DP-GEN

DeepModeling

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CHAPTER

ONE

OVERVIEW

1.1 About DP-GEN

DP-GEN (Deep Generator) is a software written in Python, delicately designed to generate a deep learning based model of interatomic potential energy and force field. DP-GEN is dependent on DeepMD-kit. With highly scalable interface with common softwares for molecular simulation, DP-GEN is capable to automatically prepare scripts and maintain job queues on HPC machines (High Performance Cluster) and analyze results.

If you use this software in any publication, please cite:

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, 107206.

1.1.1 Highlighted features

- **Accurate and efficient**: DP-GEN is capable to sample more than tens of million structures and select only a few for first principles calculation. DP-GEN will finally obtain a uniformly accurate model.
- **User-friendly and automatic**: Users may install and run DP-GEN easily. Once succusefully running, DP-GEN can dispatch and handle all jobs on HPCs, and thus there's no need for any personal effort.
- **Highly scalable**: With modularized code structures, users and developers can easily extend DP-GEN for their most relevant needs. DP-GEN currently supports for HPC systems (Slurm, PBS, LSF and cloud machines), Deep Potential interface with DeePMD-kit, MD interface with LAMMPS, Gromacs and *ab-initio* calculation interface with VASP, PWSCF, CP2K, SIESTA and Gaussian, Abacus, PWMAT, etc . We're sincerely welcome and embraced to users' contributions, with more possibilities and cases to use DP-GEN.

1.2 Download and install

DP-GEN only supports Python 3.9 and above. You can use one of the following methods to install DP-GEN:

- Install via pip: `pip install dpgen`
- Install via conda: `conda install -c conda-forge dpgen``
- Install from source code: `git clone https://github.com/deepmodeling/dpgen && pip install ./dpgen`

To test if the installation is successful, you may execute

```
dpgen -h
```

1.3 Use DP-GEN

A quick-start on using DPGEN can be found here. You can follow the Handson tutorial, it is friendly to new users.

1.4 Case Studies

- Practical-Guidelines-for-DP

Before starting a new Deep Potential (DP) project, we suggest people (especially those who are newbies) read the following context first to get some insights into what tools we can use, what kinds of risks and difficulties we may meet, and how we can advance a new DP project smoothly.

- Convergence-Test

to ensure the data quality, the reliability of the final model, as well as the feasibility of the project, a convergence test should be done first.

- Gas-phase

In this tutorial, we will take the simulation of methane combustion as an example and introduce the procedure of DP-based MD simulation.

- Mg-Y_alloy

We will briefly analyze the candidate configurational space of a metallic system by taking Mg-based Mg-Y binary alloy as an example. The task is divided into steps during the DP-GEN process.

- Transfer-learning

This tutorial will introduce how to implement potential energy surface (PES) transfer-learning by using the DP-GEN software. In DP-GEN (version > 0.8.0), the "simplify" module is designed for this purpose.

1.5 License

The project dpgen is licensed under GNU LGPLv3.0

CHAPTER

TWO

COMMAND LINE INTERFACE

dpgen is a convenient script that uses DeepGenerator to prepare initial data, drive DeepMDkit and analyze results. This script works based on several sub-commands with their own options. To see the options for the sub-commands, type "dpgen sub-command -h".

```
usage: dpgen [-h]
             {init_surf,init_bulk,auto_gen_param,init_reaction,run,run/report,collect,
↪simplify,autotest,db,gui}
             ...
```

2.1 Sub-commands

2.1.1 init_surf

Generating initial data for surface systems.

```
dpgen init_surf [-h] PARAM [MACHINE]
```

Positional Arguments

PARAM	parameter file, json/yaml format
MACHINE	machine file, json/yaml format

2.1.2 init_bulk

Generating initial data for bulk systems.

```
dpgen init_bulk [-h] PARAM [MACHINE]
```

Positional Arguments

PARAM parameter file, json/yaml format

MACHINE machine file, json/yaml format

2.1.3 auto_gen_param

auto gen param.json

```
dpgen auto_gen_param [-h] PARAM
```

Positional Arguments

PARAM parameter file, json/yaml format

2.1.4 init_reaction

Generating initial data for reactive systems.

```
dpgen init_reaction [-h] PARAM [MACHINE]
```

Positional Arguments

PARAM parameter file, json/yaml format

MACHINE machine file, json/yaml format

2.1.5 run

Main process of Deep Potential Generator.

```
dpgen run [-h] [-d] PARAM MACHINE
```

Positional Arguments

PARAM parameter file, json/yaml format

MACHINE machine file, json/yaml format

Named Arguments

-d, --debug log debug info

Default: False

2.1.6 run/report

Report the systems and the thermodynamic conditions of the labeled frames.

```
dpgen run/report [-h] [-s] [-i] [-t] [-p PARAM] [-v] JOB_DIR
```

Positional Arguments

JOB_DIR the directory of the DP-GEN job,

Named Arguments

-s, --stat-sys count the labeled frames for each system

Default: False

-i, --stat-iter print the iteration candidate,failed,accurate count and fp calculation,success and fail count

Default: False

-t, --stat-time print the iteration time, warning!! assume model_devi parallel cores == 1

Default: False

-p, --param the json file provides DP-GEN paramters, should be located in JOB_DIR

Default: "param.json"

-v, --verbose being loud

Default: False

2.1.7 collect

Collect data.

```
dpgen collect [-h] [-p PARAMETER] [-v] [-m] [-s] JOB_DIR OUTPUT
```

Positional Arguments

JOB_DIR the directory of the DP-GEN job

OUTPUT the output directory of data

Named Arguments

-p, --parameter	the json file provides DP-GEN paramters, should be located in JOB_DIR Default: "param.json"
-v, --verbose	print number of data in each system Default: False
-m, --merge	merge the systems with the same chemical formula Default: False
-s, --shuffle	shuffle the data systems Default: False

2.1.8 simplify

Simplify data.

```
dpgen simplify [-h] [-d] PARAM MACHINE
```

Positional Arguments

PARAM	parameter file, json/yaml format
MACHINE	machine file, json/yaml format

Named Arguments

-d, --debug	log debug info Default: False

2.1.9 autotest

Auto-test for Deep Potential.

```
dpgen autotest [-h] [-d] TASK PARAM [MACHINE]
```

Positional Arguments

TASK	task can be make, run or post
PARAM	parameter file, json/yaml format
MACHINE	machine file, json/yaml format

Named Arguments

-d, --debug log debug info

Default: False

2.1.10 db

Collecting data from DP-GEN.

```
dpgen db [-h] PARAM
```

Positional Arguments

PARAM parameter file, json format

2.1.11 gui

Serve DP-GUI.

```
dpgen gui [-h] [-p PORT] [--bind_all]
```

Named Arguments

-p, --port The port to serve DP-GUI on.

