class **DeepPot**

Deep Potential.

Public Functions

`inline DeepPot()`

DP constructor without initialization.

`inline ~DeepPot()`

`inline DeepPot(const std::string &model, const int &gpu_rank = 0, const std::string &file_content = "")`

DP constructor with initialization.

Parameters

- **model** – [in] The name of the frozen model file.
- **gpu_rank** – [in] The GPU rank.
- **file_content** – [in] The content of the frozen model file.

`inline void init(const std::string &model, const int &gpu_rank = 0, const std::string &file_content = "")`

Initialize the DP.

Parameters

- **model** – [in] The name of the frozen model file.
- **gpu_rank** – [in] The GPU rank.
- **file_content** – [in] The content of the frozen model file.

`template<typename VALUETYPE, typename ENERGYVTYPE>`

```
inline void compute(ENERGYVTYPE &ener, std::vector<VALUETYPE> &force,
                  std::vector<VALUETYPE> &virial, const std::vector<VALUETYPE> &coord,
                  const std::vector<int> &atype, const std::vector<VALUETYPE> &box, const
                  std::vector<VALUETYPE> &fparam = std::vector<VALUETYPE>(), const
                  std::vector<VALUETYPE> &aparam = std::vector<VALUETYPE>())
```

Evaluate the energy, force and virial by using this DP.

Parameters

- **ener** – [out] The system energy.
- **force** – [out] The force on each atom.
- **virial** – [out] The virial.
- **coord** – [in] The coordinates of atoms. The array should be of size nframes x natoms x 3.
- **atype** – [in] The atom types. The list should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size nframes x 9 (PBC) or empty (no PBC).
- **fparam** – [in] The frame parameter. The array can be of size : nframes x dim_fparam. dim_fparam. Then all frames are assumed to be provided with the same fparam.
- **aparam** – [in] The atomic parameter The array can be of size : nframes x natoms x dim_aparam. natoms x dim_aparam. Then all frames are assumed to be provided with the same aparam.

```
template<typename VALUETYPE, typename ENERGYVTYPE>
inline void compute(ENERGYVTYPE &ener, std::vector<VALUETYPE> &force,
                  std::vector<VALUETYPE> &virial, std::vector<VALUETYPE>
                  &atom_energy, std::vector<VALUETYPE> &atom_virial, const
                  std::vector<VALUETYPE> &coord, const std::vector<int> &atype, const
                  std::vector<VALUETYPE> &box, const std::vector<VALUETYPE> &fparam
                  = std::vector<VALUETYPE>(), const std::vector<VALUETYPE> &aparam =
                  std::vector<VALUETYPE>())
```

Evaluate the energy, force, virial, atomic energy, and atomic virial by using this DP.

Parameters

- **ener** – [out] The system energy.
- **force** – [out] The force on each atom.
- **virial** – [out] The virial.
- **atom_energy** – [out] The atomic energy.
- **atom_virial** – [out] The atomic virial.
- **coord** – [in] The coordinates of atoms. The array should be of size nframes x natoms x 3.
- **atype** – [in] The atom types. The list should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size nframes x 9 (PBC) or empty (no PBC).

- **fparam** – [in] The frame parameter. The array can be of size : nframes x dim_fparam. dim_fparam. Then all frames are assumed to be provided with the same fparam.
- **aparam** – [in] The atomic parameter The array can be of size : nframes x natoms x dim_aparam. natoms x dim_aparam. Then all frames are assumed to be provided with the same aparam.

```
template<typename VALUETYPE, typename ENERGYVTYPE>
inline void compute(ENERGYVTYPE &ener, std::vector<VALUETYPE> &force,
    std::vector<VALUETYPE> &virial, const std::vector<VALUETYPE> &coord,
    const std::vector<int> &atype, const std::vector<VALUETYPE> &box, const
    int nghost, const InputNlist &tmp_list, const int &ago, const
    std::vector<VALUETYPE> &fparam = std::vector<VALUETYPE>(), const
    std::vector<VALUETYPE> &aparam = std::vector<VALUETYPE>())
```

Evaluate the energy, force and virial by using this DP with the neighbor list.

Parameters

- **ener** – [out] The system energy.
- **force** – [out] The force on each atom.
- **virial** – [out] The virial.
- **coord** – [in] The coordinates of atoms. The array should be of size nframes x natoms x 3.
- **atype** – [in] The atom types. The list should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size nframes x 9 (PBC) or empty (no PBC).
- **nghost** – [in] The number of ghost atoms.
- **nlist** – [in] The neighbor list.
- **ago** – [in] Update the internal neighbour list if ago is 0.
- **fparam** – [in] The frame parameter. The array can be of size : nframes x dim_fparam. dim_fparam. Then all frames are assumed to be provided with the same fparam.
- **aparam** – [in] The atomic parameter The array can be of size : nframes x natoms x dim_aparam. natoms x dim_aparam. Then all frames are assumed to be provided with the same aparam.

```
template<typename VALUETYPE, typename ENERGYVTYPE>
inline void compute(ENERGYVTYPE &ener, std::vector<VALUETYPE> &force,
    std::vector<VALUETYPE> &virial, std::vector<VALUETYPE>
    &atom_energy, std::vector<VALUETYPE> &atom_virial, const
    std::vector<VALUETYPE> &coord, const std::vector<int> &atype, const
    std::vector<VALUETYPE> &box, const int nghost, const InputNlist &tmp_list,
    const int &ago, const std::vector<VALUETYPE> &fparam =
    std::vector<VALUETYPE>(), const std::vector<VALUETYPE> &aparam =
    std::vector<VALUETYPE>())
```

Evaluate the energy, force, virial, atomic energy, and atomic virial by using this DP with the neighbor list.

Parameters

- **ener** – [out] The system energy.

- **force** – [out] The force on each atom.
- **virial** – [out] The virial.
- **atom_energy** – [out] The atomic energy.
- **atom_virial** – [out] The atomic virial.
- **coord** – [in] The coordinates of atoms. The array should be of size nframes x natoms x 3.
- **atype** – [in] The atom types. The list should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size nframes x 9 (PBC) or empty (no PBC).
- **nghost** – [in] The number of ghost atoms.
- **nlist** – [in] The neighbor list.
- **ago** – [in] Update the internal neighbour list if ago is 0.
- **fparam** – [in] The frame parameter. The array can be of size : nframes x dim_fparam. dim_fparam. Then all frames are assumed to be provided with the same fparam.
- **aparam** – [in] The atomic parameter The array can be of size : nframes x natoms x dim_aparam. natoms x dim_aparam. Then all frames are assumed to be provided with the same aparam.

```
template<typename VALUETYPE, typename ENERGYVTYPE>
inline void compute_mixed_type(ENERGYVTYPE &ener, std::vector<VALUETYPE> &force,
                               std::vector<VALUETYPE> &virial, const int &nframes, const
                               std::vector<VALUETYPE> &coord, const std::vector<int>
                               &atype, const std::vector<VALUETYPE> &box, const
                               std::vector<VALUETYPE> &fparam =
                               std::vector<VALUETYPE>(), const std::vector<VALUETYPE>
                               &aparam = std::vector<VALUETYPE>())
```

Evaluate the energy, force and virial by using this DP with the mixed type.

Parameters

- **ener** – [out] The system energy.
- **force** – [out] The force on each atom.
- **virial** – [out] The virial.
- **nframes** – [in] The number of frames.
- **coord** – [in] The coordinates of atoms. The array should be of size nframes x natoms x 3.
- **atype** – [in] The atom types. The list should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size nframes x 9 (PBC) or empty (no PBC).
- **fparam** – [in] The frame parameter. The array can be of size : nframes x dim_fparam. dim_fparam. Then all frames are assumed to be provided with the same fparam.
- **aparam** – [in] The atomic parameter The array can be of size : nframes x natoms x dim_aparam. natoms x dim_aparam. Then all frames are assumed to be provided with the same aparam.


```
template<typename VALUETYPE, typename ENERGYVTYPE>
inline void compute_mixed_type(ENERGYVTYPE &ener, std::vector<VALUETYPE> &force,
                             std::vector<VALUETYPE> &virial, std::vector<VALUETYPE>
                             &atom_energy, std::vector<VALUETYPE> &atom_virial, const
                             int &nframes, const std::vector<VALUETYPE> &coord, const
                             std::vector<int> &atype, const std::vector<VALUETYPE> &box,
                             const std::vector<VALUETYPE> &fparam =
                             std::vector<VALUETYPE>(), const std::vector<VALUETYPE>
                             &aparam = std::vector<VALUETYPE>())
```

Evaluate the energy, force, virial, atomic energy, and atomic virial by using this DP with the mixed type.

Parameters

- **ener** – [out] The system energy.
- **force** – [out] The force on each atom.
- **virial** – [out] The virial.
- **atom_energy** – [out] The atomic energy.
- **atom_virial** – [out] The atomic virial.
- **nframes** – [in] The number of frames.
- **coord** – [in] The coordinates of atoms. The array should be of size nframes x natoms x 3.
- **atype** – [in] The atom types. The list should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size nframes x 9 (PBC) or empty (no PBC).
- **fparam** – [in] The frame parameter. The array can be of size : nframes x dim_fparam. dim_fparam. Then all frames are assumed to be provided with the same fparam.
- **aparam** – [in] The atomic parameter The array can be of size : nframes x natoms x dim_aparam. natoms x dim_aparam. Then all frames are assumed to be provided with the same aparam.

```
inline double cutoff() const
```

Get the cutoff radius.

Returns

The cutoff radius.

```
inline int numb_types() const
```

Get the number of types.

Returns

The number of types.

```
inline int numb_types_spin() const
```

Get the number of types with spin.

Returns

The number of types with spin.

```
inline void get_type_map(std::string &type_map)
```

Get the type map (element name of the atom types) of this model.

Parameters

type_map – [out] The type map of this model.

```
inline void print_summary(const std::string &pre) const
```

Print the summary of DeePMD-kit, including the version and the build information.

Parameters

pre – [in] The prefix to each line.

```
inline int dim_fparam() const
```

Get the dimension of the frame parameter.

Returns

The dimension of the frame parameter.

```
inline int dim_aparam() const
```

Get the dimension of the atomic parameter.

Returns

The dimension of the atomic parameter.

Class DeepPotModelDevi

- Defined in file_source_api_c_include_deepmd.hpp

Class Documentation

```
class DeepPotModelDevi
```

Deep Potential model deviation.

Public Functions

```
inline DeepPotModelDevi()
```

DP model deviation constructor without initialization.

```
inline ~DeepPotModelDevi()
```

```
inline DeepPotModelDevi(const std::vector<std::string> &models)
```

DP model deviation constructor with initialization.

Parameters

models – [in] The names of the frozen model file.

```
inline void init(const std::vector<std::string> &models, const int &gpu_rank = 0, const  
std::vector<std::string> &file_content = std::vector<std::string>())
```

Initialize the DP model deviation.

Parameters

- **model** – [in] The name of the frozen model file.
- **gpu_rank** – [in] The GPU rank.

- **file_content** – [in] The content of the frozen model file.

```
template<typename VALUETYPE>
inline void compute(std::vector<double> &ener, std::vector<std::vector<VALUETYPE>>> &force,
                  std::vector<std::vector<VALUETYPE>>> &virial, const
                  std::vector<VALUETYPE> &coord, const std::vector<int> &atype, const
                  std::vector<VALUETYPE> &box, const int nghost, const InputNlist &imp_list,
                  const int &ago, const std::vector<VALUETYPE> &fparam =
                  std::vector<VALUETYPE>(), const std::vector<VALUETYPE> &aparam =
                  std::vector<VALUETYPE>())
```

Evaluate the energy, force and virial by using this DP model deviation.

Parameters

- **ener** – [out] The system energy.
- **force** – [out] The force on each atom.
- **virial** – [out] The virial.
- **coord** – [in] The coordinates of atoms. The array should be of size nframes x natoms x 3.
- **atype** – [in] The atom types. The list should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size nframes x 9 (PBC) or empty (no PBC).

```
template<typename VALUETYPE>
inline void compute(std::vector<double> &ener, std::vector<std::vector<VALUETYPE>>> &force,
                  std::vector<std::vector<VALUETYPE>>> &virial,
                  std::vector<std::vector<VALUETYPE>>> &atom_energy,
                  std::vector<std::vector<VALUETYPE>>> &atom_virial, const
                  std::vector<VALUETYPE> &coord, const std::vector<int> &atype, const
                  std::vector<VALUETYPE> &box, const int nghost, const InputNlist &imp_list,
                  const int &ago, const std::vector<VALUETYPE> &fparam =
                  std::vector<VALUETYPE>(), const std::vector<VALUETYPE> &aparam =
                  std::vector<VALUETYPE>())
```

Evaluate the energy, force, virial, atomic energy, and atomic virial by using this DP model deviation.

Parameters

- **ener** – [out] The system energy.
- **force** – [out] The force on each atom.
- **virial** – [out] The virial.
- **atom_energy** – [out] The atomic energy.
- **atom_virial** – [out] The atomic virial.
- **coord** – [in] The coordinates of atoms. The array should be of size nframes x natoms x 3.
- **atype** – [in] The atom types. The list should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size nframes x 9 (PBC) or empty (no PBC).

```
inline double cutoff() const
```

Get the cutoff radius.

Returns

The cutoff radius.

```
inline int numb_types() const
```

Get the number of types.

Returns

The number of types.

```
inline int numb_types_spin() const
```

Get the number of types with spin.

Returns

The number of types with spin.

```
inline int dim_fparam() const
```

Get the dimension of the frame parameter.

Returns

The dimension of the frame parameter.

```
inline int dim_aparam() const
```

Get the dimension of the atomic parameter.

Returns

The dimension of the atomic parameter.

```
template<typename VALUETYPE>
```

```
inline void compute_avg(std::vector<VALUETYPE> &avg, const  
                        std::vector<std::vector<VALUETYPE>> &xx)
```

Compute the average of vectors.

Parameters

- **avg** – [out] The average of vectors.
- **xx** – [in] The vectors of all models.

```
template<typename VALUETYPE>
```

```
inline void compute_std(std::vector<VALUETYPE> &std, const std::vector<VALUETYPE> &avg,  
                        const std::vector<std::vector<VALUETYPE>> &xx, const int &stride)
```

Compute the standard deviation of vectors.

Parameters

- **std** – [out] The standard deviation of vectors.
- **avg** – [in] The average of vectors.
- **xx** – [in] The vectors of all models.
- **stride** – [in] The stride to compute the deviation.

```
template<typename VALUETYPE>
```

```
inline void compute_relative_std(std::vector<VALUETYPE> &std, const  
                                std::vector<VALUETYPE> &avg, const VALUETYPE eps,  
                                const int &stride)
```

Compute the relative standard deviation of vectors.

Parameters

- **std** – [out] The standard deviation of vectors.
- **avg** – [in] The average of vectors.
- **eps** – [in] The level parameter for computing the deviation.
- **stride** – [in] The stride to compute the deviation.

```
template<typename VALUETYPE>
inline void compute_std_f(std::vector<VALUETYPE> &std, const std::vector<VALUETYPE>
                        &avg, const std::vector<std::vector<VALUETYPE>> &xx)
```

Compute the standard deviation of forces.

Parameters

- **std** – [out] The standard deviation of forces.
- **avg** – [in] The average of forces.
- **xx** – [in] The vectors of all forces.

```
template<typename VALUETYPE>
inline void compute_relative_std_f(std::vector<VALUETYPE> &std, const
                                  std::vector<VALUETYPE> &avg, const VALUETYPE eps)
```

Compute the relative standard deviation of forces.

Parameters

- **std** – [out] The relative standard deviation of forces.
- **avg** – [in] The relative average of forces.
- **eps** – [in] The level parameter for computing the deviation.

Class DeepTensor

- Defined in file_source_api_c_include_deepmd.hpp

Class Documentation

class **DeepTensor**

Deep Tensor.

Public Functions

```
inline DeepTensor()
```

Deep Tensor constructor without initialization.

```
inline ~DeepTensor()
```

```
inline DeepTensor(const std::string &model, const int &gpu_rank = 0, const std::string &name_scope
                  = "")
```

[DeepTensor](#) constructor with initialization.

Parameters

- model** – [in] The name of the frozen model file.

```
inline void init(const std::string &model, const int &gpu_rank = 0, const std::string &name_scope =
    "")
```

Initialize the [DeepTensor](#).

Parameters

model – [in] The name of the frozen model file.

```
template<typename VALUETYPE>
```

```
inline void compute(std::vector<VALUETYPE> &tensor, const std::vector<VALUETYPE> &coord,
    const std::vector<int> &atype, const std::vector<VALUETYPE> &box)
```

Evaluate the tensor, force and virial by using this Deep Tensor.

Parameters

- **tensor** – [out] The atomic tensor.
- **coord** – [in] The coordinates of atoms. The array should be of size nframes x natoms x 3.
- **atype** – [in] The atom types. The list should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size nframes x 9 (PBC) or empty (no PBC).

```
template<typename VALUETYPE>
```

```
inline void compute(std::vector<VALUETYPE> &tensor, const std::vector<VALUETYPE> &coord,
    const std::vector<int> &atype, const std::vector<VALUETYPE> &box, const
    int nghost, const InputNlist &tmp_list)
```

Evaluate the tensor, force and virial by using this Deep Tensor with the neighbor list.

Parameters

- **tensor** – [out] The tensor.
- **coord** – [in] The coordinates of atoms. The array should be of size nframes x natoms x 3.
- **atype** – [in] The atom types. The list should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size nframes x 9 (PBC) or empty (no PBC).
- **nghost** – [in] The number of ghost atoms.
- **nlist** – [in] The neighbor list.

```
template<typename VALUETYPE>
```

```
inline void compute(std::vector<VALUETYPE> &global_tensor, std::vector<VALUETYPE>
    &force, std::vector<VALUETYPE> &virial, const std::vector<VALUETYPE>
    &coord, const std::vector<int> &atype, const std::vector<VALUETYPE>
    &box)
```

Evaluate the global tensor, force and virial by using this Deep Tensor.

Parameters

- **global_tensor** – [out] The global tensor.
- **force** – [out] The force on each atom.
- **virial** – [out] The virial.
- **coord** – [in] The coordinates of atoms. The array should be of size nframes x natoms x 3.

- **atype** – [in] The atom types. The list should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size nframes x 9 (PBC) or empty (no PBC).

```
template<typename VALUETYPE>
inline void compute(std::vector<VALUETYPE> &global_tensor, std::vector<VALUETYPE>
    &force, std::vector<VALUETYPE> &virial, std::vector<VALUETYPE>
    &atom_tensor, std::vector<VALUETYPE> &atom_virial, const
    std::vector<VALUETYPE> &coord, const std::vector<int> &atype, const
    std::vector<VALUETYPE> &box)
```

Evaluate the global tensor, force, virial, atomic tensor, and atomic virial by using this Deep Tensor.

Parameters

- **global_tensor** – [out] The global tensor.
- **force** – [out] The force on each atom.
- **virial** – [out] The virial.
- **atom_tensor** – [out] The atomic tensor.
- **atom_virial** – [out] The atomic virial.
- **coord** – [in] The coordinates of atoms. The array should be of size nframes x natoms x 3.
- **atype** – [in] The atom types. The list should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size nframes x 9 (PBC) or empty (no PBC).

```
template<typename VALUETYPE>
inline void compute(std::vector<VALUETYPE> &global_tensor, std::vector<VALUETYPE>
    &force, std::vector<VALUETYPE> &virial, const std::vector<VALUETYPE>
    &coord, const std::vector<int> &atype, const std::vector<VALUETYPE>
    &box, const int nghost, const InputNlist &lmp_list)
```

Evaluate the global tensor, force and virial by using this Deep Tensor with the neighbor list.

Parameters

- **global_tensor** – [out] The global tensor.
- **force** – [out] The force on each atom.
- **virial** – [out] The virial.
- **coord** – [in] The coordinates of atoms. The array should be of size nframes x natoms x 3.
- **atype** – [in] The atom types. The list should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size nframes x 9 (PBC) or empty (no PBC).
- **nghost** – [in] The number of ghost atoms.
- **nlist** – [in] The neighbor list.

```
template<typename VALUETYPE>
```

```
inline void compute(std::vector<VALUETYPE> &global_tensor, std::vector<VALUETYPE>
    &force, std::vector<VALUETYPE> &virial, std::vector<VALUETYPE>
    &atom_tensor, std::vector<VALUETYPE> &atom_virial, const
    std::vector<VALUETYPE> &coord, const std::vector<int> &atype, const
    std::vector<VALUETYPE> &box, const int nghost, const InputNlist &imp_list)
```

Evaluate the global tensor, force, virial, atomic tensor, and atomic virial by using this Deep Tensor with the neighbor list.

Parameters

- **global_tensor** – [out] The global tensor.
- **force** – [out] The force on each atom.
- **virial** – [out] The virial.
- **atom_tensor** – [out] The atomic tensor.
- **atom_virial** – [out] The atomic virial.
- **coord** – [in] The coordinates of atoms. The array should be of size nframes x natoms x 3.
- **atype** – [in] The atom types. The list should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size nframes x 9 (PBC) or empty (no PBC).
- **nghost** – [in] The number of ghost atoms.
- **nlist** – [in] The neighbor list.

```
inline double cutoff() const
```

Get the cutoff radius.

Returns

The cutoff radius.

```
inline int numb_types() const
```

Get the number of types.

Returns

The number of types.

```
inline int output_dim() const
```

Get the output dimension.

Returns

The output dimension.

```
inline std::vector<int> sel_types() const
```

```
inline void print_summary(const std::string &pre) const
```

Print the summary of DeePMD-kit, including the version and the build information.

Parameters

pre – [in] The prefix to each line.

Class DipoleChargeModifier

- Defined in file `_source_api_c_include_deepmd.hpp`

Class Documentation

class `DipoleChargeModifier`

Public Functions

`inline DipoleChargeModifier()`

`DipoleChargeModifier` constructor without initialization.

`inline ~DipoleChargeModifier()`

`inline DipoleChargeModifier(const std::string &model, const int &gpu_rank = 0, const std::string &name_scope = "")`

`DipoleChargeModifier` constructor with initialization.

Parameters

- `model` – [in] The name of the frozen model file.
- `gpu_rank` – [in] The rank of the GPU to be used.
- `name_scope` – [in] The name scope of the model.

`inline void init(const std::string &model, const int &gpu_rank = 0, const std::string &name_scope = "")`

Initialize the `DipoleChargeModifier`.

Parameters

- `model` – [in] The name of the frozen model file.
- `gpu_rank` – [in] The rank of the GPU to be used.
- `name_scope` – [in] The name scope of the model.

`template<typename VALUETYPE>`

`inline void compute(std::vector<VALUETYPE> &dfcorr_, std::vector<VALUETYPE> &dvcorr_, const std::vector<VALUETYPE> &dcoord_, const std::vector<int> &dtype_, const std::vector<VALUETYPE> &dbox, const std::vector<std::pair<int, int>> &pairs, const std::vector<VALUETYPE> &delef_, const int nghost, const InputNlist &imp_list)`

Evaluate the force and virial correction by using this dipole charge modifier.

Parameters

- `dfcorr_` – [out] The force correction on each atom.
- `dvcorr_` – [out] The virial correction.
- `dcoord_` – [in] The coordinates of atoms. The array should be of size `natoms x 3`.
- `dtype_` – [in] The atom types. The list should contain `natoms` ints.
- `dbox` – [in] The cell of the region. The array should be of size 9.

- **pairs** – [in] The pairs of atoms. The list should contain npairs pairs of ints.
- **delef_** – [in] The electric field on each atom. The array should be of size natoms x 3.
- **nghost** – [in] The number of ghost atoms.
- **lmp_list** – [in] The neighbor list.

inline double **cutoff**() const

Get the cutoff radius.

Returns

The cutoff radius.

inline int **numb_types**() const

Get the number of types.

Returns

The number of types.

inline std::vector<int> **sel_types**() const

inline void **print_summary**(const std::string &pre) const

Print the summary of DeePMD-kit, including the version and the build information.

Parameters

pre – [in] The prefix to each line.

20.3.3 Functions

Template Function **_DP_DeepPotCompute**

- Defined in file `_source_api_c_include_deepmd.hpp`

Function Documentation

template<typename **FPTYPE**>

inline void **_DP_DeepPotCompute**(**DP_DeepPot** *dp, const int nframes, const int natom, const **FPTYPE** *coord, const int *atype, const **FPTYPE** *cell, const **FPTYPE** *fparam, const **FPTYPE** *aparam, double *energy, **FPTYPE** *force, **FPTYPE** *virial, **FPTYPE** *atomic_energy, **FPTYPE** *atomic_virial)

Specialized Template Function **_DP_DeepPotCompute< double >**

- Defined in file `_source_api_c_include_deepmd.hpp`

Function Documentation

```
template<>
inline void _DP_DeepPotCompute<double>(DP_DeepPot *dp, const int nframes, const int natom, const
double *coord, const int *atype, const double *cell, const double
*fparam, const double *aparam, double *energy, double *force,
double *virial, double *atomic_energy, double *atomic_virial)
```

Specialized Template Function `_DP_DeepPotCompute< float >`

- Defined in file_source_api_c_include_deepmd.hpp

Function Documentation

```
template<>
inline void _DP_DeepPotCompute<float>(DP_DeepPot *dp, const int nframes, const int natom, const float
*coord, const int *atype, const float *cell, const float *fparam,
const float *aparam, double *energy, float *force, float *virial,
float *atomic_energy, float *atomic_virial)
```

Template Function `_DP_DeepPotComputeMixedType`

- Defined in file_source_api_c_include_deepmd.hpp

Function Documentation

```
template<typename FPTYPE>
inline void _DP_DeepPotComputeMixedType(DP_DeepPot *dp, const int nframes, const int natom, const
FPTYPE *coord, const int *atype, const FPTYPE *cell, const
FPTYPE *fparam, const FPTYPE *aparam, double *energy,
FPTYPE *force, FPTYPE *virial, FPTYPE *atomic_energy,
FPTYPE *atomic_virial)
```

Specialized Template Function `_DP_DeepPotComputeMixedType< double >`

- Defined in file_source_api_c_include_deepmd.hpp

Function Documentation

```
template<>
inline void _DP_DeepPotComputeMixedType<double>(DP_DeepPot *dp, const int nframes, const int
natom, const double *coord, const int *atype, const
double *cell, const double *fparam, const double
*aparam, double *energy, double *force, double
*virial, double *atomic_energy, double
*atomic_virial)
```

Specialized Template Function `_DP_DeepPotComputeMixedType< float >`

- Defined in file `_source_api_c_include_deepmd.hpp`

Function Documentation

```
template<>
inline void _DP_DeepPotComputeMixedType<float>(DP_DeepPot *dp, const int nframes, const int natom,
                                                const float *coord, const int *atype, const float *cell,
                                                const float *fparam, const float *aparam, double
                                                *energy, float *force, float *virial, float
                                                *atomic_energy, float *atomic_virial)
```

Template Function `_DP_DeepPotComputeNList`

- Defined in file `_source_api_c_include_deepmd.hpp`

Function Documentation

```
template<typename FPTYPE>
inline void _DP_DeepPotComputeNList(DP_DeepPot *dp, const int nframes, const int natom, const
FPTYPE *coord, const int *atype, const FPTYPE *cell, const int
nghost, const DP_Nlist *nlist, const int ngo, const FPTYPE
*fparam, const FPTYPE *aparam, double *energy, FPTYPE
*force, FPTYPE *virial, FPTYPE *atomic_energy, FPTYPE
*atomic_virial)
```

Specialized Template Function `_DP_DeepPotComputeNList< double >`

- Defined in file `_source_api_c_include_deepmd.hpp`

Function Documentation

```
template<>
inline void _DP_DeepPotComputeNList<double>(DP_DeepPot *dp, const int nframes, const int natom,
                                              const double *coord, const int *atype, const double *cell,
                                              const int nghost, const DP_Nlist *nlist, const int ngo,
                                              const double *fparam, const double *aparam, double
                                              *energy, double *force, double *virial, double
                                              *atomic_energy, double *atomic_virial)
```

Specialized Template Function `_DP_DeepPotComputeNList< float >`

- Defined in file `_source_api_c_include_deepmd.hpp`

Function Documentation

```
template<>
inline void _DP_DeepPotComputeNList<float>(DP_DeepPot *dp, const int nframes, const int natom, const
float *coord, const int *atype, const float *cell, const int
nghost, const DP_Nlist *nlist, const int ago, const float
*fparam, const float *aparam, double *energy, float *force,
float *virial, float *atomic_energy, float *atomic_virial)
```

Template Function `_DP_DeepPotModelDeviComputeNList`

- Defined in file `_source_api_c_include_deepmd.hpp`

Function Documentation

```
template<typename FPTYPE>
inline void _DP_DeepPotModelDeviComputeNList(DP_DeepPotModelDevi *dp, const int natom, const
FPTYPE *coord, const int *atype, const FPTYPE *cell,
const int nghost, const DP_Nlist *nlist, const int ago,
const FPTYPE *fparam, const FPTYPE *aparam,
double *energy, FPTYPE *force, FPTYPE *virial,
FPTYPE *atomic_energy, FPTYPE *atomic_virial)
```

Specialized Template Function `_DP_DeepPotModelDeviComputeNList< double >`

- Defined in file `_source_api_c_include_deepmd.hpp`

Function Documentation

```
template<>
inline void _DP_DeepPotModelDeviComputeNList<double>(DP_DeepPotModelDevi *dp, const int natom,
const double *coord, const int *atype, const
double *cell, const int nghost, const DP_Nlist
*nlist, const int ago, const double *fparam,
const double *aparam, double *energy, double
*force, double *virial, double *atomic_energy,
double *atomic_virial)
```

Specialized Template Function `_DP_DeepPotModelDeviComputeNList< float >`

- Defined in file `_source_api_c_include_deepmd.hpp`

Function Documentation

```
template<>
inline void _DP_DeepPotModelDeviComputeNList<float>(DP_DeepPotModelDevi *dp, const int natom,
                                                    const float *coord, const int *atype, const float
                                                    *cell, const int nghost, const DP_Nlist *nlist,
                                                    const int ago, const float *fparam, const float
                                                    *aparam, double *energy, float *force, float
                                                    *virial, float *atomic_energy, float
                                                    *atomic_virial)
```

Template Function `_DP_DeepTensorCompute`

- Defined in file `_source_api_c_include_deepmd.hpp`

Function Documentation

```
template<typename FPTYPE>
inline void _DP_DeepTensorCompute(DP_DeepTensor *dt, const int natom, const FPTYPE *coord, const int
                                  *atype, const FPTYPE *cell, FPTYPE *global_tensor, FPTYPE
                                  *force, FPTYPE *virial, FPTYPE **atomic_energy, FPTYPE
                                  *atomic_virial, int *size_at)
```

Specialized Template Function `_DP_DeepTensorCompute< double >`

- Defined in file `_source_api_c_include_deepmd.hpp`

Function Documentation

```
template<>
inline void _DP_DeepTensorCompute<double>(DP_DeepTensor *dt, const int natom, const double *coord,
                                           const int *atype, const double *cell, double *global_tensor,
                                           double *force, double *virial, double **atomic_tensor,
                                           double *atomic_virial, int *size_at)
```

Specialized Template Function `_DP_DeepTensorCompute< float >`

- Defined in file `_source_api_c_include_deepmd.hpp`

Function Documentation

```
template<>
inline void _DP_DeepTensorCompute<float>(DP_DeepTensor *dt, const int natom, const float *coord,
                                         const int *atype, const float *cell, float *global_tensor, float
                                         *force, float *virial, float **atomic_tensor, float
                                         *atomic_virial, int *size_at)
```

Template Function `_DP_DeepTensorComputeNList`

- Defined in file `_source_api_c_include_deepmd.hpp`

Function Documentation

```
template<typename FPTYPE>
inline void _DP_DeepTensorComputeNList(DP_DeepTensor *dt, const int natom, const FPTYPE *coord,
                                       const int *atype, const FPTYPE *cell, const int nghost, const
                                       DP_Nlist *nlist, FPTYPE *global_tensor, FPTYPE *force,
                                       FPTYPE *virial, FPTYPE **atomic_energy, FPTYPE
                                       *atomic_virial, int *size_at)
```

Specialized Template Function `_DP_DeepTensorComputeNList< double >`

- Defined in file `_source_api_c_include_deepmd.hpp`

Function Documentation

```
template<>
inline void _DP_DeepTensorComputeNList<double>(DP_DeepTensor *dt, const int natom, const double
                                                *coord, const int *atype, const double *cell, const int
                                                nghost, const DP_Nlist *nlist, double *global_tensor,
                                                double *force, double *virial, double
                                                **atomic_tensor, double *atomic_virial, int *size_at)
```

Specialized Template Function `_DP_DeepTensorComputeNList< float >`

- Defined in file `_source_api_c_include_deepmd.hpp`

Function Documentation

```
template<>
inline void _DP_DeepTensorComputeNList<float>(DP_DeepTensor *dt, const int natom, const float
                                             *coord, const int *atype, const float *cell, const int
                                             nghost, const DP_Nlist *nlist, float *global_tensor, float
                                             *force, float *virial, float **atomic_tensor, float
                                             *atomic_virial, int *size_at)
```

Template Function `_DP_DeepTensorComputeTensor`

- Defined in file `_source_api_c_include_deepmd.hpp`

Function Documentation

```
template<typename FPTYPE>
inline void _DP_DeepTensorComputeTensor(DP_DeepTensor *dt, const int natom, const FPTYPE *coord,
                                         const int *atype, const FPTYPE *cell, FPTYPE **tensor, int
                                         *size)
```

Specialized Template Function `_DP_DeepTensorComputeTensor< double >`

- Defined in file `_source_api_c_include_deepmd.hpp`

Function Documentation

```
template<>
inline void _DP_DeepTensorComputeTensor<double>(DP_DeepTensor *dt, const int natom, const double
                                             *coord, const int *atype, const double *cell, double
                                             **tensor, int *size)
```

Specialized Template Function `_DP_DeepTensorComputeTensor< float >`

- Defined in file `_source_api_c_include_deepmd.hpp`

Function Documentation

```
template<>
inline void _DP_DeepTensorComputeTensor<float>(DP_DeepTensor *dt, const int natom, const float
                                                *coord, const int *atype, const float *cell, float
                                                **tensor, int *size)
```

Template Function _DP_DeepTensorComputeTensorNList

- Defined in file_source_api_c_include_deepmd.hpp

Function Documentation

```
template<typename FPTYPE>
inline void _DP_DeepTensorComputeTensorNList(DP_DeepTensor *dt, const int natom, const FPTYPE
                                                *coord, const int *atype, const FPTYPE *cell, const int
                                                nghost, const DP_Nlist *nlist, FPTYPE **tensor, int
                                                *size)
```

Specialized Template Function _DP_DeepTensorComputeTensorNList< double >

- Defined in file_source_api_c_include_deepmd.hpp

Function Documentation

```
template<>
inline void _DP_DeepTensorComputeTensorNList<double>(DP_DeepTensor *dt, const int natom, const
                                                       double *coord, const int *atype, const double
                                                       *cell, const int nghost, const DP_Nlist *nlist,
                                                       double **tensor, int *size)
```

Specialized Template Function _DP_DeepTensorComputeTensorNList< float >

- Defined in file_source_api_c_include_deepmd.hpp

Function Documentation

```
template<>
inline void _DP_DeepTensorComputeTensorNList<float>(DP_DeepTensor *dt, const int natom, const float
                                                       *coord, const int *atype, const float *cell, const
                                                       int nghost, const DP_Nlist *nlist, float **tensor,
                                                       int *size)
```

Template Function `_DP_DipoleChargeModifierComputeNList`

- Defined in file `_source_api_c_include_deepmd.hpp`

Function Documentation

```
template<typename FPTYPE>
inline void _DP_DipoleChargeModifierComputeNList(DP_DipoleChargeModifier *dcm, const int natom,
                                                  const FPTYPE *coord, const int *atype, const
                                                  FPTYPE *cell, const int *pairs, const int npairs,
                                                  const FPTYPE *delef_, const int nghost, const
                                                  DP_Nlist *nlist, FPTYPE *dfcorr_, FPTYPE
                                                  *dvcorr_)
```

Specialized Template Function `_DP_DipoleChargeModifierComputeNList< double >`

- Defined in file `_source_api_c_include_deepmd.hpp`

Function Documentation

```
template<>
inline void _DP_DipoleChargeModifierComputeNList<double>(DP_DipoleChargeModifier *dcm, const
                                                          int natom, const double *coord, const int
                                                          *atype, const double *cell, const int
                                                          *pairs, const int npairs, const double
                                                          *delef_, const int nghost, const DP_Nlist
                                                          *nlist, double *dfcorr_, double *dvcorr_)
```

Specialized Template Function `_DP_DipoleChargeModifierComputeNList< float >`

- Defined in file `_source_api_c_include_deepmd.hpp`

Function Documentation

```
template<>
inline void _DP_DipoleChargeModifierComputeNList<float>(DP_DipoleChargeModifier *dcm, const int
                                                         natom, const float *coord, const int *atype,
                                                         const float *cell, const int *pairs, const int
                                                         npairs, const float *delef_, const int nghost,
                                                         const DP_Nlist *nlist, float *dfcorr_, float
                                                         *dvcorr_)
```

Function `_DP_Get_Energy_Pointer(std::vector<double>&, const int)`

- Defined in file `_source_api_c_include_deepmd.hpp`

Function Documentation

inline double `*_DP_Get_Energy_Pointer`(std::vector<double> &vec, const int nframes)

Function `_DP_Get_Energy_Pointer(double&, const int)`

- Defined in file `_source_api_c_include_deepmd.hpp`

Function Documentation

inline double `*_DP_Get_Energy_Pointer`(double &vec, const int nframes)

Function `deepmd::hpp::convert_nlist`

- Defined in file `_source_api_c_include_deepmd.hpp`

Function Documentation

inline void `deepmd::hpp::convert_nlist`([InputNlist](#) &to_nlist, std::vector<std::vector<int>> &from_nlist)

Convert int vector to [InputNlist](#).

Parameters

- `to_nlist` – [out] [InputNlist](#).
- `from_nlist` – [in] 2D int vector. The first axis represents the central atoms and the second axis represents the neighbor atoms.

Function `deepmd::hpp::convert_pbtxt_to_pb`

- Defined in file `_source_api_c_include_deepmd.hpp`

Function Documentation

inline void `deepmd::hpp::convert_pbtxt_to_pb`(std::string fn_pb_txt, std::string fn_pb)

Convert pbtxt to pb.

Parameters

- `fn_pb_txt` – [in] Filename of the pb txt file.
- `fn_pb` – [in] Filename of the pb file.

Function `deepmd::hpp::read_file_to_string`

- Defined in `file_source_api_c_include_deepmd.hpp`

Function Documentation

`inline void deepmd::hpp::read_file_to_string(std::string model, std::string &file_content)`

Read model file to a string.

Parameters

- **model** – [in] Path to the model.
- **file_content** – [out] Content of the model file.

Template Function `deepmd::hpp::select_by_type`

- Defined in `file_source_api_c_include_deepmd.hpp`

Function Documentation

`template<typename VALUETYPE>`

`void deepmd::hpp::select_by_type(std::vector<int> &fwd_map, std::vector<int> &bkw_map, int
 &nghost_real, const std::vector<VALUETYPE> &dcoord_, const
 std::vector<int> &dtype_, const int &nghost, const
 std::vector<int> &sel_type_)`

Get forward and backward map of selected atoms by atom types.

Parameters

- **fwd_map** – [out] The forward map with size `natoms`.
- **bkw_map** – [out] The backward map with size `nreal`.
- **nghost_real** – [out] The number of selected ghost atoms.
- **dcoord_** – [in] The coordinates of all atoms. Reserved for compatibility.
- **dtype_** – [in] The atom types of all atoms.
- **nghost** – [in] The number of ghost atoms.
- **sel_type_** – [in] The selected atom types.

Template Function `deepmd::hpp::select_map`

- Defined in `file_source_api_c_include_deepmd.hpp`

Function Documentation

```
template<typename VT>
void deepmd::hpp::select_map(std::vector<VT> &out, const std::vector<VT> &in, const
                             std::vector<int> &fwd_map, const int &stride)
```

Apply the given map to a vector. Assume nframes is 1.

Template Parameters

VT – The value type of the vector. Only support int.

Parameters

- **out** – [out] The output vector.
- **in** – [in] The input vector.
- **fwd_map** – [in] The map.
- **stride** – [in] The stride of the input vector.

Function DP_ConvertPbtxtToPb

- Defined in file_source_api_c_include_c_api.h

Function Documentation

```
void DP_ConvertPbtxtToPb(const char *c_pbtxt, const char *c_pb)
```

Convert PBtxt to PB.

Parameters

- **c_pbtxt** – [in] The name of the PBtxt file.
- **c_pb** – [in] The name of the PB file.

Function DP_DeepPotCheckOK

- Defined in file_source_api_c_include_c_api.h

Function Documentation

```
const char *DP_DeepPotCheckOK(DP_DeepPot *dp)
```

Check if there is any exceptions throw.

Parameters

dp – The DP to use.

Returns

const char* error message.

Function DP_DeepPotCompute

- Defined in file `_source_api_c_include_c_api.h`

Function Documentation

```
void DP_DeepPotCompute(DP_DeepPot *dp, const int natom, const double *coord, const int *atype, const
                        double *cell, double *energy, double *force, double *virial, double
                        *atomic_energy, double *atomic_virial)
```

Evaluate the energy, force and virial by using a DP. (double version)

Attention

The number of frames is assumed to be 1.

Warning: The output arrays should be allocated before calling this function. Pass NULL if not required.

Parameters

- **dp** – [in] The DP to use.
- **natoms** – [in] The number of atoms.
- **coord** – [in] The coordinates of atoms. The array should be of size `natoms x 3`.
- **atype** – [in] The atom types. The array should contain `natoms` ints.
- **box** – [in] The cell of the region. The array should be of size 9. Pass NULL if pbc is not used.
- **energy** – [out] Output energy.
- **force** – [out] Output force. The array should be of size `natoms x 3`.
- **virial** – [out] Output virial. The array should be of size 9.
- **atomic_energy** – [out] Output atomic energy. The array should be of size `natoms`.
- **atomic_virial** – [out] Output atomic virial. The array should be of size `natoms x 9`.

Function DP_DeepPotCompute2

- Defined in file `_source_api_c_include_c_api.h`

Function Documentation

```
void DP_DeepPotCompute2(DP_DeepPot *dp, const int nframes, const int natom, const double *coord, const
                        int *atype, const double *cell, const double *fparam, const double *aparam,
                        double *energy, double *force, double *virial, double *atomic_energy, double
                        *atomic_virial)
```

Evaluate the energy, force and virial by using a DP. (double version)

Version
2

Warning: The output arrays should be allocated before calling this function. Pass NULL if not required.

Parameters

- **dp** – [in] The DP to use.
- **nframes** – [in] The number of frames.
- **natoms** – [in] The number of atoms.
- **coord** – [in] The coordinates of atoms. The array should be of size natoms x 3.
- **atype** – [in] The atom types. The array should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size 9. Pass NULL if pbc is not used.
- **fparam** – [in] The frame parameters. The array can be of size nframes x dim_fparam.
- **aparam** – [in] The atom parameters. The array can be of size nframes x dim_aparam.
- **energy** – [out] Output energy.
- **force** – [out] Output force. The array should be of size natoms x 3.
- **virial** – [out] Output virial. The array should be of size 9.
- **atomic_energy** – [out] Output atomic energy. The array should be of size natoms.
- **atomic_virial** – [out] Output atomic virial. The array should be of size natoms x 9.

Function DP_DeepPotComputeF

- Defined in file_source_api_c_include_c_api.h

Function Documentation

```
void DP_DeepPotComputeF(DP_DeepPot *dp, const int natom, const float *coord, const int *atype, const
                        float *cell, double *energy, float *force, float *virial, float *atomic_energy, float
                        *atomic_virial)
```

Evaluate the energy, force and virial by using a DP. (float version)

Attention

The number of frames is assumed to be 1.

Warning: The output arrays should be allocated before calling this function. Pass NULL if not required.

Parameters

- **dp** – [in] The DP to use.
- **natoms** – [in] The number of atoms.
- **coord** – [in] The coordinates of atoms. The array should be of size natoms x 3.
- **atype** – [in] The atom types. The array should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size 9. Pass NULL if pbc is not used.
- **energy** – [out] Output energy.
- **force** – [out] Output force. The array should be of size natoms x 3.
- **virial** – [out] Output virial. The array should be of size 9.
- **atomic_energy** – [out] Output atomic energy. The array should be of size natoms.
- **atomic_virial** – [out] Output atomic virial. The array should be of size natoms x 9.

Function DP_DeepPotComputeF2

- Defined in file_source_api_c_include_c_api.h

Function Documentation

```
void DP_DeepPotComputeF2(DP_DeepPot *dp, const int nframes, const int natom, const float *coord, const
                        int *atype, const float *cell, const float *fparam, const float *aparam, double
                        *energy, float *force, float *virial, float *atomic_energy, float *atomic_virial)
```

Evaluate the energy, force and virial by using a DP. (float version)

Version

2

Warning: The output arrays should be allocated before calling this function. Pass NULL if not required.

Parameters

- **dp** – [in] The DP to use.
- **nframes** – [in] The number of frames.
- **natoms** – [in] The number of atoms.
- **coord** – [in] The coordinates of atoms. The array should be of size natoms x 3.
- **atype** – [in] The atom types. The array should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size 9. Pass NULL if pbc is not used.
- **fparam** – [in] The frame parameters. The array can be of size nframes x dim_fparam.
- **aparam** – [in] The atom parameters. The array can be of size nframes x dim_aparam.
- **energy** – [out] Output energy.
- **force** – [out] Output force. The array should be of size natoms x 3.
- **virial** – [out] Output virial. The array should be of size 9.
- **atomic_energy** – [out] Output atomic energy. The array should be of size natoms.
- **atomic_virial** – [out] Output atomic virial. The array should be of size natoms x 9.

Function DP_DeepPotComputeMixedType

- Defined in file_source_api_c_include_c_api.h

Function Documentation

```
void DP_DeepPotComputeMixedType(DP_DeepPot *dp, const int nframes, const int natoms, const double
                                *coord, const int *atype, const double *cell, const double *fparam,
                                const double *aparam, double *energy, double *force, double *virial,
                                double *atomic_energy, double *atomic_virial)
```

Evaluate the energy, force and virial by using a DP with the mixed type. (double version)

Warning: The output arrays should be allocated before calling this function. Pass NULL if not required.

Parameters

- **dp** – [in] The DP to use.
- **nframes** – [in] The number of frames.
- **natoms** – [in] The number of atoms.
- **coord** – [in] The coordinates of atoms. The array should be of size natoms x 3.
- **atype** – [in] The atom types. The array should contain nframes x natoms ints.

- **box** – [in] The cell of the region. The array should be of size 9. Pass NULL if pbc is not used.
- **fparam** – [in] The frame parameters. The array can be of size nframes x dim_fparam.
- **aparam** – [in] The atom parameters. The array can be of size nframes x dim_aparam.
- **energy** – [out] Output energy.
- **force** – [out] Output force. The array should be of size natoms x 3.
- **virial** – [out] Output virial. The array should be of size 9.
- **atomic_energy** – [out] Output atomic energy. The array should be of size natoms.
- **atomic_virial** – [out] Output atomic virial. The array should be of size natoms x 9.

Function DP_DeepPotComputeMixedTypef

- Defined in file_source_api_c_include_c_api.h

Function Documentation

```
void DP_DeepPotComputeMixedTypef (DP_DeepPot *dp, const int nframes, const int natoms, const float
                                   *coord, const int *atype, const float *cell, const float *fparam, const
                                   float *aparam, double *energy, float *force, float *virial, float
                                   *atomic_energy, float *atomic_virial)
```

Evaluate the energy, force and virial by using a DP with the mixed type. (float version)

Warning: The output arrays should be allocated before calling this function. Pass NULL if not required.

Parameters

- **dp** – [in] The DP to use.
- **nframes** – [in] The number of frames.
- **natoms** – [in] The number of atoms.
- **coord** – [in] The coordinates of atoms. The array should be of size natoms x 3.
- **atype** – [in] The atom types. The array should contain nframes x natoms ints.
- **box** – [in] The cell of the region. The array should be of size 9. Pass NULL if pbc is not used.
- **fparam** – [in] The frame parameters. The array can be of size nframes x dim_fparam.
- **aparam** – [in] The atom parameters. The array can be of size nframes x dim_aparam.
- **energy** – [out] Output energy.
- **force** – [out] Output force. The array should be of size natoms x 3.
- **virial** – [out] Output virial. The array should be of size 9.
- **atomic_energy** – [out] Output atomic energy. The array should be of size natoms.
- **atomic_virial** – [out] Output atomic virial. The array should be of size natoms x 9.

Function DP_DeepPotComputeNList

- Defined in file `_source_api_c_include_c_api.h`

Function Documentation

```
void DP_DeepPotComputeNList(DP_DeepPot *dp, const int natom, const double *coord, const int *atype,
                           const double *cell, const int nghost, const DP_Nlist *nlist, const int ago,
                           double *energy, double *force, double *virial, double *atomic_energy,
                           double *atomic_virial)
```

Evaluate the energy, force and virial by using a DP with the neighbor list. (double version)

Attention

The number of frames is assumed to be 1.

Warning: The output arrays should be allocated before calling this function. Pass NULL if not required.

Parameters

- **dp** – [in] The DP to use.
- **natoms** – [in] The number of atoms.
- **coord** – [in] The coordinates of atoms. The array should be of size `natoms x 3`.
- **atype** – [in] The atom types. The array should contain `natoms` ints.
- **box** – [in] The cell of the region. The array should be of size 9. Pass NULL if pbc is not used.
- **nghost** – [in] The number of ghost atoms.
- **nlist** – [in] The neighbor list.
- **ago** – [in] Update the internal neighbour list if ago is 0.
- **energy** – [out] Output energy.
- **force** – [out] Output force. The array should be of size `natoms x 3`.
- **virial** – [out] Output virial. The array should be of size 9.
- **atomic_energy** – [out] Output atomic energy. The array should be of size `natoms`.
- **atomic_virial** – [out] Output atomic virial. The array should be of size `natoms x 9`.

Function DP_DeepPotComputeNList2

- Defined in file `_source_api_c_include_c_api.h`

Function Documentation

```
void DP_DeepPotComputeNList2(DP_DeepPot *dp, const int nframes, const int natom, const double
                             *coord, const int *atype, const double *cell, const int nghost, const
                             DP_Nlist *nlist, const int ago, const double *fparam, const double
                             *aparam, double *energy, double *force, double *virial, double
                             *atomic_energy, double *atomic_virial)
```

Evaluate the energy, force and virial by using a DP with the neighbor list. (double version)

Version
2

Warning: The output arrays should be allocated before calling this function. Pass NULL if not required.

Parameters

- **dp** – [in] The DP to use.
- **nframes** – [in] The number of frames.
- **natoms** – [in] The number of atoms.
- **coord** – [in] The coordinates of atoms. The array should be of size `natoms x 3`.
- **atype** – [in] The atom types. The array should contain `natoms` ints.
- **box** – [in] The cell of the region. The array should be of size 9. Pass NULL if pbc is not used.
- **nghost** – [in] The number of ghost atoms.
- **nlist** – [in] The neighbor list.
- **ago** – [in] Update the internal neighbour list if ago is 0.
- **fparam** – [in] The frame parameters. The array can be of size `nframes x dim_fparam`.
- **aparam** – [in] The atom parameters. The array can be of size `nframes x dim_aparam`.
- **energy** – [out] Output energy.
- **force** – [out] Output force. The array should be of size `natoms x 3`.
- **virial** – [out] Output virial. The array should be of size 9.
- **atomic_energy** – [out] Output atomic energy. The array should be of size `natoms`.
- **atomic_virial** – [out] Output atomic virial. The array should be of size `natoms x 9`.

Function DP_DeepPotComputeNListf

- Defined in file `_source_api_c_include_c_api.h`

Function Documentation

```
void DP_DeepPotComputeNListf(DP_DeepPot *dp, const int natom, const float *coord, const int *atype,
                             const float *cell, const int nghost, const DP_Nlist *nlist, const int ago,
                             double *energy, float *force, float *virial, float *atomic_energy, float
                             *atomic_virial)
```

Evaluate the energy, force and virial by using a DP with the neighbor list. (float version)

Attention

The number of frames is assumed to be 1.

Warning: The output arrays should be allocated before calling this function. Pass NULL if not required.

Parameters

- **dp** – [in] The DP to use.
- **natoms** – [in] The number of atoms.
- **coord** – [in] The coordinates of atoms. The array should be of size `natoms x 3`.
- **atype** – [in] The atom types. The array should contain `natoms` ints.
- **box** – [in] The cell of the region. The array should be of size 9. Pass NULL if pbc is not used.
- **nghost** – [in] The number of ghost atoms.
- **nlist** – [in] The neighbor list.
- **ago** – [in] Update the internal neighbour list if ago is 0.
- **energy** – [out] Output energy.
- **force** – [out] Output force. The array should be of size `natoms x 3`.
- **virial** – [out] Output virial. The array should be of size 9.
- **atomic_energy** – [out] Output atomic energy. The array should be of size `natoms`.
- **atomic_virial** – [out] Output atomic virial. The array should be of size `natoms x 9`.

Function DP_DeepPotComputeNListf2

- Defined in file `_source_api_c_include_c_api.h`

Function Documentation

```
void DP_DeepPotComputeNListf2(DP_DeepPot *dp, const int nframes, const int natom, const float *coord,
                             const int *atype, const float *cell, const int nghost, const DP_Nlist *nlist,
                             const int ago, const float *fparam, const float *aparam, double *energy,
                             float *force, float *virial, float *atomic_energy, float *atomic_virial)
```

Evaluate the energy, force and virial by using a DP with the neighbor list. (float version)

Version
2

Warning: The output arrays should be allocated before calling this function. Pass NULL if not required.

Parameters

- **dp** – [in] The DP to use.
- **nframes** – [in] The number of frames.
- **natoms** – [in] The number of atoms.
- **coord** – [in] The coordinates of atoms. The array should be of size `natoms x 3`.
- **atype** – [in] The atom types. The array should contain `natoms` ints.
- **box** – [in] The cell of the region. The array should be of size 9. Pass NULL if pbc is not used.
- **nghost** – [in] The number of ghost atoms.
- **nlist** – [in] The neighbor list.
- **ago** – [in] Update the internal neighbour list if ago is 0.
- **fparam** – [in] The frame parameters. The array can be of size `nframes x dim_fparam`.
- **aparam** – [in] The atom parameters. The array can be of size `nframes x dim_aparam`.
- **energy** – [out] Output energy.
- **force** – [out] Output force. The array should be of size `natoms x 3`.
- **virial** – [out] Output virial. The array should be of size 9.
- **atomic_energy** – [out] Output atomic energy. The array should be of size `natoms`.
- **atomic_virial** – [out] Output atomic virial. The array should be of size `natoms x 9`.

Function DP_DeepPotGetCutoff

- Defined in file_source_api_c_include_c_api.h

Function Documentation

double DP_DeepPotGetCutoff(DP_DeepPot *dp)

Get the type map of a DP.

Parameters

dp – [in] The DP to use.

Returns

The cutoff radius.

Function DP_DeepPotGetDimAParam

- Defined in file_source_api_c_include_c_api.h

Function Documentation

int DP_DeepPotGetDimAParam(DP_DeepPot *dp)

Get the dimension of atomic parameters of a DP.

Parameters

dp – [in] The DP to use.

Returns

The dimension of atomic parameters of the DP.

Function DP_DeepPotGetDimFParam

- Defined in file_source_api_c_include_c_api.h

Function Documentation

int DP_DeepPotGetDimFParam(DP_DeepPot *dp)

Get the dimension of frame parameters of a DP.

Parameters

dp – [in] The DP to use.

Returns

The dimension of frame parameters of the DP.

Function DP_DeepPotGetNumbTypes

- Defined in file_source_api_c_include_c_api.h

Function Documentation

int DP_DeepPotGetNumbTypes(DP_DeepPot *dp)

Get the number of types of a DP.

Parameters

dp – [in] The DP to use.

Returns

The number of types of the DP.

Function DP_DeepPotGetNumbTypesSpin

- Defined in file_source_api_c_include_c_api.h

Function Documentation

int DP_DeepPotGetNumbTypesSpin(DP_DeepPot *dp)

Get the number of types with spin of a DP.

Parameters

dp – [in] The DP to use.

Returns

The number of types with spin of the DP.

Function DP_DeepPotGetTypeMap

- Defined in file_source_api_c_include_c_api.h

Function Documentation

const char *DP_DeepPotGetTypeMap(DP_DeepPot *dp)

Get the type map of a DP.

Parameters

dp – [in] The DP to use.

Returns

The type map of the DP.

Function DP_DeepPotModelDeviCheckOK

- Defined in file_source_api_c_include_c_api.h

Function Documentation

```
const char *DP_DeepPotModelDeviCheckOK(DP_DeepPotModelDevi *dp)
```

Check if there is any exceptions throw.

Parameters

dp – The DP model deviation to use.

Returns

const char* error message.

Function DP_DeepPotModelDeviComputeNList

- Defined in file_source_api_c_include_c_api.h

Function Documentation

```
void DP_DeepPotModelDeviComputeNList(DP_DeepPotModelDevi *dp, const int natom, const double
                                     *coord, const int *atype, const double *cell, const int nghost,
                                     const DP_Nlist *nlist, const int ago, double *energy, double
                                     *force, double *virial, double *atomic_energy, double
                                     *atomic_virial)
```

Evaluate the energy, force and virial by using a DP model deviation with neighbor list. (double version)

Warning: The output arrays should be allocated before calling this function. Pass NULL if not required.

Parameters

- **dp** – [in] The DP model deviation to use.
- **natoms** – [in] The number of atoms.
- **coord** – [in] The coordinates of atoms. The array should be of size natoms x 3.
- **atype** – [in] The atom types. The array should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size 9. Pass NULL if pbc is not used.
- **nghost** – [in] The number of ghost atoms.
- **nlist** – [in] The neighbor list.
- **ago** – [in] Update the internal neighbour list if ago is 0.
- **energy** – [out] Output energy.
- **force** – [out] Output force. The array should be of size natoms x 3.
- **virial** – [out] Output virial. The array should be of size 9.

- **atomic_energy** – [out] Output atomic energy. The array should be of size natoms.
- **atomic_virial** – [out] Output atomic virial. The array should be of size natoms x 9.

Function DP_DeepPotModelDeviComputeNList2

- Defined in file_source_api_c_include_c_api.h

Function Documentation

```
void DP_DeepPotModelDeviComputeNList2(DP_DeepPotModelDevi *dp, const int nframes, const int
natoms, const double *coord, const int *atype, const double
*cell, const int nghost, const DP_Nlist *nlist, const int ago,
const double *fparam, const double *aparam, double *energy,
double *force, double *virial, double *atomic_energy, double
*atomic_virial)
```

Evaluate the energy, force and virial by using a DP model deviation with neighbor list. (double version)

Version
2

Warning: The output arrays should be allocated before calling this function. Pass NULL if not required.

Parameters

- **dp** – [in] The DP model deviation to use.
- **nframes** – [in] The number of frames. Only support 1 for now.
- **natoms** – [in] The number of atoms.
- **coord** – [in] The coordinates of atoms. The array should be of size natoms x 3.
- **atype** – [in] The atom types. The array should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size 9. Pass NULL if pbc is not used.
- **nghost** – [in] The number of ghost atoms.
- **nlist** – [in] The neighbor list.
- **ago** – [in] Update the internal neighbour list if ago is 0.
- **fparam** – [in] The frame parameters. The array can be of size nframes x dim_fparam.
- **aparam** – [in] The atom parameters. The array can be of size nframes x natoms x dim_aparam.
- **energy** – [out] Output energy.
- **force** – [out] Output force. The array should be of size natoms x 3.
- **virial** – [out] Output virial. The array should be of size 9.
- **atomic_energy** – [out] Output atomic energy. The array should be of size natoms.

- **atomic_virial** – [out] Output atomic virial. The array should be of size natoms x 9.

Function DP_DeepPotModelDeviComputeNListf

- Defined in file_source_api_c_include_c_api.h

Function Documentation

```
void DP_DeepPotModelDeviComputeNListf(DP_DeepPotModelDevi *dp, const int natom, const float
                                     *coord, const int *atype, const float *cell, const int nghost,
                                     const DP_Nlist *nlist, const int ago, double *energy, float
                                     *force, float *virial, float *atomic_energy, float *atomic_virial)
```

Evaluate the energy, force and virial by using a DP model deviation with neighbor list. (float version)

Warning: The output arrays should be allocated before calling this function. Pass NULL if not required.

Parameters

- **dp** – [in] The DP model deviation to use.
- **natoms** – [in] The number of atoms.
- **coord** – [in] The coordinates of atoms. The array should be of size natoms x 3.
- **atype** – [in] The atom types. The array should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size 9. Pass NULL if pbc is not used.
- **nghost** – [in] The number of ghost atoms.
- **nlist** – [in] The neighbor list.
- **ago** – [in] Update the internal neighbour list if ago is 0.
- **energy** – [out] Output energy.
- **force** – [out] Output force. The array should be of size natoms x 3.
- **virial** – [out] Output virial. The array should be of size 9.
- **atomic_energy** – [out] Output atomic energy. The array should be of size natoms.
- **atomic_virial** – [out] Output atomic virial. The array should be of size natoms x 9.

Function DP_DeepPotModelDeviComputeNListf2

- Defined in file_source_api_c_include_c_api.h

Function Documentation

```
void DP_DeepPotModelDeviComputeNListf2(DP_DeepPotModelDevi *dp, const int nframes, const int
    natoms, const float *coord, const int *atype, const float *cell,
    const int nghost, const DP_Nlist *nlist, const int ago, const
    float *fparam, const float *aparam, double *energy, float
    *force, float *virial, float *atomic_energy, float
    *atomic_virial)
```

Evaluate the energy, force and virial by using a DP model deviation with neighbor list. (float version)

Version
2

Warning: The output arrays should be allocated before calling this function. Pass NULL if not required.

Parameters

- **dp** – [in] The DP model deviation to use.
- **nframes** – [in] The number of frames. Only support 1 for now.
- **natoms** – [in] The number of atoms.
- **coord** – [in] The coordinates of atoms. The array should be of size natoms x 3.
- **atype** – [in] The atom types. The array should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size 9. Pass NULL if pbc is not used.
- **nghost** – [in] The number of ghost atoms.
- **nlist** – [in] The neighbor list.
- **ago** – [in] Update the internal neighbour list if ago is 0.
- **fparam** – [in] The frame parameters. The array can be of size nframes x dim_fparam.
- **aparam** – [in] The atom parameters. The array can be of size nframes x natoms x dim_aparam.
- **energy** – [out] Output energy.
- **force** – [out] Output force. The array should be of size natoms x 3.
- **virial** – [out] Output virial. The array should be of size 9.
- **atomic_energy** – [out] Output atomic energy. The array should be of size natoms.
- **atomic_virial** – [out] Output atomic virial. The array should be of size natoms x 9.

Function DP_DeepPotModelDeviGetCutoff

- Defined in file `_source_api_c_include_c_api.h`

Function Documentation

`double DP_DeepPotModelDeviGetCutoff(DP_DeepPotModelDevi *dp)`

Get the type map of a DP model deviation.

Parameters

dp – [in] The DP model deviation to use.

Returns

The cutoff radius.

Function DP_DeepPotModelDeviGetDimAParam

- Defined in file `_source_api_c_include_c_api.h`

Function Documentation

`int DP_DeepPotModelDeviGetDimAParam(DP_DeepPotModelDevi *dp)`

Get the dimension of atomic parameters of a DP Model Deviation.

Parameters

dp – [in] The DP Model Deviation to use.

Returns

The dimension of atomic parameters of the DP Model Deviation.

Function DP_DeepPotModelDeviGetDimFParam

- Defined in file `_source_api_c_include_c_api.h`

Function Documentation

`int DP_DeepPotModelDeviGetDimFParam(DP_DeepPotModelDevi *dp)`

Get the dimension of frame parameters of a DP Model Deviation.

Parameters

dp – [in] The DP Model Deviation to use.

Returns

The dimension of frame parameters of the DP Model Deviation.

Function DP_DeepPotModelDeviGetNumbTypes

- Defined in file_source_api_c_include_c_api.h

Function Documentation

```
int DP_DeepPotModelDeviGetNumbTypes(DP_DeepPotModelDevi *dp)
```

Get the number of types of a DP model deviation.

Parameters

dp – [in] The DP model deviation to use.

Returns

The number of types of the DP model deviation.

Function DP_DeepPotModelDeviGetNumbTypesSpin

- Defined in file_source_api_c_include_c_api.h

Function Documentation

```
int DP_DeepPotModelDeviGetNumbTypesSpin(DP_DeepPotModelDevi *dp)
```

Get the number of types with spin of a DP model deviation.

Parameters

dp – [in] The DP model deviation to use.

Returns

The number of types with spin of the DP model deviation.

Function DP_DeepTensorCheckOK

- Defined in file_source_api_c_include_c_api.h

Function Documentation

```
const char *DP_DeepTensorCheckOK(DP_DeepTensor *dt)
```

Check if there is any exceptions throw.

Parameters

dt – The Deep Tensor to use.

Returns

const char* error message.

Function DP_DeepTensorCompute

- Defined in file_source_api_c_include_c_api.h

Function Documentation

```
void DP_DeepTensorCompute(DP_DeepTensor *dt, const int natom, const double *coord, const int *atype,
                          const double *cell, double *global_tensor, double *force, double *virial,
                          double **atomic_tensor, double *atomic_virial, int *size_at)
```

Evaluate the global tensor, force and virial by using a DP. (double version)

Warning: The output arrays should be allocated before calling this function. Pass NULL if not required.

Parameters

- **dt** – [in] The Deep Tensor to use.
- **natoms** – [in] The number of atoms.
- **coord** – [in] The coordinates of atoms. The array should be of size natoms x 3.
- **atype** – [in] The atom types. The array should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size 9. Pass NULL if pbc is not used.
- **global_tensor** – [out] Output global tensor.
- **force** – [out] Output force. The array should be of size natoms x 3.
- **virial** – [out] Output virial. The array should be of size 9.
- **atomic_tensor** – [out] Output atomic tensor. The array should be of size natoms.
- **atomic_virial** – [out] Output atomic virial. The array should be of size natoms x 9.
- **size_at** – [out] Output size of atomic tensor.

Function DP_DeepTensorComputef

- Defined in file_source_api_c_include_c_api.h

Function Documentation

```
void DP_DeepTensorComputef(DP_DeepTensor *dt, const int natom, const float *coord, const int *atype,
                           const float *cell, float *global_tensor, float *force, float *virial, float
                           **atomic_tensor, float *atomic_virial, int *size_at)
```

Evaluate the global tensor, force and virial by using a DP. (float version)

Warning: The output arrays should be allocated before calling this function. Pass NULL if not required.

Parameters

- **dt** – [in] The Deep Tensor to use.
- **natoms** – [in] The number of atoms.
- **coord** – [in] The coordinates of atoms. The array should be of size natoms x 3.
- **atype** – [in] The atom types. The array should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size 9. Pass NULL if pbc is not used.
- **global_tensor** – [out] Output global tensor.
- **force** – [out] Output force. The array should be of size natoms x 3.
- **virial** – [out] Output virial. The array should be of size 9.
- **atomic_tensor** – [out] Output atomic tensor. The array should be of size natoms.
- **atomic_virial** – [out] Output atomic virial. The array should be of size natoms x 9.
- **size_at** – [out] Output size of atomic tensor.

Function DP_DeepTensorComputeNList

- Defined in file_source_api_c_include_c_api.h

Function Documentation

```
void DP_DeepTensorComputeNList(DP_DeepTensor *dt, const int natom, const double *coord, const int
                               *atype, const double *cell, const int nghost, const DP_Nlist *nlist,
                               double *global_tensor, double *force, double *virial, double
                               **atomic_tensor, double *atomic_virial, int *size_at)
```

Evaluate the global tensor, force and virial by using a DP with the neighbor list. (double version)

Warning: The output arrays should be allocated before calling this function. Pass NULL if not required.

Parameters

- **dt** – [in] The Deep Tensor to use.
- **natoms** – [in] The number of atoms.
- **coord** – [in] The coordinates of atoms. The array should be of size natoms x 3.
- **atype** – [in] The atom types. The array should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size 9. Pass NULL if pbc is not used.
- **nghost** – [in] The number of ghost atoms.
- **nlist** – [in] The neighbor list.
- **global_tensor** – [out] Output global tensor.
- **force** – [out] Output force. The array should be of size natoms x 3.

- **virial** – [out] Output virial. The array should be of size 9.
- **atomic_tensor** – [out] Output atomic tensor. The array should be of size natoms.
- **atomic_virial** – [out] Output atomic virial. The array should be of size natoms x 9.
- **size_at** – [out] Output size of atomic tensor.

Function DP_DeepTensorComputeNListf

- Defined in file_source_api_c_include_c_api.h

Function Documentation

```
void DP_DeepTensorComputeNListf(DP_DeepTensor *dt, const int natom, const float *coord, const int
                                *atype, const float *cell, const int nghost, const DP_Nlist *nlist, float
                                *global_tensor, float *force, float *virial, float **atomic_tensor, float
                                *atomic_virial, int *size_at)
```

Evaluate the global tensor, force and virial by using a DP with the neighbor list. (float version)

Warning: The output arrays should be allocated before calling this function. Pass NULL if not required.

Parameters

- **dt** – [in] The Deep Tensor to use.
- **natoms** – [in] The number of atoms.
- **coord** – [in] The coordinates of atoms. The array should be of size natoms x 3.
- **atype** – [in] The atom types. The array should contain natoms ints.
- **box** – [in] The cell of the region. The array should be of size 9. Pass NULL if pbc is not used.
- **nghost** – [in] The number of ghost atoms.
- **nlist** – [in] The neighbor list.
- **global_tensor** – [out] Output global tensor.
- **force** – [out] Output force. The array should be of size natoms x 3.
- **virial** – [out] Output virial. The array should be of size 9.
- **atomic_tensor** – [out] Output atomic tensor. The array should be of size natoms.
- **atomic_virial** – [out] Output atomic virial. The array should be of size natoms x 9.
- **size_at** – [out] Output size of atomic tensor.

Function `DP_DeepTensorComputeTensor`

- Defined in file `_source_api_c_include_c_api.h`

Function Documentation

```
void DP_DeepTensorComputeTensor(DP_DeepTensor *dt, const int natom, const double *coord, const int
                                *atype, const double *cell, double **tensor, int *size)
```

Evaluate the tensor by using a DP. (double version)

Parameters

- **dt** – [in] The Deep Tensor to use.
- **natoms** – [in] The number of atoms.
- **coord** – [in] The coordinates of atoms. The array should be of size `natoms x 3`.
- **atype** – [in] The atom types. The array should contain `natoms` ints.
- **box** – [in] The cell of the region. The array should be of size 9. Pass NULL if pbc is not used.
- **tensor** – [out] Output tensor.

Function `DP_DeepTensorComputeTensorf`

- Defined in file `_source_api_c_include_c_api.h`

Function Documentation

```
void DP_DeepTensorComputeTensorf(DP_DeepTensor *dt, const int natom, const float *coord, const int
                                  *atype, const float *cell, float **tensor, int *size)
```

Evaluate the tensor by using a DP. (float version)

Parameters

- **dt** – [in] The Deep Tensor to use.
- **natoms** – [in] The number of atoms.
- **coord** – [in] The coordinates of atoms. The array should be of size `natoms x 3`.
- **atype** – [in] The atom types. The array should contain `natoms` ints.
- **box** – [in] The cell of the region. The array should be of size 9. Pass NULL if pbc is not used.
- **tensor** – [out] Output tensor.
- **size** – [out] Output size of the tensor.

Function DP_DeepTensorComputeTensorNList

- Defined in file `_source_api_c_include_c_api.h`

Function Documentation

```
void DP_DeepTensorComputeTensorNList(DP_DeepTensor *dt, const int natom, const double *coord,
                                     const int *atype, const double *cell, const int nghost, const
                                     DP_Nlist *nlist, double **tensor, int *size)
```

Evaluate the tensor by using a DP with the neighbor list. (double version)

Parameters

- **dt** – [in] The Deep Tensor to use.
- **natoms** – [in] The number of atoms.
- **coord** – [in] The coordinates of atoms. The array should be of size `natoms x 3`.
- **atype** – [in] The atom types. The array should contain `natoms` ints.
- **box** – [in] The cell of the region. The array should be of size 9. Pass NULL if pbc is not used.
- **nghost** – [in] The number of ghost atoms.
- **nlist** – [in] The neighbor list.
- **tensor** – [out] Output tensor.
- **size** – [out] Output size of the tensor.

Function DP_DeepTensorComputeTensorNListf

- Defined in file `_source_api_c_include_c_api.h`

Function Documentation

```
void DP_DeepTensorComputeTensorNListf(DP_DeepTensor *dt, const int natom, const float *coord, const
                                       int *atype, const float *cell, const int nghost, const DP_Nlist
                                       *nlist, float **tensor, int *size)
```

Evaluate the tensor by using a DP with the neighbor list. (float version)

Parameters

- **dt** – [in] The Deep Tensor to use.
- **natoms** – [in] The number of atoms.
- **coord** – [in] The coordinates of atoms. The array should be of size `natoms x 3`.
- **atype** – [in] The atom types. The array should contain `natoms` ints.
- **box** – [in] The cell of the region. The array should be of size 9. Pass NULL if pbc is not used.
- **nghost** – [in] The number of ghost atoms.
- **nlist** – [in] The neighbor list.

- **tensor** – [out] Output tensor.
- **size** – [out] Output size of the tensor.

Function `DP_DeepTensorGetCutoff`

- Defined in `file_source_api_c_include_c_api.h`

Function Documentation

`double DP_DeepTensorGetCutoff(DP_DeepTensor *dt)`

Get the type map of a Deep Tensor.

Parameters

dt – [in] The Deep Tensor to use.

Returns

The cutoff radius.

Function `DP_DeepTensorGetNumbSelTypes`

- Defined in `file_source_api_c_include_c_api.h`

Function Documentation

`int DP_DeepTensorGetNumbSelTypes(DP_DeepTensor *dt)`

Get the number of sel types of a Deep Tensor.

Parameters

dt – [in] The Deep Tensor to use.

Returns

The number of sel types

Function `DP_DeepTensorGetNumbTypes`

- Defined in `file_source_api_c_include_c_api.h`

Function Documentation

`int DP_DeepTensorGetNumbTypes(DP_DeepTensor *dt)`

Get the type map of a Deep Tensor.

Parameters

dt – [in] The Deep Tensor to use.

Returns

The number of types of the Deep Tensor.

Function DP_DeepTensorGetOutputDim

- Defined in file_source_api_c_include_c_api.h

Function Documentation

int DP_DeepTensorGetOutputDim(DP_DeepTensor *dt)

Get the output dimension of a Deep Tensor.

Parameters

dt – [in] The Deep Tensor to use.

Returns

The output dimension of the Deep Tensor.

Function DP_DeepTensorGetSelTypes

- Defined in file_source_api_c_include_c_api.h

Function Documentation

int *DP_DeepTensorGetSelTypes(DP_DeepTensor *dt)

Get sel types of a Deep Tensor.

Parameters

dt – [in] The Deep Tensor to use.

Returns

The sel types

Function DP_DipoleChargeModifierCheckOK

- Defined in file_source_api_c_include_c_api.h

Function Documentation

const char *DP_DipoleChargeModifierCheckOK(DP_DipoleChargeModifier *dcm)

Check if there is any exceptions throw.

Parameters

dcm – The DipoleChargeModifier to use.

Returns

const char* error message.

Function `DP_DipoleChargeModifierComputeNList`

- Defined in file `_source_api_c_include_c_api.h`

Function Documentation

```
void DP_DipoleChargeModifierComputeNList(DP_DipoleChargeModifier *dcm, const int natom, const
                                         double *coord, const int *atype, const double *cell, const
                                         int *pairs, const int npairs, const double *delef_, const int
                                         nghost, const DP_Nlist *nlist, double *dfcorr_, double
                                         *dvcorr_)
```

Evaluate the force and virial correction by using a dipole charge modifier with the neighbor list. (double version)

Warning: The output arrays should be allocated before calling this function. Pass NULL if not required.

Parameters

- **dcm** – [in] The dipole charge modifier to use.
- **natoms** – [in] The number of atoms.
- **coord** – [in] The coordinates of atoms. The array should be of size `natoms x 3`.
- **atype** – [in] The atom types. The array should contain `natoms` ints.
- **cell** – [in] The cell of the region. The array should be of size 9. Pass NULL if pbc is not used.
- **pairs** – [in] The pairs of atoms. The list should contain `npairs` pairs of ints.
- **npairs** – [in] The number of pairs.
- **delef_** – [in] The electric field on each atom. The array should be of size `nframes x natoms x 3`.
- **nghost** – [in] The number of ghost atoms.
- **nlist** – [in] The neighbor list.
- **dfcorr_** – [out] Output force correction. The array should be of size `natoms x 3`.
- **dvcorr_** – [out] Output virial correction. The array should be of size 9.

Function `DP_DipoleChargeModifierComputeNListf`

- Defined in file `_source_api_c_include_c_api.h`

Function Documentation

```
void DP_DipoleChargeModifierComputeNListf(DP_DipoleChargeModifier *dcm, const int natom, const
float *coord, const int *atype, const float *cell, const int
*pairs, const int npairs, const float *delef_, const int
nghost, const DP_Nlist *nlist, float *dfcorr_, float
*dvcorr_)
```

Evaluate the force and virial correction by using a dipole charge modifier with the neighbor list. (float version)

Warning: The output arrays should be allocated before calling this function. Pass NULL if not required.

Parameters

- **dcm** – [in] The dipole charge modifier to use.
- **natoms** – [in] The number of atoms.
- **coord** – [in] The coordinates of atoms. The array should be of size natoms x 3.
- **atype** – [in] The atom types. The array should contain natoms ints.
- **cell** – [in] The cell of the region. The array should be of size 9. Pass NULL if pbc is not used.
- **pairs** – [in] The pairs of atoms. The list should contain npairs pairs of ints.
- **npairs** – [in] The number of pairs.
- **delef_** – [in] The electric field on each atom. The array should be of size nframes x natoms x 3.
- **nghost** – [in] The number of ghost atoms.
- **nlist** – [in] The neighbor list.
- **dfcorr_** – [out] Output force correction. The array should be of size natoms x 3.
- **dvcorr_** – [out] Output virial correction. The array should be of size 9.

Function DP_DipoleChargeModifierGetCutoff

- Defined in file_source_api_c_include_c_api.h

Function Documentation

```
double DP_DipoleChargeModifierGetCutoff(DP_DipoleChargeModifier *dt)
```

Get the type map of a DipoleChargeModifier.

Parameters

- dcm** – [in] The DipoleChargeModifier to use.

Returns

The cutoff radius.

Function DP_DipoleChargeModifierGetNumbSelTypes

- Defined in file `_source_api_c_include_c_api.h`

Function Documentation

```
int DP_DipoleChargeModifierGetNumbSelTypes(DP_DipoleChargeModifier *dt)
```

Get the number of sel types of a DipoleChargeModifier.

Parameters

dcm – [in] The DipoleChargeModifier to use.

Returns

The number of sel types

Function DP_DipoleChargeModifierGetNumbTypes

- Defined in file `_source_api_c_include_c_api.h`

Function Documentation

```
int DP_DipoleChargeModifierGetNumbTypes(DP_DipoleChargeModifier *dt)
```

Get the type map of a DipoleChargeModifier.

Parameters

dcm – [in] The DipoleChargeModifier to use.

Returns

The number of types of the DipoleChargeModifier.

Function DP_DipoleChargeModifierGetSelTypes

- Defined in file `_source_api_c_include_c_api.h`

Function Documentation

```
int *DP_DipoleChargeModifierGetSelTypes(DP_DipoleChargeModifier *dt)
```

Get sel types of a DipoleChargeModifier.

Parameters

dcm – [in] The DipoleChargeModifier to use.

Returns

The sel types

Function DP_NewDeepPot

- Defined in file_source_api_c_include_c_api.h

Function Documentation

`DP_DeepPot *DP_NewDeepPot(const char *c_model)`

DP constructor with initialization.

Parameters

c_model – [in] The name of the frozen model file.

Returns

A pointer to the deep potential.

Function DP_NewDeepPotModelDevi

- Defined in file_source_api_c_include_c_api.h

Function Documentation

`DP_DeepPotModelDevi *DP_NewDeepPotModelDevi(const char **c_models, int n_models)`

DP model deviation constructor with initialization.

Parameters

- **c_models** – [in] The array of the name of the frozen model file.
- **nmodels** – [in] The number of models.

Function DP_NewDeepPotModelDeviWithParam

- Defined in file_source_api_c_include_c_api.h

Function Documentation

`DP_DeepPotModelDevi *DP_NewDeepPotModelDeviWithParam(const char **c_model, const int n_models, const int gpu_rank, const char **c_file_contents, const int n_file_contents, const int *size_file_contents)`

DP model deviation constructor with initialization.

Parameters

- **c_models** – [in] The array of the name of the frozen model file.
- **nmodels** – [in] The number of models.
- **gpu_rank** – [in] The rank of the GPU.
- **c_file_contents** – [in] The contents of the model file.
- **n_file_contents** – [in] The number of the contents of the model file.

- **size_file_contents** – [in] The sizes of the contents of the model file.

Returns

DP_DeepPotModelDevi* A pointer to the deep potential model deviation.

Function DP_NewDeepPotWithParam

- Defined in file_source_api_c_include_c_api.h

Function Documentation

DP_DeepPot *DP_NewDeepPotWithParam(const char *c_model, const int gpu_rank, const char *c_file_content)

DP constructor with initialization.

Parameters

- **c_model** – The name of the frozen model file.
- **gpu_rank** – The rank of the GPU.
- **c_file_content** – Broken implementation. Use DP_NewDeepPotWithParam2 instead.

Returns

DP_DeepPot* A pointer to the deep potential.

Function DP_NewDeepPotWithParam2

- Defined in file_source_api_c_include_c_api.h

Function Documentation

DP_DeepPot *DP_NewDeepPotWithParam2(const char *c_model, const int gpu_rank, const char *c_file_content, const int size_file_content)

DP constructor with initialization.

Version

2

Parameters

- **c_model** – The name of the frozen model file.
- **gpu_rank** – The rank of the GPU.
- **c_file_content** – The content of the model file.
- **size_file_content** – The size of the model file.

Returns

DP_DeepPot* A pointer to the deep potential.

Function DP_NewDeepTensor

- Defined in file_source_api_c_include_c_api.h

Function Documentation

DP_DeepTensor *DP_NewDeepTensor(const char *c_model)

Deep Tensor constructor with initialization.

Parameters

c_model – [in] The name of the frozen model file.

Returns

A pointer to the deep tensor.

Function DP_NewDeepTensorWithParam

- Defined in file_source_api_c_include_c_api.h

Function Documentation

DP_DeepTensor *DP_NewDeepTensorWithParam(const char *c_model, const int gpu_rank, const char *c_name_scope)

Deep Tensor constructor with initialization.

Parameters

- **c_model** – The name of the frozen model file.
- **gpu_rank** – The rank of the GPU.
- **c_name_scope** – The name scope.

Returns

DP_DeepTensor* A pointer to the deep tensor.

Function DP_NewDipoleChargeModifier

- Defined in file_source_api_c_include_c_api.h

Function Documentation

DP_DipoleChargeModifier *DP_NewDipoleChargeModifier(const char *c_model)

Dipole charge modifier constructor with initialization.

Parameters

c_model – [in] The name of the frozen model file.

Returns

A pointer to the dipole charge modifier.

Function DP_NewDipoleChargeModifierWithParam

- Defined in file `_source_api_c_include_c_api.h`

Function Documentation

`DP_DipoleChargeModifier *DP_NewDipoleChargeModifierWithParam(const char *c_model, const int gpu_rank, const char *c_name_scope)`

Dipole charge modifier constructor with initialization.

Parameters

- **c_model** – The name of the frozen model file.
- **gpu_rank** – The rank of the GPU.
- **c_name_scope** – The name scope.

Returns

`DP_DipoleChargeModifier*` A pointer to the dipole charge modifier.

Function DP_NewNlist

- Defined in file `_source_api_c_include_c_api.h`

Function Documentation

`DP_Nlist *DP_NewNlist(int inum_, int *ilist_, int *numneigh_, int **firstneigh_)`

Create a new neighbor list.

Parameters

- **inum_** – [in] Number of core region atoms
- **Array** – [in] stores the core region atom's index
- **Array** – [in] stores the core region atom's neighbor atom number
- **Array** – [in] stores the core region atom's neighbor index

Returns

A pointer to the neighbor list.

Function DP_NlistCheckOK

- Defined in file `_source_api_c_include_c_api.h`

Function Documentation

const char ***DP_NlistCheckOK**(DP_Nlist *dp)

Check if there is any exceptions throw.

Parameters

dp – The neighbor list to use.

Returns

const char* error message.

Function DP_PrintSummary

- Defined in file_source_api_c_include_c_api.h

Function Documentation

void **DP_PrintSummary**(const char *c_pre)

Print the summary of DeePMD-kit, including the version and the build information.

Parameters

c_pre – [in] The prefix to each line.

Function DP_ReadFileToChar

- Defined in file_source_api_c_include_c_api.h

Function Documentation

const char ***DP_ReadFileToChar**(const char *c_model)

Read a file to a char array.

Parameters

c_model – [in] The name of the file.

Returns

const char* The char array.

Function DP_ReadFileToChar2

- Defined in file_source_api_c_include_c_api.h

Function Documentation

`const char *DP_ReadFileToChar2(const char *c_model, int *size)`

Read a file to a char array. This version can handle string with '\0'.

Version

2

Parameters

- **c_model** – [in] The name of the file.
- **size** – [out] The size of the char array.

Returns

`const char*` The char array.

Function DP_SelectByType

- Defined in `file_source_api_c_include_c_api.h`

Function Documentation

`void DP_SelectByType(const int natoms, const int *atype, const int nghost, const int nsel_type, const int *sel_type, int *fwd_map, int *nreal, int *bkw_map, int *nghost_real)`

Get forward and backward map of selected atoms by atom types.

Parameters

- **natoms** – [in] The number of atoms.
- **atype** – [in] The atom types of all atoms.
- **nghost** – [in] The number of ghost atoms.
- **nsel_type** – [in] The number of selected atom types.
- **sel_type** – [in] The selected atom types.
- **fwd_map** – [out] The forward map with size natoms.
- **nreal** – [out] The number of selected real atoms.
- **bkw_map** – [out] The backward map with size nreal.
- **nghost_real** – [out] The number of selected ghost atoms.

Function DP_SelectMapInt

- Defined in file_source_api_c_include_c_api.h

Function Documentation

void **DP_SelectMapInt**(const int *in, const int *fwd_map, const int stride, const int nall1, const int nall2, int *out)

Apply the given map to a vector. Assume nframes is 1.

Parameters

- **in** – [in] The input vector.
- **fwd_map** – [in] The map.
- **stride** – [in] The stride of the input vector.
- **nall1** – [in] The number of atoms in the input vector.
- **nall2** – [out] The number of atoms in the output vector.
- **out** – [out] The output vector.

20.3.4 Defines

Define DP_CHECK_OK

- Defined in file_source_api_c_include_deepmd.hpp

Define Documentation

DP_CHECK_OK(check_func, dp)

Check if any exceptions throw in the C++ API. Throw if possible.

Define DP_NEW_OK

- Defined in file_source_api_c_include_c_api_internal.h

Define Documentation

DP_NEW_OK(dpcls, xx)

Define DP_REQUIRES_OK

- Defined in file `_source_api_c_include_c_api_internal.h`

Define Documentation

`DP_REQUIRES_OK(dp, xx)`

20.3.5 Typedefs**Typedef DP_DeepPot**

- Defined in file `_source_api_c_include_c_api.h`

Typedef Documentation

typedef struct `DP_DeepPot` `DP_DeepPot`
The deep potential.

Typedef DP_DeepPotModelDevi

- Defined in file `_source_api_c_include_c_api.h`

Typedef Documentation

typedef struct `DP_DeepPotModelDevi` `DP_DeepPotModelDevi`
The deep potential model deviation.

Typedef DP_DeepTensor

- Defined in file `_source_api_c_include_c_api.h`

Typedef Documentation

typedef struct `DP_DeepTensor` `DP_DeepTensor`
The deep tensor.

Typedef DP_DipoleChargeModifier

- Defined in file_source_api_c_include_c_api.h

Typedef Documentation

typedef struct DP_DipoleChargeModifier DP_DipoleChargeModifier

The dipole charge modifier.

Typedef DP_Nlist

- Defined in file_source_api_c_include_c_api.h

Typedef Documentation

typedef struct DP_Nlist DP_Nlist

Neighbor list.