Default: 6042

--bind_all Serve on all public interfaces. This will expose your DP-GUI instance to the network on both IPv4 and IPv6 (where available).

Default: False

CHAPTER

THREE

CODE STRUCTURE

Let's look at the home page of DP-GEN. https://github.com/deepmodeling/dpgen

```
├── build
├── CITATION.cff
├── conda
├── dist
├── doc
├── dpgen
├── dpgen.egg-info
├── examples
├── LICENSE
├── README.md
├── requirements.txt
├── setup.py
└── tests
```

- `tests` : unittest tools for developers.
- `examples`: templates for PARAM and MACHINE files for different software, versions and tasks. For details of the parameters in PARAM, you can refer to `TASK parameters` chapters in this document. If you are confused about how to set up a JSON file, you can also use dpgui

Most of the code related to DP-GEN functions is in the `dpgen` directory. Open the `dpgen` directory, and we can see

```
├── arginfo.py
├── auto_test
├── collect
├── data
├── database
├── _date.py
├── dispatcher
├── generator
├── __init__.py
├── main.py
├── __pycache__
├── remote
├── simplify
├── tools
├── util.py
└── _version.py
```

- `auto_test` corresponds to `dpgen autotest`, for undertaking materials property analysis.

- `collect` corresponds to `dpgen collect`.
- `data` corresponds to `dpgen init_bulk`, `dpgen init_surf` and `dpgen init_reaction`, for preparing initial data of bulk and surf systems.
- `database` is the source code for collecting data generated by DP-GEN and interface with database.
- `simplify` corresponds to `dpgen simplify`.
- `remote` and `dispatcher` : source code for automatically submiting scripts,maintaining job queues and collecting results. **Notice this part hase been integrated into dpdispatcher** `generator` is the core part of DP-GEN. It's for main process of deep generator. Let's open this folder.

```
├── arginfo.py
├── ch4
├── __init__.py
├── lib
└── run.py
```

`run.py` is the core of DP-GEN, corresponding to `dpgen run`. We can find `make_train`, `run_train`, ... `post_fp`, and other steps related functions here.

CHAPTER

FOUR

RUN

4.1 Overview of the Run process

The run process contains a series of successive iterations, undertaken in order such as heating the system to certain temperatures. Each iteration is composed of three steps: exploration, labeling, and training. Accordingly, there are three sub-folders: 00.train, 01.model_devi, and 02.fp in each iteration.

00.train: DP-GEN will train several (default 4) models based on initial and generated data. The only difference between these models is the random seed for neural network initialization.

01.model_devi : represent for model-deviation. DP-GEN will use models obtained from 00.train to run Molecular Dynamics(default LAMMPS). Larger deviation for structure properties (default is the force of atoms) means less accuracy of the models. Using this criterion, a few structures will be selected and put into the next stage 02.fp for more accurate calculation based on First Principles.

02.fp : Selected structures will be calculated by first-principles methods(default VASP). DP-GEN will obtain some new data and put them together with initial data and data generated in previous iterations. After that, new training will be set up and DP-GEN will enter the next iteration!

In the run process of the DP-GEN, we need to specify the basic information about the system, the initial data, and details of the training, exploration, and labeling tasks. In addition, we need to specify the software, machine environment, and computing resource and enable the process of job generation, submission, query, and collection automatically. We can perform the run process as we expect by specifying the keywords in param.json and machine.json, and they will be introduced in detail in the following sections.

Here, we give a general description of the run process. We can execute the run process of DP-GEN easily by:

```
dpgen run param.json machine.json
```

The following files or folders will be created and upgraded by codes

- iter.00000x contains the main results that DP-GEN generates in the first iteration.
- record.dpgen records the current stage of the run process.
- dpgen.log includes time and iteration information.

When the first iteration is completed, the folder structure of iter.000000 is like this:

```
$ ls iter.000000
00.train 01.model_devi 02.fp
```

In folder iter.000000/ 00.train:

- Folder 00x contains the input and output files of the DeePMD-kit, in which a model is trained.

- graph.00x.pb is the model DeePMD-kit generates. The only difference between these models is the random seed for neural network initialization.

In folder iter.000000/ 01.model_devi

- Folder confs contains the initial configurations for LAMMPS MD converted from POSCAR you set in *sys_configs* of param.json.
- Folder task.000.00000x contains the input and output files of the LAMMPS. In folder task.000.00000x, file model_devi.out records the model deviation of concerned labels, energy and force in MD. It serves as the criterion for selecting which structures and doing first-principle calculations.

In folder iter.000000/ 02.fp

- candidate.shuffle.000.out records which structures will be selected from last step 01.model_devi. There are always far more candidates than the maximum you expect to calculate at one time. In this condition, DP-GEN will randomly choose up to *fp_task_max* structures and form the folder task.*.
- rest_accurate.shuffle.000.out records the other structures where our model is accurate (`max_devi_f` is less than *model_devi_f_trust_lo*, no need to calculate any more),
- rest_failed.shuffled.000.out records the other structures where our model is too inaccurate (larger than *model_devi_f_trust_hi*, there may be some error).
- data.000: After first-principle calculations, DP-GEN will collect these data and change them into the format DeePMD-kit needs. In the next iteration's 00.train, these data will be trained together as well as the initial data.