21.1 Class Hierarchy

- Namespace deepmd
 - Struct deepmd_exception
 - Struct deepmd_exception_oom
 - Template Struct EwaldParameters
 - Struct InputNlist
 - Template Struct Region
- Template Struct DescrptSeRGPUExecuteFunctor
- Template Struct GeluGPUExecuteFunctor
- Template Struct GeluGradGPUExecuteFunctor
- Template Struct GeluGradGradGPUExecuteFunctor
- Template Struct ProdForceSeAGPUExecuteFunctor
- Template Struct ProdForceSeRGPUExecuteFunctor
- Template Struct ProdVirialSeAGPUExecuteFunctor
- Template Struct ProdVirialSeRGPUExecuteFunctor
- Template Struct TabulateCheckerGPUExecuteFunctor
- Template Struct TabulateFusionGPUExecuteFunctor
- Template Struct TabulateFusionGradGPUExecuteFunctor
- Template Class SimulationRegion
- Union U_Flt64_Int64

21.2 File Hierarchy

- dir_source

- dir_source_lib

- *dir_source_lib_include

- file_source_lib_include_ComputeDescriptor.h
 - file_source_lib_include_coord.h
 - file_source_lib_include_device.h
 - file_source_lib_include_DeviceFunctor.h
 - file_source_lib_include_env_mat.h
 - file_source_lib_include_env_mat_nvnmd.h
 - file_source_lib_include_errors.h
 - file_source_lib_include_ewald.h
 - file_source_lib_include_fmt_nlist.h
 - file_source_lib_include_gelu.h
 - file_source_lib_include_gpu_cuda.h
 - file_source_lib_include_gpu_rocm.h
 - file_source_lib_include_map_aparam.h
 - file_source_lib_include_neighbor_list.h
 - file_source_lib_include_pair_tab.h
 - file_source_lib_include_pairwise.h
 - file_source_lib_include_prod_env_mat.h
 - file_source_lib_include_prod_env_mat_nvnmd.h
 - file_source_lib_include_prod_force.h
 - file_source_lib_include_prod_force_grad.h
 - file_source_lib_include_prod_virial.h
 - file_source_lib_include_prod_virial_grad.h
 - file_source_lib_include_region.h
 - file_source_lib_include_SimulationRegion.h
 - file_source_lib_include_SimulationRegion_Impl.h
 - file_source_lib_include_soft_min_switch.h
 - file_source_lib_include_soft_min_switch_force.h
 - file_source_lib_include_soft_min_switch_force_grad.h
 - file_source_lib_include_soft_min_switch_virial.h
 - file_source_lib_include_soft_min_switch_virial_grad.h
 - file_source_lib_include_switcher.h

- file_source_lib_include_tabulate.h
- file_source_lib_include_utilities.h

21.3 Full API

21.3.1 Namespaces

Namespace deepmd

Contents

- Classes
- Functions
- Variables

Classes

- Struct deepmd_exception
- Struct deepmd_exception_oom
- Template Struct EwaldParameters
- Struct InputNlist
- Template Struct Region

Functions

- Template Function deepmd::build_nlist_cpu
- Template Function deepmd::build_nlist_gpu
- Template Function deepmd::compute_cell_info
- Function deepmd::convert_nlist
- Function deepmd::convert_nlist_gpu_device
- Template Function deepmd::convert_to_inter_cpu
- Template Function deepmd::convert_to_inter_gpu
- Template Function deepmd::convert_to_phys_cpu
- Template Function deepmd::convert_to_phys_gpu
- Template Function deepmd::copy_coord_cpu
- Template Function deepmd::copy_coord_gpu
- Function deepmd::cos_switch(const double&, const double&, const double&)
- Function deepmd::cos_switch(double&, double&, const double&, const double&, const double&)

- Template Function `deepmd::cprod`
- Function `deepmd::cum_sum`
- Template Function `deepmd::delete_device_memory`
- Template Function `deepmd::dot1`
- Template Function `deepmd::dot2`
- Template Function `deepmd::dot3`
- Template Function `deepmd::dot4`
- Template Function `deepmd::dotmv3`
- Function `deepmd::DPGetDeviceCount`
- Function `deepmd::dprc_pairwise_map_cpu`
- Function `deepmd::DPSetDevice`
- Template Function `deepmd::env_mat_a_cpu`
- Template Function `deepmd::env_mat_a_nvnmnd_quantize_cpu`
- Function `deepmd::env_mat_nbor_update`
- Template Function `deepmd::env_mat_r_cpu`
- Template Function `deepmd::ewald_recip`
- Function `deepmd::filter_ftype_gpu_cuda`
- Template Function `deepmd::format_nbor_list_gpu_cuda`
- Template Function `deepmd::format_nlist_cpu`
- Function `deepmd::free_nlist_gpu_device`
- Template Function `deepmd::gelu_cpu`
- Template Function `deepmd::gelu_gpu_cuda`
- Template Function `deepmd::gelu_grad_cpu`
- Template Function `deepmd::gelu_grad_gpu_cuda`
- Template Function `deepmd::gelu_grad_grad_cpu`
- Template Function `deepmd::gelu_grad_grad_gpu_cuda`
- Function `deepmd::group_atoms_cpu`
- Template Function `deepmd::init_region_cpu`
- Template Function `deepmd::invsqrt`
- Specialized Template Function `deepmd::invsqrt< double >`
- Specialized Template Function `deepmd::invsqrt< float >`
- Template Function `deepmd::malloc_device_memory(FPTYPE *amp, const std::vector<FPTYPE>&)`
- Template Function `deepmd::malloc_device_memory(FPTYPE *amp, const int)`
- Template Function `deepmd::malloc_device_memory(FPTYPE *amp, std::vector<FPTYPE>&)`
- Template Function `deepmd::malloc_device_memory_sync(FPTYPE *amp, std::vector<FPTYPE>&)`

- Template Function `deepmd::malloc_device_memory_sync(FPTYPE *amp, const std::vector<FPTYPE>&)`
- Template Function `deepmd::malloc_device_memory_sync(FPTYPE *amp, const FPTYPE *, const int)`
- Template Function `deepmd::map_aparam_cpu`
- Function `deepmd::max_numneigh`
- Template Function `deepmd::memcpy_device_to_host(const FPTYPE *, std::vector<FPTYPE>&)`
- Template Function `deepmd::memcpy_device_to_host(const FPTYPE *, FPTYPE *, const int)`
- Template Function `deepmd::memcpy_device_to_host(FPTYPE *, std::vector<FPTYPE>&)`
- Template Function `deepmd::memcpy_host_to_device(FPTYPE *, const std::vector<FPTYPE>&)`
- Template Function `deepmd::memcpy_host_to_device(FPTYPE *, const FPTYPE *, const int)`
- Template Function `deepmd::memcpy_host_to_device(FPTYPE *, std::vector<FPTYPE>&)`
- Template Function `deepmd::memset_device_memory`
- Template Function `deepmd::normalize_coord_cpu`
- Template Function `deepmd::normalize_coord_gpu`
- Template Function `deepmd::pair_tab_cpu`
- Template Function `deepmd::prod_env_mat_a_cpu`
- Template Function `deepmd::prod_env_mat_a_gpu_cuda`
- Template Function `deepmd::prod_env_mat_a_nvnmmd_quantize_cpu`
- Template Function `deepmd::prod_env_mat_r_cpu`
- Template Function `deepmd::prod_env_mat_r_gpu_cuda`
- Template Function `deepmd::prod_force_a_cpu(FPTYPE *, const FPTYPE *, const FPTYPE *, const int *, const int, const int, const int, const int)`
- Template Function `deepmd::prod_force_a_cpu(FPTYPE *, const FPTYPE *, const FPTYPE *, const int *, const int, const int, const int, const int, const int, const int)`
- Template Function `deepmd::prod_force_a_gpu_cuda`
- Template Function `deepmd::prod_force_grad_a_cpu`
- Template Function `deepmd::prod_force_grad_a_gpu_cuda`
- Template Function `deepmd::prod_force_grad_r_cpu`
- Template Function `deepmd::prod_force_grad_r_gpu_cuda`
- Template Function `deepmd::prod_force_r_cpu`
- Template Function `deepmd::prod_force_r_gpu_cuda`
- Template Function `deepmd::prod_virial_a_cpu`
- Template Function `deepmd::prod_virial_a_gpu_cuda`
- Template Function `deepmd::prod_virial_grad_a_cpu`
- Template Function `deepmd::prod_virial_grad_a_gpu_cuda`
- Template Function `deepmd::prod_virial_grad_r_cpu`
- Template Function `deepmd::prod_virial_grad_r_gpu_cuda`

- Template Function `deepmd::prod_virial_r_cpu`
- Template Function `deepmd::prod_virial_r_gpu_cuda`
- Template Function `deepmd::soft_min_switch_cpu`
- Template Function `deepmd::soft_min_switch_force_cpu`
- Template Function `deepmd::soft_min_switch_force_grad_cpu`
- Template Function `deepmd::soft_min_switch_virial_cpu`
- Template Function `deepmd::soft_min_switch_virial_grad_cpu`
- Function `deepmd::spline3_switch`
- Template Function `deepmd::spline5_switch`
- Template Function `deepmd::tabulate_fusion_se_a_cpu`
- Template Function `deepmd::tabulate_fusion_se_a_gpu_cuda`
- Template Function `deepmd::tabulate_fusion_se_a_grad_cpu`
- Template Function `deepmd::tabulate_fusion_se_a_grad_gpu_cuda`
- Template Function `deepmd::tabulate_fusion_se_a_grad_grad_cpu`
- Template Function `deepmd::tabulate_fusion_se_a_grad_grad_gpu_cuda`
- Template Function `deepmd::tabulate_fusion_se_r_cpu`
- Template Function `deepmd::tabulate_fusion_se_r_gpu_cuda`
- Template Function `deepmd::tabulate_fusion_se_r_grad_cpu`
- Template Function `deepmd::tabulate_fusion_se_r_grad_gpu_cuda`
- Template Function `deepmd::tabulate_fusion_se_r_grad_grad_cpu`
- Template Function `deepmd::tabulate_fusion_se_r_grad_grad_gpu_cuda`
- Template Function `deepmd::tabulate_fusion_se_t_cpu`
- Template Function `deepmd::tabulate_fusion_se_t_gpu_cuda`
- Template Function `deepmd::tabulate_fusion_se_t_grad_cpu`
- Template Function `deepmd::tabulate_fusion_se_t_grad_gpu_cuda`
- Template Function `deepmd::tabulate_fusion_se_t_grad_grad_cpu`
- Template Function `deepmd::tabulate_fusion_se_t_grad_grad_gpu_cuda`
- Template Function `deepmd::test_encoding_decoding_nbor_info_gpu_cuda`
- Function `deepmd::use_nei_info_cpu`
- Function `deepmd::use_nei_info_gpu`
- Function `deepmd::use_nlist_map`
- Template Function `deepmd::volume_cpu`
- Template Function `deepmd::volume_gpu`

Variables

- Variable `deepmd::ElectrostaticConversion`

Namespace `std`

21.3.2 Classes and Structs

Struct `deepmd_exception`

- Defined in `file_source_lib_include_errors.h`

Inheritance Relationships

Base Type

- `public std::runtime_error`

Derived Type

- `public deepmd::deepmd_exception_oom (Struct deepmd_exception_oom)`

Struct Documentation

struct `deepmd_exception` : `public std::runtime_error`
 General DeePMD-kit exception. Throw if anything doesn't work.
 Subclassed by `deepmd::deepmd_exception_oom`

Public Functions

```
inline deepmd_exception()
inline deepmd_exception(const std::string &msg)
```

Struct `deepmd_exception_oom`

- Defined in `file_source_lib_include_errors.h`

Inheritance Relationships

Base Type

- `public deepmd::deepmd_exception (Struct deepmd_exception)`

Struct Documentation

struct `deepmd_exception_oom` : public `deepmd::deepmd_exception`

Public Functions

`inline deepmd_exception_oom()`

`inline deepmd_exception_oom(const std::string &msg)`

Template Struct `EwaldParameters`

- Defined in `file_source_lib_include_ewald.h`

Struct Documentation

template<typename `VALUETYPE`>

struct `EwaldParameters`

Public Members

`VALUETYPE rcut = 6.0`

`VALUETYPE beta = 2`

`VALUETYPE spacing = 4`

Struct `InputNlist`

- Defined in `file_source_lib_include_neighbor_list.h`

Struct Documentation

struct **InputNlist**

Construct **InputNlist** with the input LAMMPS nbor list info.

Public Functions

inline **InputNlist**()

inline **InputNlist**(int inum_, int *ilist_, int *numneigh_, int **firstneigh_)

inline ~**InputNlist**()

Public Members

int **inum**

Number of core region atoms.

int ***ilist**

Array stores the core region atom's index.

int ***numneigh**

Array stores the core region atom's neighbor atom number.

int ****firstneigh**

Array stores the core region atom's neighbor index.

Template Struct Region

- Defined in file_source_lib_include_region.h

Struct Documentation

template<typename **FPTYPE**>

struct **Region**

Public Functions

`Region()`

`~Region()`

Public Members

`FPTYPE *boxt`

`FPTYPE *rec_boxt`

Template Struct `DescrptSeRGPUExecuteFunctor`

- Defined in file `_source_lib_include_DeviceFunctor.h`

Struct Documentation

`template<typename FPTYPE>`

`struct DescrptSeRGPUExecuteFunctor`

Public Functions

`void operator() (const FPTYPE *coord, const int *type, const int *ilist, const int *jrange, const int *jlist, int *array_int, unsigned long long *array_longlong, const FPTYPE *avg, const FPTYPE *std, FPTYPE *descript, FPTYPE *descript_deriv, FPTYPE *rij, int *nlist, const int nloc, const int nall, const int nnei, const int ndescript, const float rcut_r, const float rcut_r_smth, const std::vector<int> sec_a, const bool fill_nei_a, const int MAGIC_NUMBER)`

Template Struct `GeluGPUExecuteFunctor`

- Defined in file `_source_lib_include_DeviceFunctor.h`

Struct Documentation

`template<typename FPTYPE>`

`struct GeluGPUExecuteFunctor`

Public Functions

void **operator()** (const `FPTYPE` *in, `FPTYPE` *out, const int size)

Template Struct `GeluGradGPUExecuteFunctor`

- Defined in file `_source_lib_include_DeviceFunctor.h`

Struct Documentation

```
template<typename FPTYPE>
struct GeluGradGPUExecuteFunctor
```

Public Functions

void **operator()** (const `FPTYPE` *dy, const `FPTYPE` *in, `FPTYPE` *out, const int size)

Template Struct `GeluGradGradGPUExecuteFunctor`

- Defined in file `_source_lib_include_DeviceFunctor.h`

Struct Documentation

```
template<typename FPTYPE>
struct GeluGradGradGPUExecuteFunctor
```

Public Functions

void **operator()** (const `FPTYPE` *dy, const `FPTYPE` *dy_, const `FPTYPE` *in, `FPTYPE` *out, const int size)

Template Struct `ProdForceSeAGPUExecuteFunctor`

- Defined in file `_source_lib_include_DeviceFunctor.h`

Struct Documentation

```
template<typename FPTYPE>
struct ProdForceSeAGPUExecuteFunctor
```

Public Functions

```
void operator() (FPTYPE *force, const FPTYPE *net_derive, const FPTYPE *in_deriv, const int
                 *nlist, const int nloc, const int nall, const int nnei, const int ndescript, const int
                 n_a_sel, const int n_a_shift)
```

Template Struct ProdForceSeRGPUExecuteFunctor

- Defined in file_source_lib_include_DeviceFunctor.h

Struct Documentation

```
template<typename FPTYPE>
```

```
struct ProdForceSeRGPUExecuteFunctor
```

Public Functions

```
void operator() (FPTYPE *force, const FPTYPE *net_derive, const FPTYPE *in_deriv, const int
                 *nlist, const int nloc, const int nall, const int nnei, const int ndescript)
```

Template Struct ProdVirialSeAGPUExecuteFunctor

- Defined in file_source_lib_include_DeviceFunctor.h

Struct Documentation

```
template<typename FPTYPE>
```

```
struct ProdVirialSeAGPUExecuteFunctor
```

Public Functions

```
void operator() (FPTYPE *virial, FPTYPE *atom_virial, const FPTYPE *net_deriv, const FPTYPE
                 *in_deriv, const FPTYPE *rij, const int *nlist, const int nloc, const int nall, const int
                 nnei, const int ndescript, const int n_a_sel, const int n_a_shift)
```

Template Struct ProdVirialSeRGPUExecuteFunctor

- Defined in file_source_lib_include_DeviceFunctor.h

Struct Documentation

```
template<typename FPTYPE>
```

```
struct ProdVirialSeRGPUExecuteFunctor
```

Public Functions

```
void operator() (FPTYPE *virial, FPTYPE *atom_virial, const FPTYPE *net_deriv, const FPTYPE
                *in_deriv, const FPTYPE *rij, const int *nlist, const int nloc, const int nall, const int
                nnei, const int ndescript)
```

Template Struct TabulateCheckerGPUExecuteFunctor

- Defined in file_source_lib_include_DeviceFunctor.h

Struct Documentation

```
template<typename FPTYPE>
```

```
struct TabulateCheckerGPUExecuteFunctor
```

Public Functions

```
void operator() (const FPTYPE *table_info, const FPTYPE *in, int *out, const int nloc, const int
                nnei)
```

Template Struct TabulateFusionGPUExecuteFunctor

- Defined in file_source_lib_include_DeviceFunctor.h

Struct Documentation

```
template<typename FPTYPE>
```

```
struct TabulateFusionGPUExecuteFunctor
```

Public Functions

```
void operator() (const FPTYPE *table, const FPTYPE *table_info, const FPTYPE *in, const
                FPTYPE *ff, const int nloc, const int nnei, const int last_layer_size, FPTYPE *out)
```

Template Struct `TabulateFusionGradGPUExecuteFunctor`

- Defined in file `_source_lib_include_DeviceFunctor.h`

Struct Documentation

```
template<typename FPTYPE>
struct TabulateFusionGradGPUExecuteFunctor
```

Public Functions

```
void operator() (const FPTYPE *table, const FPTYPE *table_info, const FPTYPE *in, const
                 FPTYPE *ff, const FPTYPE *dy, const int nloc, const int nnei, const int
                 last_layer_size, FPTYPE *dy_dx, FPTYPE *dy_df)
```

Template Class `SimulationRegion`

- Defined in file `_source_lib_include_SimulationRegion.h`

Class Documentation

```
template<typename VALUETYPE>
class SimulationRegion
```

Public Functions

```
inline void reinitBox(const double *boxv)
inline void affineTransform(const double *affine_map)
inline void reinitOrigin(const double *orig)
inline void reinitOrigin(const std::vector<double> &orig)
void backup()
void recover()
SimulationRegion()
~SimulationRegion()
inline double *getBoxTensor()
inline const double *getBoxTensor() const
inline double *getRecBoxTensor()
inline const double *getRecBoxTensor() const
```



```

inline double *getBoxOrigin()

inline const double *getBoxOrigin() const

inline double getVolume() const

inline void toFaceDistance(double *dd) const

inline void phys2Inter(double *i_v, const VALUETYPE *p_v) const

inline void inter2Phys(VALUETYPE *p_v, const double *i_v) const

inline bool isPeriodic(const int dim) const

inline double *getShiftVec(const int index = 0)

inline const double *getShiftVec(const int index = 0) const

inline int getShiftIndex(const int *idx) const

inline int getNullShiftIndex() const

inline void shiftCoord(const int *idx, VALUETYPE &x, VALUETYPE &y, VALUETYPE &z) const

inline void diffNearestNeighbor(const VALUETYPE *r0, const VALUETYPE *r1, VALUETYPE
                                *phys) const

inline virtual void diffNearestNeighbor(const VALUETYPE x0, const VALUETYPE y0, const
                                         VALUETYPE z0, const VALUETYPE x1, const
                                         VALUETYPE y1, const VALUETYPE z1, VALUETYPE
                                         &dx, VALUETYPE &dy, VALUETYPE &dz) const

inline virtual void diffNearestNeighbor(const VALUETYPE x0, const VALUETYPE y0, const
                                         VALUETYPE z0, const VALUETYPE x1, const
                                         VALUETYPE y1, const VALUETYPE z1, VALUETYPE
                                         &dx, VALUETYPE &dy, VALUETYPE &dz, int &shift_x,
                                         int &shift_y, int &shift_z) const

inline virtual void diffNearestNeighbor(const VALUETYPE x0, const VALUETYPE y0, const
                                         VALUETYPE z0, const VALUETYPE x1, const
                                         VALUETYPE y1, const VALUETYPE z1, VALUETYPE
                                         &dx, VALUETYPE &dy, VALUETYPE &dz,
                                         VALUETYPE &shift_x, VALUETYPE &shift_y,
                                         VALUETYPE &shift_z) const

```

Public Static Functions

```

static inline int compactIndex(const int *idx)

static inline int getNumbShiftVec()

static inline int getShiftVecTotalSize()

```

Protected Functions

```
void computeShiftVec()
```

```
inline double *getInterShiftVec(const int index = 0)
```

```
inline const double *getInterShiftVec(const int index = 0) const
```

Protected Attributes

```
double shift_vec[shift_vec_size]
```

```
double inter_shift_vec[shift_vec_size]
```

Protected Static Functions

```
static inline int index3to1(const int tx, const int ty, const int tz)
```

Protected Static Attributes

```
static const int SPACENDIM = 3
```

```
static const int DBOX_XX = 1
```

```
static const int DBOX_YY = 1
```

```
static const int DBOX_ZZ = 1
```

```
static const int NBOX_XX = DBOX_XX * 2 + 1
```

```
static const int NBOX_YY = DBOX_YY * 2 + 1
```

```
static const int NBOX_ZZ = DBOX_ZZ * 2 + 1
```

```
static const int shift_info_size = NBOX_XX * NBOX_YY * NBOX_ZZ
```

```
static const int shift_vec_size = SPACENDIM * shift_info_size
```

21.3.3 Unions

Union `U_Flt64_Int64`

- Defined in `file_source_lib_include_env_mat_nvnmd.h`

Union Documentation

```
union U_Flt64_Int64
```

Public Members

```
double nflt
```

```
int64_t nint
```

21.3.4 Functions

Template Function `add_flt_nvnmd`

- Defined in `file_source_lib_include_env_mat_nvnmd.h`

Function Documentation

```
template<class T>
void add_flt_nvnmd(T &y, T x1, T x2)
```

Function `build_nlist`(`std::vector<std::vector<int>>&`, `std::vector<std::vector<int>>&`, `const std::vector<double>&`, `const int&`, `const double&`, `const double&`, `const std::vector<int>&`, `const std::vector<int>&`, `const std::vector<int>&`, `const SimulationRegion<double>&`, `const std::vector<int>&`)

- Defined in `file_source_lib_include_neighbor_list.h`

Function Documentation

```
void build_nlist(std::vector<std::vector<int>> &nlist0, std::vector<std::vector<int>> &nlist1, const
    std::vector<double> &coord, const int &nloc, const double &rc0, const double &rc1,
    const std::vector<int> &nat_stt_, const std::vector<int> &nat_end_, const
    std::vector<int> &ext_stt_, const std::vector<int> &ext_end_, const
    SimulationRegion<double> &region, const std::vector<int> &global_grid)
```

Function `build_nlist(std::vector<std::vector<int>>&, std::vector<std::vector<int>>&, const std::vector<double>&, const double&, const double&, const std::vector<int>&, const SimulationRegion<double>&)`

- Defined in file_source_lib_include_neighbor_list.h

Function Documentation

void **build_nlist**(std::vector<std::vector<int>> &nlist0, std::vector<std::vector<int>> &nlist1, const std::vector<double> &coord, const double &rc0, const double &rc1, const std::vector<int> &grid, const SimulationRegion<double> ®ion)

Function `build_nlist(std::vector<std::vector<int>>&, std::vector<std::vector<int>>&, const std::vector<double>&, const std::vector<int>&, const std::vector<int>&, const double&, const double&, const std::vector<int>&, const SimulationRegion<double>&)`

- Defined in file_source_lib_include_neighbor_list.h

Function Documentation

void **build_nlist**(std::vector<std::vector<int>> &nlist0, std::vector<std::vector<int>> &nlist1, const std::vector<double> &coord, const std::vector<int> &sel0, const std::vector<int> &sel1, const double &rc0, const double &rc1, const std::vector<int> &grid, const SimulationRegion<double> ®ion)

Function `build_nlist(std::vector<std::vector<int>>&, std::vector<std::vector<int>>&, const std::vector<double>&, const double&, const double&, const SimulationRegion<double> *)`

- Defined in file_source_lib_include_neighbor_list.h

Function Documentation

void **build_nlist**(std::vector<std::vector<int>> &nlist0, std::vector<std::vector<int>> &nlist1, const std::vector<double> &coord, const double &rc0_, const double &rc1_, const SimulationRegion<double> *region = NULL)

Function `compute_descriptor(std::vector<double>&, std::vector<double>&, std::vector<double>&, const std::vector<double>&, const int&, const std::vector<int>&, const SimulationRegion<double>&, const bool&, const int&, const std::vector<int>&, const std::vector<int>&, const std::vector<int>&, const std::vector<int>&, const int, const int, const int, const int)`

- Defined in file_source_lib_include_ComputeDescriptor.h

Function Documentation

```
inline void compute_descriptor(std::vector<double> &descript_a, std::vector<double> &descript_r,
                                std::vector<double> &rot_mat, const std::vector<double> &posi, const
                                int &ntypes, const std::vector<int> &type, const
                                SimulationRegion<double> &region, const bool &b_pbc, const int
                                &i_idx, const std::vector<int> &fmt_nlist_a, const std::vector<int>
                                &fmt_nlist_r, const std::vector<int> &sec_a, const std::vector<int>
                                &sec_r, const int axis0_type, const int axis0_idx, const int axis1_type,
                                const int axis1_idx)
```

Function `compute_descriptor`(std::vector<double>&, std::vector<double>&, std::vector<double>&, std::vector<double>&, std::vector<double>&, std::vector<double>&, const std::vector<double>&, const int&, const std::vector<int>&, const [SimulationRegion](#)<double>&, const bool&, const int&, const std::vector<int>&, const std::vector<int>&, const std::vector<int>&, const std::vector<int>&, const int, const int, const int, const int)

- Defined in file_source_lib_include_ComputeDescriptor.h

Function Documentation

```
inline void compute_descriptor(std::vector<double> &descript_a, std::vector<double>
                                &descript_a_deriv, std::vector<double> &descript_r,
                                std::vector<double> &descript_r_deriv, std::vector<double> &rrij_a,
                                std::vector<double> &rrij_r, std::vector<double> &rot_mat, const
                                std::vector<double> &posi, const int &ntypes, const std::vector<int>
                                &type, const SimulationRegion<double> &region, const bool &b_pbc,
                                const int &i_idx, const std::vector<int> &fmt_nlist_a, const
                                std::vector<int> &fmt_nlist_r, const std::vector<int> &sec_a, const
                                std::vector<int> &sec_r, const int axis0_type, const int axis0_idx, const
                                int axis1_type, const int axis1_idx)
```

Function `compute_descriptor_se_a_ef_para`

- Defined in file_source_lib_include_ComputeDescriptor.h

Function Documentation

```
inline void compute_descriptor_se_a_ef_para(std::vector<double> &descript_a, std::vector<double>
                                &descript_a_deriv, std::vector<double> &rrij_a, const
                                std::vector<double> &posi, const int &ntypes, const
                                std::vector<int> &type, const
                                SimulationRegion<double> &region, const bool &b_pbc,
                                const std::vector<double> &efield, const int &i_idx, const
                                std::vector<int> &fmt_nlist_a, const std::vector<int>
                                &sec_a, const double &rmin, const double &rmax)
```

Function `compute_descriptor_se_a_ef_vert`

- Defined in file `_source_lib_include_ComputeDescriptor.h`

Function Documentation

```
inline void compute_descriptor_se_a_ef_vert(std::vector<double> &descript_a, std::vector<double>
&descript_a_deriv, std::vector<double> &rij_a, const
std::vector<double> &posi, const int &ntypes, const
std::vector<int> &type, const
SimulationRegion<double> &region, const bool &b_pbc,
const std::vector<double> &efield, const int &i_idx, const
std::vector<int> &fmt_nlist_a, const std::vector<int>
&sec_a, const double &rmin, const double &rmax)
```

Function `compute_descriptor_se_a_extf`

- Defined in file `_source_lib_include_ComputeDescriptor.h`

Function Documentation

```
inline void compute_descriptor_se_a_extf(std::vector<double> &descript_a, std::vector<double>
&descript_a_deriv, std::vector<double> &rij_a, const
std::vector<double> &posi, const int &ntypes, const
std::vector<int> &type, const SimulationRegion<double>
&region, const bool &b_pbc, const std::vector<double>
&efield, const int &i_idx, const std::vector<int>
&fmt_nlist_a, const std::vector<int> &sec_a, const double
&rmin, const double &rmax)
```

Function `compute_dRdT`

- Defined in file `_source_lib_include_ComputeDescriptor.h`

Function Documentation

Warning: doxygenfunction: Unable to resolve function “compute_dRdT” with arguments (double (*), const double*, const double*, const double*) in doxygen xml output for project “core” from directory: `_build/core/xml/`. Potential matches:

```
- void compute_dRdT(double (*dRdT)[9], const double *r1, const double *r2, const double *rot)
```

Function compute_dRdT_1

- Defined in file_source_lib_include_ComputeDescriptor.h

Function Documentation

Warning: doxygenfunction: Unable to resolve function “compute_dRdT_1” with arguments (double (*), const double*, const double*, const double*) in doxygen xml output for project “core” from directory: _build/core/xml/. Potential matches:

```
- void compute_dRdT_1(double (*dRdT)[9], const double *r1, const double *r2, const double *rot)
```

Function compute_dRdT_2

- Defined in file_source_lib_include_ComputeDescriptor.h

Function Documentation

Warning: doxygenfunction: Unable to resolve function “compute_dRdT_2” with arguments (double (*), const double*, const double*, const double*) in doxygen xml output for project “core” from directory: _build/core/xml/. Potential matches:

```
- void compute_dRdT_2(double (*dRdT)[9], const double *r1, const double *r2, const double *rot)
```

Function copy_coord

- Defined in file_source_lib_include_neighbor_list.h

Function Documentation

```
void copy_coord(std::vector<double> &out_c, std::vector<int> &out_t, std::vector<int> &mapping,
               std::vector<int> &ncell, std::vector<int> &ngcell, const std::vector<double> &in_c,
               const std::vector<int> &in_t, const double &rc, const SimulationRegion<double>
               &region)
```

Template Function `deepmd::build_nlist_cpu`

- Defined in file `_source_lib_include_neighbor_list.h`

Function Documentation

```
template<typename FPTYPE>
int deepmd::build_nlist_cpu(InputNlist &nlist, int *max_list_size, const FPTYPE *c_cpy, const int
                           &nloc, const int &nall, const int &mem_size, const float &rcut)
```

Template Function `deepmd::build_nlist_gpu`

- Defined in file `_source_lib_include_neighbor_list.h`

Function Documentation

```
template<typename FPTYPE>
int deepmd::build_nlist_gpu(InputNlist &nlist, int *max_list_size, int *nlist_data, const FPTYPE
                           *c_cpy, const int &nloc, const int &nall, const int &mem_size, const float
                           &rcut)
```

Template Function `deepmd::compute_cell_info`

- Defined in file `_source_lib_include_coord.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::compute_cell_info(int *cell_info, const float &rcut, const deepmd::Region<FPTYPE>
                              &region)
```

Function `deepmd::convert_nlist`

- Defined in file `_source_lib_include_neighbor_list.h`

Function Documentation

```
void deepmd::convert_nlist(InputNlist &to_nlist, std::vector<std::vector<int>> &from_nlist)
```

Construct the `InputNlist` with a two-dimensional vector.

Parameters

- **to_nlist** – `InputNlist` struct which stores the neighbor information of the core region atoms.
- **from_nlist** – Vector which stores the neighbor information of the core region atoms.

Function `deepmd::convert_nlist_gpu_device`

- Defined in file `_source_lib_include_neighbor_list.h`

Function Documentation

```
void deepmd::convert_nlist_gpu_device(InputNlist &gpu_nlist, InputNlist &cpu_nlist, int
                                     *&gpu_memory, const int &max_nbor_size)
```

Convert the a host memory `InputNlist` to a device memory `InputNlist`.

Parameters

- `cpu_nlist` – Host memory `InputNlist` struct which stores the neighbor information of the core region atoms
- `gpu_nlist` – Device memory `InputNlist` struct which stores the neighbor information of the core region atoms
- `gpu_memory` – Device array which stores the elements of `gpu_nlist`
- `max_nbor_size` –

Template Function `deepmd::convert_to_inter_cpu`

- Defined in file `_source_lib_include_region.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::convert_to_inter_cpu(FPTYPE *ri, const Region<FPTYPE> &region, const FPTYPE
                                  *rp)
```

Template Function `deepmd::convert_to_inter_gpu`

- Defined in file `_source_lib_include_region.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::convert_to_inter_gpu(FPTYPE *ri, const Region<FPTYPE> &region, const FPTYPE
                                  *rp)
```

Template Function `deepmd::convert_to_phys_cpu`

- Defined in `file_source_lib_include_region.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::convert_to_phys_cpu(FPTYPE *rp, const Region<FPTYPE> &region, const FPTYPE *ri)
```

Template Function `deepmd::convert_to_phys_gpu`

- Defined in `file_source_lib_include_region.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::convert_to_phys_gpu(FPTYPE *rp, const Region<FPTYPE> &region, const FPTYPE *ri)
```

Template Function `deepmd::copy_coord_cpu`

- Defined in `file_source_lib_include_coord.h`

Function Documentation

```
template<typename FPTYPE>
int deepmd::copy_coord_cpu(FPTYPE *out_c, int *out_t, int *mapping, int *nall, const FPTYPE *in_c,
                           const int *in_t, const int &nloc, const int &mem_nall, const float &rcut,
                           const deepmd::Region<FPTYPE> &region)
```

Template Function `deepmd::copy_coord_gpu`

- Defined in `file_source_lib_include_coord.h`

Function Documentation

```
template<typename FPTYPE>
int deepmd::copy_coord_gpu(FPTYPE *out_c, int *out_t, int *mapping, int *nall, int *int_data, const
                           FPTYPE *in_c, const int *in_t, const int &nloc, const int &mem_nall, const
                           int &loc_cellnum, const int &total_cellnum, const int *cell_info, const
                           deepmd::Region<FPTYPE> &region)
```

Function `deepmd::cos_switch(const double&, const double&, const double&)`

- Defined in `file_source_lib_include_switcher.h`

Function Documentation

```
inline double deepmd::cos_switch(const double &xxx, const double &rmin, const double &rmax)
```

Function `deepmd::cos_switch(double&, double&, const double&, const double&, const double&)`

- Defined in `file_source_lib_include_switcher.h`

Function Documentation

```
inline void deepmd::cos_switch(double &vv, double &dd, const double &xxx, const double &rmin, const
                                double &rmax)
```

Template Function `deepmd::cprod`

- Defined in `file_source_lib_include_utilities.h`

Function Documentation

```
template<typename TYPE>
inline void deepmd::cprod(const TYPE *r0, const TYPE *r1, TYPE *r2)
```

Function `deepmd::cum_sum`

- Defined in `file_source_lib_include_utilities.h`

Function Documentation

```
void deepmd::cum_sum(std::vector<int> &zsec, const std::vector<int> &n_sel)
```

Template Function `deepmd::delete_device_memory`

- Defined in `file_source_lib_include_gpu_cuda.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::delete_device_memory(FPTYPE *&device)
```

Template Function `deepmd::dot1`

- Defined in `file_source_lib_include_utilities.h`

Function Documentation

```
template<typename TYPE>
inline TYPE deepmd::dot1(const TYPE *r0, const TYPE *r1)
```

Template Function `deepmd::dot2`

- Defined in `file_source_lib_include_utilities.h`

Function Documentation

```
template<typename TYPE>
inline TYPE deepmd::dot2(const TYPE *r0, const TYPE *r1)
```

Template Function `deepmd::dot3`

- Defined in `file_source_lib_include_utilities.h`

Function Documentation

```
template<typename TYPE>
inline TYPE deepmd::dot3(const TYPE *r0, const TYPE *r1)
```

Template Function `deepmd::dot4`

- Defined in `file_source_lib_include_utilities.h`

Function Documentation

```
template<typename TYPE>
inline TYPE deepmd::dot4(const TYPE *r0, const TYPE *r1)
```

Template Function `deepmd::dotmv3`

- Defined in file `_source_lib_include_utilities.h`

Function Documentation

```
template<typename TYPE>
inline void deepmd::dotmv3(TYPE *vec_o, const TYPE *tensor, const TYPE *vec_i)
```

Function `deepmd::DPGetDeviceCount`

- Defined in file `_source_lib_include_gpu_cuda.h`

Function Documentation

```
inline void deepmd::DPGetDeviceCount(int &gpu_num)
```

Function `deepmd::dprc_pairwise_map_cpu`

- Defined in file `_source_lib_include_pairwise.h`

Function Documentation

```
void deepmd::dprc_pairwise_map_cpu(std::vector<int> &forward_qm_map, std::vector<int>
                                   &backward_qm_map, std::vector<int> &forward_qmmm_map,
                                   std::vector<int> &backward_qmmm_map, int &nloc_qm, int
                                   &nloc_qmmm, int &nall_qm, int &nall_qmmm, const
                                   std::vector<std::vector<int>> &fragments, const int nloc, const
                                   int nall)
```

DPRc pairwise map.

Parameters

- **forward_qm_map** – [out] Forward map for QM atoms.
- **backward_qm_map** – [out] Backward map for QM atoms.
- **forward_qmmm_map** – [out] Forward map for QM/MM atoms.
- **backward_qmmm_map** – [out] Backward map for QM/MM atoms.
- **nloc_qm** – [out] The number of local QM atoms.
- **nloc_qmmm** – [out] The number of local QM/MM atoms.
- **nall_qm** – [out] The number of all QM atoms, including local and ghost atoms.
- **nall_qmmm** – [out] The number of all QM/MM atoms, including local and ghost atoms.
- **fragments** – [in] The indexes of atoms that each fragment contains. Assume that only the first fragment consists of QM atoms.
- **nloc** – [in] The number of local atoms.
- **nall** – [in] The number of all atoms, including local and ghost atoms.

Function `deepmd::DPSetDevice`

- Defined in `file_source_lib_include_gpu_cuda.h`

Function Documentation

```
inline cudaError_t deepmd::DPSetDevice(int rank)
```

Template Function `deepmd::env_mat_a_cpu`

- Defined in `file_source_lib_include_env_mat.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::env_mat_a_cpu(std::vector<FPTYPE> &descript_a, std::vector<FPTYPE>
    &descript_a_deriv, std::vector<FPTYPE> &rij_a, const
    std::vector<FPTYPE> &posi, const std::vector<int> &type, const int
    &i_idx, const std::vector<int> &fmt_nlist, const std::vector<int> &sec,
    const float &rmin, const float &rmax)
```

Template Function `deepmd::env_mat_a_nvnmnd_quantize_cpu`

- Defined in `file_source_lib_include_env_mat_nvnmnd.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::env_mat_a_nvnmnd_quantize_cpu(std::vector<FPTYPE> &descript_a,
    std::vector<FPTYPE> &descript_a_deriv,
    std::vector<FPTYPE> &rij_a, const
    std::vector<FPTYPE> &posi, const std::vector<int>
    &type, const int &i_idx, const std::vector<int>
    &fmt_nlist, const std::vector<int> &sec, const float
    &rmin, const float &rmax)
```

Function `deepmd::env_mat_nbor_update`

- Defined in `file_source_lib_include_prod_env_mat.h`

Function Documentation

void deepmd::env_mat_nbor_update(InputNlist &inlist, InputNlist &gpu_inlist, int &max_nbor_size, int *&nbor_list_dev, const int *mesh, const int size)

Template Function deepmd::env_mat_r_cpu

- Defined in file_source_lib_include_env_mat.h

Function Documentation

```
template<typename FPTYPE>
void deepmd::env_mat_r_cpu(std::vector<FPTYPE> &descript_a, std::vector<FPTYPE>
    &descript_a_deriv, std::vector<FPTYPE> &rij_a, const
    std::vector<FPTYPE> &posi, const std::vector<int> &type, const int
    &i_idx, const std::vector<int> &fmt_nlist_a, const std::vector<int>
    &sec_a, const float &rmin, const float &rmax)
```

Template Function deepmd::ewald_recp

- Defined in file_source_lib_include_ewald.h

Function Documentation

```
template<typename VALUETYPE>
void deepmd::ewald_recp(VALUETYPE &ener, std::vector<VALUETYPE> &force,
    std::vector<VALUETYPE> &virial, const std::vector<VALUETYPE>
    &coord, const std::vector<VALUETYPE> &charge, const
    deepmd::Region<VALUETYPE> &region, const
    EwaldParameters<VALUETYPE> &param)
```

Function deepmd::filter_ftype_gpu_cuda

- Defined in file_source_lib_include_neighbor_list.h

Function Documentation

void deepmd::filter_ftype_gpu_cuda(int *ftype_out, const int *ftype_in, const int nloc)

Filter the fake atom type.

If ≥ 0 , set to 0; if < 0 , set to -1.

Parameters

- **ftype_out** – The output filtered atom type.
- **ftype_in** – The input atom type.
- **nloc** – The number of atoms.

Template Function `deepmd::format_nbor_list_gpu_cuda`

- Defined in `file_source_lib_include_fmt_nlist.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::format_nbor_list_gpu_cuda(int *nlist, const FPTYPE *coord, const int *type, const
                                     deepmd::InputNlist &gpu_inlist, int *array_int, uint_64
                                     *array_longlong, const int max_nbor_size, const int nloc,
                                     const int nall, const float rcut, const std::vector<int> sec)
```

Template Function `deepmd::format_nlist_cpu`

- Defined in `file_source_lib_include_fmt_nlist.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::format_nlist_cpu(int *nlist, const InputNlist &in_nlist, const FPTYPE *coord, const int
                             *type, const int nloc, const int nall, const float rcut, const
                             std::vector<int> sec)
```

Function `deepmd::free_nlist_gpu_device`

- Defined in `file_source_lib_include_neighbor_list.h`

Function Documentation

```
void deepmd::free_nlist_gpu_device(InputNlist &gpu_nlist)
```

Reclaim the allocated device memory of struct `InputNlist`.

Parameters

gpu_nlist – Device memory `InputNlist` struct which stores the neighbor information of the core region atoms

Template Function `deepmd::gelu_cpu`

- Defined in `file_source_lib_include_gelu.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::gelu_cpu(FPTYPE *out, const FPTYPE *xx, const int_64 size)
```

Template Function deepmd::gelu_gpu_cuda

- Defined in file_source_lib_include_gelu.h

Function Documentation

```
template<typename FPTYPE>
void deepmd::gelu_gpu_cuda(FPTYPE *out, const FPTYPE *xx, const int_64 size)
```

Template Function deepmd::gelu_grad_cpu

- Defined in file_source_lib_include_gelu.h

Function Documentation

```
template<typename FPTYPE>
void deepmd::gelu_grad_cpu(FPTYPE *out, const FPTYPE *xx, const FPTYPE *dy, const int_64 size)
```

Template Function deepmd::gelu_grad_gpu_cuda

- Defined in file_source_lib_include_gelu.h

Function Documentation

```
template<typename FPTYPE>
void deepmd::gelu_grad_gpu_cuda(FPTYPE *out, const FPTYPE *xx, const FPTYPE *dy, const int_64
                                size)
```

Template Function deepmd::gelu_grad_grad_cpu

- Defined in file_source_lib_include_gelu.h

Function Documentation

```
template<typename FPTYPE>
void deepmd::gelu_grad_grad_cpu(FPTYPE *out, const FPTYPE *xx, const FPTYPE *dy, const
                                FPTYPE *dy_2, const int_64 size)
```

Template Function `deepmd::gelu_grad_grad_gpu_cuda`

- Defined in `file_source_lib_include_gelu.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::gelu_grad_grad_gpu_cuda(FPTYPE *out, const FPTYPE *xx, const FPTYPE *dy, const
                                      FPTYPE *dy_2, const int_64 size)
```

Function `deepmd::group_atoms_cpu`

- Defined in `file_source_lib_include_pairwise.h`

Function Documentation

```
void deepmd::group_atoms_cpu(std::vector<std::vector<int>> &fragments, const std::vector<int>
                              &idxs)
```

Group atoms into different fragments according to indexes.

Parameters

- **fragments** – [out] The indexes of atoms that each fragment contains. Fragment has been sorted.
- **idxs** – [in] The indexes of the fragment that each atom belongs to. -1 will be ignored.