DP-GEN identifies the stage of the run process by a record file, record.dpgen, which will be created and upgraded by codes. Each line contains two numbers: the first is the index of iteration, and the second, ranging from 0 to 9, records which stage in each iteration is currently running.

Index of iterations	Stage in eachiteration	Process
0	0	make_train
0	1	run_train
0	2	post_train
0	3	make_model_devi
0	4	run_model_devi
0	5	post_model_devi
0	6	make_fp
0	7	run_fp
0	8	post_fp

0,1,2 correspond to make_train, run_train, post_train. DP-GEN will write scripts in make_train, run the task by specific machine in run_train and collect result in post_train. The records for model_devi and fp stage follow similar rules.

If the process of DP-GEN stops for some reasons, DP-GEN will automatically recover the main process by record.dpgen. You may also change it manually for your purpose, such as removing the last iterations and recovering from one checkpoint. When re-running dpgen, the process will start from the stage that the last line record.

4.2 Example-of-param.json

We have provided different examples of param.json in dpgen/examples/run/. In this section, we give a description of the param.json, taking dpgen/examples/run/dp2.x-lammps-vasp/param_CH4_deepmd-kit-2.0.1.json as an example. This is a param.json for a gas-phase methane molecule. Here, DeePMD-kit (v2.x), LAMMPS and VASP codes are used for training, exploration and labeling respectively.

4.2.1 basics

The basics related keys in param.json are given as follows

```
"type_map": [
  "H",
  "C"
],
"mass_map": [
  1,
  12
],
```

The basics related keys specify the basic information about the system. *type_map* gives the atom types, i.e. "H" and "C". *mass_map* gives the standard atom weights, i.e. "1" and "12".

4.2.2 data

The data related keys in param.json are given as follows

```
"init_data_prefix": "....../init/",
"init_data_sys": [
  "CH4.POSCAR.01x01x01/02.md/sys-0004-0001/deepmd"
],

"sys_configs_prefix": "....../init/",
"sys_configs": [
  [
    "CH4.POSCAR.01x01x01/01.scale_pert/sys-0004-0001/scale*/00000*/POSCAR"
  ],
  [
    "CH4.POSCAR.01x01x01/01.scale_pert/sys-0004-0001/scale*/00001*/POSCAR"
  ]
],
```

The data related keys specify the init data for training initial DP models and structures used for model_devi calculations. *init_data_prefix* and *init_data_sys* specify the location of the init data. *sys_configs_prefix* and *sys_configs* specify the location of the structures.

Here, the init data is provided at "..... /init/CH4.POSCAR.01x01x01/02.md/sys-0004-0001/deepmd". These structures are divided into two groups and provided at ".....init/CH4.POSCAR.01x01x01/01.scale_pert/sys-0004-0001/scale*/00000*/POSCAR" and ".....init/CH4.POSCAR.01x01x01/01.scale_pert/sys-0004-0001/scale*/00001*/POSCAR".

4.2.3 training

The training related keys in param.json are given as follows

```
"numb_models": 4,
"default_training_param": {
},
```

The training related keys specify the details of training tasks. *numb_models* specifies the number of models to be trained. "default_training_param" specifies the training parameters for `deepmd-kit`.

Here, 4 DP models will be trained in `00.train`. A detailed explanation of training parameters can be found in DeePMD-kit's documentation (https://docs.deepmodeling.com/projects/deepmd/en/master/).

4.2.4 exploration

The exploration related keys in param.json are given as follows

```
"model_devi_dt": 0.002,
"model_devi_skip": 0,
"model_devi_f_trust_lo": 0.05,
"model_devi_f_trust_hi": 0.15,
"model_devi_clean_traj": true,
"model_devi_jobs": [
  {
    "sys_idx": [
      0
    ],
    "temps": [
      100
    ],
    "press": [
      1.0
    ],
    "trj_freq": 10,
    "nsteps": 300,
    "ensemble": "nvt",
    "_idx": "00"
  },
  {
    "sys_idx": [
      1
    ],
    "temps": [
      100
    ],
    "press": [
      1.0
    ],
    "trj_freq": 10,
    "nsteps": 3000,
    "ensemble": "nvt",
    "_idx": "01"
```

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```
    }
  ],
```

The exploration related keys specify the details of exploration tasks. *model_devi_dt* specifies timestep for MD simulation. *model_devi_skip* specifies the number of structures skipped for saving in each MD. *model_devi_f_trust_lo* and *model_devi_f_trust_hi* specify the lower and upper bound of model_devi of forces for the selection. *model_devi_clean_traj* specifies whether to clean traj folders in MD. If type of model_devi_clean_traj is boolean type then it denote whether to clean traj folders in MD since they are too large. In *model_devi_jobs*, *sys_idx* specifies the group of structures used for model_devi calculations, *temps* specifies the temperature (K) in MD, *press* specifies the pressure (Bar) in MD, *trj_freq* specifies the frequency of trajectory saved in MD, *nsteps* specifies the running steps of MD, *ensemble* specifies the ensemble used in MD, and "_idx" specifies the index of iteration.

Here, MD simulations are performed at the temperature of 100 K and the pressure of 1.0 Bar with an integrator time of 2 fs under the nvt ensemble. Two iterations are set in *model_devi_jobs*. MD simulations are run for 300 and 3000 time steps with the first and second groups of structures in *sys_configs* in 00 and 01 iterations. We choose to save all structures generated in MD simulations and have set *trj_freq* as 10, so 30 and 300 structures are saved in 00 and 01 iterations. If the "max_devi_f" of saved structure falls between 0.05 and 0.15, DP-GEN will treat the structure as a candidate. We choose to clean traj folders in MD since they are too large. If you want to save the most recent n iterations of traj folders, you can set *model_devi_clean_traj* to be an integer.

4.2.5 labeling

The labeling related keys in param.json are given as follows

```
  "fp_style": "vasp",
  "shuffle_poscar": false,
  "fp_task_max": 20,
  "fp_task_min": 1,
  "fp_pp_path": "....../methane/",
  "fp_pp_files": [
    "POTCAR"
  ],
  "fp_incar": "....../INCAR_methane"
```

The labeling related keys specify the details of labeling tasks. *fp_style* specifies software for First Principles. *fp_task_max* and *fp_task_min* specify the minimum and maximum of structures to be calculated in `02.fp` of each iteration. *fp_pp_path* and *fp_pp_files* specify the location of the psuedo-potential file to be used for 02.fp. *run_jdata[fp_style=vasp]/fp_incar* specifies input file for VASP. INCAR must specify KSPACING and KGAMMA.

Here, a minimum of 1 and a maximum of 20 structures will be labeled using the VASP code with the INCAR provided at "....../INCAR_methane" and POTCAR provided at "....../methane/POTCAR" in each iteration. Note that the order of elements in POTCAR should correspond to the order in *type_map*.

All the keys of the DP-GEN are explained in detail in the section Parameters.

4.3 Example of machine.json

4.3.1 DPDispatcher Update Note

DPDispatcher has updated and the api of machine.json is changed. DP-GEN will use the new DPDispatcher if the value of key *api_version* in machine.json is equal to or large than 1.0. And for now, DPDispatcher is maintained on a separate repo (https://github.com/deepmodeling/dpdispatcher). Please check the documents (https://deepmd.readthedocs.io/projects/dpdispatcher/en/latest/) for more information about the new DPDispatcher.

DP-GEN will use the old DPDispatcher if the key *api_version* is not specified in machine.json or the *api_version* is smaller than 1.0. This gurantees that the old machine.json still works.

4.3.2 New DPDispatcher

Each iteration in the run process of DP-GEN is composed of three steps: exploration, labeling, and training. Accordingly, machine.json is composed of three parts: train, model_devi, and fp. Each part is a list of dicts. Each dict can be considered as an independent environment for calculation.

In this section, we will show you how to perform train task at a local workstation, model_devi task at a local Slurm cluster, and fp task at a remote PBS cluster using the new DPDispatcher. For each task, three types of keys are needed:

- Command: provides the command used to execute each step.
- Machine: specifies the machine environment (local workstation, local or remote cluster, or cloud server).
- Resources: specify the number of groups, nodes, CPU, and GPU; enable the virtual environment.

Performing train task at a local workstation

In this example, we perform the `train` task on a local workstation.

```
"train":
    {
      "command": "dp",
      "machine": {
        "batch_type": "Shell",
        "context_type": "local",
        "local_root": "./",
        "remote_root": "/home/user1234/work_path"
      },
      "resources": {
        "number_node": 1,
        "cpu_per_node": 4,
        "gpu_per_node": 1,
        "group_size": 1,
        "source_list": ["/home/user1234/deepmd.env"]
      }
    },
```

The *command* for the train task in the DeePMD-kit is "dp".

In machine parameters, *batch_type* specifies the type of job scheduling system. If there is no job scheduling system, we can use the "Shell" to perform the task. *context_type* specifies the method of data transfer, and "local" means copying and moving data via local file storage systems (e.g. cp, mv, etc.). In DP-GEN, the paths of all tasks are

automatically located and set by the software, and therefore *local_root* is always set to "./". The input file for each task will be sent to the *remote_root* and the task will be performed there, so we need to make sure that the path exists.

In the resources parameter, *number_node*, *cpu_per_node*, and *gpu_per_node* specify the number of nodes, the number of CPUs, and the number of GPUs required for a task respectively. *group_size*, which needs to be highlighted, specifies how many tasks will be packed into a group. In the training tasks, we need to train 4 models. If we only have one GPU, we can set the *group_size* to 4. If *group_size* is set to 1, 4 models will be trained on one GPU at the same time, as there is no job scheduling system. Finally, the environment variables can be activated by *source_list*. In this example, "source /home/user1234/deepmd.env" is executed before "dp" to load the environment variables necessary to perform the training task.

Perform model_devi task at a local Slurm cluster

In this example, we perform the model_devi task at a local Slurm workstation.

```
"model_devi":
    {
      "command": "lmp",
      "machine": {
       "context_type": "local",
        "batch_type": "Slurm",
        "local_root": "./",
        "remote_root": "/home/user1234/work_path"
      },
      "resources": {
        "number_node": 1,
        "cpu_per_node": 4,
        "gpu_per_node": 1,
        "queue_name": "QueueGPU",
        "custom_flags" : ["#SBATCH --mem=32G"],
        "group_size": 10,
        "source_list": ["/home/user1234/lammps.env"]
      }
    }
```

The *command* for the model_devi task in the LAMMPS is "lmp".

In the machine parameter, we specify the type of job scheduling system by changing the *batch_type* to "Slurm".

In the resources parameter, we specify the name of the queue to which the task is submitted by adding *queue_name*. We can add additional lines to the calculation script via the *custom_flags*. In the model_devi steps, there are frequently many short tasks, so we usually pack multiple tasks (e.g. 10) into a group for submission. Other parameters are similar to that of the local workstation.

Perform fp task in a remote PBS cluster

In this example, we perform the fp task at a remote PBS cluster that can be accessed via SSH.

```
"fp":
    {
      "command": "mpirun -n 32 vasp_std",
      "machine": {
       "context_type": "SSHContext",
        "batch_type": "PBS",
```

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```
        "local_root": "./",
        "remote_root": "/home/user1234/work_path",
        "remote_profile": {
          "hostname": "39.xxx.xx.xx",
          "username": "user1234"
         }
      },
      "resources": {
        "number_node": 1,
        "cpu_per_node": 32,
        "gpu_per_node": 0,
        "queue_name": "QueueCPU",
        "group_size": 5,
        "source_list": ["/home/user1234/vasp.env"]
      }
    }
```

VASP code is used for fp task and mpi is used for parallel computing, so "mpirun -n 32" is added to specify the number of parallel threads.

In the machine parameter, *context_type* is modified to "SSHContext" and *batch_type* is modified to "PBS". It is worth noting that *remote_root* should be set to an accessible path on the remote PBS cluster. *remote_profile* is added to specify the information used to connect the remote cluster, including hostname, username, port, etc.

In the resources parameter, we set *gpu_per_node* to 0 since it is cost-effective to use the CPU for VASP calculations.