Template Function `deepmd::init_region_cpu`

- Defined in `file_source_lib_include_region.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::init_region_cpu(Region<FPTYPE> &region, const FPTYPE *boxt)
```

Template Function `deepmd::invsqrt`

- Defined in file `_source_lib_include_utilities.h`

Function Documentation

```
template<typename TYPE>
inline TYPE deepmd::invsqrt(const TYPE x)
```

Specialized Template Function `deepmd::invsqrt< double >`

- Defined in file `_source_lib_include_utilities.h`

Function Documentation

```
template<>
inline double deepmd::invsqrt<double>(const double x)
```

Specialized Template Function `deepmd::invsqrt< float >`

- Defined in file `_source_lib_include_utilities.h`

Function Documentation

```
template<>
inline float deepmd::invsqrt<float>(const float x)
```

Template Function `deepmd::malloc_device_memory(FPTYPE *&, const std::vector<FPTYPE>&)`

- Defined in file `_source_lib_include_gpu_cuda.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::malloc_device_memory(FPTYPE *&device, const std::vector<FPTYPE> &host)
```

Template Function `deepmd::malloc_device_memory(FPTYPE *&, const int)`

- Defined in file `_source_lib_include_gpu_cuda.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::malloc_device_memory(FPTYPE *&device, const int size)
```

Template Function `deepmd::malloc_device_memory(FPTYPE *&, std::vector<FPTYPE>&)`

- Defined in `file_source_lib_include_gpu_rocm.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::malloc_device_memory(FPTYPE *&device, std::vector<FPTYPE> &host)
```

Template Function `deepmd::malloc_device_memory_sync(FPTYPE *&, const`
`std::vector<FPTYPE>&)`

- Defined in `file_source_lib_include_gpu_cuda.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::malloc_device_memory_sync(FPTYPE *&device, const std::vector<FPTYPE> &host)
```

Template Function `deepmd::malloc_device_memory_sync(FPTYPE *&, const FPTYPE *, const int)`

- Defined in `file_source_lib_include_gpu_cuda.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::malloc_device_memory_sync(FPTYPE *&device, const FPTYPE *host, const int size)
```

Template Function `deepmd::malloc_device_memory_sync(FPTYPE *&, std::vector<FPTYPE>&)`

- Defined in `file_source_lib_include_gpu_rocm.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::malloc_device_memory_sync(FPTYPE *&device, std::vector<FPTYPE> &host)
```

Template Function deepmd::map_aparam_cpu

- Defined in file_source_lib_include_map_aparam.h

Function Documentation

```
template<typename FPTYPE>
void deepmd::map_aparam_cpu(FPTYPE *output, const FPTYPE *aparam, const int *nlist, const int
                             &nloc, const int &nei, const int &numb_aparam)
```

Function deepmd::max_numneigh

- Defined in file_source_lib_include_neighbor_list.h

Function Documentation

```
int deepmd::max_numneigh(const InputNlist &to_nlist)
```

Compute the max number of neighbors within the core region atoms.

Parameters

to_nlist – InputNlist struct which stores the neighbor information of the core region atoms.

Return values

max – number of neighbors

Returns

integer

Template Function deepmd::memcpy_device_to_host(const FPTYPE *, std::vector<FPTYPE>&)

- Defined in file_source_lib_include_gpu_cuda.h

Function Documentation

```
template<typename FPTYPE>
void deepmd::memcpy_device_to_host(const FPTYPE *device, std::vector<FPTYPE> &host)
```

Template Function `deepmd::memcpy_device_to_host(const FPTYPE *, FPTYPE *, const int)`

- Defined in file `_source_lib_include_gpu_cuda.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::memcpy_device_to_host(const FPTYPE *device, FPTYPE *host, const int size)
```

Template Function `deepmd::memcpy_device_to_host(FPTYPE *, std::vector<FPTYPE>&)`

- Defined in file `_source_lib_include_gpu_rocm.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::memcpy_device_to_host(FPTYPE *device, std::vector<FPTYPE> &host)
```

Template Function `deepmd::memcpy_host_to_device(FPTYPE *, const std::vector<FPTYPE>&)`

- Defined in file `_source_lib_include_gpu_cuda.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::memcpy_host_to_device(FPTYPE *device, const std::vector<FPTYPE> &host)
```

Template Function `deepmd::memcpy_host_to_device(FPTYPE *, const FPTYPE *, const int)`

- Defined in file `_source_lib_include_gpu_cuda.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::memcpy_host_to_device(FPTYPE *device, const FPTYPE *host, const int size)
```

Template Function `deepmd::memcpy_host_to_device(FPTYPE *, std::vector<FPTYPE>&)`

- Defined in file `_source_lib_include_gpu_rocm.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::memcpy_host_to_device(FPTYPE *device, std::vector<FPTYPE> &host)
```

Template Function deepmd::memset_device_memory

- Defined in file_source_lib_include_gpu_cuda.h

Function Documentation

```
template<typename FPTYPE>
void deepmd::memset_device_memory(FPTYPE *device, const int var, const int size)
```

Template Function deepmd::normalize_coord_cpu

- Defined in file_source_lib_include_coord.h

Function Documentation

```
template<typename FPTYPE>
void deepmd::normalize_coord_cpu(FPTYPE *coord, const int natom, const
                                deepmd::Region<FPTYPE> &region)
```

Template Function deepmd::normalize_coord_gpu

- Defined in file_source_lib_include_coord.h

Function Documentation

```
template<typename FPTYPE>
void deepmd::normalize_coord_gpu(FPTYPE *coord, const int natom, const
                                deepmd::Region<FPTYPE> &region)
```

Template Function deepmd::pair_tab_cpu

- Defined in file_source_lib_include_pair_tab.h

Function Documentation

```
template<typename FPTYPE>
void deepmd::pair_tab_cpu(FPTYPE *energy, FPTYPE *force, FPTYPE *virial, const double
                          *table_info, const double *table_data, const FPTYPE *rij, const FPTYPE
                          *scale, const int *type, const int *nlist, const int *natoms, const
                          std::vector<int> &sel_a, const std::vector<int> &sel_r)
```

Template Function deepmd::prod_env_mat_a_cpu

- Defined in file_source_lib_include_prod_env_mat.h

Function Documentation

```
template<typename FPTYPE>
void deepmd::prod_env_mat_a_cpu(FPTYPE *em, FPTYPE *em_deriv, FPTYPE *rij, int *nlist, const
                                FPTYPE *coord, const int *type, const InputNlist &inlist, const int
                                max_nbor_size, const FPTYPE *avg, const FPTYPE *std, const int
                                nloc, const int nall, const float rcut, const float rcut_smth, const
                                std::vector<int> sec, const int *f_type = NULL)
```

Template Function deepmd::prod_env_mat_a_gpu_cuda

- Defined in file_source_lib_include_prod_env_mat.h

Function Documentation

```
template<typename FPTYPE>
void deepmd::prod_env_mat_a_gpu_cuda(FPTYPE *em, FPTYPE *em_deriv, FPTYPE *rij, int *nlist,
                                      const FPTYPE *coord, const int *type, const InputNlist
                                      &gpu_inlist, int *array_int, unsigned long long
                                      *array_longlong, const int max_nbor_size, const FPTYPE *avg,
                                      const FPTYPE *std, const int nloc, const int nall, const float
                                      rcut, const float rcut_smth, const std::vector<int> sec, const int
                                      *f_type = NULL)
```

Template Function deepmd::prod_env_mat_a_nvnmmd_quantize_cpu

- Defined in file_source_lib_include_prod_env_mat_nvnmmd.h

Function Documentation

```
template<typename FPTYPE>
void deepmd::prod_env_mat_a_nvnmmd_quantize_cpu(FPTYPE *em, FPTYPE *em_deriv, FPTYPE *rij,
int *nlist, const FPTYPE *coord, const int *type,
const InputNlist &inlist, const int max_nbor_size,
const FPTYPE *avg, const FPTYPE *std, const int
nloc, const int nall, const float rcut, const float
rcut_smth, const std::vector<int> sec, const int
*f_type = NULL)
```

Template Function deepmd::prod_env_mat_r_cpu

- Defined in file_source_lib_include_prod_env_mat.h

Function Documentation

```
template<typename FPTYPE>
void deepmd::prod_env_mat_r_cpu(FPTYPE *em, FPTYPE *em_deriv, FPTYPE *rij, int *nlist, const
FPTYPE *coord, const int *type, const InputNlist &inlist, const int
max_nbor_size, const FPTYPE *avg, const FPTYPE *std, const int
nloc, const int nall, const float rcut, const float rcut_smth, const
std::vector<int> sec)
```

Template Function deepmd::prod_env_mat_r_gpu_cuda

- Defined in file_source_lib_include_prod_env_mat.h

Function Documentation

```
template<typename FPTYPE>
void deepmd::prod_env_mat_r_gpu_cuda(FPTYPE *em, FPTYPE *em_deriv, FPTYPE *rij, int *nlist,
const FPTYPE *coord, const int *type, const InputNlist
&gpu_inlist, int *array_int, unsigned long long
*array_longlong, const int max_nbor_size, const FPTYPE *avg,
const FPTYPE *std, const int nloc, const int nall, const float
rcut, const float rcut_smth, const std::vector<int> sec)
```

Template Function deepmd::prod_force_a_cpu(FPTYPE *, const FPTYPE *, const FPTYPE *, const int *, const int, const int, const int, const int)

- Defined in file_source_lib_include_prod_force.h

Function Documentation

```
template<typename FPTYPE>
void deepmd::prod_force_a_cpu(FPTYPE *force, const FPTYPE *net_deriv, const FPTYPE *in_deriv,
                             const int *nlist, const int nloc, const int nall, const int nnei, const int
                             nframes)
```

Produce force from `net_deriv` and `in_deriv`.

Template Parameters

FPTYPE – float or double

Parameters

- **force** – [out] Atomic forces.
- **net_deriv** – [in] Net derivative.
- **in_deriv** – [in] Environmental derivative.
- **nlist** – [in] Neighbor list.
- **nloc** – [in] The number of local atoms.
- **nall** – [in] The number of all atoms, including ghost atoms.
- **nnei** – [in] The number of neighbors.
- **nframes** – [in] The number of frames.

Template Function `deepmd::prod_force_a_cpu(FPTYPE *, const FPTYPE *, const FPTYPE *, const int *, const int, const int, const int, const int, const int, const int)`

- Defined in `file_source_lib_include_prod_force.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::prod_force_a_cpu(FPTYPE *force, const FPTYPE *net_deriv, const FPTYPE *in_deriv,
                             const int *nlist, const int nloc, const int nall, const int nnei, const int
                             nframes, const int thread_nloc, const int thread_start_index)
```

Produce force from `net_deriv` and `in_deriv`.

This function is used for multi-threading. Only part of atoms are computed in this thread. They will be computed in parallel.

Template Parameters

FPTYPE – float or double

Parameters

- **force** – [out] Atomic forces.
- **net_deriv** – [in] Net derivative.
- **in_deriv** – [in] Environmental derivative.
- **nlist** – [in] Neighbor list.
- **nloc** – [in] The number of local atoms.
- **nall** – [in] The number of all atoms, including ghost atoms.

- **nnei** – [in] The number of neighbors.
- **nframes** – [in] The number of frames.
- **thread_nloc** – [in] The number of local atoms to be computed in this thread.
- **thread_start_index** – [in] The start index of local atoms to be computed in this thread. The index should be in [0, nloc).

Template Function `deepmd::prod_force_a_gpu_cuda`

- Defined in `file_source_lib_include_prod_force.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::prod_force_a_gpu_cuda(FPTYPE *force, const FPTYPE *net_deriv, const FPTYPE
                                   *in_deriv, const int *nlist, const int nloc, const int nall, const int
                                   nnei, const int nframes)
```

Template Function `deepmd::prod_force_grad_a_cpu`

- Defined in `file_source_lib_include_prod_force_grad.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::prod_force_grad_a_cpu(FPTYPE *grad_net, const FPTYPE *grad, const FPTYPE
                                   *env_deriv, const int *nlist, const int nloc, const int nnei, const int
                                   nframes)
```

Template Function `deepmd::prod_force_grad_a_gpu_cuda`

- Defined in `file_source_lib_include_prod_force_grad.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::prod_force_grad_a_gpu_cuda(FPTYPE *grad_net, const FPTYPE *grad, const FPTYPE
                                         *env_deriv, const int *nlist, const int nloc, const int nnei,
                                         const int nframes)
```

Template Function `deepmd::prod_force_grad_r_cpu`

- Defined in file `_source_lib_include_prod_force_grad.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::prod_force_grad_r_cpu(FPTYPE *grad_net, const FPTYPE *grad, const FPTYPE
                                   *env_deriv, const int *nlist, const int nloc, const int nnei, const int
                                   nframes)
```

Template Function `deepmd::prod_force_grad_r_gpu_cuda`

- Defined in file `_source_lib_include_prod_force_grad.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::prod_force_grad_r_gpu_cuda(FPTYPE *grad_net, const FPTYPE *grad, const FPTYPE
                                         *env_deriv, const int *nlist, const int nloc, const int nnei,
                                         const int nframes)
```

Template Function `deepmd::prod_force_r_cpu`

- Defined in file `_source_lib_include_prod_force.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::prod_force_r_cpu(FPTYPE *force, const FPTYPE *net_deriv, const FPTYPE *in_deriv,
                              const int *nlist, const int nloc, const int nall, const int nnei, const int
                              nframes)
```

Template Function `deepmd::prod_force_r_gpu_cuda`

- Defined in file `_source_lib_include_prod_force.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::prod_force_r_gpu_cuda(FPTYPE *force, const FPTYPE *net_deriv, const FPTYPE
                                   *in_deriv, const int *nlist, const int nloc, const int nall, const int
                                   nnei, const int nframes)
```

Template Function `deepmd::prod_virial_a_cpu`

- Defined in file `_source_lib_include_prod_virial.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::prod_virial_a_cpu(FPTYPE *virial, FPTYPE *atom_virial, const FPTYPE *net_deriv,
                              const FPTYPE *env_deriv, const FPTYPE *rij, const int *nlist, const
                              int nloc, const int nall, const int nnei)
```

Template Function `deepmd::prod_virial_a_gpu_cuda`

- Defined in file `_source_lib_include_prod_virial.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::prod_virial_a_gpu_cuda(FPTYPE *virial, FPTYPE *atom_virial, const FPTYPE
                                     *net_deriv, const FPTYPE *env_deriv, const FPTYPE *rij, const
                                     int *nlist, const int nloc, const int nall, const int nnei)
```

Template Function `deepmd::prod_virial_grad_a_cpu`

- Defined in file `_source_lib_include_prod_virial_grad.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::prod_virial_grad_a_cpu(FPTYPE *grad_net, const FPTYPE *grad, const FPTYPE
                                     *env_deriv, const FPTYPE *rij, const int *nlist, const int nloc,
                                     const int nnei)
```

Template Function `deepmd::prod_virial_grad_a_gpu_cuda`

- Defined in file `_source_lib_include_prod_virial_grad.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::prod_virial_grad_a_gpu_cuda(FPTYPE *grad_net, const FPTYPE *grad, const FPTYPE
                                           *env_deriv, const FPTYPE *rij, const int *nlist, const int
                                           nloc, const int nnei)
```

Template Function `deepmd::prod_virial_grad_r_cpu`

- Defined in file `file_source_lib_include_prod_virial_grad.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::prod_virial_grad_r_cpu(FPTYPE *grad_net, const FPTYPE *grad, const FPTYPE
                                   *env_deriv, const FPTYPE *rij, const int *nlist, const int nloc,
                                   const int nnei)
```

Template Function `deepmd::prod_virial_grad_r_gpu_cuda`

- Defined in file `file_source_lib_include_prod_virial_grad.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::prod_virial_grad_r_gpu_cuda(FPTYPE *grad_net, const FPTYPE *grad, const FPTYPE
                                         *env_deriv, const FPTYPE *rij, const int *nlist, const int
                                         nloc, const int nnei)
```

Template Function `deepmd::prod_virial_r_cpu`

- Defined in file `file_source_lib_include_prod_virial.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::prod_virial_r_cpu(FPTYPE *virial, FPTYPE *atom_virial, const FPTYPE *net_deriv,
                              const FPTYPE *env_deriv, const FPTYPE *rij, const int *nlist, const
                              int nloc, const int nall, const int nnei)
```

Template Function `deepmd::prod_virial_r_gpu_cuda`

- Defined in file `file_source_lib_include_prod_virial.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::prod_virial_r_gpu_cuda(FPTYPE *virial, FPTYPE *atom_virial, const FPTYPE
                                    *net_deriv, const FPTYPE *env_deriv, const FPTYPE *rij, const
                                    int *nlist, const int nloc, const int nall, const int nnei)
```

Template Function `deepmd::soft_min_switch_cpu`

- Defined in file `_source_lib_include_soft_min_switch.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::soft_min_switch_cpu(FPTYPE *sw_value, FPTYPE *sw_deriv, const FPTYPE *rij, const
                                int *nlist, const int &nloc, const int &nnei, const FPTYPE &alpha,
                                const FPTYPE &rmin, const FPTYPE &rmax)
```

Template Function `deepmd::soft_min_switch_force_cpu`

- Defined in file `_source_lib_include_soft_min_switch_force.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::soft_min_switch_force_cpu(FPTYPE *force, const FPTYPE *du, const FPTYPE
                                        *sw_deriv, const int *nlist, const int nloc, const int nall, const
                                        int nnei)
```

Template Function `deepmd::soft_min_switch_force_grad_cpu`

- Defined in file `_source_lib_include_soft_min_switch_force_grad.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::soft_min_switch_force_grad_cpu(FPTYPE *grad_net, const FPTYPE *grad, const
                                             FPTYPE *sw_deriv, const int *nlist, const int nloc,
                                             const int nnei)
```

Template Function `deepmd::soft_min_switch_virial_cpu`

- Defined in file `_source_lib_include_soft_min_switch_virial.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::soft_min_switch_virial_cpu(FPTYPE *virial, FPTYPE *atom_virial, const FPTYPE
                                        *du, const FPTYPE *sw_deriv, const FPTYPE *rij, const int
                                        *nlist, const int nloc, const int nall, const int nnei)
```

Template Function `deepmd::soft_min_switch_virial_grad_cpu`

- Defined in file `_source_lib_include_soft_min_switch_virial_grad.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::soft_min_switch_virial_grad_cpu(FPTYPE *grad_net, const FPTYPE *grad, const
                                             FPTYPE *sw_deriv, const FPTYPE *rij, const int
                                             *nlist, const int nloc, const int nnei)
```

Function `deepmd::spline3_switch`

- Defined in file `_source_lib_include_switcher.h`

Function Documentation

```
inline void deepmd::spline3_switch(double &vv, double &dd, const double &xx, const double &rmin,
                                   const double &rmax)
```

Template Function `deepmd::spline5_switch`

- Defined in file `_source_lib_include_switcher.h`

Function Documentation

```
template<typename FPTYPE>
inline void deepmd::spline5_switch(FPTYPE &vv, FPTYPE &dd, const FPTYPE &xx, const float
                                   &rmin, const float &rmax)
```

Template Function `deepmd::tabulate_fusion_se_a_cpu`

- Defined in file `_source_lib_include_tabulate.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::tabulate_fusion_se_a_cpu(FPTYPE *out, const FPTYPE *table, const FPTYPE
                                       *table_info, const FPTYPE *em_x, const FPTYPE *em, const
                                       FPTYPE *two_embed, const int nloc, const int nnei, const int
                                       last_layer_size, const bool is_sorted = true)
```


Template Function `deepmd::tabulate_fusion_se_a_gpu_cuda`

- Defined in file `_source_lib_include_tabulate.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::tabulate_fusion_se_a_gpu_cuda(FPTYPE *out, const FPTYPE *table, const FPTYPE
                                           *table_info, const FPTYPE *em_x, const FPTYPE *em,
                                           const FPTYPE *two_embed, const int nloc, const int
                                           nnei, const int last_layer_size, const bool is_sorted =
                                           true)
```

Template Function `deepmd::tabulate_fusion_se_a_grad_cpu`

- Defined in file `_source_lib_include_tabulate.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::tabulate_fusion_se_a_grad_cpu(FPTYPE *dy_dem_x, FPTYPE *dy_dem, const
                                           FPTYPE *table, const FPTYPE *table_info, const
                                           FPTYPE *em_x, const FPTYPE *em, const FPTYPE
                                           *two_embed, const FPTYPE *dy, const int nloc, const
                                           int nnei, const int last_layer_size, const bool is_sorted =
                                           true)
```

Template Function `deepmd::tabulate_fusion_se_a_grad_gpu_cuda`

- Defined in file `_source_lib_include_tabulate.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::tabulate_fusion_se_a_grad_gpu_cuda(FPTYPE *dy_dem_x, FPTYPE *dy_dem, const
                                                 FPTYPE *table, const FPTYPE *table_info, const
                                                 FPTYPE *em_x, const FPTYPE *em, const
                                                 FPTYPE *two_embed, const FPTYPE *dy, const
                                                 int nloc, const int nnei, const int last_layer_size,
                                                 const bool is_sorted = true)
```

Template Function `deepmd::tabulate_fusion_se_a_grad_grad_cpu`

- Defined in file `_source_lib_include_tabulate.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::tabulate_fusion_se_a_grad_grad_cpu(FPTYPE *dz_dy, const FPTYPE *table, const
                                                FPTYPE *table_info, const FPTYPE *em_x, const
                                                FPTYPE *em, const FPTYPE *dz_dy_dem_x,
                                                const FPTYPE *dz_dy_dem, const int nloc, const
                                                int nnei, const int last_layer_size, const bool
                                                is_sorted = true)
```

Template Function `deepmd::tabulate_fusion_se_a_grad_grad_gpu_cuda`

- Defined in file `_source_lib_include_tabulate.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::tabulate_fusion_se_a_grad_grad_gpu_cuda(FPTYPE *dz_dy, const FPTYPE *table,
                                                       const FPTYPE *table_info, const FPTYPE
                                                       *em_x, const FPTYPE *em, const FPTYPE
                                                       *dz_dy_dem_x, const FPTYPE *dz_dy_dem,
                                                       const int nloc, const int nnei, const int
                                                       last_layer_size, const bool is_sorted = true)
```

Template Function `deepmd::tabulate_fusion_se_r_cpu`

- Defined in file `_source_lib_include_tabulate.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::tabulate_fusion_se_r_cpu(FPTYPE *out, const FPTYPE *table, const FPTYPE
                                       *table_info, const FPTYPE *em, const int nloc, const int nnei,
                                       const int last_layer_size)
```

Template Function `deepmd::tabulate_fusion_se_r_gpu_cuda`

- Defined in file `_source_lib_include_tabulate.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::tabulate_fusion_se_r_gpu_cuda(FPTYPE *out, const FPTYPE *table, const FPTYPE
                                           *table_info, const FPTYPE *em, const int nloc, const int
                                           nnei, const int last_layer_size)
```

Template Function `deepmd::tabulate_fusion_se_r_grad_cpu`

- Defined in file `_source_lib_include_tabulate.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::tabulate_fusion_se_r_grad_cpu(FPTYPE *dy_dem, const FPTYPE *table, const
                                           FPTYPE *table_info, const FPTYPE *em, const
                                           FPTYPE *dy, const int nloc, const int nnei, const int
                                           last_layer_size)
```

Template Function `deepmd::tabulate_fusion_se_r_grad_gpu_cuda`

- Defined in file `_source_lib_include_tabulate.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::tabulate_fusion_se_r_grad_gpu_cuda(FPTYPE *dy_dem, const FPTYPE *table, const
                                                FPTYPE *table_info, const FPTYPE *em, const
                                                FPTYPE *dy, const int nloc, const int nnei, const
                                                int last_layer_size)
```

Template Function `deepmd::tabulate_fusion_se_r_grad_grad_cpu`

- Defined in file `_source_lib_include_tabulate.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::tabulate_fusion_se_r_grad_grad_cpu(FPTYPE *dz_dy, const FPTYPE *table, const
FPTYPE *table_info, const FPTYPE *em, const
FPTYPE *dz_dy_dem, const int nloc, const int
nnei, const int last_layer_size)
```

Template Function deepmd::tabulate_fusion_se_r_grad_grad_gpu_cuda

- Defined in file_source_lib_include_tabulate.h

Function Documentation

```
template<typename FPTYPE>
void deepmd::tabulate_fusion_se_r_grad_grad_gpu_cuda(FPTYPE *dz_dy, const FPTYPE *table,
const FPTYPE *table_info, const FPTYPE
*em, const FPTYPE *dz_dy_dem, const int
nloc, const int nnei, const int last_layer_size)
```

Template Function deepmd::tabulate_fusion_se_t_cpu

- Defined in file_source_lib_include_tabulate.h

Function Documentation

```
template<typename FPTYPE>
void deepmd::tabulate_fusion_se_t_cpu(FPTYPE *out, const FPTYPE *table, const FPTYPE
*table_info, const FPTYPE *em_x, const FPTYPE *em, const
int nloc, const int nnei_i, const int nnei_j, const int
last_layer_size)
```

Template Function deepmd::tabulate_fusion_se_t_gpu_cuda

- Defined in file_source_lib_include_tabulate.h

Function Documentation

```
template<typename FPTYPE>
void deepmd::tabulate_fusion_se_t_gpu_cuda(FPTYPE *out, const FPTYPE *table, const FPTYPE
*table_info, const FPTYPE *em_x, const FPTYPE *em,
const int nloc, const int nnei_i, const int nnei_j, const int
last_layer_size)
```

Template Function `deepmd::tabulate_fusion_se_t_grad_cpu`

- Defined in `file_source_lib_include_tabulate.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::tabulate_fusion_se_t_grad_cpu(FPTYPE *dy_dem_x, FPTYPE *dy_dem, const
                                           FPTYPE *table, const FPTYPE *table_info, const
                                           FPTYPE *em_x, const FPTYPE *em, const FPTYPE
                                           *dy, const int nloc, const int nnei_i, const int nnei_j,
                                           const int last_layer_size)
```

Template Function `deepmd::tabulate_fusion_se_t_grad_gpu_cuda`

- Defined in `file_source_lib_include_tabulate.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::tabulate_fusion_se_t_grad_gpu_cuda(FPTYPE *dy_dem_x, FPTYPE *dy_dem, const
                                                  FPTYPE *table, const FPTYPE *table_info, const
                                                  FPTYPE *em_x, const FPTYPE *em, const
                                                  FPTYPE *dy, const int nloc, const int nnei_i, const
                                                  int nnei_j, const int last_layer_size)
```

Template Function `deepmd::tabulate_fusion_se_t_grad_grad_cpu`

- Defined in `file_source_lib_include_tabulate.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::tabulate_fusion_se_t_grad_grad_cpu(FPTYPE *dz_dy, const FPTYPE *table, const
                                                  FPTYPE *table_info, const FPTYPE *em_x, const
                                                  FPTYPE *em, const FPTYPE *dz_dy_dem_x,
                                                  const FPTYPE *dz_dy_dem, const int nloc, const
                                                  int nnei_i, const int nnei_j, const int
                                                  last_layer_size)
```

Template Function `deepmd::tabulate_fusion_se_t_grad_grad_gpu_cuda`

- Defined in file `_source_lib_include_tabulate.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::tabulate_fusion_se_t_grad_grad_gpu_cuda(FPTYPE *dz_dy, const FPTYPE *table,
                                                    const FPTYPE *table_info, const FPTYPE
                                                    *em_x, const FPTYPE *em, const FPTYPE
                                                    *dz_dy_dem_x, const FPTYPE *dz_dy_dem,
                                                    const int nloc, const int nnei_i, const int
                                                    nnei_j, const int last_layer_size)
```

Template Function `deepmd::test_encoding_decoding_nbor_info_gpu_cuda`

- Defined in file `_source_lib_include_fmt_nlist.h`

Function Documentation

```
template<typename FPTYPE>
void deepmd::test_encoding_decoding_nbor_info_gpu_cuda(uint_64 *key, int *out_type, int
                                                    *out_index, const int *in_type, const
                                                    FPTYPE *in_dist, const int *in_index,
                                                    const int size_of_array)
```

Function `deepmd::use_nei_info_cpu`

- Defined in file `_source_lib_include_neighbor_list.h`

Function Documentation

```
void deepmd::use_nei_info_cpu(int *nlist, int *ntype, bool *nmask, const int *type, const int *nlist_map,
                              const int nloc, const int nnei, const int ntypes, const bool b_nlist_map)
```

Function `deepmd::use_nei_info_gpu`

- Defined in file `_source_lib_include_neighbor_list.h`

Function Documentation

```
void deepmd::use_nei_info_gpu(int *nlist, int *ntype, bool *nmask, const int *type, const int *nlist_map,
                             const int nloc, const int nnei, const int ntypes, const bool b_nlist_map)
```

Function deepmd::use_nlist_map

- Defined in file_source_lib_include_neighbor_list.h

Function Documentation

```
void deepmd::use_nlist_map(int *nlist, const int *nlist_map, const int nloc, const int nnei)
```

Template Function deepmd::volume_cpu

- Defined in file_source_lib_include_region.h

Function Documentation

```
template<typename FPTYPE>
FPTYPE deepmd::volume_cpu(const Region<FPTYPE> &region)
```

Template Function deepmd::volume_gpu

- Defined in file_source_lib_include_region.h

Function Documentation

```
template<typename FPTYPE>
void deepmd::volume_gpu(FPTYPE *volume, const Region<FPTYPE> &region)
```

Template Function dotmul_flt_nvnmmd

- Defined in file_source_lib_include_env_mat_nvnmmd.h

Function Documentation

```
template<class T>
void dotmul_flt_nvnmmd(T &y, T *x1, T *x2, int64_t M)
```

Function DPAssert(cudaError_t, const char *, int, bool)

- Defined in file_source_lib_include_gpu_cuda.h

Function Documentation

```
inline void DPAssert(cudaError_t code, const char *file, int line, bool abort = true)
```

Function DPAssert(hipError_t, const char *, int, bool)

- Defined in file_source_lib_include_gpu_rocm.h

Function Documentation

```
inline void DPAssert(hipError_t code, const char *file, int line, bool abort = true)
```

Function env_mat_a

- Defined in file_source_lib_include_env_mat.h

Function Documentation

```
void env_mat_a(std::vector<double> &descript_a, std::vector<double> &descript_a_deriv,  
               std::vector<double> &rij_a, const std::vector<double> &posi, const int &ntypes, const  
               std::vector<int> &type, const SimulationRegion<double> &region, const bool &b_pbc,  
               const int &i_idx, const std::vector<int> &fmt_nlist, const std::vector<int> &sec, const  
               double &rmin, const double &rmax)
```

Function env_mat_r

- Defined in file_source_lib_include_env_mat.h

Function Documentation

```
void env_mat_r(std::vector<double> &descript_r, std::vector<double> &descript_r_deriv,  
               std::vector<double> &rij_r, const std::vector<double> &posi, const int &ntypes, const  
               std::vector<int> &type, const SimulationRegion<double> &region, const bool &b_pbc,  
               const int &i_idx, const std::vector<int> &fmt_nlist, const std::vector<int> &sec, const  
               double &rmin, const double &rmax)
```


Template Function `find_max_expo(int64_t&, T *, int64_t)`

- Defined in file `_source_lib_include_env_mat_nvnmd.h`

Function Documentation

```
template<class T>
void find_max_expo(int64_t &max_expo, T *x, int64_t M)
```

Template Function `find_max_expo(int64_t&, T *, int64_t, int64_t)`

- Defined in file `_source_lib_include_env_mat_nvnmd.h`

Function Documentation

```
template<class T>
void find_max_expo(int64_t &max_expo, T *x, int64_t N, int64_t M)
```

Template Function `format_nlist_i_cpu`

- Defined in file `_source_lib_include_fmt_nlist.h`

Function Documentation

```
template<typename FPTYPE>
int format_nlist_i_cpu(std::vector<int> &fmt_nei_idx_a, const std::vector<FPTYPE> &posi, const
                      std::vector<int> &type, const int &i_idx, const std::vector<int> &nei_idx_a,
                      const float &rcut, const std::vector<int> &sec_a)
```

Function `format_nlist_i_fill_a`

- Defined in file `_source_lib_include_fmt_nlist.h`

Function Documentation

```
int format_nlist_i_fill_a(std::vector<int> &fmt_nei_idx_a, std::vector<int> &fmt_nei_idx_r, const
                          std::vector<double> &posi, const int &ntypes, const std::vector<int> &type,
                          const SimulationRegion<double> &region, const bool &b_pbc, const int
                          &i_idx, const std::vector<int> &nei_idx_a, const std::vector<int>
                          &nei_idx_r, const double &rcut, const std::vector<int> &sec_a, const
                          std::vector<int> &sec_r)
```

Template Function `mul_flt_nvnmmd`

- Defined in file `_source_lib_include_env_mat_nvnmmd.h`

Function Documentation

```
template<class T>
void mul_flt_nvnmmd(T &y, T x1, T x2)
```

Function `nborAssert(cudaError_t, const char *, int, bool)`

- Defined in file `_source_lib_include_gpu_cuda.h`

Function Documentation

```
inline void nborAssert(cudaError_t code, const char *file, int line, bool abort = true)
```

Function `nborAssert(hipError_t, const char *, int, bool)`

- Defined in file `_source_lib_include_gpu_rocm.h`

Function Documentation

```
inline void nborAssert(hipError_t code, const char *file, int line, bool abort = true)
```

Function `omp_get_num_threads`

- Defined in file `_source_lib_include_ewald.h`

Function Documentation

```
int omp_get_num_threads()
```

Function `omp_get_thread_num`

- Defined in file `_source_lib_include_ewald.h`

Function Documentation

int **omp_get_thread_num**()

Template Function **splitflt**

- Defined in file_source_lib_include_env_mat_nvnmd.h

Function Documentation

template<class T>
void **splitflt**(T x, int64_t &sign, int64_t &expo, int64_t &mant)

21.3.5 Variables

Variable **deepmd::ElectrostaticConversion**

- Defined in file_source_lib_include_ewald.h

Variable Documentation

const double **deepmd::ElectrostaticConversion** = 14.39964535475696995031

21.3.6 Defines

Define **DPErrcheck**

- Defined in file_source_lib_include_gpu_cuda.h

Define Documentation

DPErrcheck(res)

Define **DPErrcheck**

- Defined in file_source_lib_include_gpu_rocm.h

Define Documentation

`DPErrcheck(res)`

Define `FLT_MASK`

- Defined in `file_source_lib_include_env_mat_nvnmd.h`

Define Documentation

`FLT_MASK`

Define `GPU_MAX_NBOR_SIZE`

- Defined in `file_source_lib_include_gpu_cuda.h`

Define Documentation

`GPU_MAX_NBOR_SIZE`

Define `GPU_MAX_NBOR_SIZE`

- Defined in `file_source_lib_include_gpu_rocm.h`

Define Documentation

`GPU_MAX_NBOR_SIZE`

Define `MOASPNDIM`

- Defined in `file_source_lib_include_SimulationRegion.h`

Define Documentation

`MOASPNDIM`

Define NBIT_CUTF

- Defined in file_source_lib_include_env_mat_nvnmd.h

Define Documentation

NBIT_CUTF

Define NBIT_FLTF

- Defined in file_source_lib_include_env_mat_nvnmd.h

Define Documentation

NBIT_FLTF

Define nborErrcheck

- Defined in file_source_lib_include_gpu_cuda.h

Define Documentation

nborErrcheck(res)

Define nborErrcheck

- Defined in file_source_lib_include_gpu_rocm.h

Define Documentation

nborErrcheck(res)

Define SQRT_2_PI

- Defined in file_source_lib_include_device.h

Define Documentation

SQRT_2_PI

Define TPB

- Defined in file_source_lib_include_device.h

Define Documentation

TPB

21.3.7 Typedefs

Typedef int_64

- Defined in file_source_lib_include_device.h

Typedef Documentation

typedef long long **int_64**

Typedef uint_64

- Defined in file_source_lib_include_device.h

Typedef Documentation

typedef unsigned long long **uint_64**

LICENSE

The project DeePMD-kit is licensed under [GNU LGPLv3.0](#).

AUTHORS AND CREDITS

23.1 Cite DeePMD-kit and methods

- For general purpose,
- If GPU version is used,
- If local frame (loc_frame) is used,
- If DeepPot-SE (se_e2_a, se_e2_r, se_e3, se_atten) is used,
- If three-body embedding DeepPot-SE (se_e3) is used,
- If attention-based descriptor (se_atten, se_atten_v2) is used,
- If fitting dipole,
- If fitting polarizability,
- If fitting density of states,
- If fitting relative energies,
- If DPLR is used, or se_e2_r and hybrid are used,
- If DPRc is used,
- If interpolation with a pair-wise potential is used,
- If the model is compressed (dp compress),
- If model deviation is computed,
- If relative or atomic model deviation is computed,
- If NVNMD is used,

23.2 Package Contributors

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- wsyxbcl
- ziyao

23.3 Other Credits

- Zhang ZiXuan for designing the Deepmodeling logo.
- Everyone on the Deepmodeling mailing list for contributing to many discussions and decisions!

LOGO

The logo of DeePMD-kit is a beaver. Beavers were widely distributed in Europe and Asia but became nearly extinct due to hunting. Listed as a first-class state-protected animal in China, the population of beavers in China is less than the giant pandas. We hope that users of DeePMD-kit can enhance the awareness to protect beavers.

- [genindex](#)
- [modindex](#)
- [search](#)

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PYTHON MODULE INDEX

d

deepmd, 195
deepmd.calculator, 501
deepmd.cluster, 200
deepmd.cluster.local, 200
deepmd.cluster.slurm, 201
deepmd.common, 503
deepmd.descriptor, 201
deepmd.descriptor.descriptor, 249
deepmd.descriptor.hybrid, 256
deepmd.descriptor.loc_frame, 261
deepmd.descriptor.se, 264
deepmd.descriptor.se_a, 266
deepmd.descriptor.se_a_ebd, 272
deepmd.descriptor.se_a_ef, 274
deepmd.descriptor.se_a_mask, 279
deepmd.descriptor.se_atten, 283
deepmd.descriptor.se_atten_v2, 288
deepmd.descriptor.se_r, 290
deepmd.descriptor.se_t, 295
deepmd.entrypoints, 299
deepmd.entrypoints.compress, 303
deepmd.entrypoints.convert, 304
deepmd.entrypoints.doc, 304
deepmd.entrypoints.freeze, 304
deepmd.entrypoints.ipi, 305
deepmd.entrypoints.main, 305
deepmd.entrypoints.neighbor_stat, 306
deepmd.entrypoints.test, 306
deepmd.entrypoints.train, 307
deepmd.entrypoints.transfer, 308
deepmd.env, 508
deepmd.env.op_grads_module, 560
deepmd.env.op_module, 511
deepmd.fit, 308
deepmd.fit.dipole, 323
deepmd.fit.dos, 325
deepmd.fit.ener, 328
deepmd.fit.fitting, 332
deepmd.fit.polar, 333
deepmd.infer, 338
deepmd.infer.data_modifier, 356
deepmd.infer.deep_dipole, 358
deepmd.infer.deep_dos, 359
deepmd.infer.deep_eval, 362
deepmd.infer.deep_polar, 365
deepmd.infer.deep_pot, 367
deepmd.infer.deep_tensor, 371
deepmd.infer.deep_wfc, 374
deepmd.infer.ewald_recip, 375
deepmd.infer.model_devi, 376
deepmd.lmp, 508
deepmd.loggers, 379
deepmd.loggers.loggers, 380
deepmd.loss, 381
deepmd.loss.dos, 387
deepmd.loss.ener, 388
deepmd.loss.loss, 392
deepmd.loss.tensor, 393
deepmd.model, 394
deepmd.model.dos, 405
deepmd.model.ener, 407
deepmd.model.model, 411
deepmd.model.model_stat, 417
deepmd.model.multi, 417
deepmd.model.pairwise_dprc, 420
deepmd.model.tensor, 423
deepmd.nvnmd, 427
deepmd.nvnmd.data, 427
deepmd.nvnmd.data.data, 428
deepmd.nvnmd.descriptor, 428
deepmd.nvnmd.descriptor.se_a, 429
deepmd.nvnmd.descriptor.se_atten, 429
deepmd.nvnmd.entrypoints, 430
deepmd.nvnmd.entrypoints.freeze, 434
deepmd.nvnmd.entrypoints.mapt, 434
deepmd.nvnmd.entrypoints.train, 437
deepmd.nvnmd.entrypoints.wrap, 438
deepmd.nvnmd.fit, 439
deepmd.nvnmd.fit.ener, 439
deepmd.nvnmd.utils, 440
deepmd.nvnmd.utils.argcheck, 444
deepmd.nvnmd.utils.config, 444
deepmd.nvnmd.utils.encode, 447

- deepmd.nvnmd.utils.fio, 449
- deepmd.nvnmd.utils.network, 451
- deepmd.nvnmd.utils.op, 452
- deepmd.nvnmd.utils.weight, 452
- deepmd.op, 454
- deepmd.train, 454
- deepmd.train.run_options, 454
- deepmd.train.trainer, 455
- deepmd.utils, 457
 - deepmd.utils.argcheck, 466
 - deepmd.utils.batch_size, 468
 - deepmd.utils.compat, 470
 - deepmd.utils.convert, 471
 - deepmd.utils.data, 473
 - deepmd.utils.data_system, 476
 - deepmd.utils.errors, 479
 - deepmd.utils.finetune, 480
 - deepmd.utils.graph, 480
 - deepmd.utils.learning_rate, 484
 - deepmd.utils.multi_init, 485
 - deepmd.utils.neighbor_stat, 486
 - deepmd.utils.network, 487
 - deepmd.utils.pair_tab, 488
 - deepmd.utils.parallel_op, 489
 - deepmd.utils.path, 490
 - deepmd.utils.plugin, 494
 - deepmd.utils.random, 495
 - deepmd.utils.sess, 496
 - deepmd.utils.spin, 496
 - deepmd.utils.tabulate, 497
 - deepmd.utils.type_embed, 499
 - deepmd.utils.weight_avg, 501

Symbols

[_DP_DeepPotCompute](#) (C++ function), [618](#)
[_DP_DeepPotCompute<double>](#) (C++ function), [619](#)
[_DP_DeepPotCompute<float>](#) (C++ function), [619](#)
[_DP_DeepPotComputeMixedType](#) (C++ function), [619](#)
[_DP_DeepPotComputeMixedType<double>](#) (C++ function), [619](#)
[_DP_DeepPotComputeMixedType<float>](#) (C++ function), [620](#)
[_DP_DeepPotComputeNList](#) (C++ function), [620](#)
[_DP_DeepPotComputeNList<double>](#) (C++ function), [620](#)
[_DP_DeepPotComputeNList<float>](#) (C++ function), [621](#)
[_DP_DeepPotModelDeviComputeNList](#) (C++ function), [621](#)
[_DP_DeepPotModelDeviComputeNList<double>](#) (C++ function), [621](#)
[_DP_DeepPotModelDeviComputeNList<float>](#) (C++ function), [622](#)
[_DP_DeepTensorCompute](#) (C++ function), [622](#)
[_DP_DeepTensorCompute<double>](#) (C++ function), [622](#)
[_DP_DeepTensorCompute<float>](#) (C++ function), [623](#)
[_DP_DeepTensorComputeNList](#) (C++ function), [623](#)
[_DP_DeepTensorComputeNList<double>](#) (C++ function), [623](#)
[_DP_DeepTensorComputeNList<float>](#) (C++ function), [624](#)
[_DP_DeepTensorComputeTensor](#) (C++ function), [624](#)
[_DP_DeepTensorComputeTensor<double>](#) (C++ function), [624](#)
[_DP_DeepTensorComputeTensor<float>](#) (C++ function), [625](#)
[_DP_DeepTensorComputeTensorNList](#) (C++ function), [625](#)
[_DP_DeepTensorComputeTensorNList<double>](#) (C++ function), [625](#)
[_DP_DeepTensorComputeTensorNList<float>](#)

(C++ function), [625](#)
[_DP_DipoleChargeModifierComputeNList](#) (C++ function), [626](#)
[_DP_DipoleChargeModifierComputeNList<double>](#) (C++ function), [626](#)
[_DP_DipoleChargeModifierComputeNList<float>](#) (C++ function), [626](#)
[_DP_Get_Energy_Pointer](#) (C++ function), [627](#)