Explicit descriptions of keys in machine.json will be given in the following section.

4.4 dpgen run param parameters

Note: One can load, modify, and export the input file by using our effective web-based tool DP-GUI online or hosted using the *command line interface* `dpgen gui`. All parameters below can be set in DP-GUI. By clicking "SAVE JSON", one can download the input file.

run_jdata:

type: `dict`
argument path: `run_jdata`

param.json file

type_map:

type: `list[str]`
argument path: `run_jdata/type_map`

Atom types. Reminder: The elements in param.json, type.raw and data.lmp(when using lammps) should be in the same order.

mass_map:

type: `str | list[float]`, optional, default: `auto`
argument path: `run_jdata/mass_map`

Standard atomic weights (default: "auto"). if one want to use isotopes, or non-standard element names, chemical symbols, or atomic number in the type_map list, please customize the mass_map list instead of using "auto".

use_ele_temp:

type: `int`, optional, default: `0`

argument path: `run_jdata/use_ele_temp`

Currently only support fp_style vasp.
- 0: no electron temperature.
- 1: eletron temperature as frame parameter.
- 2: electron temperature as atom parameter.

init_data_prefix:

type: `str`, optional

argument path: `run_jdata/init_data_prefix`

Prefix of initial data directories.

init_data_sys:

type: `list[str]`

argument path: `run_jdata/init_data_sys`

Paths of initial data. The path can be either a system diretory containing NumPy files or an HDF5 file. You may use either absolute or relative path here. Systems will be detected recursively in the directories or the HDF5 file.

sys_format:

type: `str`, optional, default: `vasp/poscar`

argument path: `run_jdata/sys_format`

Format of sys_configs.

init_batch_size:

type: `list[typing.Union[int, str]] | str`, optional

argument path: `run_jdata/init_batch_size`

Each number is the batch_size of corresponding system for training in init_data_sys. One recommended rule for setting the sys_batch_size and init_batch_size is that batch_size mutiply number of atoms ot the stucture should be larger than 32. If set to auto, batch size will be 32 divided by number of atoms. This argument will not override the mixed batch size in *default_training_param*.

sys_configs_prefix:

type: `str`, optional

argument path: `run_jdata/sys_configs_prefix`

Prefix of sys_configs.

sys_configs:

type: `list[list[str]]`

argument path: `run_jdata/sys_configs`

2D list. Containing directories of structures to be explored in iterations for each system. Wildcard characters are supported here.

sys_batch_size:

type: `list[typing.Union[int, str]]`, optional

argument path: `run_jdata/sys_batch_size`

Each number is the batch_size for training of corresponding system in sys_configs. If set to auto, batch size will be 32 divided by number of atoms. This argument will not override the mixed batch size in *default_training_param*.

numb_models:

type: `int`

argument path: `run_jdata/numb_models`

Number of models to be trained in 00.train. 4 is recommend.

training_iter0_model_path:

type: `list[str]`, optional

argument path: `run_jdata/training_iter0_model_path`

The model used to init the first iter training. Number of element should be equal to numb_models.

training_init_model:

type: `bool`, optional

argument path: `run_jdata/training_init_model`

Iteration > 0, the model parameters will be initilized from the model trained at the previous iteration. Iteration == 0, the model parameters will be initialized from training_iter0_model_path.

default_training_param:

type: `dict`

argument path: `run_jdata/default_training_param`

Training parameters for deepmd-kit in 00.train. You can find instructions from DeePMD-kit documentation.

dp_train_skip_neighbor_stat:

type: `bool`, optional, default: `False`

argument path: `run_jdata/dp_train_skip_neighbor_stat`

Append –skip-neighbor-stat flag to dp train.

dp_compress:

type: `bool`, optional, default: `False`

argument path: `run_jdata/dp_compress`

Use dp compress to compress the model.

training_reuse_iter:

type: `int` | `NoneType`, optional

argument path: `run_jdata/training_reuse_iter`

The minimal index of iteration that continues training models from old models of last iteration.

training_reuse_old_ratio:

type: `str` | `float`, optional, default: `auto`

argument path: `run_jdata/training_reuse_old_ratio`

The probability proportion of old data during training. It can be:
- float: directly assign the probability of old data;

- *auto:f*: automatic probability, where f is the new-to-old ratio;
- *auto*: equivalent to *auto:10*.

This option is only adopted when continuing training models from old models. This option will override default parameters.

training_reuse_numb_steps:

type: int | NoneType, optional, default: None, alias: *training_reuse_stop_batch*
argument path: run_jdata/training_reuse_numb_steps

Number of training batch. This option is only adopted when continuing training models from old models. This option will override default parameters.

training_reuse_start_lr:

type: float | NoneType, optional, default: None
argument path: run_jdata/training_reuse_start_lr

The learning rate the start of the training. This option is only adopted when continuing training models from old models. This option will override default parameters.

training_reuse_start_pref_e:

type: int | float | NoneType, optional, default: None
argument path: run_jdata/training_reuse_start_pref_e

The prefactor of energy loss at the start of the training. This option is only adopted when continuing training models from old models. This option will override default parameters.

training_reuse_start_pref_f:

type: int | float | NoneType, optional, default: None
argument path: run_jdata/training_reuse_start_pref_f

The prefactor of force loss at the start of the training. This option is only adopted when continuing training models from old models. This option will override default parameters.

model_devi_activation_func:

type: list[list[str]] | NoneType, optional
argument path: run_jdata/model_devi_activation_func

The activation function in the model. The shape of list should be (N_models, 2), where 2 represents the embedding and fitting network. This option will override default parameters.

srtab_file_path:

type: str, optional
argument path: run_jdata/srtab_file_path

The path of the table for the short-range pairwise interaction which is needed when using DP-ZBL potential

one_h5:

type: bool, optional, default: False
argument path: run_jdata/one_h5

When using DeePMD-kit, all of the input data will be merged into one HDF5 file.

training_init_frozen_model:

type: list[str], optional

argument path: run_jdata/training_init_frozen_model

At interation 0, initilize the model parameters from the given frozen models. Number of element should be equal to numb_models.