A

[activation_function:](#)
 [model/type_embedding/activation_function](#) (Argument), [80](#)
 [model\[standard\]/descriptor\[se_a_mask\]/activation_function](#) (Argument), [97](#)
 [model\[standard\]/descriptor\[se_a_tpe\]/activation_function](#) (Argument), [88](#)
 [model\[standard\]/descriptor\[se_atten_v2\]/activation_function](#) (Argument), [95](#)
 [model\[standard\]/descriptor\[se_atten\]/activation_function](#) (Argument), [92](#)
 [model\[standard\]/descriptor\[se_e2_a\]/activation_function](#) (Argument), [84](#)
 [model\[standard\]/descriptor\[se_e2_r\]/activation_function](#) (Argument), [90](#)
 [model\[standard\]/descriptor\[se_e3\]/activation_function](#) (Argument), [86](#)
 [model\[standard\]/fitting_net\[dipole\]/activation_function](#) (Argument), [103](#)
 [model\[standard\]/fitting_net\[dos\]/activation_function](#) (Argument), [101](#)
 [model\[standard\]/fitting_net\[ener\]/activation_function](#) (Argument), [99](#)
 [model\[standard\]/fitting_net\[polar\]/activation_function](#) (Argument), [102](#)
[add\(\)](#) (deepmd.utils.data.DeepmdData method), [474](#)
[add\(\)](#) (deepmd.utils.data_system.DeepmdDataSystem method), [477](#)
[add\(\)](#) (deepmd.utils.DeepmdData method), [458](#)
[add\(\)](#) (deepmd.utils.DeepmdDataSystem method), [461](#)
[add_data_requirement\(\)](#) (in module

deepmd.common), 503
 add_dict() (deepmd.utils.data_system.DeepmdDataSystem method), 478
 add_dict() (deepmd.utils.DeepmdDataSystem method), 461
 add_flt_nvnmd(C++ function), 683
 add_flt_nvnmd() (in module deepmd.env.op_module), 535
 AddFltNvnmd() (in module deepmd.env.op_module), 511
 ArgsPlugin (class in deepmd.utils.argcheck), 466
 atom_ener:
 model[standard]/fitting_net[ener]/atom_ener (Argument), 100
 attn:
 model[standard]/descriptor[se_atten_v2]/attn (Argument), 96
 model[standard]/descriptor[se_atten]/attn (Argument), 93
 attn_dotr:
 model[standard]/descriptor[se_atten_v2]/attn_dotr (Argument), 96
 model[standard]/descriptor[se_atten]/attn_dotr (Argument), 93
 attn_layer:
 model[standard]/descriptor[se_atten_v2]/attn_layer (Argument), 96
 model[standard]/descriptor[se_atten]/attn_layer (Argument), 93
 attn_mask:
 model[standard]/descriptor[se_atten_v2]/attn_mask (Argument), 96
 model[standard]/descriptor[se_atten]/attn_mask (Argument), 93
 auto_prob:
 training/training_data/auto_prob (Argument), 112
 training/validation_data/auto_prob (Argument), 113
 AutoBatchSize (class in deepmd.utils.batch_size), 468
 avg() (deepmd.utils.data.DeepmdData method), 475
 avg() (deepmd.utils.DeepmdData method), 459
 axis_neuron:
 model[standard]/descriptor[se_a_mask]/axis_neuron (Argument), 97
 model[standard]/descriptor[se_a_tpe]/axis_neuron (Argument), 87
 model[standard]/descriptor[se_atten_v2]/axis_neuron (Argument), 95
 model[standard]/descriptor[se_atten]/axis_neuron (Argument), 92
 model[standard]/descriptor[se_e2_a]/axis_neuron (Argument), 84
 axis_rule:
 model[standard]/descriptor[loc_frame]/axis_rule (Argument), 83
 B
 batch_size:
 training/training_data/batch_size (Argument), 112
 training/validation_data/batch_size (Argument), 113
 bin2hex() (deepmd.nvnmd.utils.Encode method), 440
 bin2hex() (deepmd.nvnmd.utils.encode.Encode method), 447
 bin2hex_str() (deepmd.nvnmd.utils.Encode method), 440
 bin2hex_str() (deepmd.nvnmd.utils.encode.Encode method), 447
 build() (deepmd.descriptor.Descriptor method), 202
 build() (deepmd.descriptor.descriptor.Descriptor method), 250
 build() (deepmd.descriptor.DescriptHybrid method), 208
 build() (deepmd.descriptor.DescriptLocFrame method), 214
 build() (deepmd.descriptor.DescriptSeA method), 218
 build() (deepmd.descriptor.DescriptSeAEbd method), 223
 build() (deepmd.descriptor.DescriptSeAEf method), 225
 build() (deepmd.descriptor.DescriptSeAEfLower method), 228
 build() (deepmd.descriptor.DescriptSeAMask method), 231
 build() (deepmd.descriptor.DescriptSeAtten method), 235
 build() (deepmd.descriptor.DescriptSeR method), 242
 build() (deepmd.descriptor.DescriptSeT method), 246
 build() (deepmd.descriptor.hybrid.DescriptHybrid method), 257
 build() (deepmd.descriptor.loc_frame.DescriptLocFrame method), 262
 build() (deepmd.descriptor.se_a.DescriptSeA method), 268
 build() (deepmd.descriptor.se_a_ebd.DescriptSeAEbd method), 273
 build() (deepmd.descriptor.se_a_ef.DescriptSeAEf method), 275
 build() (deepmd.descriptor.se_a_ef.DescriptSeAEfLower method), 278

`build()` (deepmd.descriptor.se_a_mask.DescriptSeAMask method), 281
`build()` (deepmd.descriptor.se_atten.DescriptSeAtten method), 285
`build()` (deepmd.descriptor.se_r.DescriptSeR method), 292
`build()` (deepmd.descriptor.se_t.DescriptSeT method), 296
`build()` (deepmd.fit.dipole.DipoleFittingSeA method), 323
`build()` (deepmd.fit.DipoleFittingSeA method), 312
`build()` (deepmd.fit.dos.DOSFitting method), 326
`build()` (deepmd.fit.DOSFitting method), 309
`build()` (deepmd.fit.ener.EnerFitting method), 329
`build()` (deepmd.fit.EnerFitting method), 315
`build()` (deepmd.fit.GlobalPolarFittingSeA method), 319
`build()` (deepmd.fit.polar.GlobalPolarFittingSeA method), 334
`build()` (deepmd.fit.polar.PolarFittingSeA method), 336
`build()` (deepmd.fit.PolarFittingSeA method), 321
`build()` (deepmd.loss.dos.DOSLoss method), 387
`build()` (deepmd.loss.DOSLoss method), 381
`build()` (deepmd.loss.ener.EnerDipoleLoss method), 388
`build()` (deepmd.loss.ener.EnerSpinLoss method), 389
`build()` (deepmd.loss.ener.EnerStdLoss method), 391
`build()` (deepmd.loss.EnerDipoleLoss method), 382
`build()` (deepmd.loss.EnerSpinLoss method), 383
`build()` (deepmd.loss.EnerStdLoss method), 385
`build()` (deepmd.loss.loss.Loss method), 392
`build()` (deepmd.loss.tensor.TensorLoss method), 393
`build()` (deepmd.loss.TensorLoss method), 386
`build()` (deepmd.model.dos.DOSModel method), 406
`build()` (deepmd.model.DOSModel method), 395
`build()` (deepmd.model.ener.EnerModel method), 409
`build()` (deepmd.model.EnerModel method), 398
`build()` (deepmd.model.model.Model method), 412
`build()` (deepmd.model.multi.MultiModel method), 418
`build()` (deepmd.model.MultiModel method), 402
`build()` (deepmd.model.pairwise_dprc.PairwiseDPRC method), 420
`build()` (deepmd.model.tensor.TensorModel method), 426
`build()` (deepmd.train.trainer.DatasetLoader method), 456
`build()` (deepmd.train.trainer.DPTrainer method), 455
`build()` (deepmd.utils.learning_rate.LearningRateExp method), 485
`build()` (deepmd.utils.LearningRateExp method), 463
`build()` (deepmd.utils.spin.Spin method), 497
`build()` (deepmd.utils.tabulate.DPTabulate method), 498
`build()` (deepmd.utils.type_embed.TypeEmbedNet method), 499
`build_davg_dstd()` (deepmd.nvnmd.entrypoints.mapt.MapTable method), 436
`build_davg_dstd()` (deepmd.nvnmd.entrypoints.MapTable method), 431
`build_davg_dstd()` (in module deepmd.nvnmd.descriptor.se_a), 429
`build_davg_dstd()` (in module deepmd.nvnmd.descriptor.se_atten), 429
`build_descript()` (deepmd.model.model.Model method), 413
`build_embedding_net()` (deepmd.nvnmd.entrypoints.mapt.MapTable method), 436
`build_embedding_net()` (deepmd.nvnmd.entrypoints.MapTable method), 431
`build_fv_graph()` (deepmd.DipoleChargeModifier method), 199
`build_fv_graph()` (deepmd.infer.data_modifier.DipoleChargeModifier method), 357
`build_fv_graph()` (deepmd.infer.DipoleChargeModifier method), 353
`build_grad()` (deepmd.nvnmd.entrypoints.mapt.MapTable method), 436
`build_grad()` (deepmd.nvnmd.entrypoints.MapTable method), 431
`build_map()` (deepmd.nvnmd.entrypoints.mapt.MapTable method), 436
`build_map()` (deepmd.nvnmd.entrypoints.MapTable method), 431
`build_map_coef()` (deepmd.nvnmd.entrypoints.mapt.MapTable method), 436
`build_map_coef()` (deepmd.nvnmd.entrypoints.MapTable method), 431
`build_nlist` (C++ function), 683, 684
`build_op_descriptor()` (in module deepmd.nvnmd.descriptor.se_a), 429
`build_op_descriptor()` (in module deepmd.nvnmd.descriptor.se_atten), 429
`build_s2g()` (deepmd.nvnmd.entrypoints.mapt.MapTable method), 436
`build_s2g()` (deepmd.nvnmd.entrypoints.MapTable method), 431
`build_s2g_grad()` (deepmd.nvnmd.entrypoints.mapt.MapTable method), 436

`build_s2g_grad()` (deepmd.nvnmd.entrypoints.MapTable (deepmd.model.ener.EnerModel method), 431
`build_t2g()` (deepmd.nvnmd.entrypoints.maptable (deepmd.model.ener.EnerModel method), 436
`build_t2g()` (deepmd.nvnmd.entrypoints.MapTable change_energy_bias() (deepmd.model.ener.EnerModel method), 431
`build_type_exclude_mask()` (deepmd.descriptor.Descriptor method), 203
`build_type_exclude_mask()` (deepmd.descriptor.descriptor.Descriptor method), 251
`build_type_exclude_mask()` (deepmd.descriptor.DescriptSeAtten method), 236
`build_type_exclude_mask()` (deepmd.descriptor.se_atten.DescriptSeAtten method), 286
`build_u2s()` (deepmd.nvnmd.entrypoints.maptable (deepmd.nvnmd.descriptor.se_atten), 437
`build_u2s()` (deepmd.nvnmd.entrypoints.MapTable method), 432
`build_u2s_grad()` (deepmd.nvnmd.entrypoints.maptable (deepmd.nvnmd.descriptor.se_atten), 437
`build_u2s_grad()` (deepmd.nvnmd.entrypoints.MapTable method), 432
`byte2hex()` (deepmd.nvnmd.utils.Encode method), 440
`byte2hex()` (deepmd.nvnmd.utils.encode.Encode method), 447

C

`cal_coef4()` (deepmd.nvnmd.entrypoints.maptable (deepmd.infer.model_devi), 437
`cal_coef4()` (deepmd.nvnmd.entrypoints.MapTable method), 432
`calc_model_devi()` (in module deepmd.infer), 355
`calc_model_devi()` (in module deepmd.infer.model_devi), 376
`calc_model_devi_e()` (in module deepmd.infer.model_devi), 377
`calc_model_devi_f()` (in module deepmd.infer.model_devi), 377
`calc_model_devi_v()` (in module deepmd.infer.model_devi), 377
`calculate()` (deepmd.calculator.DP method), 503
`cast_precision()` (in module deepmd.common), 504
`change_energy_bias()` (deepmd.fit.ener.EnerFitting method), 330
`change_energy_bias()` (deepmd.fit.EnerFitting method), 315
`change_energy_bias()` (deepmd.model.ener.EnerModel method), 410
`change_energy_bias()` (deepmd.model.ener.EnerModel method), 399
`change_energy_bias()` (deepmd.model.model.Model method), 413
`check_batch_size()` (deepmd.utils.data.DeepmdData method), 475
`check_batch_size()` (deepmd.utils.DeepmdData method), 459
`check_dec()` (deepmd.nvnmd.utils.Encode method), 441
`check_dec()` (deepmd.nvnmd.utils.encode.Encode method), 447
`check_switch_range()` (in module deepmd.nvnmd.descriptor.se_a), 429
`check_switch_range()` (in module deepmd.nvnmd.descriptor.se_atten), 429
`check_test_size()` (deepmd.utils.data.DeepmdData method), 475
`check_test_size()` (deepmd.utils.DeepmdData method), 459
`choice()` (in module deepmd.utils.random), 495
`clear_session()` (in module deepmd.common), 504
`compress()` (in module deepmd.entrypoints), 299
`compress()` (in module deepmd.entrypoints.compress), 303
`compress:`
`model/compress` (Argument), 81
`compute_descriptor` (C++ function), 685
`compute_descriptor_se_a_ef_para` (C++ function), 685
`compute_descriptor_se_a_ef_vert` (C++ function), 686
`compute_descriptor_se_a_extf` (C++ function), 686
`compute_energy_shift()` (deepmd.utils.data_system.DeepmdDataSystem method), 478
`compute_energy_shift()` (deepmd.utils.DeepmdDataSystem method), 461
`compute_input_stats()` (deepmd.descriptor.Descriptor method), 204
`compute_input_stats()` (deepmd.descriptor.descriptor.Descriptor method), 252
`compute_input_stats()` (deepmd.descriptor.DescriptHybrid method), 209
`compute_input_stats()` (deepmd.descriptor.DescriptLocFrame

method), 215

`compute_input_stats()` (deepmd.descriptor.DescriptSeA method), 219

`compute_input_stats()` (deepmd.descriptor.DescriptSeAEf method), 226

`compute_input_stats()` (deepmd.descriptor.DescriptSeAEfLower method), 229

`compute_input_stats()` (deepmd.descriptor.DescriptSeAMask method), 232

`compute_input_stats()` (deepmd.descriptor.DescriptSeAtten method), 237

`compute_input_stats()` (deepmd.descriptor.DescriptSeR method), 243

`compute_input_stats()` (deepmd.descriptor.DescriptSeT method), 247

`compute_input_stats()` (deepmd.descriptor.hybrid.DescriptHybrid method), 257

`compute_input_stats()` (deepmd.descriptor.loc_frame.DescriptLocFrame method), 263

`compute_input_stats()` (deepmd.descriptor.se_a.DescriptSeA method), 269

`compute_input_stats()` (deepmd.descriptor.se_a_ef.DescriptSeAEf method), 276

`compute_input_stats()` (deepmd.descriptor.se_a_ef.DescriptSeAEfLower method), 279

`compute_input_stats()` (deepmd.descriptor.se_a_mask.DescriptSeAMask method), 282

`compute_input_stats()` (deepmd.descriptor.se_atten.DescriptSeAtten method), 287

`compute_input_stats()` (deepmd.descriptor.se_r.DescriptSeR method), 293

`compute_input_stats()` (deepmd.descriptor.se_t.DescriptSeT method), 297

`compute_input_stats()` (deepmd.fit.dos.DOSFitting method), 326

`compute_input_stats()` (deepmd.fit.DOSFitting method), 310

`compute_input_stats()` (deepmd.fit.ener.EnerFitting method), 330

`compute_input_stats()` (deepmd.fit.EnerFitting method), 316

`compute_input_stats()` (deepmd.fit.polar.PolarFittingSeA method), 337

`compute_input_stats()` (deepmd.fit.PolarFittingSeA method), 322

`compute_output_stats()` (deepmd.fit.dos.DOSFitting method), 327

`compute_output_stats()` (deepmd.fit.DOSFitting method), 310

`compute_output_stats()` (deepmd.fit.ener.EnerFitting method), 330

`compute_output_stats()` (deepmd.fit.EnerFitting method), 316

`compute_prec:`
training/mixed_precision/compute_prec (Argument), 114

`config_file:`
nvnmd/config_file (Argument), 116

`convert()` (in module deepmd.entypoints), 300

`convert()` (in module deepmd.entypoints.convert), 304

`convert_012_to_21()` (in module deepmd.utils.convert), 471

`convert_10_to_21()` (in module deepmd.utils.convert), 471

`convert_12_to_21()` (in module deepmd.utils.convert), 471

`convert_13_to_21()` (in module deepmd.utils.convert), 471

`convert_20_to_21()` (in module deepmd.utils.convert), 471

`convert_dp012_to_dp10()` (in module deepmd.utils.convert), 472

`convert_dp10_to_dp11()` (in module deepmd.utils.convert), 472

`convert_dp12_to_dp13()` (in module deepmd.utils.convert), 472

`convert_dp13_to_dp20()` (in module deepmd.utils.convert), 472

`convert_dp20_to_dp21()` (in module deepmd.utils.convert), 472

`convert_input_v0_v1()` (in module deepmd.utils.compat), 470

`convert_input_v1_v2()` (in module deepmd.utils.compat), 470

`convert_pb_to_pbtxt()` (in module

deepmd.utils.convert), 472
 convert_pbtxt_to_pb() (in module
 deepmd.utils.convert), 472
 convert_to_21() (in module deepmd.utils.convert),
 472
 copy_coord (C++ function), 687
 copy_flt_nvnmmd() (in module
 deepmd.env.op_module), 536
 CopyFltNvnmd() (in module
 deepmd.env.op_module), 511
 create_file_path() (deepmd.nvnmd.utils.fio.Fio
 method), 449

D

data_bias_nsample:
 model/data_bias_nsample (Argument), 79
 data_dict:
 training/data_dict (Argument), 115
 data_stat() (deepmd.model.dos.DOSModel
 method), 407
 data_stat() (deepmd.model.DOSModel method),
 396
 data_stat() (deepmd.model.ener.EnerModel
 method), 410
 data_stat() (deepmd.model.EnerModel method),
 399
 data_stat() (deepmd.model.model.Model method),
 414
 data_stat() (deepmd.model.multi.MultiModel
 method), 419
 data_stat() (deepmd.model.MultiModel method),
 403
 data_stat() (deepmd.model.pairwise_dprc.PairwiseDPRC
 method), 421
 data_stat() (deepmd.model.tensor.TensorModel
 method), 426
 data_stat_nbatch:
 model/data_stat_nbatch (Argument), 78
 data_stat_protect:
 model/data_stat_protect (Argument), 78
 DatasetLoader (class in deepmd.train.trainer), 456
 dec2bin() (deepmd.nvnmd.utils.Encode method),
 441
 dec2bin() (deepmd.nvnmd.utils.encode.Encode
 method), 447
 decay_steps:
 learning_rate[exp]/decay_steps
 (Argument), 105
 DeepDipole (class in deepmd.infer), 341
 DeepDipole (class in deepmd.infer.deep_dipole), 358
 DeepDOS (class in deepmd.infer), 338
 DeepDOS (class in deepmd.infer.deep_dos), 359
 DeepEval (class in deepmd), 195
 DeepEval (class in deepmd.infer), 342
 DeepEval (class in deepmd.infer.deep_eval), 362
 DeepGlobalPolar (class in deepmd.infer), 345
 DeepGlobalPolar (class in
 deepmd.infer.deep_polar), 365
 deepmd
 module, 195
 deepmd.calculator
 module, 501
 deepmd.cluster
 module, 200
 deepmd.cluster.local
 module, 200
 deepmd.cluster.slurm
 module, 201
 deepmd.common
 module, 503
 deepmd.descriptor
 module, 201
 deepmd.descriptor.descriptor
 module, 249
 deepmd.descriptor.hybrid
 module, 256
 deepmd.descriptor.loc_frame
 module, 261
 deepmd.descriptor.se
 module, 264
 deepmd.descriptor.se_a
 module, 266
 deepmd.descriptor.se_a_ebd
 module, 272
 deepmd.descriptor.se_a_ef
 module, 274
 deepmd.descriptor.se_a_mask
 module, 279
 deepmd.descriptor.se_atten
 module, 283
 deepmd.descriptor.se_atten_v2
 module, 288
 deepmd.descriptor.se_r
 module, 290
 deepmd.descriptor.se_t
 module, 295
 deepmd.entrypoints
 module, 299
 deepmd.entrypoints.compress
 module, 303
 deepmd.entrypoints.convert
 module, 304
 deepmd.entrypoints.doc
 module, 304
 deepmd.entrypoints.freeze
 module, 304
 deepmd.entrypoints.ipi
 module, 305

```

deepmd.entrypoints.main
  module, 305
deepmd.entrypoints.neighbor_stat
  module, 306
deepmd.entrypoints.test
  module, 306
deepmd.entrypoints.train
  module, 307
deepmd.entrypoints.transfer
  module, 308
deepmd.env
  module, 508
deepmd.env.op_grads_module
  module, 560
deepmd.env.op_module
  module, 511
deepmd.fit
  module, 308
deepmd.fit.dipole
  module, 323
deepmd.fit.dos
  module, 325
deepmd.fit.ener
  module, 328
deepmd.fit.fitting
  module, 332
deepmd.fit.polar
  module, 333
deepmd.infer
  module, 338
deepmd.infer.data_modifier
  module, 356
deepmd.infer.deep_dipole
  module, 358
deepmd.infer.deep_dos
  module, 359
deepmd.infer.deep_eval
  module, 362
deepmd.infer.deep_polar
  module, 365
deepmd.infer.deep_pot
  module, 367
deepmd.infer.deep_tensor
  module, 371
deepmd.infer.deep_wfc
  module, 374
deepmd.infer.ewald_recip
  module, 375
deepmd.infer.model_devi
  module, 376
deepmd.lmp
  module, 508
deepmd.loggers
  module, 379
deepmd.loggers.loggers
  module, 380
deepmd.loss
  module, 381
deepmd.loss.dos
  module, 387
deepmd.loss.ener
  module, 388
deepmd.loss.loss
  module, 392
deepmd.loss.tensor
  module, 393
deepmd.model
  module, 394
deepmd.model.dos
  module, 405
deepmd.model.ener
  module, 407
deepmd.model.model
  module, 411
deepmd.model.model_stat
  module, 417
deepmd.model.multi
  module, 417
deepmd.model.pairwise_dprc
  module, 420
deepmd.model.tensor
  module, 423
deepmd.nvnmd
  module, 427
deepmd.nvnmd.data
  module, 427
deepmd.nvnmd.data.data
  module, 428
deepmd.nvnmd.descriptor
  module, 428
deepmd.nvnmd.descriptor.se_a
  module, 429
deepmd.nvnmd.descriptor.se_atten
  module, 429
deepmd.nvnmd.entrypoints
  module, 430
deepmd.nvnmd.entrypoints.freeze
  module, 434
deepmd.nvnmd.entrypoints.mapt
  module, 434
deepmd.nvnmd.entrypoints.train
  module, 437
deepmd.nvnmd.entrypoints.wrap
  module, 438
deepmd.nvnmd.fit
  module, 439
deepmd.nvnmd.fit.ener
  module, 439

```

| | |
|-----------------------------|---|
| deepmd.nvnmd.utils | deepmd.utils.parallel_op |
| module, 440 | module, 489 |
| deepmd.nvnmd.utils.argcheck | deepmd.utils.path |
| module, 444 | module, 490 |
| deepmd.nvnmd.utils.config | deepmd.utils.plugin |
| module, 444 | module, 494 |
| deepmd.nvnmd.utils.encode | deepmd.utils.random |
| module, 447 | module, 495 |
| deepmd.nvnmd.utils.fio | deepmd.utils.sess |
| module, 449 | module, 496 |
| deepmd.nvnmd.utils.network | deepmd.utils.spin |
| module, 451 | module, 496 |
| deepmd.nvnmd.utils.op | deepmd.utils.tabulate |
| module, 452 | module, 497 |
| deepmd.nvnmd.utils.weight | deepmd.utils.type_embed |
| module, 452 | module, 499 |
| deepmd.op | deepmd.utils.weight_avg |
| module, 454 | module, 501 |
| deepmd.train | deepmd::AtomMap (C++ class), 573 |
| module, 454 | deepmd::AtomMap::AtomMap (C++ function), 573 |
| deepmd.train.run_options | deepmd::AtomMap::backward (C++ function), 573 |
| module, 454 | deepmd::AtomMap::forward (C++ function), 573 |
| deepmd.train.trainer | deepmd::AtomMap::get_bkw_map (C++ function), |
| module, 455 | 574 |
| deepmd.utils | deepmd::AtomMap::get_fwd_map (C++ function), |
| module, 457 | 574 |
| deepmd.utils.argcheck | deepmd::AtomMap::get_type (C++ function), 573 |
| module, 466 | deepmd::build_nlist_cpu (C++ function), 688 |
| deepmd.utils.batch_size | deepmd::build_nlist_gpu (C++ function), 688 |
| module, 468 | deepmd::check_status (C++ function), 588 |
| deepmd.utils.compat | deepmd::compute_cell_info (C++ function), 688 |
| module, 470 | deepmd::convert_nlist (C++ function), 688 |
| deepmd.utils.convert | deepmd::convert_nlist_gpu_device (C++ func- |
| module, 471 | tion), 689 |
| deepmd.utils.data | deepmd::convert_pbtxt_to_pb (C++ function), |
| module, 473 | 588 |
| deepmd.utils.data_system | deepmd::convert_to_inter_cpu (C++ function), |
| module, 476 | 689 |
| deepmd.utils.errors | deepmd::convert_to_inter_gpu (C++ function), |
| module, 479 | 689 |
| deepmd.utils.finetune | deepmd::convert_to_phys_cpu (C++ function), |
| module, 480 | 690 |
| deepmd.utils.graph | deepmd::convert_to_phys_gpu (C++ function), |
| module, 480 | 690 |
| deepmd.utils.learning_rate | deepmd::copy_coord_cpu (C++ function), 690 |
| module, 484 | deepmd::copy_coord_gpu (C++ function), 690 |
| deepmd.utils.multi_init | deepmd::cos_switch (C++ function), 691 |
| module, 485 | deepmd::cprod (C++ function), 691 |
| deepmd.utils.neighbor_stat | deepmd::cum_sum (C++ function), 691 |
| module, 486 | deepmd::deepmd_exception (C++ struct), 572, 673 |
| deepmd.utils.network | deepmd::deepmd_exception::deepmd_exception |
| module, 487 | (C++ function), 673 |
| deepmd.utils.pair_tab | deepmd::deepmd_exception_oom (C++ struct), 674 |
| module, 488 | |

```

deepmd::deepmd_exception_oom::deepmd_exception_oom
    (C++ function), 674
deepmd::DeepPot (C++ class), 574
deepmd::DeepPot::~~DeepPot (C++ function), 574
deepmd::DeepPot::compute (C++ function), 574--576
deepmd::DeepPot::compute_mixed_type (C++ function), 577
deepmd::DeepPot::cutoff (C++ function), 578
deepmd::DeepPot::DeepPot (C++ function), 574
deepmd::DeepPot::dim_aparam (C++ function), 578
deepmd::DeepPot::dim_fparam (C++ function), 578
deepmd::DeepPot::get_type_map (C++ function), 579
deepmd::DeepPot::init (C++ function), 574
deepmd::DeepPot::numb_types (C++ function), 578
deepmd::DeepPot::numb_types_spin (C++ function), 578
deepmd::DeepPot::print_summary (C++ function), 574
deepmd::DeepPotModelDevi (C++ class), 579
deepmd::DeepPotModelDevi::~~DeepPotModelDevi
    (C++ function), 579
deepmd::DeepPotModelDevi::compute (C++ function), 579, 580
deepmd::DeepPotModelDevi::compute_avg (C++ function), 581
deepmd::DeepPotModelDevi::compute_relative_std
    (C++ function), 582
deepmd::DeepPotModelDevi::compute_relative_std_e
    (C++ function), 582
deepmd::DeepPotModelDevi::compute_std (C++ function), 582
deepmd::DeepPotModelDevi::compute_std_e
    (C++ function), 582
deepmd::DeepPotModelDevi::compute_std_f
    (C++ function), 582
deepmd::DeepPotModelDevi::cutoff (C++ function), 581
deepmd::DeepPotModelDevi::DeepPotModelDevi
    (C++ function), 579
deepmd::DeepPotModelDevi::dim_aparam (C++ function), 581
deepmd::DeepPotModelDevi::dim_fparam (C++ function), 581
deepmd::DeepPotModelDevi::init (C++ function), 579
deepmd::DeepPotModelDevi::numb_types (C++ function), 581
deepmd::DeepPotModelDevi::numb_types_spin
    (C++ function), 581
deepmd::DeepTensor (C++ class), 583
deepmd::DeepTensor::~~DeepTensor (C++ function), 583
deepmd::DeepTensor::compute (C++ function), 583--585
deepmd::DeepTensor::cutoff (C++ function), 586
deepmd::DeepTensor::DeepTensor (C++ function), 583
deepmd::DeepTensor::init (C++ function), 583
deepmd::DeepTensor::numb_types (C++ function), 586
deepmd::DeepTensor::output_dim (C++ function), 586
deepmd::DeepTensor::print_summary (C++ function), 583
deepmd::DeepTensor::sel_types (C++ function), 586
deepmd::delete_device_memory (C++ function), 692
deepmd::DipoleChargeModifier (C++ class), 586
deepmd::DipoleChargeModifier::~~DipoleChargeModifier
    (C++ function), 586
deepmd::DipoleChargeModifier::compute (C++ function), 587
deepmd::DipoleChargeModifier::cutoff (C++ function), 587
deepmd::DipoleChargeModifier::DipoleChargeModifier
    (C++ function), 586
deepmd::DipoleChargeModifier::init (C++ function), 587
deepmd::DipoleChargeModifier::numb_types
    (C++ function), 587
deepmd::DipoleChargeModifier::print_summary
    (C++ function), 587
deepmd::DipoleChargeModifier::sel_types
    (C++ function), 587
deepmd::dot1 (C++ function), 692
deepmd::dot2 (C++ function), 692
deepmd::dot3 (C++ function), 692
deepmd::dot4 (C++ function), 692
deepmd::dotmv3 (C++ function), 693
deepmd::DPGetDeviceCount (C++ function), 693
deepmd::dprc_pairwise_map_cpu (C++ function), 693
deepmd::DPSetDevice (C++ function), 694
deepmd::ElectrostaticConversion (C++ member), 723
deepmd::ENERGYTYPE (C++ type), 597
deepmd::env_mat_a_cpu (C++ function), 694
deepmd::env_mat_a_nvnmmd_quantize_cpu (C++ function), 694
deepmd::env_mat_nbor_update (C++ function), 695
deepmd::env_mat_r_cpu (C++ function), 695

```

deepmd::ewald_recip (C++ function), 695
 deepmd::EwaldParameters (C++ struct), 674
 deepmd::EwaldParameters::beta (C++ member), 674
 deepmd::EwaldParameters::rcut (C++ member), 674
 deepmd::EwaldParameters::spacing (C++ member), 674
 deepmd::filter_ftype_gpu_cuda (C++ function), 695
 deepmd::format_nbor_list_gpu_cuda (C++ function), 696
 deepmd::format_nlist_cpu (C++ function), 696
 deepmd::free_nlist_gpu_device (C++ function), 696
 deepmd::gelu_cpu (C++ function), 697
 deepmd::gelu_gpu_cuda (C++ function), 697
 deepmd::gelu_grad_cpu (C++ function), 697
 deepmd::gelu_grad_gpu_cuda (C++ function), 697
 deepmd::gelu_grad_grad_cpu (C++ function), 698
 deepmd::gelu_grad_grad_gpu_cuda (C++ function), 698
 deepmd::get_env_nthreads (C++ function), 588
 deepmd::group_atoms_cpu (C++ function), 698
 deepmd::hpp::convert_nlist (C++ function), 627
 deepmd::hpp::convert_pbtxt_to_pb (C++ function), 627
 deepmd::hpp::deepmd_exception (C++ struct), 601
 deepmd::hpp::deepmd_exception::deepmd_exception (C++ function), 601
 deepmd::hpp::DeepPot (C++ class), 605
 deepmd::hpp::DeepPot::~DeepPot (C++ function), 605
 deepmd::hpp::DeepPot::compute (C++ function), 605–607
 deepmd::hpp::DeepPot::compute_mixed_type (C++ function), 608, 609
 deepmd::hpp::DeepPot::cutoff (C++ function), 609
 deepmd::hpp::DeepPot::DeepPot (C++ function), 605
 deepmd::hpp::DeepPot::dim_aparam (C++ function), 610
 deepmd::hpp::DeepPot::dim_fparam (C++ function), 610
 deepmd::hpp::DeepPot::get_type_map (C++ function), 609
 deepmd::hpp::DeepPot::init (C++ function), 605
 deepmd::hpp::DeepPot::numb_types (C++ function), 609
 deepmd::hpp::DeepPot::numb_types_spin (C++ function), 609
 deepmd::hpp::DeepPot::print_summary (C++ function), 610
 deepmd::hpp::DeepPotModelDevi (C++ class), 610
 deepmd::hpp::DeepPotModelDevi::~DeepPotModelDevi (C++ function), 610
 deepmd::hpp::DeepPotModelDevi::compute (C++ function), 611
 deepmd::hpp::DeepPotModelDevi::compute_avg (C++ function), 612
 deepmd::hpp::DeepPotModelDevi::compute_relative_std (C++ function), 612
 deepmd::hpp::DeepPotModelDevi::compute_relative_std_f (C++ function), 613
 deepmd::hpp::DeepPotModelDevi::compute_std (C++ function), 612
 deepmd::hpp::DeepPotModelDevi::compute_std_f (C++ function), 613
 deepmd::hpp::DeepPotModelDevi::cutoff (C++ function), 611
 deepmd::hpp::DeepPotModelDevi::DeepPotModelDevi (C++ function), 610
 deepmd::hpp::DeepPotModelDevi::dim_aparam (C++ function), 612
 deepmd::hpp::DeepPotModelDevi::dim_fparam (C++ function), 612
 deepmd::hpp::DeepPotModelDevi::init (C++ function), 610
 deepmd::hpp::DeepPotModelDevi::numb_types (C++ function), 612
 deepmd::hpp::DeepPotModelDevi::numb_types_spin (C++ function), 612
 deepmd::hpp::DeepTensor (C++ class), 613
 deepmd::hpp::DeepTensor::~DeepTensor (C++ function), 613
 deepmd::hpp::DeepTensor::compute (C++ function), 614, 615
 deepmd::hpp::DeepTensor::cutoff (C++ function), 616
 deepmd::hpp::DeepTensor::DeepTensor (C++ function), 613
 deepmd::hpp::DeepTensor::init (C++ function), 614
 deepmd::hpp::DeepTensor::numb_types (C++ function), 616
 deepmd::hpp::DeepTensor::output_dim (C++ function), 616
 deepmd::hpp::DeepTensor::print_summary (C++ function), 616
 deepmd::hpp::DeepTensor::sel_types (C++ function), 616
 deepmd::hpp::DipoleChargeModifier (C++ class), 617
 deepmd::hpp::DipoleChargeModifier::~DipoleChargeModifier (C++ function), 617
 deepmd::hpp::DipoleChargeModifier::compute (C++ function), 617

| | | |
|--|----------|--|
| deepmd::hpp::DipoleChargeModifier::cutoff (C++ function), 618 | 702, 703 | deepmd::memset_device_memory (C++ function), 563 |
| deepmd::hpp::DipoleChargeModifier::DipoleChargeModifier (C++ function), 617 | | deepmd::model_compatible (C++ function), 589 |
| deepmd::hpp::DipoleChargeModifier::init (C++ function), 617 | | deepmd::name_prefix (C++ function), 589 |
| deepmd::hpp::DipoleChargeModifier::numb_types (C++ function), 618 | | deepmd::NeighborListData (C++ struct), 572 |
| deepmd::hpp::DipoleChargeModifier::print_summary (C++ function), 618 | | deepmd::NeighborListData::copy_from_nlist (C++ function), 572 |
| deepmd::hpp::DipoleChargeModifier::sel_types (C++ function), 618 | | deepmd::NeighborListData::firstneigh (C++ member), 572 |
| deepmd::hpp::InputNlist (C++ struct), 601 | | deepmd::NeighborListData::ilist (C++ mem- ber), 572 |
| deepmd::hpp::InputNlist::firstneigh (C++ member), 602 | | deepmd::NeighborListData::jlist (C++ mem- ber), 572 |
| deepmd::hpp::InputNlist::ilist (C++ member), 602 | | deepmd::NeighborListData::make_inlist (C++ function), 572 |
| deepmd::hpp::InputNlist::InputNlist (C++ function), 601 | | deepmd::NeighborListData::numneigh (C++ member), 572 |
| deepmd::hpp::InputNlist::inum (C++ member), 602 | | deepmd::NeighborListData::shuffle (C++ func- tion), 572 |
| deepmd::hpp::InputNlist::nl (C++ member), 602 | | deepmd::NeighborListData::shuffle_exclude_empty (C++ function), 572 |
| deepmd::hpp::InputNlist::numneigh (C++ mem- ber), 602 | | deepmd::normalize_coord_cpu (C++ function), 703 |
| deepmd::hpp::read_file_to_string (C++ func- tion), 628 | | deepmd::normalize_coord_gpu (C++ function), 703 |
| deepmd::hpp::select_by_type (C++ function), 628 | | deepmd::pair_tab_cpu (C++ function), 704 |
| deepmd::hpp::select_map (C++ function), 629 | | deepmd::print_summary (C++ function), 589 |
| deepmd::init_region_cpu (C++ function), 698 | | deepmd::prod_env_mat_a_cpu (C++ function), 704 |
| deepmd::InputNlist (C++ struct), 675 | | deepmd::prod_env_mat_a_gpu_cuda (C++ func- tion), 704 |
| deepmd::InputNlist::~InputNlist (C++ func- tion), 675 | | deepmd::prod_env_mat_a_nvnmmd_quantize_cpu (C++ function), 705 |
| deepmd::InputNlist::firstneigh (C++ member), 675 | | deepmd::prod_env_mat_r_cpu (C++ function), 705 |
| deepmd::InputNlist::ilist (C++ member), 675 | | deepmd::prod_env_mat_r_gpu_cuda (C++ func- tion), 705 |
| deepmd::InputNlist::InputNlist (C++ function), 675 | | deepmd::prod_force_a_cpu (C++ function), 706 |
| deepmd::InputNlist::inum (C++ member), 675 | | deepmd::prod_force_a_gpu_cuda (C++ function), 707 |
| deepmd::InputNlist::numneigh (C++ member), 675 | | deepmd::prod_force_grad_a_cpu (C++ function), 707 |
| deepmd::invsqrt (C++ function), 699 | | deepmd::prod_force_grad_a_gpu_cuda (C++ function), 707 |
| deepmd::invsqrt<double> (C++ function), 699 | | deepmd::prod_force_grad_r_cpu (C++ function), 708 |
| deepmd::invsqrt<float> (C++ function), 699 | | deepmd::prod_force_grad_r_gpu_cuda (C++ function), 708 |
| deepmd::load_op_library (C++ function), 589 | | deepmd::prod_force_r_cpu (C++ function), 708 |
| deepmd::malloc_device_memory (C++ function), 699, 700 | | deepmd::prod_force_r_gpu_cuda (C++ function), 708 |
| deepmd::malloc_device_memory_sync (C++ func- tion), 700, 701 | | deepmd::prod_virial_a_cpu (C++ function), 709 |
| deepmd::map_aparam_cpu (C++ function), 701 | | deepmd::prod_virial_a_gpu_cuda (C++ function), 709 |
| deepmd::max_numneigh (C++ function), 701 | | deepmd::prod_virial_grad_a_cpu (C++ function), |
| deepmd::memcpy_device_to_host (C++ function), 701, 702 | | |
| deepmd::memcpy_host_to_device (C++ function), | | |

709

deepmd::prod_virial_grad_a_gpu_cuda (C++ function), 709

deepmd::prod_virial_grad_r_cpu (C++ function), 710

deepmd::prod_virial_grad_r_gpu_cuda (C++ function), 710

deepmd::prod_virial_r_cpu (C++ function), 710

deepmd::prod_virial_r_gpu_cuda (C++ function), 710

deepmd::read_file_to_string (C++ function), 590

deepmd::Region (C++ struct), 675

deepmd::Region::~Region (C++ function), 676

deepmd::Region::boxt (C++ member), 676

deepmd::Region::rec_boxt (C++ member), 676

deepmd::Region::Region (C++ function), 676

deepmd::select_by_type (C++ function), 590

deepmd::select_map (C++ function), 591

deepmd::select_map_inv (C++ function), 592

deepmd::select_real_atoms (C++ function), 592

deepmd::select_real_atoms_coord (C++ function), 593

deepmd::session_get_dtype (C++ function), 593

deepmd::session_get_scalar (C++ function), 593

deepmd::session_get_vector (C++ function), 594

deepmd::session_input_tensors (C++ function), 594, 595

deepmd::session_input_tensors_mixed_type (C++ function), 596

deepmd::soft_min_switch_cpu (C++ function), 711

deepmd::soft_min_switch_force_cpu (C++ function), 711

deepmd::soft_min_switch_force_grad_cpu (C++ function), 711

deepmd::soft_min_switch_virial_cpu (C++ function), 711

deepmd::soft_min_switch_virial_grad_cpu (C++ function), 712

deepmd::spline3_switch (C++ function), 712

deepmd::spline5_switch (C++ function), 712

deepmd::STRINGTYPE (C++ type), 597

deepmd::tabulate_fusion_se_a_cpu (C++ function), 712

deepmd::tabulate_fusion_se_a_gpu_cuda (C++ function), 713

deepmd::tabulate_fusion_se_a_grad_cpu (C++ function), 713

deepmd::tabulate_fusion_se_a_grad_gpu_cuda (C++ function), 713

deepmd::tabulate_fusion_se_a_grad_grad_cpu (C++ function), 714

deepmd::tabulate_fusion_se_a_grad_grad_gpu_cuda (C++ function), 714

deepmd::tabulate_fusion_se_r_cpu (C++ function), 714

deepmd::tabulate_fusion_se_r_gpu_cuda (C++ function), 715

deepmd::tabulate_fusion_se_r_grad_cpu (C++ function), 715

deepmd::tabulate_fusion_se_r_grad_gpu_cuda (C++ function), 715

deepmd::tabulate_fusion_se_r_grad_grad_cpu (C++ function), 716

deepmd::tabulate_fusion_se_r_grad_grad_gpu_cuda (C++ function), 716

deepmd::tabulate_fusion_se_t_cpu (C++ function), 716

deepmd::tabulate_fusion_se_t_gpu_cuda (C++ function), 716

deepmd::tabulate_fusion_se_t_grad_cpu (C++ function), 717

deepmd::tabulate_fusion_se_t_grad_gpu_cuda (C++ function), 717

deepmd::tabulate_fusion_se_t_grad_grad_cpu (C++ function), 717

deepmd::tabulate_fusion_se_t_grad_grad_gpu_cuda (C++ function), 718

deepmd::test_encoding_decoding_nbor_info_gpu_cuda (C++ function), 718

deepmd::tf_exception (C++ struct), 573

deepmd::tf_exception::tf_exception (C++ function), 573

deepmd::use_nei_info_cpu (C++ function), 718

deepmd::use_nei_info_gpu (C++ function), 719

deepmd::use_nlist_map (C++ function), 719

deepmd::volume_cpu (C++ function), 719

deepmd::volume_gpu (C++ function), 719

DeepmdData (class in deepmd.utils), 457

DeepmdData (class in deepmd.utils.data), 473

DeepmdDataSystem (class in deepmd.utils), 460

DeepmdDataSystem (class in deepmd.utils.data_system), 476

DeepPolar (class in deepmd.infer), 346

DeepPolar (class in deepmd.infer.deep_polar), 366

DeepPot (class in deepmd.infer), 347

DeepPot (class in deepmd.infer.deep_pot), 367

DeepPotential () (in module deepmd), 198

DeepPotential () (in module deepmd.infer), 351

DeepTensor (class in deepmd.infer.deep_tensor), 371

DeepWFC (class in deepmd.infer), 351

DeepWFC (class in deepmd.infer.deep_wfc), 374

default_mesh (deepmd.utils.data_system.DeepmdDataSystem property), 478

default_mesh (deepmd.utils.DeepmdDataSystem property), 461

deprecate_numb_test () (in module

deepmd.utils.compat), 470
 Descriptor (class in deepmd.descriptor), 201
 Descriptor (class in deepmd.descriptor.descriptor), 249
 descriptor:
 model[multi]/descriptor (Argument), 104
 model[standard]/descriptor (Argument), 82
 Descript() (in module deepmd.env.op_module), 511
 descript() (in module deepmd.env.op_module), 536
 descript2r4() (in module deepmd.nvnmd.descriptor.se_a), 429
 descript2r4() (in module deepmd.nvnmd.descriptor.se_atten), 429
 descript_hybrid_args() (in module deepmd.utils.argcheck), 466
 descript_local_frame_args() (in module deepmd.utils.argcheck), 466
 descript_norot() (in module deepmd.env.op_module), 536
 descript_se_a() (in module deepmd.env.op_module), 537
 descript_se_a_args() (in module deepmd.utils.argcheck), 466
 descript_se_a_ef() (in module deepmd.env.op_module), 537
 descript_se_a_ef_para() (in module deepmd.env.op_module), 538
 descript_se_a_ef_vert() (in module deepmd.env.op_module), 539
 descript_se_a_mask() (in module deepmd.env.op_module), 539
 descript_se_a_mask_args() (in module deepmd.utils.argcheck), 466
 descript_se_a_tpe_args() (in module deepmd.utils.argcheck), 466
 descript_se_atten_args() (in module deepmd.utils.argcheck), 467
 descript_se_atten_common_args() (in module deepmd.utils.argcheck), 467
 descript_se_atten_v2_args() (in module deepmd.utils.argcheck), 467
 descript_se_r() (in module deepmd.env.op_module), 540
 descript_se_r_args() (in module deepmd.utils.argcheck), 467
 descript_se_t_args() (in module deepmd.utils.argcheck), 467
 descript_variant_type_args() (in module deepmd.utils.argcheck), 467
 DescriptHybrid (class in deepmd.descriptor), 208
 DescriptHybrid (class in deepmd.descriptor.hybrid), 256
 DescriptLocFrame (class in deepmd.descriptor), 212
 DescriptLocFrame (class in deepmd.descriptor.loc_frame), 261
 DescriptNorot() (in module deepmd.env.op_module), 512
 DescriptSe (class in deepmd.descriptor.se), 264
 DescriptSeA (class in deepmd.descriptor), 216
 DescriptSeA (class in deepmd.descriptor.se_a), 266
 DescriptSeA() (in module deepmd.env.op_module), 512
 DescriptSeAEbd (class in deepmd.descriptor), 222
 DescriptSeAEbd (class in module deepmd.descriptor.se_a_ebd), 272
 DescriptSeAEf (class in deepmd.descriptor), 224
 DescriptSeAEf (class in deepmd.descriptor.se_a_ef), 274
 DescriptSeAEf() (in module deepmd.env.op_module), 513
 DescriptSeAEfLower (class in deepmd.descriptor), 227
 DescriptSeAEfLower (class in module deepmd.descriptor.se_a_ef), 277
 DescriptSeAEfPara() (in module deepmd.env.op_module), 514
 DescriptSeAEfVert() (in module deepmd.env.op_module), 514
 DescriptSeAMask (class in deepmd.descriptor), 229
 DescriptSeAMask (class in module deepmd.descriptor.se_a_mask), 279
 DescriptSeAMask() (in module deepmd.env.op_module), 515
 DescriptSeAtten (class in deepmd.descriptor), 233
 DescriptSeAtten (class in module deepmd.descriptor.se_atten), 283
 DescriptSeAttenV2 (class in deepmd.descriptor), 238
 DescriptSeAttenV2 (class in module deepmd.descriptor.se_atten_v2), 288
 DescriptSeR (class in deepmd.descriptor), 240
 DescriptSeR (class in deepmd.descriptor.se_r), 290
 DescriptSeR() (in module deepmd.env.op_module), 515
 DescriptSeRGPUExecuteFunctor (C++ struct), 676
 DescriptSeRGPUExecuteFunctor::operator() (C++ function), 676
 DescriptSeT (class in deepmd.descriptor), 245
 DescriptSeT (class in deepmd.descriptor.se_t), 295
 detect_model_version() (in module deepmd.utils.convert), 473
 DipoleChargeModifier (class in deepmd), 198
 DipoleChargeModifier (class in deepmd.infer), 352
 DipoleChargeModifier (class in module deepmd.infer.data_modifier), 356
 DipoleFittingSeA (class in deepmd.fit), 311
 DipoleFittingSeA (class in deepmd.fit.dipole), 323
 DipoleModel (class in deepmd.model), 396
 DipoleModel (class in deepmd.model.tensor), 423

disp_file:
 training/disp_file (Argument), 114
 disp_freq:
 training/disp_freq (Argument), 114
 disp_message() (deepmd.nvnmd.utils.config.NvnmdConfig method), 445
 disp_training:
 training/disp_training (Argument), 114
 doc_train_input() (in module deepmd.entypoints), 300
 doc_train_input() (in module deepmd.entypoints.doc), 304
 DOSFitting (class in deepmd.fit), 308
 DOSFitting (class in deepmd.fit.dos), 325
 DOSLoss (class in deepmd.loss), 381
 DOSLoss (class in deepmd.loss.dos), 387
 DOSModel (class in deepmd.model), 394
 DOSModel (class in deepmd.model.dos), 405
 dotmul_flt_nvnmd (C++ function), 719
 dotmul_flt_nvnmd() (in module deepmd.env.op_module), 540
 DotmulFltNvnmd() (in module deepmd.env.op_module), 516
 DP (class in deepmd.calculator), 501
 DP_CHECK_OK (C macro), 663
 DP_ConvertPbtxtToPb (C++ function), 629
 DP_DeepPot (C++ struct), 602
 DP_DeepPot (C++ type), 664
 DP_DeepPot::daparam (C++ member), 602
 DP_DeepPot::dfparam (C++ member), 602
 DP_DeepPot::dp (C++ member), 602
 DP_DeepPot::DP_DeepPot (C++ function), 602
 DP_DeepPot::exception (C++ member), 602
 DP_DeepPotCheckOK (C++ function), 629
 DP_DeepPotCompute (C++ function), 630
 DP_DeepPotCompute2 (C++ function), 631
 DP_DeepPotComputef (C++ function), 632
 DP_DeepPotComputef2 (C++ function), 632
 DP_DeepPotComputeMixedType (C++ function), 633
 DP_DeepPotComputeMixedTypef (C++ function), 634
 DP_DeepPotComputeNList (C++ function), 635
 DP_DeepPotComputeNList2 (C++ function), 636
 DP_DeepPotComputeNListf (C++ function), 637
 DP_DeepPotComputeNListf2 (C++ function), 638
 DP_DeepPotGetCutoff (C++ function), 639
 DP_DeepPotGetDimAParam (C++ function), 639
 DP_DeepPotGetDimFParam (C++ function), 639
 DP_DeepPotGetNumbTypes (C++ function), 640
 DP_DeepPotGetNumbTypesSpin (C++ function), 640
 DP_DeepPotGetTypeMap (C++ function), 640
 DP_DeepPotModelDevi (C++ struct), 603
 DP_DeepPotModelDevi (C++ type), 664
 DP_DeepPotModelDevi::daparam (C++ member), 603
 DP_DeepPotModelDevi::dfparam (C++ member), 603
 DP_DeepPotModelDevi::dp (C++ member), 603
 DP_DeepPotModelDevi::DP_DeepPotModelDevi (C++ function), 603
 DP_DeepPotModelDevi::exception (C++ member), 603
 DP_DeepPotModelDeviCheckOK (C++ function), 641
 DP_DeepPotModelDeviComputeNList (C++ function), 641
 DP_DeepPotModelDeviComputeNList2 (C++ function), 642
 DP_DeepPotModelDeviComputeNListf (C++ function), 643
 DP_DeepPotModelDeviComputeNListf2 (C++ function), 644
 DP_DeepPotModelDeviGetCutoff (C++ function), 645
 DP_DeepPotModelDeviGetDimAParam (C++ function), 645
 DP_DeepPotModelDeviGetDimFParam (C++ function), 645
 DP_DeepPotModelDeviGetNumbTypes (C++ function), 646
 DP_DeepPotModelDeviGetNumbTypesSpin (C++ function), 646
 DP_DeepTensor (C++ struct), 603
 DP_DeepTensor (C++ type), 664
 DP_DeepTensor::DP_DeepTensor (C++ function), 603
 DP_DeepTensor::dt (C++ member), 604
 DP_DeepTensor::exception (C++ member), 604
 DP_DeepTensorCheckOK (C++ function), 646
 DP_DeepTensorCompute (C++ function), 647
 DP_DeepTensorComputef (C++ function), 647
 DP_DeepTensorComputeNList (C++ function), 648
 DP_DeepTensorComputeNListf (C++ function), 649
 DP_DeepTensorComputeTensor (C++ function), 650
 DP_DeepTensorComputeTensorf (C++ function), 650
 DP_DeepTensorComputeTensorNList (C++ function), 651
 DP_DeepTensorComputeTensorNListf (C++ function), 651
 DP_DeepTensorGetCutoff (C++ function), 652
 DP_DeepTensorGetNumbSelTypes (C++ function), 652
 DP_DeepTensorGetNumbTypes (C++ function), 652
 DP_DeepTensorGetOutputDim (C++ function), 653
 DP_DeepTensorGetSelTypes (C++ function), 653
 DP_DipoleChargeModifier (C++ struct), 604
 DP_DipoleChargeModifier (C++ type), 665

DP_DipoleChargeModifier::dcm (C++ member), 604
 DP_DipoleChargeModifier::DP_DipoleChargeModifier (C++ function), 604
 DP_DipoleChargeModifier::exception (C++ member), 604
 DP_DipoleChargeModifierCheckOK (C++ function), 653
 DP_DipoleChargeModifierComputeNList (C++ function), 654
 DP_DipoleChargeModifierComputeNListf (C++ function), 655
 DP_DipoleChargeModifierGetCutoff (C++ function), 655
 DP_DipoleChargeModifierGetNumbSelTypes (C++ function), 656
 DP_DipoleChargeModifierGetNumbTypes (C++ function), 656
 DP_DipoleChargeModifierGetSelTypes (C++ function), 656
 dp_ipi() (in module deepmd.entrypoints.ipi), 305
 DP_NEW_OK (C macro), 663
 DP_NewDeepPot (C++ function), 657
 DP_NewDeepPotModelDevi (C++ function), 657
 DP_NewDeepPotModelDeviWithParam (C++ function), 657
 DP_NewDeepPotWithParam (C++ function), 658
 DP_NewDeepPotWithParam2 (C++ function), 658
 DP_NewDeepTensor (C++ function), 659
 DP_NewDeepTensorWithParam (C++ function), 659
 DP_NewDipoleChargeModifier (C++ function), 659
 DP_NewDipoleChargeModifierWithParam (C++ function), 660
 DP_NewNlist (C++ function), 660
 DP_Nlist (C++ struct), 604
 DP_Nlist (C++ type), 665
 DP_Nlist::DP_Nlist (C++ function), 605
 DP_Nlist::exception (C++ member), 605
 DP_Nlist::nl (C++ member), 605
 DP_NlistCheckOK (C++ function), 661
 DP_PrintSummary (C++ function), 661
 DP_ReadFileToChar (C++ function), 661
 DP_ReadFileToChar2 (C++ function), 662
 DP_REQUIRES_OK (C macro), 664
 DP_SelectByType (C++ function), 662
 DP_SelectMapInt (C++ function), 663
 DPAssert (C++ function), 720
 DPErrcheck (C macro), 723, 724
 DPH5Path (class in deepmd.utils.path), 490
 DPOSPath (class in deepmd.utils.path), 491
 DPPPath (class in deepmd.utils.path), 492
 dprc_pairwise_idx() (in module deepmd.env.op_module), 540
 DprcPairwiseIdx() (in module deepmd.env.op_module), 516
 DPTabulate (class in deepmd.utils.tabulate), 497
 DPTrainer (class in deepmd.train.trainer), 455
E
 embed_atom_type() (in module deepmd.utils.type_embed), 500
 embedding_net() (in module deepmd.utils.network), 487
 embedding_net_rand_seed_shift() (in module deepmd.utils.network), 488
 enable:
 nvnmd/enable (Argument), 116
 enable_atom_ener_coeff:
 loss[ener_spin]/enable_atom_ener_coeff (Argument), 109
 loss[ener]/enable_atom_ener_coeff (Argument), 107
 enable_compression() (deepmd.descriptor.Descriptor method), 204
 enable_compression() (deepmd.descriptor.descriptor.Descriptor method), 252
 enable_compression() (deepmd.descriptor.DescriptHybrid method), 210
 enable_compression() (deepmd.descriptor.DescriptSeA method), 219
 enable_compression() (deepmd.descriptor.DescriptSeAtten method), 237
 enable_compression() (deepmd.descriptor.DescriptSeR method), 243
 enable_compression() (deepmd.descriptor.DescriptSeT method), 247
 enable_compression() (deepmd.descriptor.hybrid.DescriptHybrid method), 258
 enable_compression() (deepmd.descriptor.se_a.DescriptSeA method), 269
 enable_compression() (deepmd.descriptor.se_atten.DescriptSeAtten method), 287
 enable_compression() (deepmd.descriptor.se_r.DescriptSeR method), 293
 enable_compression() (deepmd.descriptor.se_t.DescriptSeT

method), 297

enable_compression()
(deepmd.model.model.Model method), 414

enable_compression()
(deepmd.model.model.StandardModel method), 416

enable_compression()
(deepmd.model.pairwise_dprc.PairwiseDPRC method), 421

enable_mixed_precision()
(deepmd.descriptor.Descriptor method), 205

enable_mixed_precision()
(deepmd.descriptor.descriptor.Descriptor method), 253

enable_mixed_precision()
(deepmd.descriptor.DescriptHybrid method), 210

enable_mixed_precision()
(deepmd.descriptor.DescriptSeA method), 220

enable_mixed_precision()
(deepmd.descriptor.hybrid.DescriptHybrid method), 258

enable_mixed_precision()
(deepmd.descriptor.se_a.DescriptSeA method), 270

enable_mixed_precision()
(deepmd.fit.dipole.DipoleFittingSeA method), 324

enable_mixed_precision()
(deepmd.fit.DipoleFittingSeA method), 312

enable_mixed_precision()
(deepmd.fit.dos.DOSFitting method), 327

enable_mixed_precision() (deepmd.fit.DOSFitting method), 310

enable_mixed_precision()
(deepmd.fit.ener.EnerFitting method), 331

enable_mixed_precision()
(deepmd.fit.EnerFitting method), 316

enable_mixed_precision()
(deepmd.fit.GlobalPolarFittingSeA method), 319

enable_mixed_precision()
(deepmd.fit.polar.GlobalPolarFittingSeA method), 334

enable_mixed_precision()
(deepmd.fit.polar.PolarFittingSeA method), 337

enable_mixed_precision()
(deepmd.fit.PolarFittingSeA method), 322

enable_mixed_precision()
(deepmd.model.model.Model method), 414

enable_mixed_precision()
(deepmd.model.model.StandardModel method), 416

enable_mixed_precision()
(deepmd.model.multi.MultiModel method), 419

enable_mixed_precision()
(deepmd.model.MultiModel method), 403

enable_profiler:
training/enable_profiler (Argument), 115

Encode (class in deepmd.nvnmd.utils), 440

Encode (class in deepmd.nvnmd.utils.encode), 447

EnerDipoleLoss (class in deepmd.loss), 382

EnerDipoleLoss (class in deepmd.loss.ener), 388

EnerFitting (class in deepmd.fit), 313

EnerFitting (class in deepmd.fit.ener), 328

EnerModel (class in deepmd.model), 397

EnerModel (class in deepmd.model.ener), 407

EnerSpinLoss (class in deepmd.loss), 383

EnerSpinLoss (class in deepmd.loss.ener), 389

EnerStdLoss (class in deepmd.loss), 384

EnerStdLoss (class in deepmd.loss.ener), 390

env_mat_a (C++ function), 720

env_mat_r (C++ function), 720

eval() (deepmd.DipoleChargeModifier method), 199

eval() (deepmd.infer.data_modifier.DipoleChargeModifier method), 357

eval() (deepmd.infer.deep_dos.DeepDOS method), 360

eval() (deepmd.infer.deep_polar.DeepGlobalPolar method), 365

eval() (deepmd.infer.deep_pot.DeepPot method), 369

eval() (deepmd.infer.deep_tensor.DeepTensor method), 372

eval() (deepmd.infer.DeepDOS method), 339

eval() (deepmd.infer.DeepGlobalPolar method), 345

eval() (deepmd.infer.DeepPot method), 349

eval() (deepmd.infer.DipoleChargeModifier method), 353

eval() (deepmd.infer.ewald_recip.EwaldRecp method), 375

eval() (deepmd.infer.EwaldRecp method), 354

eval() (deepmd.loss.dos.DOSLoss method), 387

eval() (deepmd.loss.DOSLoss method), 381

eval() (deepmd.loss.ener.EnerDipoleLoss method), 389

eval() (deepmd.loss.ener.EnerSpinLoss method),

390
 eval() (deepmd.loss.ener.EnerStdLoss method), 392
 eval() (deepmd.loss.ener.DipoleLoss method), 382
 eval() (deepmd.loss.ener.SpinLoss method), 383
 eval() (deepmd.loss.ener.StdLoss method), 385
 eval() (deepmd.loss.loss.Loss method), 393
 eval() (deepmd.loss.tensor.TensorLoss method), 394
 eval() (deepmd.loss.TensorLoss method), 386
 eval_descriptor() (deepmd.infer.deep_dos.DeepDOS method), 361
 eval_descriptor() (deepmd.infer.deep_pot.DeepPot method), 370
 eval_descriptor() (deepmd.infer.DeepDOS method), 340
 eval_descriptor() (deepmd.infer.DeepPot method), 350
 eval_full() (deepmd.infer.deep_tensor.DeepTensor method), 373
 eval_single_list() (deepmd.train.trainer.DPTrainer static method), 455
 eval_typeebd() (deepmd.DeepEval method), 196
 eval_typeebd() (deepmd.infer.deep_eval.DeepEval method), 363
 eval_typeebd() (deepmd.infer.DeepEval method), 343
 ewald_beta:
 model/modifier[dipole_charge]/ewald_beta (Argument), 81
 ewald_h:
 model/modifier[dipole_charge]/ewald_h (Argument), 81
 ewald_recip() (in module deepmd.env.op_module), 541
 EwaldRecip (class in deepmd.infer), 354
 EwaldRecip (class in deepmd.infer.ewald_recip), 375
 EwaldRecip() (in module deepmd.env.op_module), 516
 exclude_types:
 model[standard]/descriptor[se_a_mask]/exclude_types (Argument), 97
 model[standard]/descriptor[se_a_tpe]/exclude_types (Argument), 88
 model[standard]/descriptor[se_atten_v2]/exclude_types (Argument), 96
 model[standard]/descriptor[se_atten]/exclude_types (Argument), 93
 model[standard]/descriptor[se_e2_a]/exclude_types (Argument), 85
 model[standard]/descriptor[se_e2_r]/exclude_types (Argument), 91
 execute() (deepmd.utils.batch_size.AutoBatchSize method), 469
 execute_all() (deepmd.utils.batch_size.AutoBatchSize method), 469
 exits() (deepmd.nvnmd.utils.fio.Fio method), 449
 expand_sys_str() (in module deepmd.common), 504
 explicit_ntypes (deepmd.descriptor.Descriptor property), 205
 explicit_ntypes(deepmd.descriptor.descriptor.Descriptor property), 253
 explicit_ntypes(deepmd.descriptor.DescriptHybrid property), 210
 explicit_ntypes(deepmd.descriptor.DescriptSeAtten property), 238
 explicit_ntypes(deepmd.descriptor.hybrid.DescriptHybrid property), 258
 explicit_ntypes(deepmd.descriptor.se_atten.DescriptSeAtten property), 288
 extend_bin() (deepmd.nvnmd.utils.Encode method), 441
 extend_bin() (deepmd.nvnmd.utils.encode.Encode method), 448
 extend_hex() (deepmd.nvnmd.utils.Encode method), 441
 extend_hex() (deepmd.nvnmd.utils.encode.Encode method), 448
 extend_list() (deepmd.nvnmd.utils.Encode method), 441
 extend_list() (deepmd.nvnmd.utils.encode.Encode method), 448
F
 filter_GR2D() (in module deepmd.nvnmd.descriptor.se_a), 429
 filter_GR2D() (in module deepmd.nvnmd.descriptor.se_atten), 429
 filter_lower_R42GR() (in module deepmd.nvnmd.descriptor.se_a), 429
 filter_lower_R42GR() (in module deepmd.nvnmd.descriptor.se_atten), 429
 filter_tensorVariableList() (in module deepmd.nvnmd.entrypoints.freeze), 434
 find_max_expo (C++ function), 721
 find_max_expo() (deepmd.nvnmd.utils.Encode method), 441
 find_max_expo() (deepmd.nvnmd.utils.encode.Encode method), 448
 fio in deepmd.nvnmd.utils.fio, 449
 FioBin (class in deepmd.nvnmd.utils.fio), 442
 FioBin (class in deepmd.nvnmd.utils.fio), 449
 FioDic (class in deepmd.nvnmd.utils.fio), 442
 FioDic (class in deepmd.nvnmd.utils.fio), 450
 FioJsonDic (class in deepmd.nvnmd.utils.fio), 450
 FioNpyDic (class in deepmd.nvnmd.utils.fio), 451
 FioTxt (class in deepmd.nvnmd.utils.fio), 443
 FioTxt (class in deepmd.nvnmd.utils.fio), 451
 fit_diag:

model[standard]/fitting_net[polar]/fit_diagelu_grad_grad_custom() (in module
 (Argument), 102 deepmd.env.op_module), 542
 Fitting (class in deepmd.fit), 317
 Fitting (class in deepmd.fit.fitting), 332
 fitting_dipole() (in module deepmd.utils.argcheck), 467
 fitting_dos() (in module deepmd.utils.argcheck), 467
 fitting_ener() (in module deepmd.utils.argcheck), 467
 fitting_net:
 model[standard]/fitting_net (Argument), 98
 fitting_net_dict:
 model[multi]/fitting_net_dict (Argument), 104
 fitting_polar() (in module deepmd.utils.argcheck), 467
 fitting_variant_type_args() (in module deepmd.utils.argcheck), 467
 fitting_weight:
 training/fitting_weight (Argument), 115
 flt2bin() (deepmd.nvnmd.utils.Encode method), 441
 flt2bin() (deepmd.nvnmd.utils.encode.Encode method), 448
 flt2bin_one() (deepmd.nvnmd.utils.Encode method), 441
 flt2bin_one() (deepmd.nvnmd.utils.encode.Encode method), 448
 FLT_MASK (C macro), 724
 flt_nvnmd() (in module deepmd.env.op_module), 541
 FltNvnmd() (in module deepmd.env.op_module), 517
 format_nlist_i_cpu (C++ function), 721
 format_nlist_i_fill_a (C++ function), 721
 freeze() (in module deepmd.entrypoints), 300
 freeze() (in module deepmd.entrypoints.freeze), 304

G

gather_placeholder() (in module deepmd.model.pairwise_dprc), 422
 gelu() (in module deepmd.common), 505
 Gelu() (in module deepmd.env.op_module), 517
 gelu() (in module deepmd.env.op_module), 541
 gelu_custom() (in module deepmd.env.op_module), 541
 gelu_grad() (in module deepmd.env.op_module), 542
 gelu_grad_custom() (in module deepmd.env.op_module), 542
 gelu_grad_grad() (in module deepmd.env.op_module), 542
 gelu_tf() (in module deepmd.common), 505
 GeluCustom() (in module deepmd.env.op_module), 517
 GeluGPUExecuteFunctor (C++ struct), 676
 GeluGPUExecuteFunctor::operator() (C++ function), 677
 GeluGrad() (in module deepmd.env.op_module), 517
 GeluGradCustom() (in module deepmd.env.op_module), 517
 GeluGradGPUExecuteFunctor (C++ struct), 677
 GeluGradGPUExecuteFunctor::operator() (C++ function), 677
 GeluGradGrad() (in module deepmd.env.op_module), 518
 GeluGradGradCustom() (in module deepmd.env.op_module), 518
 GeluGradGradGPUExecuteFunctor (C++ struct), 677
 GeluGradGradGPUExecuteFunctor::operator() (C++ function), 677
 gen_args() (in module deepmd.utils.argcheck), 467
 gen_doc() (in module deepmd.utils.argcheck), 467
 gen_json() (in module deepmd.utils.argcheck), 467
 generate() (deepmd.utils.parallel_op.ParallelOp method), 490
 get() (deepmd.nvnmd.utils.fio.FioDic method), 450
 get() (deepmd.nvnmd.utils.FioDic method), 442
 get() (deepmd.utils.pair_tab.PairTab method), 488
 get() (deepmd.utils.PairTab method), 464
 get_activation_func() (in module deepmd.common), 505
 get_all_argument() (deepmd.utils.argcheck.ArgsPlugin method), 466
 get_atom_type() (deepmd.utils.data.DeepmdData method), 475
 get_atom_type() (deepmd.utils.DeepmdData method), 459
 get_attention_layer_nodes_from_graph_def() (in module deepmd.utils.graph), 480
 get_attention_layer_variables_from_graph_def() (in module deepmd.utils.graph), 480
 get_batch() (deepmd.utils.data.DeepmdData method), 475
 get_batch() (deepmd.utils.data_system.DeepmdDataSystem method), 478
 get_batch() (deepmd.utils.DeepmdData method), 459
 get_batch() (deepmd.utils.DeepmdDataSystem method), 461
 get_batch_mixed() (deepmd.utils.data_system.DeepmdDataSystem method), 478
 get_batch_mixed() (deepmd.utils.DeepmdDataSystem method), 462

`get_batch_size()` (deepmd.utils.data_system.DeepmdDataSystem method), 352
`get_batch_size()` (deepmd.utils.DeepmdDataSystem method), 478
`get_batch_size()` (deepmd.utils.DeepmdDataSystem method), 462
`get_batch_standard()` (deepmd.utils.data_system.DeepmdDataSystem method), 478
`get_batch_standard()` (deepmd.utils.DeepmdDataSystem method), 462
`get_constant_initializer()` (in module deepmd.nvnmd.utils.weight), 452
`get_data_dict()` (deepmd.train.trainer.DatasetLoader method), 456
`get_data_dict()` (deepmd.utils.data.DeepmdData method), 475
`get_data_dict()` (deepmd.utils.data_system.DeepmdDataSystem method), 478
`get_data_dict()` (deepmd.utils.DeepmdData method), 459
`get_data_dict()` (deepmd.utils.DeepmdDataSystem method), 462
`get_deepmd_jdata()` (deepmd.nvnmd.utils.config.NvnmdConfig method), 445
`get_descriptor_type()` (deepmd.infer.deep_pot.DeepPot method), 370
`get_descriptor_type()` (deepmd.infer.DeepPot method), 350
`get_dim_aparam()` (deepmd.infer.deep_dipole.DeepDipole method), 359
`get_dim_aparam()` (deepmd.infer.deep_dos.DeepDOS method), 361
`get_dim_aparam()` (deepmd.infer.deep_polar.DeepGlobalPolar method), 366
`get_dim_aparam()` (deepmd.infer.deep_polar.DeepPolar method), 367
`get_dim_aparam()` (deepmd.infer.deep_pot.DeepPot method), 371
`get_dim_aparam()` (deepmd.infer.deep_tensor.DeepTensor method), 373
`get_dim_aparam()` (deepmd.infer.deep_wfc.DeepWFC method), 375
`get_dim_aparam()` (deepmd.infer.DeepDipole method), 342
`get_dim_aparam()` (deepmd.infer.DeepDOS method), 340
`get_dim_aparam()` (deepmd.infer.DeepGlobalPolar method), 346
`get_dim_aparam()` (deepmd.infer.DeepPolar method), 347
`get_dim_aparam()` (deepmd.infer.DeepPot method), 351
`get_dim_aparam()` (deepmd.infer.DeepWFC method), 352
`get_dim_out()` (deepmd.descriptor.Descriptor method), 205
`get_dim_out()` (deepmd.descriptor.descriptor.Descriptor method), 253
`get_dim_out()` (deepmd.descriptor.DescriptHybrid method), 210
`get_dim_out()` (deepmd.descriptor.DescriptLocFrame method), 215
`get_dim_out()` (deepmd.descriptor.DescriptSeA method), 220
`get_dim_out()` (deepmd.descriptor.DescriptSeAEf method), 226
`get_dim_out()` (deepmd.descriptor.DescriptSeR method), 244
`get_dim_out()` (deepmd.descriptor.DescriptSeT method), 248
`get_dim_out()` (deepmd.descriptor.hybrid.DescriptHybrid method), 258
`get_dim_out()` (deepmd.descriptor.loc_frame.DescriptLocFrame method), 263
`get_dim_out()` (deepmd.descriptor.se_a.DescriptSeA method), 270
`get_dim_out()` (deepmd.descriptor.se_a_ef.DescriptSeAEf method), 276
`get_dim_out()` (deepmd.descriptor.se_r.DescriptSeR method), 294
`get_dim_out()` (deepmd.descriptor.se_t.DescriptSeT method), 294

method), 298

get_dim_rot_mat_1() (deepmd.descriptor.Descriptor method), 205

get_dim_rot_mat_1() (deepmd.descriptor.descriptor.Descriptor method), 253

get_dim_rot_mat_1() (deepmd.descriptor.DescriptSeA method), 220

get_dim_rot_mat_1() (deepmd.descriptor.DescriptSeAEf method), 226

get_dim_rot_mat_1() (deepmd.descriptor.se_a.DescriptSeA method), 270

get_dim_rot_mat_1() (deepmd.descriptor.se_a_ef.DescriptSeAEf method), 276

get_dp_init_weights() (deepmd.nvnmd.utils.config.NvnmdConfig method), 445

get_dscp_jdata() (deepmd.nvnmd.utils.config.NvnmdConfig method), 445

get_embedding_net_nodes() (in module deepmd.utils.graph), 480

get_embedding_net_nodes_from_graph_def() (in module deepmd.utils.graph), 481

get_embedding_net_variables() (in module deepmd.utils.graph), 481

get_embedding_net_variables_from_graph_def() (in module deepmd.utils.graph), 481

get_env() (in module deepmd.lmp), 508

get_evaluation_results() (deepmd.train.trainer.DPTrainer method), 455

get_feed_dict() (deepmd.model.model.Model method), 414

get_feed_dict() (deepmd.model.pairwise_dprc.PairwiseDPRc method), 421

get_feed_dict() (deepmd.train.trainer.DPTrainer method), 455

get_file_list() (deepmd.nvnmd.utils.fio.Fio method), 449

get_filter_type_weight() (in module deepmd.nvnmd.utils.weight), 452

get_filter_weight() (in module deepmd.nvnmd.utils), 443

get_filter_weight() (in module deepmd.nvnmd.utils.weight), 452

get_fitn_jdata() (deepmd.nvnmd.utils.config.NvnmdConfig method), 445

get_fitnet_weight() (in module deepmd.nvnmd.utils), 443

get_fitnet_weight() (in module deepmd.nvnmd.utils.weight), 453

get_fitting() (deepmd.model.model.Model method), 415

get_fitting() (deepmd.model.model.StandardModel method), 416

get_fitting() (deepmd.model.multi.MultiModel method), 419

get_fitting() (deepmd.model.MultiModel method), 403

get_fitting() (deepmd.model.pairwise_dprc.PairwiseDPRc method), 422

get_fitting_net_nodes() (in module deepmd.utils.graph), 481

get_fitting_net_nodes_from_graph_def() (in module deepmd.utils.graph), 482

get_fitting_net_variables() (in module deepmd.utils.graph), 482

get_fitting_net_variables_from_graph_def() (in module deepmd.utils.graph), 482

get_global_step() (deepmd.train.trainer.DPTrainer method), 455

get_configs() (in module deepmd.cluster.local), 200

get_learning_rate_jdata() (deepmd.nvnmd.utils.config.NvnmdConfig method), 445

get_library_path() (in module deepmd.lmp), 508

get_ll() (in module deepmd.entrypoints.main), 305

get_loss() (deepmd.fit.dipole.DipoleFittingSeA method), 324

get_loss() (deepmd.fit.DipoleFittingSeA method), 313

get_loss() (deepmd.fit.dos.DOSFitting method), 327

get_loss() (deepmd.fit.DOSFitting method), 310

get_loss() (deepmd.fit.ener.EnerFitting method), 331

get_loss() (deepmd.fit.EnerFitting method), 316

get_loss() (deepmd.fit.Fitting method), 317

get_loss() (deepmd.fit.fitting.Fitting method), 332

get_loss() (deepmd.fit.GlobalPolarFittingSeA method), 320

get_loss() (deepmd.fit.polar.GlobalPolarFittingSeA method), 334

get_loss() (deepmd.fit.polar.PolarFittingSeA method), 337

get_loss() (deepmd.fit.PolarFittingSeA method), 322

get_loss() (deepmd.model.model.Model method), 415

get_loss() (deepmd.model.model.StandardModel method), 416

get_loss() (deepmd.model.multi.MultiModel method), 419

`get_loss()` (deepmd.model.MultiModel method), 403
`get_loss()` (deepmd.model.pairwise_dprc.PairwiseDP method), 422
`get_loss_jdata()` (deepmd.nvnmd.utils.config.NvnmdConfig method), 445
`get_model_jdata()` (deepmd.nvnmd.utils.config.NvnmdConfig method), 445
`get_natoms()` (deepmd.utils.data.DeepmdData method), 475
`get_natoms()` (deepmd.utils.DeepmdData method), 459
`get_natoms_vec()` (deepmd.utils.data.DeepmdData method), 475
`get_natoms_vec()` (deepmd.utils.DeepmdData method), 459
`get_nbatches()` (deepmd.utils.data_system.DeepmdDataSystem method), 478
`get_nbatches()` (deepmd.utils.DeepmdDataSystem method), 462
`get_nlist()` (deepmd.descriptor.Descriptor method), 205
`get_nlist()` (deepmd.descriptor.descriptor.Descriptor method), 253
`get_nlist()` (deepmd.descriptor.DescriptHybrid method), 210
`get_nlist()` (deepmd.descriptor.DescriptLocFrame method), 215
`get_nlist()` (deepmd.descriptor.DescriptSeA method), 220
`get_nlist()` (deepmd.descriptor.DescriptSeAEf method), 226
`get_nlist()` (deepmd.descriptor.DescriptSeR method), 244
`get_nlist()` (deepmd.descriptor.DescriptSeT method), 248
`get_nlist()` (deepmd.descriptor.hybrid.DescriptHybrid method), 258
`get_nlist()` (deepmd.descriptor.loc_frame.DescriptLocFrame method), 263
`get_nlist()` (deepmd.descriptor.se_a.DescriptSeA method), 270
`get_nlist()` (deepmd.descriptor.se_a_ef.DescriptSeAEf method), 276
`get_nlist()` (deepmd.descriptor.se_r.DescriptSeR method), 294
`get_nlist()` (deepmd.descriptor.se_t.DescriptSeT method), 298
`get_nlist_i()` (deepmd.descriptor.DescriptHybrid method), 211
`get_nlist_i()` (deepmd.descriptor.hybrid.DescriptHybrid method), 259
`get_normalize()` (in module deepmd.nvnmd.utils.weight), 453
`get_np_precision()` (in module deepmd.common), 505
`get_nsymbols()` (deepmd.utils.data_system.DeepmdDataSystem method), 479
`get_nsymbols()` (deepmd.utils.DeepmdDataSystem method), 462
`get_ntypes()` (deepmd.descriptor.Descriptor method), 206
`get_ntypes()` (deepmd.descriptor.descriptor.Descriptor method), 254
`get_ntypes()` (deepmd.descriptor.DescriptHybrid method), 211
`get_ntypes()` (deepmd.descriptor.DescriptLocFrame method), 215
`get_ntypes()` (deepmd.descriptor.DescriptSeA method), 220
`get_ntypes()` (deepmd.descriptor.DescriptSeAEf method), 227
`get_ntypes()` (deepmd.descriptor.DescriptSeR method), 244
`get_ntypes()` (deepmd.descriptor.DescriptSeT method), 248
`get_ntypes()` (deepmd.descriptor.hybrid.DescriptHybrid method), 259
`get_ntypes()` (deepmd.descriptor.loc_frame.DescriptLocFrame method), 263
`get_ntypes()` (deepmd.descriptor.se_a.DescriptSeA method), 270
`get_ntypes()` (deepmd.descriptor.se_a_ef.DescriptSeAEf method), 277
`get_ntypes()` (deepmd.descriptor.se_r.DescriptSeR method), 294
`get_ntypes()` (deepmd.descriptor.se_t.DescriptSeT method), 298
`get_ntypes()` (deepmd.infer.deep_dos.DeepDOS method), 362
`get_ntypes()` (deepmd.infer.deep_pot.DeepPot method), 371
`get_ntypes()` (deepmd.infer.deep_tensor.DeepTensor method), 374
`get_ntypes()` (deepmd.infer.DeepDOS method), 340
`get_ntypes()` (deepmd.infer.DeepPot method), 351
`get_ntypes()` (deepmd.model.dos.DOSModel method), 407
`get_ntypes()` (deepmd.model.DOSModel method), 396
`get_ntypes()` (deepmd.model.ener.EnerModel method), 410
`get_ntypes()` (deepmd.model.EnerModel method), 399
`get_ntypes()` (deepmd.model.model.Model method), 415
`get_ntypes()` (deepmd.model.model.StandardModel method), 416

`get_ntypes()` (deepmd.model.multi.MultiModel method), 419
`get_ntypes()` (deepmd.model.MultiModel method), 403
`get_ntypes()` (deepmd.model.pairwise_dprc.PairwiseDPRC method), 422
`get_ntypes()` (deepmd.model.tensor.TensorModel method), 426
`get_ntypes()` (deepmd.utils.data.DeepmdData method), 475
`get_ntypes()` (deepmd.utils.data_system.DeepmdDataSystem method), 479
`get_ntypes()` (deepmd.utils.DeepmdData method), 459
`get_ntypes()` (deepmd.utils.DeepmdDataSystem method), 462
`get_ntypes_spin()` (deepmd.infer.deep_pot.DeepPot method), 371
`get_ntypes_spin()` (deepmd.infer.DeepPot method), 351
`get_ntypes_spin()` (deepmd.utils.spin.Spin method), 497
`get_num_aparam()` (deepmd.fit.dos.DOSFitting method), 327
`get_num_aparam()` (deepmd.fit.DOSFitting method), 311
`get_num_aparam()` (deepmd.fit.ener.EnerFitting method), 331
`get_num_aparam()` (deepmd.fit.EnerFitting method), 316
`get_num_aparam()` (deepmd.model.dos.DOSModel method), 407
`get_num_aparam()` (deepmd.model.DOSModel method), 396
`get_num_aparam()` (deepmd.model.ener.EnerModel method), 410
`get_num_aparam()` (deepmd.model.EnerModel method), 400
`get_num_aparam()` (deepmd.model.model.Model method), 415
`get_num_aparam()` (deepmd.model.multi.MultiModel method), 419
`get_num_aparam()` (deepmd.model.MultiModel method), 403
`get_num_batch()` (deepmd.utils.data.DeepmdData method), 475
`get_num_batch()` (deepmd.utils.DeepmdData method), 459
`get_num_dos()` (deepmd.fit.dos.DOSFitting method), 327
`get_num_dos()` (deepmd.fit.DOSFitting method), 311
`get_num_dos()` (deepmd.infer.deep_dos.DeepDOS method), 362
`get_num_dos()` (deepmd.infer.DeepDOS method), 340
`get_num_dos()` (deepmd.model.dos.DOSModel method), 407
`get_num_dos()` (deepmd.model.DOSModel method), 396
`get_num_dos()` (deepmd.model.model.Model method), 415
`get_num_dos()` (deepmd.model.multi.MultiModel method), 419
`get_num_dos()` (deepmd.model.MultiModel method), 403
`get_num_fparam()` (deepmd.fit.dos.DOSFitting method), 327
`get_num_fparam()` (deepmd.fit.DOSFitting method), 311
`get_num_fparam()` (deepmd.fit.ener.EnerFitting method), 331
`get_num_fparam()` (deepmd.fit.EnerFitting method), 317
`get_num_fparam()` (deepmd.model.dos.DOSModel method), 407
`get_num_fparam()` (deepmd.model.DOSModel method), 396
`get_num_fparam()` (deepmd.model.ener.EnerModel method), 410
`get_num_fparam()` (deepmd.model.EnerModel method), 400
`get_num_fparam()` (deepmd.model.model.Model method), 415
`get_num_fparam()` (deepmd.model.multi.MultiModel method), 419
`get_num_fparam()` (deepmd.model.MultiModel method), 403
`get_num_set()` (deepmd.utils.data.DeepmdData method), 475
`get_num_set()` (deepmd.utils.DeepmdData method), 459
`get_nvnm_jdata()` (deepmd.nvnm.utils.config.NvnmConfig method), 446
`get_op_dir()` (in module deepmd.lmp), 509
`get_out_size()` (deepmd.fit.dipole.DipoleFittingSeA method), 324
`get_out_size()` (deepmd.fit.DipoleFittingSeA method), 313
`get_out_size()` (deepmd.fit.GlobalPolarFittingSeA method), 320
`get_out_size()` (deepmd.fit.polar.GlobalPolarFittingSeA method), 335
`get_out_size()` (deepmd.fit.polar.PolarFittingSeA method), 337
`get_out_size()` (deepmd.fit.PolarFittingSeA method), 322
`get_out_size()` (deepmd.model.tensor.TensorModel

method), 426

`get_pattern_nodes_from_graph_def()` (in module `deepmd.utils.graph`), 482

`get_plugin()` (`deepmd.utils.Plugin` method), 465

`get_plugin()` (`deepmd.utils.plugin.Plugin` method), 494

`get_precision()` (in module `deepmd.common`), 506

`get_rcut()` (`deepmd.descriptor.Descriptor` method), 206

`get_rcut()` (`deepmd.descriptor.descriptor.Descriptor` method), 254

`get_rcut()` (`deepmd.descriptor.DescriptHybrid` method), 211

`get_rcut()` (`deepmd.descriptor.DescriptLocFrame` method), 215

`get_rcut()` (`deepmd.descriptor.DescriptSeA` method), 221

`get_rcut()` (`deepmd.descriptor.DescriptSeAEf` method), 227

`get_rcut()` (`deepmd.descriptor.DescriptSeAMask` method), 232

`get_rcut()` (`deepmd.descriptor.DescriptSeR` method), 244

`get_rcut()` (`deepmd.descriptor.DescriptSeT` method), 248

`get_rcut()` (`deepmd.descriptor.hybrid.DescriptHybrid` method), 259

`get_rcut()` (`deepmd.descriptor.loc_frame.DescriptLocFrame` method), 263

`get_rcut()` (`deepmd.descriptor.se_a.DescriptSeA` method), 270

`get_rcut()` (`deepmd.descriptor.se_a_ef.DescriptSeAEf` method), 277

`get_rcut()` (`deepmd.descriptor.se_a_mask.DescriptSeAMask` method), 282

`get_rcut()` (`deepmd.descriptor.se_r.DescriptSeR` method), 294

`get_rcut()` (`deepmd.descriptor.se_t.DescriptSeT` method), 298

`get_rcut()` (`deepmd.infer.deep_dos.DeepDOS` method), 362

`get_rcut()` (`deepmd.infer.deep_pot.DeepPot` method), 371

`get_rcut()` (`deepmd.infer.deep_tensor.DeepTensor` method), 374

`get_rcut()` (`deepmd.infer.DeepDOS` method), 340

`get_rcut()` (`deepmd.infer.DeepPot` method), 351

`get_rcut()` (`deepmd.model.dos.DOSModel` method), 407

`get_rcut()` (`deepmd.model.DOSModel` method), 396

`get_rcut()` (`deepmd.model.ener.EnerModel` method), 410

`get_rcut()` (`deepmd.model.EnerModel` method), 400

`get_rcut()` (`deepmd.model.model.Model` method), 415

`get_rcut()` (`deepmd.model.model.StandardModel` method), 416

`get_rcut()` (`deepmd.model.multi.MultiModel` method), 419

`get_rcut()` (`deepmd.model.MultiModel` method), 403

`get_rcut()` (`deepmd.model.pairwise_dprc.PairwiseDPRc` method), 422

`get_rcut()` (`deepmd.model.tensor.TensorModel` method), 426

`get_resource()` (in module `deepmd.cluster`), 200

`get_resource()` (in module `deepmd.cluster.local`), 200

`get_resource()` (in module `deepmd.cluster.slurm`), 201

`get_rot_mat()` (`deepmd.descriptor.DescriptLocFrame` method), 215

`get_rot_mat()` (`deepmd.descriptor.DescriptSeA` method), 221

`get_rot_mat()` (`deepmd.descriptor.DescriptSeAEf` method), 227

`get_rot_mat()` (`deepmd.descriptor.loc_frame.DescriptLocFrame` method), 263

`get_rot_mat()` (`deepmd.descriptor.se_a.DescriptSeA` method), 270

`get_rot_mat()` (`deepmd.descriptor.se_a_ef.DescriptSeAEf` method), 277

`get_s_range()` (`deepmd.nvnmd.utils.config.NvnmdConfig` method), 446

`get_sel_type()` (`deepmd.fit.dipole.DipoleFittingSeA` method), 324

`get_sel_type()` (`deepmd.fit.DipoleFittingSeA` method), 313

`get_sel_type()` (`deepmd.fit.GlobalPolarFittingSeA` method), 320

`get_sel_type()` (`deepmd.fit.polar.GlobalPolarFittingSeA` method), 335

`get_sel_type()` (`deepmd.fit.polar.PolarFittingSeA` method), 337

`get_sel_type()` (`deepmd.fit.PolarFittingSeA` method), 322

`get_sel_type()` (`deepmd.infer.deep_dos.DeepDOS` method), 362

`get_sel_type()` (`deepmd.infer.deep_pot.DeepPot` method), 371

`get_sel_type()` (`deepmd.infer.deep_tensor.DeepTensor` method), 374

`get_sel_type()` (`deepmd.infer.DeepDOS` method), 341

`get_sel_type()` (`deepmd.infer.DeepPot` method), 351

`get_sel_type()` (`deepmd.model.tensor.TensorModel`

method), 426

get_sess() (in module deepmd.nvnmd.utils.network), 451

get_spin_norm() (deepmd.utils.spin.Spin method), 497

get_stat() (deepmd.utils.neighbor_stat.NeighborStat method), 486

get_sys() (deepmd.utils.data_system.DeepmdDataSystem method), 479

get_sys() (deepmd.utils.DeepmdDataSystem method), 462

get_sys_n_test() (deepmd.utils.data_system.DeepmdDataSystem method), 479

get_sys_n_test() (deepmd.utils.DeepmdDataSystem method), 462

get_sys_numb_batch() (deepmd.utils.data.DeepmdData method), 475

get_sys_numb_batch() (deepmd.utils.DeepmdData method), 459

get_tensor_by_name() (in module deepmd.utils.graph), 483

get_tensor_by_name_from_graph() (in module deepmd.utils.graph), 483

get_tensor_by_type() (in module deepmd.utils.graph), 483

get_tensor_names() (deepmd.descriptor.Descriptor method), 206

get_tensor_names() (deepmd.descriptor.descriptor.Descriptor method), 254

get_tensor_names() (deepmd.descriptor.DescriptHybrid method), 211

get_tensor_names() (deepmd.descriptor.hybrid.DescriptHybrid method), 259

get_tensor_names() (deepmd.descriptor.se.DescriptSe method), 265

get_test() (deepmd.utils.data.DeepmdData method), 475

get_test() (deepmd.utils.data_system.DeepmdDataSystem method), 479

get_test() (deepmd.utils.DeepmdData method), 459

get_test() (deepmd.utils.DeepmdDataSystem method), 462

get_training_jdata() (deepmd.nvnmd.utils.config.NvnmdConfig method), 446

get_type_embedding_net_nodes_from_graph_def() (in module deepmd.utils.graph), 483