training_finetune_model:

type: list[str], optional

argument path: run_jdata/training_finetune_model

At interation 0, finetune the model parameters from the given frozen models. Number of element should be equal to numb_models.

fp_task_max:

type: int

argument path: run_jdata/fp_task_max

Maximum number of structures to be calculated in each system in 02.fp of each iteration. If the number of candidate structures exceeds *fp_task_max*, *fp_task_max* structures will be randomly picked from the candidates and labeled.

fp_task_min:

type: int

argument path: run_jdata/fp_task_min

Skip the training in the next iteration if the number of structures is no more than *fp_task_min*.

fp_accurate_threshold:

type: float, optional

argument path: run_jdata/fp_accurate_threshold

If the accurate ratio is larger than this number, no fp calculation will be performed, i.e. fp_task_max = 0.

fp_accurate_soft_threshold:

type: float, optional

argument path: run_jdata/fp_accurate_soft_threshold

If the accurate ratio is between this number and fp_accurate_threshold, the fp_task_max linearly decays to zero.

fp_cluster_vacuum:

type: float, optional

argument path: run_jdata/fp_cluster_vacuum

If the vacuum size is smaller than this value, this cluster will not be chosen for labeling.

detailed_report_make_fp:

type: bool, optional, default: True

argument path: run_jdata/detailed_report_make_fp

If set to true, a detailed report will be generated for each iteration.

ratio_failed:

type: float, optional

argument path: `run_jdata/ratio_failed`

Check the ratio of unsuccessfully terminated jobs. If too many FP tasks are not converged, RuntimeError will be raised.

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

model_devi_engine:

type: `str` (flag key), default: `lammps`

argument path: `run_jdata/model_devi_engine`

possible choices: *lammps*, *amber*, *calypso*, *gromacs*

Engine for the model deviation task.

When model_devi_engine is set to `lammps`:

LAMMPS

model_devi_jobs:

type: `list`

argument path: `run_jdata[model_devi_engine=lammps]/model_devi_jobs`

Settings for exploration in 01.model_devi. Each dict in the list corresponds to one iteration. The index of model_devi_jobs exactly accord with index of iterations

This argument takes a list with each element containing the following:

template:

type: `dict`, optional

argument path: `run_jdata[model_devi_engine=lammps]/model_devi_jobs/template`

Give an input file template for the supported engine software adopted in 01.model_devi. Through user-defined template, any freedom (function) that is permitted by the engine software could be inherited (invoked) in the workflow.

lmp:

type: `str`, optional

argument path: `run_jdata[model_devi_engine=lammps]/model_devi_jobs/template/lmp`

The path to input.lammps template. Instructions can be found in LAMMPS documentation.

plm:

type: `str`, optional

argument path: `run_jdata[model_devi_engine=lammps]/model_devi_jobs/template/plm`

The path to input.plumed template. Instructions can be found in PLUMED documentation.

rev_mat:

type: `dict`, optional

argument path: `run_jdata[model_devi_engine=lammps]/model_devi_jobs/rev_mat`

revise matrix for revising variable(s) defined in the template into the specific values (iteration-resolved). Values will be broadcasted for all tasks within the iteration invoking this key.

lmp:

type: dict, optional

argument path: run_jdata[model_devi_engine=lammps]/model_devi_jobs/rev_mat/lmp

revise matrix for revising variable(s) defined in the lammps template into the specific values (iteration-resolved).

plm:

type: dict, optional

argument path: run_jdata[model_devi_engine=lammps]/model_devi_jobs/rev_mat/plm

revise matrix for revising variable(s) defined in the plumed template into specific values(iteration-resolved)

sys_rev_mat:

type: dict, optional

argument path: run_jdata[model_devi_engine=lammps]/model_devi_jobs/sys_rev_mat

system-resolved revise matrix for revising variable(s) defined in the template into specific values. Values should be individually assigned to each system adopted by this iteration, through a dictionary where first-level keys are values of sys_idx of this iteration.

sys_idx:

type: list[int]

argument path: run_jdata[model_devi_engine=lammps]/model_devi_jobs/sys_idx

Systems to be selected as the initial structure of MD and be explored. The index corresponds exactly to the sys_configs.

temps:

type: list[float], optional

argument path: run_jdata[model_devi_engine=lammps]/model_devi_jobs/temps

Temperature (K) in MD.

press:

type: list[float], optional

argument path: run_jdata[model_devi_engine=lammps]/model_devi_jobs/press

Pressure (Bar) in MD. Required when ensemble is npt.

trj_freq:

type: int

argument path: run_jdata[model_devi_engine=lammps]/model_devi_jobs/trj_freq

Frequecy of trajectory saved in MD.

nsteps:

type: int, optional

argument path: run_jdata[model_devi_engine=lammps]/model_devi_jobs/nsteps

Running steps of MD. It is not optional when not using a template.

nbeads:

type: int, optional

argument path: run_jdata[model_devi_engine=lammps]/model_devi_jobs/nbeads

Number of beads in PIMD. If not given, classical MD will be performed. Only supported for LAMMPS version >= 20230615.

ensemble:

type: str, optional

argument path: run_jdata[model_devi_engine=lammps]/model_devi_jobs/ensemble

Determining which ensemble used in MD, options include "npt" and "nvt". It is not optional when not using a template.

neidelay:

type: int, optional

argument path: run_jdata[model_devi_engine=lammps]/model_devi_jobs/neidelay

delay building until this many steps since last build.

taut:

type: float, optional

argument path: run_jdata[model_devi_engine=lammps]/model_devi_jobs/taut

Coupling time of thermostat (ps).

taup:

type: float, optional

argument path: run_jdata[model_devi_engine=lammps]/model_devi_jobs/taup

Coupling time of barostat (ps).

model_devi_f_trust_lo:

type: dict | float, optional

argument path: run_jdata[model_devi_engine=lammps]/model_devi_jobs/model_devi_f_trust_lo

Lower bound of forces for the selection. If dict, should be set for each index in sys_idx, respectively.

model_devi_f_trust_hi:

type: dict | float, optional

argument path: run_jdata[model_devi_engine=lammps]/model_devi_jobs/model_devi_f_trust_hi

Upper bound of forces for the selection. If dict, should be set for each index in sys_idx, respectively.

model_devi_v_trust_lo:

type: dict | float, optional

argument path: run_jdata[model_devi_engine=lammps]/model_devi_jobs/model_devi_v_trust_lo

Lower bound of virial for the selection. If dict, should be set for each index in sys_idx, respectively. Should be used with DeePMD-kit v2.x.

model_devi_v_trust_hi:

type: dict | float, optional

argument path: run_jdata[model_devi_engine=lammps]/model_devi_jobs/model_devi_v_trust_hi

Upper bound of virial for the selection. If dict, should be set for each index in sys_idx, respectively. Should be used with DeePMD-kit v2.x.

model_devi_dt:

type: float

argument path: run_jdata[model_devi_engine=lammps]/model_devi_dt

Timestep for MD. 0.002 is recommend.

model_devi_skip:

type: int

argument path: run_jdata[model_devi_engine=lammps]/model_devi_skip

Number of structures skipped for fp in each MD.

model_devi_f_trust_lo:

type: dict | list[float] | float

argument path: run_jdata[model_devi_engine=lammps]/model_devi_f_trust_lo

Lower bound of forces for the selection. If list or dict, should be set for each index in sys_configs, respectively.

model_devi_f_trust_hi:

type: dict | list[float] | float

argument path: run_jdata[model_devi_engine=lammps]/model_devi_f_trust_hi

Upper bound of forces for the selection. If list or dict, should be set for each index in sys_configs, respectively.

model_devi_v_trust_lo:

type: dict | list[float] | float, optional, default: 10000000000.0
argument path:
run_jdata[model_devi_engine=lammps]/model_devi_v_trust_lo

Lower bound of virial for the selection. If list or dict, should be set for each index in sys_configs, respectively. Should be used with DeePMD-kit v2.x.

model_devi_v_trust_hi:

type: dict | list[float] | float, optional, default: 10000000000.0
argument path:
run_jdata[model_devi_engine=lammps]/model_devi_v_trust_hi

Upper bound of virial for the selection. If list or dict, should be set for each index in sys_configs, respectively. Should be used with DeePMD-kit v2.x.

model_devi_adapt_trust_lo:

type: bool, optional
argument path:
run_jdata[model_devi_engine=lammps]/model_devi_adapt_trust_lo

Adaptively determines the lower trust levels of force and virial. This option should be used together with model_devi_numb_candi_f, model_devi_numb_candi_v and optionally with model_devi_perc_candi_f and model_devi_perc_candi_v. dpgen will make two sets:

- 1. From the frames with force model deviation lower than model_devi_f_trust_hi, select max(model_devi_numb_candi_f, model_devi_perc_candi_f*n_frames) frames with largest force model deviation.
- 2. From the frames with virial model deviation lower than model_devi_v_trust_hi, select max(model_devi_numb_candi_v, model_devi_perc_candi_v*n_frames) frames with largest virial model deviation.

The union of the two sets is made as candidate dataset.

model_devi_numb_candi_f:

type: int, optional
argument path:
run_jdata[model_devi_engine=lammps]/model_devi_numb_candi_f

See model_devi_adapt_trust_lo.

model_devi_numb_candi_v:

type: int, optional
argument path:
run_jdata[model_devi_engine=lammps]/model_devi_numb_candi_v

See model_devi_adapt_trust_lo.

model_devi_perc_candi_f:

type: float, optional

argument path:
run_jdata[model_devi_engine=lammps]/model_devi_perc_candi_f

See model_devi_adapt_trust_lo.

model_devi_perc_candi_v:

type: float, optional
argument path:
run_jdata[model_devi_engine=lammps]/model_devi_perc_candi_v

See model_devi_adapt_trust_lo.

model_devi_f_avg_relative:

type: bool, optional
argument path:
run_jdata[model_devi_engine=lammps]/model_devi_f_avg_relative

Normalized the force model deviations by the RMS force magnitude along the trajectory. This key should not be used with use_relative.

model_devi_clean_traj:

type: bool | int, optional, default: True
argument path:
run_jdata[model_devi_engine=lammps]/model_devi_clean_traj

If type of model_devi_clean_traj is bool type then it denote whether to clean traj folders in MD since they are too large. If it is Int type, then the most recent n iterations of traj folders will be retained, others will be removed.

model_devi_merge_traj:

type: bool, optional, default: False
argument path:
run_jdata[model_devi_engine=lammps]/model_devi_merge_traj

If model_devi_merge_traj is set as True, only all.lammpstrj will be generated, instead of lots of small traj files.

model_devi_nopbc:

type: bool, optional, default: False
argument path:
run_jdata[model_devi_engine=lammps]/model_devi_nopbc

Assume open boundary condition in MD simulations.

model_devi_plumed:

type: bool, optional, default: False
argument path:
run_jdata[model_devi_engine=lammps]/model_devi_plumed

model_devi_plumed_path:

type: bool, optional, default: False
argument path:
run_jdata[model_devi_engine=lammps]/model_devi_plumed_path

shuffle_poscar:

type: bool, optional, default: False
argument path: run_jdata[model_devi_engine=lammps]/shuffle_poscar

Shuffle atoms of each frame before running simulations. The purpose is to sample the element occupation of alloys.

use_relative:

type: bool, optional, default: False
argument path: run_jdata[model_devi_engine=lammps]/use_relative

Calculate relative force model deviation.

epsilon:

type: float, optional
argument path: run_jdata[model_devi_engine=lammps]/epsilon

The level parameter for computing the relative force model deviation.

use_relative_v:

type: bool, optional, default: False
argument path: run_jdata[model_devi_engine=lammps]/use_relative_v

Calculate relative virial model deviation.

epsilon_v:

type: float, optional
argument path: run_jdata[model_devi_engine=lammps]/epsilon_v

The level parameter for computing the relative virial model deviation.