get_type_embedding_net_variables_from_graph_def() (in module deepmd.utils.graph), 484

get_type_embedding_weight() (in module deepmd.nvnmd.utils.weight), 453

get_type_map() (deepmd.infer.deep_dos.DeepDOS method), 362

get_type_map() (deepmd.infer.deep_pot.DeepPot method), 371

get_type_map() (deepmd.infer.deep_tensor.DeepTensor method), 374

get_type_map() (deepmd.infer.DeepDOS method), 341

get_type_map() (deepmd.infer.DeepPot method), 351

get_type_map() (deepmd.model.dos.DOSModel method), 407

get_type_map() (deepmd.model.DOSModel method), 396

get_type_map() (deepmd.model.ener.EnerModel method), 410

get_type_map() (deepmd.model.EnerModel method), 400

get_type_map() (deepmd.model.model.Model method), 415

get_type_map() (deepmd.model.multi.MultiModel method), 419

get_type_map() (deepmd.model.MultiModel method), 403

get_type_map() (deepmd.model.tensor.TensorModel method), 426

get_type_map() (deepmd.utils.data.DeepmdData method), 476

get_type_map() (deepmd.utils.data_system.DeepmdDataSystem method), 479

get_type_map() (deepmd.utils.DeepmdData method), 460

get_type_map() (deepmd.utils.DeepmdDataSystem method), 463

get_type_weight() (in module deepmd.nvnmd.utils.weight), 453

get_use_spin() (deepmd.utils.spin.Spin method), 497

get_virtual_len() (deepmd.utils.spin.Spin method), 497

get_weight() (in module deepmd.nvnmd.utils.weight), 453

glob() (deepmd.utils.path.DPH5Path method), 490

glob() (deepmd.utils.path.DPOSPath method), 492

glob() (deepmd.utils.path.DPPPath method), 493

global_cvt_2_ener_float() (in module deepmd.env), 508

global_cvt_2_tf_float() (in module deepmd.env), 508

GLOBAL_ENER_FLOAT_PRECISION (in module deepmd.env), 508

GLOBAL_NP_FLOAT_PRECISION (in module deepmd.env), 508

GlobalPolarFittingSeA (class in deepmd.fit), 318

GlobalPolarFittingSeA (class in deepmd.fit.polar),

- 333
- GlobalPolarModel (class in deepmd.model), 400
- GlobalPolarModel (class in deepmd.model.tensor), 423
- GPU_MAX_NBOR_SIZE (C macro), 724
- gpus (deepmd.train.run_options.RunOptions attribute), 455
- GraphTooLargeError, 479
- GraphWithoutTensorError, 479
- ## H
- hex2bin() (deepmd.nvnmd.utils.Encode method), 441
- hex2bin() (deepmd.nvnmd.utils.encode.Encode method), 448
- hex2bin_str() (deepmd.nvnmd.utils.Encode method), 441
- hex2bin_str() (deepmd.nvnmd.utils.encode.Encode method), 448
- ## I
- implemented_properties (deepmd.calculator.DP attribute), 503
- import_ops() (in module deepmd.op), 454
- init_config_by_version() (deepmd.nvnmd.utils.config.NvnmdConfig method), 446
- init_ctrl() (deepmd.nvnmd.utils.config.NvnmdConfig method), 446
- init_dpin() (deepmd.nvnmd.utils.config.NvnmdConfig method), 446
- init_dscp() (deepmd.nvnmd.utils.config.NvnmdConfig method), 446
- init_fitn() (deepmd.nvnmd.utils.config.NvnmdConfig method), 446
- init_from_config() (deepmd.nvnmd.utils.config.NvnmdConfig method), 446
- init_from_deepmd_input() (deepmd.nvnmd.utils.config.NvnmdConfig method), 446
- init_from_jdata() (deepmd.nvnmd.utils.config.NvnmdConfig method), 446
- init_nbit() (deepmd.nvnmd.utils.config.NvnmdConfig method), 446
- init_net_size() (deepmd.nvnmd.utils.config.NvnmdConfig method), 446
- init_size() (deepmd.nvnmd.utils.config.NvnmdConfig method), 446
- init_train_mode() (deepmd.nvnmd.utils.config.NvnmdConfig method), 446
- init_value() (deepmd.nvnmd.utils.config.NvnmdConfig method), 446
- init_variables() (deepmd.descriptor.Descriptor method), 206
- init_variables() (deepmd.descriptor.Descriptor.Descriptor method), 254
- init_variables() (deepmd.descriptor.DescriptHybrid method), 211
- init_variables() (deepmd.descriptor.DescriptLocFrame method), 216
- init_variables() (deepmd.descriptor.DescriptSeA method), 221
- init_variables() (deepmd.descriptor.DescriptSeAtten method), 238
- init_variables() (deepmd.descriptor.hybrid.DescriptHybrid method), 259
- init_variables() (deepmd.descriptor.loc_frame.DescriptLocFrame method), 264
- init_variables() (deepmd.descriptor.se.DescriptSe method), 265
- init_variables() (deepmd.descriptor.se_a.DescriptSeA method), 270
- init_variables() (deepmd.descriptor.se_atten.DescriptSeAtten method), 288
- init_variables() (deepmd.fit.dipole.DipoleFittingSeA method), 324
- init_variables() (deepmd.fit.DipoleFittingSeA method), 313
- init_variables() (deepmd.fit.dos.DOSFitting method), 327
- init_variables() (deepmd.fit.DOSFitting method), 311
- init_variables() (deepmd.fit.ener.EnerFitting method), 331
- init_variables() (deepmd.fit.EnerFitting method), 317
- init_variables() (deepmd.fit.Fitting method), 317
- init_variables() (deepmd.fit.fitting.Fitting method), 332
- init_variables() (deepmd.fit.GlobalPolarFittingSeA method), 320
- init_variables() (deepmd.fit.polar.GlobalPolarFittingSeA method), 335
- init_variables() (deepmd.fit.polar.PolarFittingSeA method), 337
- init_variables() (deepmd.fit.PolarFittingSeA method), 322
- init_variables() (deepmd.model.dos.DOSModel method), 407
- init_variables() (deepmd.model.DOSModel method), 396
- init_variables() (deepmd.model.ener.EnerModel method), 410
- init_variables() (deepmd.model.EnerModel method), 400
- init_variables() (deepmd.model.model.Model method), 415
- init_variables() (deepmd.model.multi.MultiModel

method), 419
 init_variables() (deepmd.model.MultiModel method), 403
 init_variables() (deepmd.model.pairwise_dprc.PairwiseDPRC method), 422
 init_variables() (deepmd.model.tensor.TensorModel method), 426
 init_variables() (deepmd.utils.type_embed.TypeEmbedder method), 500
 int_64 (C++ type), 726
 is_chief (deepmd.train.run_options.RunOptions property), 455
 is_dir() (deepmd.utils.path.DPH5Path method), 491
 is_dir() (deepmd.utils.path.DPOSPath method), 492
 is_dir() (deepmd.utils.path.DPPPath method), 493
 is_file() (deepmd.nvnmd.utils.fio.Fio method), 449
 is_file() (deepmd.utils.path.DPH5Path method), 491
 is_file() (deepmd.utils.path.DPOSPath method), 492
 is_file() (deepmd.utils.path.DPPPath method), 493
 is_path() (deepmd.nvnmd.utils.fio.Fio method), 449

J
 j_loader() (in module deepmd.common), 506
 j_must_have() (in module deepmd.common), 506

L
 layer_name:
 model[standard]/fitting_net[ener]/layer_name (Argument), 100
 learning_rate (Argument)
 learning_rate:, 104
 learning_rate/scale_by_worker (Argument)
 scale_by_worker:, 104
 learning_rate/type (Argument)
 type:, 104
 learning_rate:
 learning_rate (Argument), 104
 learning_rate_args() (in module deepmd.utils.argcheck), 467
 learning_rate_dict (Argument)
 learning_rate_dict:, 105
 learning_rate_dict:
 learning_rate_dict (Argument), 105
 learning_rate_dict_args() (in module deepmd.utils.argcheck), 467
 learning_rate_exp() (in module deepmd.utils.argcheck), 467
 learning_rate_variant_type_args() (in module deepmd.utils.argcheck), 467
 learning_rate[exp]/decay_steps (Argument)
 decay_steps:, 105
 learning_rate[exp]/start_lr (Argument)
 start_lr:, 104
 learning_rate[exp]/stop_lr (Argument)
 stop_lr:, 105
 LearningRateExp (class in deepmd.utils), 463
 LearningRateExp (class in deepmd.utils.learning_rate), 484
 limit_pref() (in module deepmd.utils.argcheck), 467
 limit_pref_acdf:
 loss[dos]/limit_pref_acdf (Argument), 110
 limit_pref_ados:
 loss[dos]/limit_pref_ados (Argument), 110
 limit_pref_ae:
 loss[ener_spin]/limit_pref_ae (Argument), 109
 loss[ener]/limit_pref_ae (Argument), 106
 limit_pref_cdf:
 loss[dos]/limit_pref_cdf (Argument), 110
 limit_pref_dos:
 loss[dos]/limit_pref_dos (Argument), 110
 limit_pref_e:
 loss[ener_spin]/limit_pref_e (Argument), 108
 loss[ener]/limit_pref_e (Argument), 105
 limit_pref_f:
 loss[ener]/limit_pref_f (Argument), 106
 limit_pref_fm:
 loss[ener_spin]/limit_pref_fm (Argument), 108
 limit_pref_fr:
 loss[ener_spin]/limit_pref_fr (Argument), 108
 limit_pref_gf:
 loss[ener]/limit_pref_gf (Argument), 107
 limit_pref_pf:
 loss[ener_spin]/limit_pref_pf (Argument), 109
 loss[ener]/limit_pref_pf (Argument), 107
 limit_pref_v:
 loss[ener_spin]/limit_pref_v (Argument), 108
 loss[ener]/limit_pref_v (Argument), 106
 list:
 model[standard]/descriptor[hybrid]/list (Argument), 91
 list_to_doc() (in module deepmd.utils.argcheck), 467
 load() (deepmd.nvnmd.utils.fio.FioBin method), 450
 load() (deepmd.nvnmd.utils.fio.FioDic method), 450

`load()` (deepmd.nvnmd.utils.fio.FioJsonDic method), 451
`load()` (deepmd.nvnmd.utils.fio.FioNpyDic method), 451
`load()` (deepmd.nvnmd.utils.fio.FioTxt method), 451
`load()` (deepmd.nvnmd.utils.FioBin method), 442
`load()` (deepmd.nvnmd.utils.FioDic method), 442
`load()` (deepmd.nvnmd.utils.FioTxt method), 443
`load_graph_def()` (in module deepmd.utils.graph), 484
`load_numpy()` (deepmd.utils.path.DPH5Path method), 491
`load_numpy()` (deepmd.utils.path.DPOSPath method), 492
`load_numpy()` (deepmd.utils.path.DPPath method), 493
`load_prefix` (deepmd.DeepEval attribute), 196
`load_prefix` (deepmd.DipoleChargeModifier attribute), 199
`load_prefix` (deepmd.infer.data_modifier.DipoleChargeModifier deepmd.utils.argcheck), 467
`load_prefix` (deepmd.infer.deep_dipole.DeepDipole attribute), 359
`load_prefix` (deepmd.infer.deep_dos.DeepDOS attribute), 362
`load_prefix` (deepmd.infer.deep_eval.DeepEval attribute), 363
`load_prefix` (deepmd.infer.deep_polar.DeepGlobalPolar attribute), 366
`load_prefix` (deepmd.infer.deep_polar.DeepPolar attribute), 367
`load_prefix` (deepmd.infer.deep_pot.DeepPot attribute), 371
`load_prefix` (deepmd.infer.deep_tensor.DeepTensor attribute), 374
`load_prefix` (deepmd.infer.deep_wfc.DeepWFC attribute), 375
`load_prefix` (deepmd.infer.DeepDipole attribute), 342
`load_prefix` (deepmd.infer.DeepDOS attribute), 341
`load_prefix` (deepmd.infer.DeepEval attribute), 343
`load_prefix` (deepmd.infer.DeepGlobalPolar attribute), 346
`load_prefix` (deepmd.infer.DeepPolar attribute), 347
`load_prefix` (deepmd.infer.DeepPot attribute), 351
`load_prefix` (deepmd.infer.DeepWFC attribute), 352
`load_prefix` (deepmd.infer.DipoleChargeModifier attribute), 354
`load_txt()` (deepmd.utils.path.DPH5Path method), 491
`load_txt()` (deepmd.utils.path.DPOSPath method), 492
`load_txt()` (deepmd.utils.path.DPPath method), 493
`loss` (Argument) `loss:`, 105
`Loss` (class in deepmd.loss.loss), 392
`loss/type` (Argument) `type:`, 105
`loss:`
`loss` (Argument), 105
`loss_args()` (in module deepmd.utils.argcheck), 467
`loss_dict` (Argument) `loss_dict:`, 111
`loss_dict:`
`loss_dict` (Argument), 111
`loss_dict_args()` (in module deepmd.utils.argcheck), 467
`loss_dos()` (in module deepmd.utils.argcheck), 467
`loss_ener()` (in module deepmd.utils.argcheck), 467
`loss_ener_spin()` (in module deepmd.utils.argcheck), 467
`loss_tensor()` (in module deepmd.utils.argcheck), 467
`loss_variant_type_args()` (in module deepmd.utils.argcheck), 467
`loss[dos]/limit_pref_acdf` (Argument) `limit_pref_acdf:`, 110
`loss[dos]/limit_pref_adof` (Argument) `limit_pref_adof:`, 110
`loss[dos]/limit_pref_cdf` (Argument) `limit_pref_cdf:`, 110
`loss[dos]/limit_pref_dof` (Argument) `limit_pref_dof:`, 110
`loss[dos]/start_pref_acdf` (Argument) `start_pref_acdf:`, 110
`loss[dos]/start_pref_adof` (Argument) `start_pref_adof:`, 110
`loss[dos]/start_pref_cdf` (Argument) `start_pref_cdf:`, 110
`loss[dos]/start_pref_dof` (Argument) `start_pref_dof:`, 109
`loss[ener_spin]/enable_atom_ener_coeff` (Argument) `enable_atom_ener_coeff:`, 109
`loss[ener_spin]/limit_pref_ae` (Argument) `limit_pref_ae:`, 109
`loss[ener_spin]/limit_pref_e` (Argument) `limit_pref_e:`, 108
`loss[ener_spin]/limit_pref_fm` (Argument) `limit_pref_fm:`, 108
`loss[ener_spin]/limit_pref_fr` (Argument) `limit_pref_fr:`, 108
`loss[ener_spin]/limit_pref_pf` (Argument) `limit_pref_pf:`, 109

`loss[ener_spin]/limit_pref_v` (Argument)
`limit_pref_v:`, 108
`loss[ener_spin]/relative_f` (Argument)
`relative_f:`, 109
`loss[ener_spin]/start_pref_ae` (Argument)
`start_pref_ae:`, 108
`loss[ener_spin]/start_pref_e` (Argument)
`start_pref_e:`, 107
`loss[ener_spin]/start_pref_fm` (Argument)
`start_pref_fm:`, 108
`loss[ener_spin]/start_pref_fr` (Argument)
`start_pref_fr:`, 108
`loss[ener_spin]/start_pref_pf` (Argument)
`start_pref_pf:`, 109
`loss[ener_spin]/start_pref_v` (Argument)
`start_pref_v:`, 108
`loss[ener]/enable_atom_ener_coeff` (Argument)
`enable_atom_ener_coeff:`, 107
`loss[ener]/limit_pref_ae` (Argument)
`limit_pref_ae:`, 106
`loss[ener]/limit_pref_e` (Argument)
`limit_pref_e:`, 105
`loss[ener]/limit_pref_f` (Argument)
`limit_pref_f:`, 106
`loss[ener]/limit_pref_gf` (Argument)
`limit_pref_gf:`, 107
`loss[ener]/limit_pref_pf` (Argument)
`limit_pref_pf:`, 107
`loss[ener]/limit_pref_v` (Argument)
`limit_pref_v:`, 106
`loss[ener]/numb_generalized_coord` (Argument)
`numb_generalized_coord:`, 107
`loss[ener]/relative_f` (Argument)
`relative_f:`, 107
`loss[ener]/start_pref_ae` (Argument)
`start_pref_ae:`, 106
`loss[ener]/start_pref_e` (Argument)
`start_pref_e:`, 105
`loss[ener]/start_pref_f` (Argument)
`start_pref_f:`, 106
`loss[ener]/start_pref_gf` (Argument)
`start_pref_gf:`, 107
`loss[ener]/start_pref_pf` (Argument)
`start_pref_pf:`, 106
`loss[ener]/start_pref_v` (Argument)
`start_pref_v:`, 106
`loss[tensor]/pref` (Argument)
`pref:`, 111
`loss[tensor]/pref_atomic` (Argument)
`pref_atomic:`, 111

M

`main()` (in module `deepmd.entrypoints.main`), 305
`main_parser()` (in module `deepmd.entrypoints.main`), 305
`make_default_mesh()` (in module `deepmd.common`), 507
`make_index()` (in module `deepmd.utils.argcheck`), 467
`make_link()` (in module `deepmd.utils.argcheck`), 467
`make_model_devi()` (in module `deepmd.entrypoints`), 300
`make_model_devi()` (in module `deepmd.infer.model_devi`), 378
`make_natoms_vec()` (`deepmd.DeepEval` method), 196
`make_natoms_vec()` (`deepmd.infer.deep_eval.DeepEval` method), 363
`make_natoms_vec()` (`deepmd.infer.DeepEval` method), 343
`make_stat_input()` (in module `deepmd.model.model_stat`), 417
`map_aparam()` (in module `deepmd.env.op_module`), 543
`map_file:`
`nvnm/``map_file` (Argument), 116
`mapflt_nvnm()` (in module `deepmd.env.op_module`), 543
`map_nvnm()` (in module `deepmd.nvnm.utils`), 443
`map_nvnm()` (in module `deepmd.nvnm.utils.op`), 452
`MapAparam()` (in module `deepmd.env.op_module`), 518
`MapFltNvnm()` (in module `deepmd.env.op_module`), 518
`mapping()` (`deepmd.nvnm.entrypoints.mapt.MapTable` method), 437
`mapping()` (`deepmd.nvnm.entrypoints.MapTable` method), 432
`mapping2()` (`deepmd.nvnm.entrypoints.mapt.MapTable` method), 437
`mapping2()` (`deepmd.nvnm.entrypoints.MapTable` method), 432
`mapt()` (in module `deepmd.nvnm.entrypoints.mapt`), 437
`MapTable` (class in `deepmd.nvnm.entrypoints`), 430
`MapTable` (class in `deepmd.nvnm.entrypoints.mapt`), 434
`matmul2_qq()` (in module `deepmd.nvnm.utils.network`), 451
`matmul3_qq()` (in module `deepmd.nvnm.utils.network`), 451
`matmul_fitnet_nvnm()` (in module `deepmd.env.op_module`), 543
`matmulflt2fix_nvnm()` (in module `deepmd.env.op_module`), 543
`matmulflt_nvnm()` (in module `deepmd.env.op_module`), 543

```

    deepmd.env.op_module), 544
MatmulFitnetNvnmd()      (in      module
    deepmd.env.op_module), 519
MatmulFlt2fixNvnmd()    (in      module
    deepmd.env.op_module), 519
MatmulFltNvnmd()        (in      module
    deepmd.env.op_module), 519
merge_bin() (deepmd.nvnmd.utils.Encode method),
    441
merge_bin() (deepmd.nvnmd.utils.encode.Encode
    method), 448
merge_input_stats()
    (deepmd.descriptor.DescrptHybrid
    method), 212
merge_input_stats()
    (deepmd.descriptor.DescrptSeA method),
    221
merge_input_stats()
    (deepmd.descriptor.DescrptSeR method),
    244
merge_input_stats()
    (deepmd.descriptor.DescrptSeT method),
    248
merge_input_stats()
    (deepmd.descriptor.hybrid.DescrptHybrid
    method), 260
merge_input_stats()
    (deepmd.descriptor.se_a.DescrptSeA
    method), 271
merge_input_stats()
    (deepmd.descriptor.se_r.DescrptSeR
    method), 294
merge_input_stats()
    (deepmd.descriptor.se_t.DescrptSeT
    method), 298
merge_sys_stat()      (in      module
    deepmd.model.model_stat), 417
mixed_precision:
    training/mixed_precision (Argument), 113
mixed_precision_args() (in      module
    deepmd.utils.argcheck), 467
mkdir() (deepmd.nvnmd.utils.fio.Fio method), 449
MOASPNDIM (C macro), 724
model (Argument)
    model:, 78
Model (class in deepmd.model.model), 411
model/compress (Argument)
    compress:, 81
model/data_bias_nsample (Argument)
    data_bias_nsample:, 79
model/data_stat_nbatch (Argument)
    data_stat_nbatch:, 78
model/data_stat_protect (Argument)
    data_stat_protect:, 78
model/modifier (Argument)
    modifier:, 80
model/modifier/type (Argument)
    type:, 80
model/modifier[dipole_charge]/ewald_beta
    (Argument)
    ewald_beta:, 81
model/modifier[dipole_charge]/ewald_h
    (Argument)
    ewald_h:, 81
model/modifier[dipole_charge]/model_charge_map
    (Argument)
    model_charge_map:, 81
model/modifier[dipole_charge]/model_name
    (Argument)
    model_name:, 81
model/modifier[dipole_charge]/sys_charge_map
    (Argument)
    sys_charge_map:, 81
model/smin_alpha (Argument)
    smin_alpha:, 79
model/spin (Argument)
    spin:, 81
model/spin/spin_norm (Argument)
    spin_norm:, 81
model/spin/use_spin (Argument)
    use_spin:, 81
model/spin/virtual_len (Argument)
    virtual_len:, 81
model/srtab_add_bias (Argument)
    srtab_add_bias:, 79
model/sw_rmax (Argument)
    sw_rmax:, 79
model/sw_rmin (Argument)
    sw_rmin:, 79
model/type (Argument)
    type:, 82
model/type_embedding (Argument)
    type_embedding:, 79
model/type_embedding/activation_function
    (Argument)
    activation_function:, 80
model/type_embedding/neuron (Argument)
    neuron:, 79
model/type_embedding/precision (Argument)
    precision:, 80
model/type_embedding/resnet_dt (Argument)
    resnet_dt:, 80
model/type_embedding/seed (Argument)
    seed:, 80
model/type_embedding/trainable (Argument)
    trainable:, 80
model/type_map (Argument)
    type_map:, 78

```

```

model/use_srtab (Argument)
    use_srtab:, 79
model:
    model (Argument), 78
model_args() (in module deepmd.utils.argcheck),
    467
model_charge_map:
    model/modifier[dipole_charge]/model_charge_map
        (Argument), 81
model_compression() (in module
    deepmd.utils.argcheck), 468
model_compression_type_args() (in module
    deepmd.utils.argcheck), 468
model_name:
    model/modifier[dipole_charge]/model_name
        (Argument), 81
model_type (deepmd.DeepEval property), 196
model_type (deepmd.infer.deep_eval.DeepEval
    property), 363
model_type (deepmd.infer.DeepEval property), 343
model_type (deepmd.model.dos.DOSModel at-
    tribute), 407
model_type (deepmd.model.DOSModel attribute),
    396
model_type (deepmd.model.ener.EnerModel at-
    tribute), 411
model_type (deepmd.model.EnerModel attribute),
    400
model_type (deepmd.model.multi.MultiModel
    attribute), 420
model_type (deepmd.model.MultiModel attribute),
    404
model_type (deepmd.model.pairwise_dprc.PairwiseDPRc
    attribute), 422
model_version (deepmd.DeepEval property), 197
model_version (deepmd.infer.deep_eval.DeepEval
    property), 364
model_version (deepmd.infer.DeepEval property),
    344
model[multi]/descriptor (Argument)
    descriptor:, 104
model[multi]/fitting_net_dict (Argument)
    fitting_net_dict:, 104
model[pairwise_dprc]/qm_model (Argument)
    qm_model:, 104
model[pairwise_dprc]/qmmm_model (Argument)
    qmmm_model:, 104
model[standard]/descriptor (Argument)
    descriptor:, 82
model[standard]/descriptor/type (Argument)
    type:, 82
model[standard]/descriptor[hybrid]/list
    (Argument)
    list:, 91
model[standard]/descriptor[loc_frame]/axis_rule
    (Argument)
    axis_rule:, 83
model[standard]/descriptor[loc_frame]/rcut
    (Argument)
    rcut:, 83
model[standard]/descriptor[loc_frame]/sel_a
    (Argument)
    sel_a:, 82
model[standard]/descriptor[loc_frame]/sel_r
    (Argument)
    sel_r:, 83
model[standard]/descriptor[se_a_mask]/activation_function
    (Argument)
    activation_function:, 97
model[standard]/descriptor[se_a_mask]/axis_neuron
    (Argument)
    axis_neuron:, 97
model[standard]/descriptor[se_a_mask]/exclude_types
    (Argument)
    exclude_types:, 97
model[standard]/descriptor[se_a_mask]/neuron
    (Argument)
    neuron:, 97
model[standard]/descriptor[se_a_mask]/precision
    (Argument)
    precision:, 98
model[standard]/descriptor[se_a_mask]/resnet_dt
    (Argument)
    resnet_dt:, 97
model[standard]/descriptor[se_a_mask]/seed
    (Argument)
    seed:, 98
model[standard]/descriptor[se_a_mask]/sel
    (Argument)
    sel:, 96
model[standard]/descriptor[se_a_mask]/trainable
    (Argument)
    trainable:, 98
model[standard]/descriptor[se_a_mask]/type_one_side
    (Argument)
    type_one_side:, 97
model[standard]/descriptor[se_a_tpe]/activation_function
    (Argument)
    activation_function:, 88
model[standard]/descriptor[se_a_tpe]/axis_neuron
    (Argument)
    axis_neuron:, 87
model[standard]/descriptor[se_a_tpe]/exclude_types
    (Argument)
    exclude_types:, 88
model[standard]/descriptor[se_a_tpe]/neuron
    (Argument)
    neuron:, 87

```

```

model[standard]/descriptor[se_a_tpe]/numb_aparam
  (Argument)
  numb_aparam: 89
model[standard]/descriptor[se_a_tpe]/precision
  (Argument)
  precision: 88
model[standard]/descriptor[se_a_tpe]/rcut
  (Argument)
  rcut: 87
model[standard]/descriptor[se_a_tpe]/rcut_smth
  (Argument)
  rcut_smth: 87
model[standard]/descriptor[se_a_tpe]/resnet_dt
  (Argument)
  resnet_dt: 88
model[standard]/descriptor[se_a_tpe]/seed
  (Argument)
  seed: 88
model[standard]/descriptor[se_a_tpe]/sel
  (Argument)
  sel: 87
model[standard]/descriptor[se_a_tpe]/set_davg_zero
  (Argument)
  set_davg_zero: 89
model[standard]/descriptor[se_a_tpe]/trainable
  (Argument)
  trainable: 88
model[standard]/descriptor[se_a_tpe]/type_nchan
  (Argument)
  type_nchan: 89
model[standard]/descriptor[se_a_tpe]/type_nlayer
  (Argument)
  type_nlayer: 89
model[standard]/descriptor[se_a_tpe]/type_one_side
  (Argument)
  type_one_side: 88
model[standard]/descriptor[se_atten_v2]/activation_function
  (Argument)
  activation_function: 95
model[standard]/descriptor[se_atten_v2]/attn
  (Argument)
  attn: 96
model[standard]/descriptor[se_atten_v2]/attn_dottr
  (Argument)
  attn_dottr: 96
model[standard]/descriptor[se_atten_v2]/attn_layer
  (Argument)
  attn_layer: 96
model[standard]/descriptor[se_atten_v2]/attn_mask
  (Argument)
  attn_mask: 96
model[standard]/descriptor[se_atten_v2]/axis_neuron
  (Argument)
  axis_neuron: 95
model[standard]/descriptor[se_atten_v2]/exclude_types
  (Argument)
  exclude_types: 96
model[standard]/descriptor[se_atten_v2]/neuron
  (Argument)
  neuron: 94
model[standard]/descriptor[se_atten_v2]/precision
  (Argument)
  precision: 95
model[standard]/descriptor[se_atten_v2]/rcut
  (Argument)
  rcut: 94
model[standard]/descriptor[se_atten_v2]/rcut_smth
  (Argument)
  rcut_smth: 94
model[standard]/descriptor[se_atten_v2]/resnet_dt
  (Argument)
  resnet_dt: 95
model[standard]/descriptor[se_atten_v2]/seed
  (Argument)
  seed: 95
model[standard]/descriptor[se_atten_v2]/sel
  (Argument)
  sel: 94
model[standard]/descriptor[se_atten_v2]/set_davg_zero
  (Argument)
  set_davg_zero: 96
model[standard]/descriptor[se_atten_v2]/trainable
  (Argument)
  trainable: 95
model[standard]/descriptor[se_atten_v2]/type_one_side
  (Argument)
  type_one_side: 95
model[standard]/descriptor[se_atten]/activation_function
  (Argument)
  activation_function: 92
model[standard]/descriptor[se_atten]/attn
  (Argument)
  attn: 93
model[standard]/descriptor[se_atten]/attn_dottr
  (Argument)
  attn_dottr: 93
model[standard]/descriptor[se_atten]/attn_layer
  (Argument)
  attn_layer: 93
model[standard]/descriptor[se_atten]/attn_mask
  (Argument)
  attn_mask: 93
model[standard]/descriptor[se_atten]/axis_neuron
  (Argument)
  axis_neuron: 92
model[standard]/descriptor[se_atten]/exclude_types
  (Argument)
  exclude_types: 93

```

```

model[standard]/descriptor[se_atten]/neuron      model[standard]/descriptor[se_e2_a]/rcut_smth
  (Argument)                                     (Argument)
  neuron:., 92                                   rcut_smth:., 84
model[standard]/descriptor[se_atten]/precision model[standard]/descriptor[se_e2_a]/resnet_dt
  (Argument)                                     (Argument)
  precision:., 92                               resnet_dt:., 84
model[standard]/descriptor[se_atten]/rcut        model[standard]/descriptor[se_e2_a]/seed
  (Argument)                                     (Argument)
  rcut:., 91                                    seed:., 85
model[standard]/descriptor[se_atten]/rcut_smth model[standard]/descriptor[se_e2_a]/sel
  (Argument)                                     (Argument)
  rcut_smth:., 92                               sel:., 83
model[standard]/descriptor[se_atten]/resnet_dt model[standard]/descriptor[se_e2_a]/set_davg_zero
  (Argument)                                     (Argument)
  resnet_dt:., 92                               set_davg_zero:., 85
model[standard]/descriptor[se_atten]/seed        model[standard]/descriptor[se_e2_a]/trainable
  (Argument)                                     (Argument)
  seed:., 93                                    trainable:., 85
model[standard]/descriptor[se_atten]/sel        model[standard]/descriptor[se_e2_a]/type_one_side
  (Argument)                                     (Argument)
  sel:., 91                                    type_one_side:., 84
model[standard]/descriptor[se_atten]/set_davg_zero model[standard]/descriptor[se_e2_r]/activation_function
  (Argument)                                     (Argument)
  set_davg_zero:., 94                           activation_function:., 90
model[standard]/descriptor[se_atten]/smooth_type_embedding model[standard]/descriptor[se_e2_r]/exclude_types
  (Argument)                                     (Argument)
  smooth_type_embedding:., 93                   exclude_types:., 91
model[standard]/descriptor[se_atten]/stripped_type_embedding model[standard]/descriptor[se_e2_r]/neuron
  (Argument)                                     (Argument)
  stripped_type_embedding:., 93                 neuron:., 90
model[standard]/descriptor[se_atten]/trainable model[standard]/descriptor[se_e2_r]/precision
  (Argument)                                     (Argument)
  trainable:., 93                               precision:., 90
model[standard]/descriptor[se_atten]/type_one_side model[standard]/descriptor[se_e2_r]/rcut
  (Argument)                                     (Argument)
  type_one_side:., 92                           rcut:., 89
model[standard]/descriptor[se_e2_a]/activation_function model[standard]/descriptor[se_e2_r]/rcut_smth
  (Argument)                                     (Argument)
  activation_function:., 84                     rcut_smth:., 89
model[standard]/descriptor[se_e2_a]/axis_neuron model[standard]/descriptor[se_e2_r]/resnet_dt
  (Argument)                                     (Argument)
  axis_neuron:., 84                             resnet_dt:., 90
model[standard]/descriptor[se_e2_a]/exclude_types model[standard]/descriptor[se_e2_r]/seed
  (Argument)                                     (Argument)
  exclude_types:., 85                           seed:., 90
model[standard]/descriptor[se_e2_a]/neuron      model[standard]/descriptor[se_e2_r]/sel
  (Argument)                                     (Argument)
  neuron:., 84                                   sel:., 89
model[standard]/descriptor[se_e2_a]/precision model[standard]/descriptor[se_e2_r]/set_davg_zero
  (Argument)                                     (Argument)
  precision:., 85                               set_davg_zero:., 91
model[standard]/descriptor[se_e2_a]/rcut        model[standard]/descriptor[se_e2_r]/trainable
  (Argument)                                     (Argument)
  rcut:., 84                                    trainable:., 90

```

```

model[standard]/descriptor[se_e2_r]/type_one_side sel_type:, 103
    (Argument)
    type_one_side:, 90
model[standard]/descriptor[se_e3]/activation_function activation_function:, 101
    (Argument)
    activation_function:, 86
model[standard]/descriptor[se_e3]/neuron
    (Argument)
    neuron:, 86
model[standard]/descriptor[se_e3]/precision
    (Argument)
    precision:, 86
model[standard]/descriptor[se_e3]/rcut
    (Argument)
    rcut:, 86
model[standard]/descriptor[se_e3]/rcut_smth
    (Argument)
    rcut_smth:, 86
model[standard]/descriptor[se_e3]/resnet_dt
    (Argument)
    resnet_dt:, 86
model[standard]/descriptor[se_e3]/seed
    (Argument)
    seed:, 86
model[standard]/descriptor[se_e3]/sel
    (Argument)
    sel:, 85
model[standard]/descriptor[se_e3]/set_davg_zero
    (Argument)
    set_davg_zero:, 87
model[standard]/descriptor[se_e3]/trainable
    (Argument)
    trainable:, 86
model[standard]/fitting_net (Argument)
    fitting_net:, 98
model[standard]/fitting_net/type (Argument)
    type:, 98
model[standard]/fitting_net[dipole]/activation_function
    (Argument)
    activation_function:, 103
model[standard]/fitting_net[dipole]/neuron
    (Argument)
    neuron:, 103
model[standard]/fitting_net[dipole]/precision
    (Argument)
    precision:, 103
model[standard]/fitting_net[dipole]/resnet_dt
    (Argument)
    resnet_dt:, 103
model[standard]/fitting_net[dipole]/seed
    (Argument)
    seed:, 103
model[standard]/fitting_net[dipole]/sel_type
    (Argument)
    model[standard]/fitting_net[dos]/activation_function
        (Argument)
        model[standard]/fitting_net[dos]/neuron
            (Argument)
            neuron:, 101
        model[standard]/fitting_net[dos]/numb_aparam
            (Argument)
            numb_aparam:, 100
        model[standard]/fitting_net[dos]/numb_dos
            (Argument)
            numb_dos:, 102
        model[standard]/fitting_net[dos]/numb_fparam
            (Argument)
            numb_fparam:, 100
        model[standard]/fitting_net[dos]/precision
            (Argument)
            precision:, 101
        model[standard]/fitting_net[dos]/rcond
            (Argument)
            rcond:, 101
        model[standard]/fitting_net[dos]/resnet_dt
            (Argument)
            resnet_dt:, 101
        model[standard]/fitting_net[dos]/seed
            (Argument)
            seed:, 101
        model[standard]/fitting_net[dos]/trainable
            (Argument)
            trainable:, 101
        model[standard]/fitting_net[ener]/activation_function
            (Argument)
            activation_function:, 99
        model[standard]/fitting_net[ener]/atom_ener
            (Argument)
            atom_ener:, 100
        model[standard]/fitting_net[ener]/layer_name
            (Argument)
            layer_name:, 100
        model[standard]/fitting_net[ener]/neuron
            (Argument)
            neuron:, 99
        model[standard]/fitting_net[ener]/numb_aparam
            (Argument)
            numb_aparam:, 99
        model[standard]/fitting_net[ener]/numb_fparam
            (Argument)
            numb_fparam:, 99
        model[standard]/fitting_net[ener]/precision
            (Argument)
            precision:, 99
        model[standard]/fitting_net[ener]/rcond
            (Argument)

```

```

    rcond:, 100
model[standard]/fitting_net[ener]/resnet_dt
    (Argument)
    resnet_dt:, 99
model[standard]/fitting_net[ener]/seed
    (Argument)
    seed:, 100
model[standard]/fitting_net[ener]/trainable
    (Argument)
    trainable:, 99
model[standard]/fitting_net[ener]/use_aparam_as_mask
    (Argument)
    use_aparam_as_mask:, 100
model[standard]/fitting_net[polar]/activation_function
    (Argument)
    activation_function:, 102
model[standard]/fitting_net[polar]/fit_diag
    (Argument)
    fit_diag:, 102
model[standard]/fitting_net[polar]/neuron
    (Argument)
    neuron:, 102
model[standard]/fitting_net[polar]/precision
    (Argument)
    precision:, 102
model[standard]/fitting_net[polar]/resnet_dt
    (Argument)
    resnet_dt:, 102
model[standard]/fitting_net[polar]/scale
    (Argument)
    scale:, 102
model[standard]/fitting_net[polar]/seed
    (Argument)
    seed:, 103
model[standard]/fitting_net[polar]/sel_type
    (Argument)
    sel_type:, 103
model[standard]/fitting_net[polar]/shift_diag
    (Argument)
    shift_diag:, 102
modifier:
    model/modifier (Argument), 80
modifier_dipole_charge() (in module
    deepmd.utils.argcheck), 468
modifier_variant_type_args() (in module
    deepmd.utils.argcheck), 468
modify_data() (deepmd.DipoleChargeModifier
    method), 200
modify_data() (deepmd.infer.data_modifier.DipoleChargeModifier
    method), 357
modify_data() (deepmd.infer.DipoleChargeModifier
    method), 354
module
    deepmd, 195
    deepmd.calculator, 501
    deepmd.cluster, 200
    deepmd.cluster.local, 200
    deepmd.cluster.slurm, 201
    deepmd.common, 503
    deepmd.descriptor, 201
    deepmd.descriptor.descriptor, 249
    deepmd.descriptor.hybrid, 256
    deepmd.descriptor.loc_frame, 261
    deepmd.descriptor.se, 264
    deepmd.descriptor.se_a, 266
    deepmd.descriptor.se_a_ebd, 272
    deepmd.descriptor.se_a_ef, 274
    deepmd.descriptor.se_a_mask, 279
    deepmd.descriptor.se_atten, 283
    deepmd.descriptor.se_atten_v2, 288
    deepmd.descriptor.se_r, 290
    deepmd.descriptor.se_t, 295
    deepmd.entrypoints, 299
    deepmd.entrypoints.compress, 303
    deepmd.entrypoints.convert, 304
    deepmd.entrypoints.doc, 304
    deepmd.entrypoints.freeze, 304
    deepmd.entrypoints.ipi, 305
    deepmd.entrypoints.main, 305
    deepmd.entrypoints.neighbor_stat, 306
    deepmd.entrypoints.test, 306
    deepmd.entrypoints.train, 307
    deepmd.entrypoints.transfer, 308
    deepmd.env, 508
    deepmd.env.op_grads_module, 560
    deepmd.env.op_module, 511
    deepmd.fit, 308
    deepmd.fit.dipole, 323
    deepmd.fit.dos, 325
    deepmd.fit.ener, 328
    deepmd.fit.fitting, 332
    deepmd.fit.polar, 333
    deepmd.infer, 338
    deepmd.infer.data_modifier, 356
    deepmd.infer.deep_dipole, 358
    deepmd.infer.deep_dos, 359
    deepmd.infer.deep_eval, 362
    deepmd.infer.deep_polar, 365
    deepmd.infer.deep_pot, 367
    deepmd.infer.deep_tensor, 371
    deepmd.infer.deep_wfc, 374
    deepmd.infer.ewald_recip, 375
    deepmd.infer.infer_model_devi, 376
    deepmd.infer, 338
    deepmd.lmp, 508
    deepmd.loggers, 379
    deepmd.loggers.loggers, 380
    deepmd.loss, 381
    deepmd.loss.dos, 387

```


deepmd.loss.ener, 388
 deepmd.loss.loss, 392
 deepmd.loss.tensor, 393
 deepmd.model, 394
 deepmd.model.dos, 405
 deepmd.model.ener, 407
 deepmd.model.model, 411
 deepmd.model.model_stat, 417
 deepmd.model.multi, 417
 deepmd.model.pairwise_dprc, 420
 deepmd.model.tensor, 423
 deepmd.nvnmd, 427
 deepmd.nvnmd.data, 427
 deepmd.nvnmd.data.data, 428
 deepmd.nvnmd.descriptor, 428
 deepmd.nvnmd.descriptor.se_a, 429
 deepmd.nvnmd.descriptor.se_atten, 429
 deepmd.nvnmd.entrypoints, 430
 deepmd.nvnmd.entrypoints.freeze, 434
 deepmd.nvnmd.entrypoints.mapt, 434
 deepmd.nvnmd.entrypoints.train, 437
 deepmd.nvnmd.entrypoints.wrap, 438
 deepmd.nvnmd.fit, 439
 deepmd.nvnmd.fit.ener, 439
 deepmd.nvnmd.utils, 440
 deepmd.nvnmd.utils.argcheck, 444
 deepmd.nvnmd.utils.config, 444
 deepmd.nvnmd.utils.encode, 447
 deepmd.nvnmd.utils.fio, 449
 deepmd.nvnmd.utils.network, 451
 deepmd.nvnmd.utils.op, 452
 deepmd.nvnmd.utils.weight, 452
 deepmd.op, 454
 deepmd.train, 454
 deepmd.train.run_options, 454
 deepmd.train.trainer, 455
 deepmd.utils, 457
 deepmd.utils.argcheck, 466
 deepmd.utils.batch_size, 468
 deepmd.utils.compat, 470
 deepmd.utils.convert, 471
 deepmd.utils.data, 473
 deepmd.utils.data_system, 476
 deepmd.utils.errors, 479
 deepmd.utils.finetune, 480
 deepmd.utils.graph, 480
 deepmd.utils.learning_rate, 484
 deepmd.utils.multi_init, 485
 deepmd.utils.neighbor_stat, 486
 deepmd.utils.network, 487
 deepmd.utils.pair_tab, 488
 deepmd.utils.parallel_op, 489
 deepmd.utils.path, 490
 deepmd.utils.plugin, 494
 deepmd.utils.random, 495
 deepmd.utils.sess, 496
 deepmd.utils.spin, 496
 deepmd.utils.tabulate, 497
 deepmd.utils.type_embed, 499
 deepmd.utils.weight_avg, 501
 mul_flt_nvnmd (C++ function), 722
 mul_flt_nvnmd() (in module deepmd.env.op_module), 544
 MulFltNvnmd() (in module deepmd.env.op_module), 519
 multi_model_args() (in module deepmd.utils.argcheck), 468
 MultiModel (class in deepmd.model), 401
 MultiModel (class in deepmd.model.multi), 417
 my_device (deepmd.train.run_options.RunOptions attribute), 455
 my_rank (deepmd.train.run_options.RunOptions attribute), 455

N

name (deepmd.calculator.DP attribute), 503
 natoms_match() (deepmd.model.ener.EnerModel method), 411
 natoms_match() (deepmd.model.EnerModel method), 400
 natoms_not_match() (deepmd.model.ener.EnerModel method), 411
 natoms_not_match() (deepmd.model.EnerModel method), 400
 NBIT_CUTF (C macro), 725
 NBIT_FLTF (C macro), 725
 nborAssert (C++ function), 722
 nborErrcheck (C macro), 725
 neighbor_stat() (in module deepmd.entrypoints), 301
 neighbor_stat() (in module deepmd.entrypoints.neighbor_stat), 306
 neighbor_stat() (in module deepmd.env.op_module), 544
 NeighborStat (class in deepmd.utils.neighbor_stat), 486
 NeighborStat() (in module deepmd.env.op_module), 520
 net_size:
 nvnmd/net_size (Argument), 116
 neuron:
 model/type_embedding/neuron (Argument), 79
 model[standard]/descriptor[se_a_mask]/neuron (Argument), 97
 model[standard]/descriptor[se_a_tpe]/neuron (Argument), 87
 model[standard]/descriptor[se_atten_v2]/neuron (Argument), 94

| | |
|--|--|
| model[standard]/descriptor[se_atten]/neuron (Argument), 92 | model[standard]/fitting_net[dos]/numb_dos (Argument), 102 |
| model[standard]/descriptor[se_e2_a]/neuron (Argument), 84 | model[standard]/fitting_net[dos]/numb_fparam (Argument), 100 |
| model[standard]/descriptor[se_e2_r]/neuron (Argument), 90 | model[standard]/fitting_net[ener]/numb_fparam (Argument), 99 |
| model[standard]/descriptor[se_e3]/neuron (Argument), 86 | numb_generalized_coord: |
| model[standard]/fitting_net[dipole]/neuron (Argument), 103 | loss[ener]/numb_generalized_coord (Argument), 107 |
| model[standard]/fitting_net[dos]/neuron (Argument), 101 | numb_steps: |
| model[standard]/fitting_net[ener]/neuron (Argument), 99 | training/numb_steps (Argument), 114 |
| model[standard]/fitting_net[polar]/neuron (Argument), 102 | nvnmmd (Argument) |
| modelist (deepmd.train.run_options.RunOptions attribute), 455 | nvnmmd:, 116 |
| nodename (deepmd.train.run_options.RunOptions attribute), 455 | nvnmmd/config_file (Argument) |
| norm_expo() (deepmd.nvnmmd.utils.Encode method), 441 | config_file:, 116 |
| norm_expo() (deepmd.nvnmmd.utils.encode.Encode method), 448 | nvnmmd/enable (Argument) |
| normalize() (in module deepmd.utils.argcheck), 468 | enable:, 116 |
| normalize_data_dict() (in module deepmd.utils.argcheck), 468 | nvnmmd/map_file (Argument) |
| normalize_fitting_net_dict() (in module deepmd.utils.argcheck), 468 | map_file:, 116 |
| normalize_fitting_weight() (in module deepmd.utils.argcheck), 468 | nvnmmd/net_size (Argument) |
| normalize_learning_rate_dict() (in module deepmd.utils.argcheck), 468 | net_size:, 116 |
| normalize_learning_rate_dict_with_single_learning_weight() (in module deepmd.utils.argcheck), 468 | nvnmmd/quantize_descriptor (Argument) |
| normalize_loss_dict() (in module deepmd.utils.argcheck), 468 | quantize_descriptor:, 117 |
| normalize_multi_task() (in module deepmd.utils.argcheck), 468 | nvnmmd/quantize_fitting_net (Argument) |
| normalized_input() (in module deepmd.nvnmmd.entrypoints.train), 437 | quantize_fitting_net:, 117 |
| normalized_input_qnn() (in module deepmd.nvnmmd.entrypoints.train), 437 | nvnmmd/restore_descriptor (Argument) |
| numb_aparam: | restore_descriptor:, 116 |
| model[standard]/descriptor[se_a_tpe]/numb_aparam (Argument), 89 | nvnmmd/restore_fitting_net (Argument) |
| model[standard]/fitting_net[dos]/numb_aparam (Argument), 100 | restore_fitting_net:, 116 |
| model[standard]/fitting_net[ener]/numb_aparam (Argument), 99 | nvnmmd/version (Argument) |
| numb_btch: | version:, 116 |
| training/validation_data/numb_btch (Argument), 113 | nvnmmd/weight_file (Argument) |
| numb_dos: | weight_file:, 116 |
| | nvnmmd: |
| | nvnmmd (Argument), 116 |
| | nvnmmd_args() (in module deepmd.nvnmmd.utils), 444 |
| | nvnmmd_args() (in module deepmd.nvnmmd.utils.argcheck), 444 |
| | NvnmmdConfig (class in deepmd.nvnmmd.utils.config), 444 |
| | O |
| | omp_get_num_threads (C++ function), 722 |
| | omp_get_thread_num (C++ function), 723 |
| | one_layer() (in module deepmd.nvnmmd.utils), 444 |
| | one_layer() (in module deepmd.nvnmmd.utils.network), 452 |
| | one_layer() (in module deepmd.utils.network), 488 |
| | one_layer_nvnmmd() (in module deepmd.nvnmmd.fit.ener), 439 |
| | one_layer_rand_seed_shift() (in module deepmd.utils.network), 488 |

`one_layer_t()` (in module `deepmd.nvnmd.utils.network`), 452
`one_layer_wb()` (in module `deepmd.nvnmd.utils.network`), 452
`OutOfMemoryError`, 479
`output_prec:`
 `training/mixed_precision/output_prec`
 (Argument), 114

P

`pair_tab()` (in module `deepmd.env.op_module`), 544
`PairTab` (class in `deepmd.utils`), 464
`PairTab` (class in `deepmd.utils.pair_tab`), 488
`PairTab()` (in module `deepmd.env.op_module`), 520
`pairwise_dprc()` (in module `deepmd.utils.argcheck`), 468
`PairwiseDPRc` (class in `deepmd.model.pairwise_dprc`), 420
`parallel_prod_force_se_a()` (in module `deepmd.env.op_module`), 545
`ParallelOp` (class in `deepmd.utils.parallel_op`), 489
`ParallelProdForceSeA()` (in module `deepmd.env.op_module`), 520
`parse_args()` (in module `deepmd.entrypoints.main`), 305
`pass_tensors_from_frz_model()`
 (`deepmd.descriptor.Descriptor` method), 207
`pass_tensors_from_frz_model()`
 (`deepmd.descriptor.descriptor.Descriptor` method), 255
`pass_tensors_from_frz_model()`
 (`deepmd.descriptor.DescriptHybrid` method), 212
`pass_tensors_from_frz_model()`
 (`deepmd.descriptor.hybrid.DescriptHybrid` method), 260
`pass_tensors_from_frz_model()`
 (`deepmd.descriptor.se.DescriptSe` method), 266
`plot_lines()` (`deepmd.nvnmd.entrypoints.map.MapTable` method), 437
`plot_lines()` (`deepmd.nvnmd.entrypoints.MapTable` method), 432
`Plugin` (class in `deepmd.utils`), 464
`Plugin` (class in `deepmd.utils.plugin`), 494
`PluginVariant` (class in `deepmd.utils`), 465
`PluginVariant` (class in `deepmd.utils.plugin`), 495
`PolarFittingSeA` (class in `deepmd.fit`), 320
`PolarFittingSeA` (class in `deepmd.fit.polar`), 335
`PolarModel` (class in `deepmd.model`), 404
`PolarModel` (class in `deepmd.model.tensor`), 424
`precision` (`deepmd.descriptor.se.DescriptSe` property), 266
`precision` (`deepmd.fit.Fitting` property), 318
`precision` (`deepmd.fit.fitting.Fitting` property), 332
`precision:`
 `model/type_embedding/precision`
 (Argument), 80
 `model[standard]/descriptor[se_a_mask]/precision`
 (Argument), 98
 `model[standard]/descriptor[se_a_tpe]/precision`
 (Argument), 88
 `model[standard]/descriptor[se_atten_v2]/precision`
 (Argument), 95
 `model[standard]/descriptor[se_atten]/precision`
 (Argument), 92
 `model[standard]/descriptor[se_e2_a]/precision`
 (Argument), 85
 `model[standard]/descriptor[se_e2_r]/precision`
 (Argument), 90
 `model[standard]/descriptor[se_e3]/precision`
 (Argument), 86
 `model[standard]/fitting_net[dipole]/precision`
 (Argument), 103
 `model[standard]/fitting_net[dos]/precision`
 (Argument), 101
 `model[standard]/fitting_net[ener]/precision`
 (Argument), 99
 `model[standard]/fitting_net[polar]/precision`
 (Argument), 102
`pref:`
 `loss[tensor]/pref` (Argument), 111
`pref_atomic:`
 `loss[tensor]/pref_atomic` (Argument), 111
`print_header()` (`deepmd.loss.ener.EnerSpinLoss` method), 390
`print_header()` (`deepmd.loss.EnerSpinLoss` method), 384
`print_header()` (`deepmd.train.trainer.DPTrainer` static method), 456
`print_on_training()`
 (`deepmd.loss.ener.EnerSpinLoss` method), 390
`print_on_training()` (`deepmd.loss.EnerSpinLoss` method), 384
`print_on_training()`
 (`deepmd.train.trainer.DPTrainer` static method), 456
`print_resource_summary()`
 (`deepmd.train.run_options.RunOptions` method), 455
`print_summary()` (`deepmd.utils.data_system.DeepmdDataSystem` method), 479
`print_summary()` (`deepmd.utils.DeepmdDataSystem` method), 463
`prod_env_mat_a()` (in module `deepmd.env.op_module`), 545

| | |
|---|--|
| <code>prod_env_mat_a_mix()</code> (in module <code>deepmd.env.op_module</code>), 546 | <code>(deepmd.descriptor.hybrid.DescriptHybrid method)</code> , 260 |
| <code>prod_env_mat_a_mix_nvnm_quantize()</code> (in module <code>deepmd.env.op_module</code>), 547 | <code>prod_force_virial()</code> (<code>deepmd.descriptor.loc_frame.DescriptLocFrame method</code>), 264 |
| <code>prod_env_mat_a_nvnm_quantize()</code> (in module <code>deepmd.env.op_module</code>), 548 | <code>prod_force_virial()</code> (<code>deepmd.descriptor.se_a.DescriptSeA method</code>), 271 |
| <code>prod_env_mat_r()</code> (in module <code>deepmd.env.op_module</code>), 548 | <code>prod_force_virial()</code> (<code>deepmd.descriptor.se_a_ef.DescriptSeAEf method</code>), 277 |
| <code>prod_force()</code> (in module <code>deepmd.env.op_module</code>), 549 | <code>prod_force_virial()</code> (<code>deepmd.descriptor.se_a_mask.DescriptSeAMask method</code>), 282 |
| <code>prod_force_grad()</code> (in module <code>deepmd.env.op_grads_module</code>), 563 | <code>prod_force_virial()</code> (<code>deepmd.descriptor.se_r.DescriptSeR method</code>), 294 |
| <code>prod_force_norot()</code> (in module <code>deepmd.env.op_module</code>), 549 | <code>prod_force_virial()</code> (<code>deepmd.descriptor.se_t.DescriptSeT method</code>), 298 |
| <code>prod_force_se_a()</code> (in module <code>deepmd.env.op_module</code>), 550 | <code>prod_virial()</code> (in module <code>deepmd.env.op_module</code>), 550 |
| <code>prod_force_se_a_grad()</code> (in module <code>deepmd.env.op_grads_module</code>), 564 | <code>prod_virial_grad()</code> (in module <code>deepmd.env.op_grads_module</code>), 565 |
| <code>prod_force_se_a_mask()</code> (in module <code>deepmd.env.op_module</code>), 550 | <code>prod_virial_norot()</code> (in module <code>deepmd.env.op_module</code>), 551 |
| <code>prod_force_se_a_mask_grad()</code> (in module <code>deepmd.env.op_grads_module</code>), 564 | <code>prod_virial_se_a()</code> (in module <code>deepmd.env.op_module</code>), 551 |
| <code>prod_force_se_r()</code> (in module <code>deepmd.env.op_module</code>), 550 | <code>prod_virial_se_a_grad()</code> (in module <code>deepmd.env.op_grads_module</code>), 565 |
| <code>prod_force_se_r_grad()</code> (in module <code>deepmd.env.op_grads_module</code>), 565 | <code>prod_virial_se_r()</code> (in module <code>deepmd.env.op_module</code>), 552 |
| <code>prod_force_virial()</code> (<code>deepmd.descriptor.Descriptor method</code>), 207 | <code>prod_virial_se_r_grad()</code> (in module <code>deepmd.env.op_grads_module</code>), 566 |
| <code>prod_force_virial()</code> (<code>deepmd.descriptor.descriptor.Descriptor method</code>), 255 | <code>ProdEnvMatA()</code> (in module <code>deepmd.env.op_module</code>), 521 |
| <code>prod_force_virial()</code> (<code>deepmd.descriptor.DescriptHybrid method</code>), 212 | <code>ProdEnvMatAMix()</code> (in module <code>deepmd.env.op_module</code>), 522 |
| <code>prod_force_virial()</code> (<code>deepmd.descriptor.DescriptLocFrame method</code>), 216 | <code>ProdEnvMatAMixNvnmdQuantize()</code> (in module <code>deepmd.env.op_module</code>), 523 |
| <code>prod_force_virial()</code> (<code>deepmd.descriptor.DescriptSeA method</code>), 221 | <code>ProdEnvMatANvnmdQuantize()</code> (in module <code>deepmd.env.op_module</code>), 523 |
| <code>prod_force_virial()</code> (<code>deepmd.descriptor.DescriptSeAEf method</code>), 227 | <code>ProdEnvMatR()</code> (in module <code>deepmd.env.op_module</code>), 524 |
| <code>prod_force_virial()</code> (<code>deepmd.descriptor.DescriptSeAMask method</code>), 232 | <code>ProdForce()</code> (in module <code>deepmd.env.op_module</code>), 524 |
| <code>prod_force_virial()</code> (<code>deepmd.descriptor.DescriptSeR method</code>), 244 | <code>ProdForceGrad()</code> (in module <code>deepmd.env.op_grads_module</code>), 560 |
| <code>prod_force_virial()</code> (<code>deepmd.descriptor.DescriptSeT method</code>), 248 | <code>ProdForceNorot()</code> (in module <code>deepmd.env.op_module</code>), 525 |
| <code>prod_force_virial()</code> | <code>ProdForceSeA()</code> (in module <code>deepmd.env.op_module</code>), 525 |
| | <code>ProdForceSeAGPUExecuteFuncutor</code> (C++ struct), 677 |
| | <code>ProdForceSeAGPUExecuteFuncutor::operator()</code> |

(C++ function), 678

ProdForceSeAGrad() (in module deepmd.env.op_grads_module), 560

ProdForceSeAMask() (in module deepmd.env.op_module), 525

ProdForceSeAMaskGrad() (in module deepmd.env.op_grads_module), 561

ProdForceSeR() (in module deepmd.env.op_module), 526

ProdForceSeRGPUExecuteFunctor (C++ struct), 678

ProdForceSeRGPUExecuteFunctor::operator() (C++ function), 678

ProdForceSeRGrad() (in module deepmd.env.op_grads_module), 561

ProdVirial() (in module deepmd.env.op_module), 526

ProdVirialGrad() (in module deepmd.env.op_grads_module), 561

ProdVirialNorot() (in module deepmd.env.op_module), 526

ProdVirialSeA() (in module deepmd.env.op_module), 527

ProdVirialSeAGPUExecuteFunctor (C++ struct), 678

ProdVirialSeAGPUExecuteFunctor::operator() (C++ function), 678

ProdVirialSeAGrad() (in module deepmd.env.op_grads_module), 562

ProdVirialSeR() (in module deepmd.env.op_module), 527

ProdVirialSeRGPUExecuteFunctor (C++ struct), 679

ProdVirialSeRGPUExecuteFunctor::operator() (C++ function), 679

ProdVirialSeRGrad() (in module deepmd.env.op_grads_module), 562

profiling:
 training/profiling (Argument), 115

profiling_file:
 training/profiling_file (Argument), 115

Q

qc() (deepmd.nvnmd.utils.Encode method), 441

qc() (deepmd.nvnmd.utils.encode.Encode method), 448

qf() (deepmd.nvnmd.utils.Encode method), 442

qf() (deepmd.nvnmd.utils.encode.Encode method), 448

qf() (in module deepmd.nvnmd.utils.network), 452

qm_model:
 model[pairwise_dprc]/qm_model (Argument), 104

qmmm_model:

 model[pairwise_dprc]/qmmm_model (Argument), 104

qr() (deepmd.nvnmd.utils.Encode method), 442

qr() (deepmd.nvnmd.utils.encode.Encode method), 448

qr() (in module deepmd.nvnmd.utils.network), 452

quantize_descriptor:
 nvnmd/quantize_descriptor (Argument), 117

quantize_fitting_net:
 nvnmd/quantize_fitting_net (Argument), 117

quantize_nvnmd() (in module deepmd.env.op_module), 552

QuantizeNvnmd() (in module deepmd.env.op_module), 528

R

r2s() (in module deepmd.nvnmd.utils.op), 452

random() (in module deepmd.utils.random), 495

rcond:
 model[standard]/fitting_net[dos]/rcond (Argument), 101

 model[standard]/fitting_net[ener]/rcond (Argument), 100

rcut:
 model[standard]/descriptor[loc_frame]/rcut (Argument), 83

 model[standard]/descriptor[se_a_tpe]/rcut (Argument), 87

 model[standard]/descriptor[se_atten_v2]/rcut (Argument), 94

 model[standard]/descriptor[se_atten]/rcut (Argument), 91

 model[standard]/descriptor[se_e2_a]/rcut (Argument), 84

 model[standard]/descriptor[se_e2_r]/rcut (Argument), 89

 model[standard]/descriptor[se_e3]/rcut (Argument), 86

rcut_smth:
 model[standard]/descriptor[se_a_tpe]/rcut_smth (Argument), 87

 model[standard]/descriptor[se_atten_v2]/rcut_smth (Argument), 94

 model[standard]/descriptor[se_atten]/rcut_smth (Argument), 92

 model[standard]/descriptor[se_e2_a]/rcut_smth (Argument), 84

 model[standard]/descriptor[se_e2_r]/rcut_smth (Argument), 89

 model[standard]/descriptor[se_e3]/rcut_smth (Argument), 86

reduce() (deepmd.utils.data.DeepmdData method), 476

`reduce()` (deepmd.utils.data_system.DeepmdDataSystem method), 479
`reduce()` (deepmd.utils.DeepmdData method), 460
`reduce()` (deepmd.utils.DeepmdDataSystem method), 463
`register()` (deepmd.descriptor.Descriptor static method), 207
`register()` (deepmd.descriptor.descriptor.Descriptor static method), 255
`register()` (deepmd.fit.Fitting static method), 318
`register()` (deepmd.fit.fitting.Fitting static method), 332
`register()` (deepmd.utils.argcheck.ArgsPlugin method), 466
`register()` (deepmd.utils.Plugin method), 465
`register()` (deepmd.utils.plugin.Plugin method), 494
`reinit()` (deepmd.utils.pair_tab.PairTab method), 488
`reinit()` (deepmd.utils.PairTab method), 464
`relative_f`:
 `loss[ener_spin]/relative_f` (Argument), 109
 `loss[ener]/relative_f` (Argument), 107
`remove_decay_rate()` (in module deepmd.utils.compat), 471
`replace_model_params_with_frz_multi_model()` (in module deepmd.utils.multi_init), 485
`replace_model_params_with_pretrained_model()` (in module deepmd.utils.finetune), 480
`reset_default_tf_session_config()` (in module deepmd.env), 508
`reset_get_batch()` (deepmd.utils.data.DeepmdData method), 476
`reset_get_batch()` (deepmd.utils.DeepmdData method), 460
`resnet_dt`:
 `model/type_embedding/resnet_dt` (Argument), 80
 `model[standard]/descriptor[se_a_mask]/resnet_dt` (Argument), 97
 `model[standard]/descriptor[se_a_tpe]/resnet_dt` (Argument), 88
 `model[standard]/descriptor[se_atten_v2]/resnet_dt` (Argument), 95
 `model[standard]/descriptor[se_atten]/resnet_dt` (Argument), 92
 `model[standard]/descriptor[se_e2_a]/resnet_dt` (Argument), 84
 `model[standard]/descriptor[se_e2_r]/resnet_dt` (Argument), 90
 `model[standard]/descriptor[se_e3]/resnet_dt` (Argument), 86
 `model[standard]/fitting_net[dipole]/resnet_dt` (Argument), 103
 `model[standard]/fitting_net[dos]/resnet_dt` (Argument), 101
 `model[standard]/fitting_net[ener]/resnet_dt` (Argument), 99
 `model[standard]/fitting_net[polar]/resnet_dt` (Argument), 102
 `restore_descriptor`:
 `nvnm/restore_descriptor` (Argument), 116
 `restore_fitting_net`:
 `nvnm/restore_fitting_net` (Argument), 116
 `reverse_bin()` (deepmd.nvnm.utils.Encode method), 442
 `reverse_bin()` (deepmd.nvnm.utils.encode.Encode method), 449
 `reverse_map()` (deepmd.DeepEval static method), 197
 `reverse_map()` (deepmd.infer.deep_eval.DeepEval static method), 364
 `reverse_map()` (deepmd.infer.DeepEval static method), 344
 `rglob()` (deepmd.utils.path.DPH5Path method), 491
 `rglob()` (deepmd.utils.path.DPOSPath method), 492
 `rglob()` (deepmd.utils.path.DPPPath method), 493
 `run_s2g()` (deepmd.nvnm.entrypoints.mapt.MapTable method), 437
 `run_s2g()` (deepmd.nvnm.entrypoints.MapTable method), 432
 `run_sess()` (in module deepmd.utils.sess), 496
 `run_t2g()` (deepmd.nvnm.entrypoints.mapt.MapTable method), 437
 `run_t2g()` (deepmd.nvnm.entrypoints.MapTable method), 432
 `run_u2s()` (deepmd.nvnm.entrypoints.mapt.MapTable method), 437
 `run_u2s()` (deepmd.nvnm.entrypoints.MapTable method), 432
 `RunOptions` (class in deepmd.train.run_options), 454
 `safe_cast_tensor()` (in module deepmd.common), 507
 `save()` (deepmd.nvnm.utils.config.NvnmConfig method), 446
 `save()` (deepmd.nvnm.utils.fio.FioBin method), 450
 `save()` (deepmd.nvnm.utils.fio.FioDic method), 450
 `save()` (deepmd.nvnm.utils.fio.FioJsonDic method), 451
 `save()` (deepmd.nvnm.utils.fio.FioNpyDic method), 451
 `save()` (deepmd.nvnm.utils.fio.FioTxt method), 451
 `save()` (deepmd.nvnm.utils.FioBin method), 442
 `save()` (deepmd.nvnm.utils.FioDic method), 442
 `save()` (deepmd.nvnm.utils.FioTxt method), 443

```

save_checkpoint() (deepmd.train.trainer.DPTrainer
    method), 456
save_ckpt:
    training/save_ckpt (Argument), 114
save_compressed() (deepmd.train.trainer.DPTrainer
    method), 456
save_freq:
    training/save_freq (Argument), 114
save_weight() (in module
    deepmd.nvnmd.entypoints), 433
save_weight() (in module
    deepmd.nvnmd.entypoints.freeze), 434
scale:
    model[standard]/fitting_net[polar]/scale
        (Argument), 102
scale_by_worker:
    learning_rate/scale_by_worker (Argument),
        104
seed() (in module deepmd.utils.random), 496
seed:
    model/type_embedding/seed (Argument), 80
    model[standard]/descriptor[se_a_mask]/seed
        (Argument), 98
    model[standard]/descriptor[se_a_tpe]/seed
        (Argument), 88
    model[standard]/descriptor[se_atten_v2]/seed
        (Argument), 95
    model[standard]/descriptor[se_atten]/seed
        (Argument), 93
    model[standard]/descriptor[se_e2_a]/seed
        (Argument), 85
    model[standard]/descriptor[se_e2_r]/seed
        (Argument), 90
    model[standard]/descriptor[se_e3]/seed
        (Argument), 86
    model[standard]/fitting_net[dipole]/seed
        (Argument), 103
    model[standard]/fitting_net[dos]/seed
        (Argument), 101
    model[standard]/fitting_net[ener]/seed
        (Argument), 100
    model[standard]/fitting_net[polar]/seed
        (Argument), 103
    training/seed (Argument), 114
sel:
    model[standard]/descriptor[se_a_mask]/sel
        (Argument), 96
    model[standard]/descriptor[se_a_tpe]/sel
        (Argument), 87
    model[standard]/descriptor[se_atten_v2]/sel
        (Argument), 94
    model[standard]/descriptor[se_atten]/sel
        (Argument), 91
    model[standard]/descriptor[se_e2_a]/sel
        (Argument), 83
    model[standard]/descriptor[se_e2_r]/sel
        (Argument), 89
    model[standard]/descriptor[se_e3]/sel
        (Argument), 85
    sel_a:
        model[standard]/descriptor[loc_frame]/sel_a
            (Argument), 82
    sel_r:
        model[standard]/descriptor[loc_frame]/sel_r
            (Argument), 83
    sel_type:
        model[standard]/fitting_net[dipole]/sel_type
            (Argument), 103
        model[standard]/fitting_net[polar]/sel_type
            (Argument), 103
    select_idx_map() (in module deepmd.common),
        507
    sess (deepmd.DeepEval property), 197
    sess (deepmd.infer.deep_eval.DeepEval property),
        364
    sess (deepmd.infer.DeepEval property), 344
    set_davg_zero:
        model[standard]/descriptor[se_a_tpe]/set_davg_zero
            (Argument), 89
        model[standard]/descriptor[se_atten_v2]/set_davg_zero
            (Argument), 96
        model[standard]/descriptor[se_atten]/set_davg_zero
            (Argument), 94
        model[standard]/descriptor[se_e2_a]/set_davg_zero
            (Argument), 85
        model[standard]/descriptor[se_e2_r]/set_davg_zero
            (Argument), 91
        model[standard]/descriptor[se_e3]/set_davg_zero
            (Argument), 87
    set_log_handles() (in module deepmd.loggers), 379
    set_log_handles() (in module
        deepmd.loggers.loggers), 380
    set_ntype() (deepmd.nvnmd.utils.config.NvnmdConfig
        method), 446
    set_prefix:
        training/training_data/set_prefix
            (Argument), 111
        training/validation_data/set_prefix
            (Argument), 113
    set_sys_probs() (deepmd.utils.data_system.DeepmdDataSystem
        method), 479
    set_sys_probs() (deepmd.utils.DeepmdDataSystem
        method), 463
    shift_diag:
        model[standard]/fitting_net[polar]/shift_diag
            (Argument), 102
    shuffle() (in module deepmd.utils.random), 496
    SimulationRegion (C++ class), 680

```


SimulationRegion::~~SimulationRegion (C++ function), 680
 SimulationRegion::~affineTransform (C++ function), 680
 SimulationRegion::~backup (C++ function), 680
 SimulationRegion::~compactIndex (C++ function), 681
 SimulationRegion::~computeShiftVec (C++ function), 682
 SimulationRegion::~DBOX_XX (C++ member), 682
 SimulationRegion::~DBOX_YY (C++ member), 682
 SimulationRegion::~DBOX_ZZ (C++ member), 682
 SimulationRegion::~diffNearestNeighbor (C++ function), 681
 SimulationRegion::~getBoxOrigin (C++ function), 680, 681
 SimulationRegion::~getBoxTensor (C++ function), 680
 SimulationRegion::~getInterShiftVec (C++ function), 682
 SimulationRegion::~getNullShiftIndex (C++ function), 681
 SimulationRegion::~getNumShiftVec (C++ function), 681
 SimulationRegion::~getRecBoxTensor (C++ function), 680
 SimulationRegion::~getShiftIndex (C++ function), 681
 SimulationRegion::~getShiftVec (C++ function), 681
 SimulationRegion::~getShiftVecTotalSize (C++ function), 681
 SimulationRegion::~getVolume (C++ function), 681
 SimulationRegion::~index3to1 (C++ function), 682
 SimulationRegion::~inter2Phys (C++ function), 681
 SimulationRegion::~inter_shift_vec (C++ member), 682
 SimulationRegion::~isPeriodic (C++ function), 681
 SimulationRegion::~NBOX_XX (C++ member), 682
 SimulationRegion::~NBOX_YY (C++ member), 682
 SimulationRegion::~NBOX_ZZ (C++ member), 682
 SimulationRegion::~phys2Inter (C++ function), 681
 SimulationRegion::~recover (C++ function), 680
 SimulationRegion::~reinitBox (C++ function), 680
 SimulationRegion::~reinitOrigin (C++ function), 680
 SimulationRegion::~shift_info_size (C++ member), 682
 SimulationRegion::~shift_vec (C++ member), 682
 SimulationRegion::~shift_vec_size (C++ member), 682
 SimulationRegion::~shiftCoord (C++ function), 681
 SimulationRegion::SimulationRegion (C++ function), 680
 SimulationRegion::SPACENDIM (C++ member), 682
 SimulationRegion::toFaceDistance (C++ function), 681
 smin_alpha:
 model/smin_alpha (Argument), 79
 smooth_type_embdding:
 model[standard]/descriptor[se_atten]/smooth_type_embdding (Argument), 93
 soft_min_force() (in module deepmd.env.op_module), 552
 soft_min_force_grad() (in module deepmd.env.op_grads_module), 566
 soft_min_switch() (in module deepmd.env.op_module), 553
 soft_min_virial() (in module deepmd.env.op_module), 553
 soft_min_virial_grad() (in module deepmd.env.op_grads_module), 566
 SoftMinForce() (in module deepmd.env.op_module), 528
 SoftMinForceGrad() (in module deepmd.env.op_grads_module), 563
 SoftMinSwitch() (in module deepmd.env.op_module), 528
 SoftMinVirial() (in module deepmd.env.op_module), 529
 SoftMinVirialGrad() (in module deepmd.env.op_grads_module), 563
 sort_input() (deepmd.DeepEval static method), 197
 sort_input() (deepmd.infer.deep_eval.DeepEval static method), 364
 sort_input() (deepmd.infer.DeepEval static method), 344
 Spin (class in deepmd.utils.spin), 496
 spin:
 model/spin (Argument), 81
 spin_args() (in module deepmd.utils.argcheck), 468
 spin_norm:
 model/spin/spin_norm (Argument), 81
 split_bin() (deepmd.nvnmd.utils.Encode method), 442
 split_bin() (deepmd.nvnmd.utils.encode.Encode method), 449
 split_expo_mant() (deepmd.nvnmd.utils.Encode method), 442
 split_expo_mant() (deepmd.nvnmd.utils.encode.Encode

method), 449
 split_flt (C++ function), 723
 SQRT_2_PI (C macro), 726
 srtab_add_bias:
 model/srtab_add_bias (Argument), 79
 standard_model_args() (in module
 deepmd.utils.argcheck), 468
 StandardModel (class in deepmd.model.model), 415
 start_lr() (deepmd.utils.learning_rate.LearningRateExp
 method), 485
 start_lr() (deepmd.utils.LearningRateExp
 method), 464
 start_lr:
 learning_rate[exp]/start_lr (Argument),
 104
 start_pref() (in module deepmd.utils.argcheck),
 468
 start_pref_acdf:
 loss[dos]/start_pref_acdf (Argument), 110
 start_pref_adof:
 loss[dos]/start_pref_adof (Argument), 110
 start_pref_ae:
 loss[ener_spin]/start_pref_ae (Argument),
 108
 loss[ener]/start_pref_ae (Argument), 106
 start_pref_cdf:
 loss[dos]/start_pref_cdf (Argument), 110
 start_pref_dof:
 loss[dos]/start_pref_dof (Argument), 109
 start_pref_e:
 loss[ener_spin]/start_pref_e (Argument),
 107
 loss[ener]/start_pref_e (Argument), 105
 start_pref_f:
 loss[ener]/start_pref_f (Argument), 106
 start_pref_fm:
 loss[ener_spin]/start_pref_fm (Argument),
 108
 start_pref_fr:
 loss[ener_spin]/start_pref_fr (Argument),
 108
 start_pref_gf:
 loss[ener]/start_pref_gf (Argument), 107
 start_pref_pf:
 loss[ener_spin]/start_pref_pf (Argument),
 109
 loss[ener]/start_pref_pf (Argument), 106
 start_pref_v:
 loss[ener_spin]/start_pref_v (Argument),
 108
 loss[ener]/start_pref_v (Argument), 106
 stop_lr:
 learning_rate[exp]/stop_lr (Argument), 105
 stripped_type_embedding:

 model[standard]/descriptor[se_atten]/stripped_type_emb
 (Argument), 93
 sw_rmax:
 model/sw_rmax (Argument), 79
 sw_rmin:
 model/sw_rmin (Argument), 79
 sys_charge_map:
 model/modifier[dipole_charge]/sys_charge_map
 (Argument), 81
 sys_probs:
 training/training_data/sys_probs
 (Argument), 112
 training/validation_data/sys_probs
 (Argument), 113
 systems:
 training/training_data/systems
 (Argument), 111
 training/validation_data/systems
 (Argument), 112

T

tabulate_fusion() (in module
 deepmd.env.op_module), 554
 tabulate_fusion_grad() (in module
 deepmd.env.op_module), 554
 tabulate_fusion_grad_grad() (in module
 deepmd.env.op_module), 554
 tabulate_fusion_se_a() (in module
 deepmd.env.op_module), 555
 tabulate_fusion_se_a_grad() (in module
 deepmd.env.op_module), 555
 tabulate_fusion_se_a_grad_grad() (in module
 deepmd.env.op_module), 555
 tabulate_fusion_se_atten() (in module
 deepmd.env.op_module), 556
 tabulate_fusion_se_atten_grad() (in module
 deepmd.env.op_module), 556
 tabulate_fusion_se_r() (in module
 deepmd.env.op_module), 557
 tabulate_fusion_se_r_grad() (in module
 deepmd.env.op_module), 557
 tabulate_fusion_se_r_grad_grad() (in module
 deepmd.env.op_module), 557
 tabulate_fusion_se_t() (in module
 deepmd.env.op_module), 557
 tabulate_fusion_se_t_grad() (in module
 deepmd.env.op_module), 558
 tabulate_fusion_se_t_grad_grad() (in module
 deepmd.env.op_module), 558
 TabulateCheckerGPUExecuteFunctor (C++ struct),
 679
 TabulateCheckerGPUExecuteFunctor::operator()
 (C++ function), 679

| | | | |
|--|--|---|---|
| TabulateFusion() | (in module deepmd.env.op_module), 529 | test() | (in module deepmd.entrypoints), 301 |
| TabulateFusionGPUExecuteFuncutor | (C++ struct), 679 | test() | (in module deepmd.entrypoints.test), 306 |
| TabulateFusionGPUExecuteFuncutor::operator() | (C++ function), 679 | time_training: | |
| TabulateFusionGrad() | (in module deepmd.env.op_module), 529 | training/time_training | (Argument), 115 |
| TabulateFusionGradGPUExecuteFuncutor | (C++ struct), 680 | TPB | (C macro), 726 |
| TabulateFusionGradGPUExecuteFuncutor::operator() | (C++ function), 680 | train() | (deepmd.train.trainer.DPTrainer method), 456 |
| TabulateFusionGradGrad() | (in module deepmd.env.op_module), 530 | train() | (in module deepmd.entrypoints.train), 307 |
| TabulateFusionSeA() | (in module deepmd.env.op_module), 530 | train_dp() | (in module deepmd.entrypoints), 302 |
| TabulateFusionSeAGrad() | (in module deepmd.env.op_module), 530 | train_nvnmd() | (in module deepmd.nvnmd.entrypoints.train), 437 |
| TabulateFusionSeAGradGrad() | (in module deepmd.env.op_module), 531 | trainable: | |
| TabulateFusionSeAtten() | (in module deepmd.env.op_module), 531 | model/type_embedding/trainable | (Argument), 80 |
| TabulateFusionSeAttenGrad() | (in module deepmd.env.op_module), 532 | model[standard]/descriptor[se_a_mask]/trainable | (Argument), 98 |
| TabulateFusionSeR() | (in module deepmd.env.op_module), 532 | model[standard]/descriptor[se_a_tpe]/trainable | (Argument), 88 |
| TabulateFusionSeRGrad() | (in module deepmd.env.op_module), 532 | model[standard]/descriptor[se_atten_v2]/trainable | (Argument), 95 |
| TabulateFusionSeRGradGrad() | (in module deepmd.env.op_module), 533 | model[standard]/descriptor[se_atten]/trainable | (Argument), 93 |
| TabulateFusionSeT() | (in module deepmd.env.op_module), 533 | model[standard]/descriptor[se_e2_a]/trainable | (Argument), 85 |
| TabulateFusionSeTGrad() | (in module deepmd.env.op_module), 533 | model[standard]/descriptor[se_e2_r]/trainable | (Argument), 90 |
| TabulateFusionSeTGradGrad() | (in module deepmd.env.op_module), 534 | model[standard]/descriptor[se_e3]/trainable | (Argument), 86 |
| tanh4() | (in module deepmd.nvnmd.utils.network), 452 | model[standard]/fitting_net[dos]/trainable | (Argument), 101 |
| tanh4_flt_nvnmd() | (in module deepmd.env.op_module), 559 | model[standard]/fitting_net[ener]/trainable | (Argument), 99 |
| Tanh4FltNvnmd() | (in module deepmd.env.op_module), 534 | training | (Argument) |
| tensorboard: | | training: | 111 |
| training/tensorboard | (Argument), 115 | training/data_dict | (Argument) |
| tensorboard_freq: | | data_dict: | 115 |
| training/tensorboard_freq | (Argument), 115 | training/disp_file | (Argument) |
| tensorboard_log_dir: | | disp_file: | 114 |
| training/tensorboard_log_dir | (Argument), 115 | training/disp_freq | (Argument) |
| TensorLoss | (class in deepmd.loss), 386 | disp_freq: | 114 |
| TensorLoss | (class in deepmd.loss.tensor), 393 | training/disp_training | (Argument) |
| TensorModel | (class in deepmd.model.tensor), 425 | disp_training: | 114 |
| tensors | (deepmd.infer.deep_tensor.DeepTensor attribute), 374 | training/enable_profiler | (Argument) |
| | | enable_profiler: | 115 |
| | | training/fitting_weight | (Argument) |
| | | fitting_weight: | 115 |
| | | training/mixed_precision | (Argument) |
| | | mixed_precision: | 113 |
| | | training/mixed_precision/compute_prec | (Argument) |
| | | compute_prec: | 114 |
| | | training/mixed_precision/output_prec | (Argument) |
| | | output_prec: | 114 |

training/numb_steps (Argument)
 numb_steps:, 114
 training/profiling (Argument)
 profiling:, 115
 training/profiling_file (Argument)
 profiling_file:, 115
 training/save_ckpt (Argument)
 save_ckpt:, 114
 training/save_freq (Argument)
 save_freq:, 114
 training/seed (Argument)
 seed:, 114
 training/tensorboard (Argument)
 tensorboard:, 115
 training/tensorboard_freq (Argument)
 tensorboard_freq:, 115
 training/tensorboard_log_dir (Argument)
 tensorboard_log_dir:, 115
 training/time_training (Argument)
 time_training:, 115
 training/training_data (Argument)
 training_data:, 111
 training/training_data/auto_prob (Argument)
 auto_prob:, 112
 training/training_data/batch_size (Argument)
 batch_size:, 112
 training/training_data/set_prefix (Argument)
 set_prefix:, 111
 training/training_data/sys_probs (Argument)
 sys_probs:, 112
 training/training_data/systems (Argument)
 systems:, 111
 training/validation_data (Argument)
 validation_data:, 112
 training/validation_data/auto_prob
 (Argument)
 auto_prob:, 113
 training/validation_data/batch_size
 (Argument)
 batch_size:, 113
 training/validation_data/numb_btch
 (Argument)
 numb_btch:, 113
 training/validation_data/set_prefix
 (Argument)
 set_prefix:, 113
 training/validation_data/sys_probs
 (Argument)
 sys_probs:, 113
 training/validation_data/systems (Argument)
 systems:, 112
 training:
 training (Argument), 111
 training_args() (in module
 deepmd.utils.argcheck), 468
 training_data:
 training/training_data (Argument), 111
 training_data_args() (in module
 deepmd.utils.argcheck), 468
 transfer() (in module deepmd.entrypoints), 303
 transfer() (in module
 deepmd.entrypoints.transfer), 308
 type:
 learning_rate/type (Argument), 104
 loss/type (Argument), 105
 model/modifier/type (Argument), 80
 model/type (Argument), 82
 model[standard]/descriptor/type
 (Argument), 82
 model[standard]/fitting_net/type
 (Argument), 98
 type_embedding:
 model/type_embedding (Argument), 79
 type_embedding_args() (in module
 deepmd.utils.argcheck), 468
 type_map:
 model/type_map (Argument), 78
 type_nchanl:
 model[standard]/descriptor[se_a_tpe]/type_nchanl
 (Argument), 89
 type_nlayer:
 model[standard]/descriptor[se_a_tpe]/type_nlayer
 (Argument), 89
 type_one_side:
 model[standard]/descriptor[se_a_mask]/type_one_side
 (Argument), 97
 model[standard]/descriptor[se_a_tpe]/type_one_side
 (Argument), 88
 model[standard]/descriptor[se_atten_v2]/type_one_side
 (Argument), 95
 model[standard]/descriptor[se_atten]/type_one_side
 (Argument), 92
 model[standard]/descriptor[se_e2_a]/type_one_side
 (Argument), 84
 model[standard]/descriptor[se_e2_r]/type_one_side
 (Argument), 90
 TypeEmbedNet (class in deepmd.utils.type_embed),
 499
U
 U_Flt64_Int64 (C++ union), 683
 U_Flt64_Int64::nflt (C++ member), 683
 U_Flt64_Int64::nint (C++ member), 683
 uint_64 (C++ type), 726
 unaggregated_dy2_dx() (in module
 deepmd.env.op_module), 559

`unaggregated_dy2_dx_s()` (in `deepmd.env.op_module`), 559
`unaggregated_dy_dx()` (in `deepmd.env.op_module`), 559
`unaggregated_dy_dx_s()` (in `deepmd.env.op_module`), 560
`UnaggregatedDy2Dx()` (in `deepmd.env.op_module`), 534
`UnaggregatedDy2DxS()` (in `deepmd.env.op_module`), 534
`UnaggregatedDyDx()` (in `deepmd.env.op_module`), 535
`UnaggregatedDyDxS()` (in `deepmd.env.op_module`), 535
`update()` (`deepmd.nvnmd.utils.fio.FioDic` method), 450
`update()` (`deepmd.nvnmd.utils.FioDic` method), 442
`update_config()` (`deepmd.nvnmd.utils.config.NvnmdConfig` method), 446
`update_deepmd_input()` (in `deepmd.utils.compat`), 471
`use_aparam_as_mask:`
 `model[standard]/fitting_net[ener]/use_aparam_as_mask` (Argument), 100
`use_spin:`
 `model/spin/use_spin` (Argument), 81
`use_srtab:`
 `model/use_srtab` (Argument), 79
V
`valid_on_the_fly()` (`deepmd.train.trainer.DPTrainer` method), 456
`validation_data:`
 `training/validation_data` (Argument), 112
`validation_data_args()` (in `deepmd.utils.argcheck`), 468
`value()` (`deepmd.utils.learning_rate.LearningRateExp` method), 485
`value()` (`deepmd.utils.LearningRateExp` method), 464
`variable_summaries()` (in `deepmd.utils.network`), 488
`VariantABCMeta` (class in `deepmd.utils.plugin`), 495
`VariantMeta` (class in `deepmd.utils.plugin`), 495
`version:`
 `nvnmd/version` (Argument), 116
`virtual_len:`
 `model/spin/virtual_len` (Argument), 81
W
`weight_file:`
 `nvnmd/weight_file` (Argument), 116
`weighted_average()` (in `deepmd.utils.weight_avg`), 501
`module WFCModel` (class in `deepmd.model`), 404
`module WFCModel` (class in `deepmd.model.tensor`), 427
`module world_size` (`deepmd.train.run_options.RunOptions` attribute), 455
`module Wrap` (class in `deepmd.nvnmd.entrypoints`), 432
`Wrap` (class in `deepmd.nvnmd.entrypoints.wrap`), 438
`module wrap()` (`deepmd.nvnmd.entrypoints.Wrap` method), 433
`module wrap()` (`deepmd.nvnmd.entrypoints.wrap.Wrap` method), 438
`module wrap()` (in `module deepmd.nvnmd.entrypoints.wrap`), 439
`module wrap_bias()` (`deepmd.nvnmd.entrypoints.Wrap` method), 433
`wrap_bias()` (`deepmd.nvnmd.entrypoints.wrap.Wrap` method), 438
`wrap_dscp()` (`deepmd.nvnmd.entrypoints.Wrap` method), 433
`wrap_dscp()` (`deepmd.nvnmd.entrypoints.wrap.Wrap` method), 438
`module wrap_fitn()` (`deepmd.nvnmd.entrypoints.Wrap` method), 433
`wrap_fitn()` (`deepmd.nvnmd.entrypoints.wrap.Wrap` method), 439
`wrap_head()` (`deepmd.nvnmd.entrypoints.Wrap` method), 433
`wrap_head()` (`deepmd.nvnmd.entrypoints.wrap.Wrap` method), 439
`wrap_lut()` (`deepmd.nvnmd.entrypoints.Wrap` method), 433
`wrap_lut()` (`deepmd.nvnmd.entrypoints.wrap.Wrap` method), 439
`wrap_map()` (`deepmd.nvnmd.entrypoints.Wrap` method), 433
`wrap_map()` (`deepmd.nvnmd.entrypoints.wrap.Wrap` method), 439
`wrap_weight()` (`deepmd.nvnmd.entrypoints.Wrap` method), 433
`wrap_weight()` (`deepmd.nvnmd.entrypoints.wrap.Wrap` method), 439
`write_model_devi_out()` (in `module deepmd.infer.model_devi`), 378