When model_devi_engine is set to amber:

Amber DPRc engine. The command argument in the machine file should be path to sander.

model_devi_jobs:

type: list
argument path: run_jdata[model_devi_engine=amber]/model_devi_jobs

List of dicts. The list including the dict for information of each cycle.

This argument takes a list with each element containing the following:

sys_idx:

type: list[int]
argument path: run_jdata[model_devi_engine=amber]/model_devi_jobs/sys_idx

List of ints. List of systems to run.

trj_freq:

type: int
argument path: run_jdata[model_devi_engine=amber]/model_devi_jobs/trj_freq

Frequency to dump trajectory.

restart_from_iter:

type: int, optional
argument path: run_jdata[model_devi_engine=amber]/model_devi_jobs/restart_from_iter

The iteration index to restart the simulation from. If not given, the simulation is restarted from *sys_configs*.

low_level:

type: str
argument path: run_jdata[model_devi_engine=amber]/low_level

Low level method. The value will be filled into mdin file as @qm_theory@.

cutoff:

type: float
argument path: run_jdata[model_devi_engine=amber]/cutoff

Cutoff radius for the DPRc model.

parm7_prefix:

type: str, optional
argument path: run_jdata[model_devi_engine=amber]/parm7_prefix

The path prefix to AMBER PARM7 files.

parm7:

type: list[str]
argument path: run_jdata[model_devi_engine=amber]/parm7

List of paths to AMBER PARM7 files. Each file maps to a system.

mdin_prefix:

type: str, optional
argument path: run_jdata[model_devi_engine=amber]/mdin_prefix

The path prefix to AMBER mdin template files.

mdin:

type: list[str]
argument path: run_jdata[model_devi_engine=amber]/mdin

List of paths to AMBER mdin template files. Each files maps to a system. In the template, the following keywords will be replaced by the actual value: @*freq*@: freq to dump trajectory; @*nstlim*@: total time step to run; @*qm_region*@: AMBER mask of the QM region; @*qm_theory*@: The low level QM theory, such as DFTB2; @*qm_charge*@: The total charge of the QM theory, such as -2; @*rcut*@: cutoff radius of the DPRc model; @*GRAPH_FILE0*@, @*GRAPH_FILE1*@, ... : graph files.

qm_region:

type: list[str]
argument path: run_jdata[model_devi_engine=amber]/qm_region

List of strings. AMBER mask of the QM region. Each mask maps to a system.

qm_charge:

type: list[int]
argument path: run_jdata[model_devi_engine=amber]/qm_charge

List of ints. Charge of the QM region. Each charge maps to a system.

nsteps:

type: list[int]
argument path: run_jdata[model_devi_engine=amber]/nsteps

List of ints. The number of steps to run. Each number maps to a system.

r:

type: list[list[typing.Union[float, list[float]]]]
argument path: run_jdata[model_devi_engine=amber]/r

2D or 3D list of floats. Constrict values for the enhanced sampling. The first dimension maps to systems. The second dimension maps to confs in each system. The third dimension is the constrict value. It can be a single float for 1D or list of floats for nD.

disang_prefix:

type: str, optional
argument path: run_jdata[model_devi_engine=amber]/disang_prefix

The path prefix to disang prefix.

disang:

type: list[str]
argument path: run_jdata[model_devi_engine=amber]/disang

List of paths to AMBER disang files. Each file maps to a sytem. The keyword RVAL will be replaced by the constrict values, or RVAL1, RVAL2, … for an nD system.

model_devi_f_trust_lo:

type: dict | list[float] | float
argument path:
run_jdata[model_devi_engine=amber]/model_devi_f_trust_lo

Lower bound of forces for the selection. If dict, should be set for each index in sys_idx, respectively.

model_devi_f_trust_hi:

type: dict | list[float] | float
argument path:
run_jdata[model_devi_engine=amber]/model_devi_f_trust_hi

Upper bound of forces for the selection. If dict, should be set for each index in sys_idx, respectively.

When model_devi_engine is set to calypso:

TODO: add doc

When model_devi_engine is set to gromacs:

TODO: add doc

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

fp_style:

type: str (flag key)
argument path: run_jdata/fp_style
possible choices: *vasp*, *gaussian*, *siesta*, *cp2k*, *abacus*, *amber/diff*, *pwmat*, *pwscf*, *custom*

Software for First Principles.

When fp_style is set to vasp:

fp_pp_path:

type: str
argument path: run_jdata[fp_style=vasp]/fp_pp_path

Directory of psuedo-potential file to be used for 02.fp exists.

fp_pp_files:

type: list[str]
argument path: run_jdata[fp_style=vasp]/fp_pp_files

Psuedo-potential file to be used for 02.fp. Note that the order of elements should correspond to the order in type_map.

fp_incar:

type: str
argument path: run_jdata[fp_style=vasp]/fp_incar

Input file for VASP. INCAR must specify KSPACING and KGAMMA.

fp_aniso_kspacing:

type: list[float], optional
argument path: run_jdata[fp_style=vasp]/fp_aniso_kspacing

Set anisotropic kspacing. Usually useful for 1-D or 2-D materials. Only support VASP. If it is setting the KSPACING key in INCAR will be ignored.

cvasp:

type: bool, optional
argument path: run_jdata[fp_style=vasp]/cvasp

If cvasp is true, DP-GEN will use Custodian to help control VASP calculation.

fp_skip_bad_box:

type: str, optional
argument path: run_jdata[fp_style=vasp]/fp_skip_bad_box

Skip the configurations that are obviously unreasonable before 02.fp

When fp_style is set to gaussian:

use_clusters:

type: bool, optional, default: False
argument path: run_jdata[fp_style=gaussian]/use_clusters

If set to true, clusters will be taken instead of the whole system.

cluster_cutoff:

type: float, optional
argument path: run_jdata[fp_style=gaussian]/cluster_cutoff

The soft cutoff radius of clusters if *use_clusters* is set to true. Molecules will be taken as whole even if part of atoms is out of the cluster. Use *cluster_cutoff_hard* to only take atoms within the hard cutoff radius.

cluster_cutoff_hard:

type: float, optional
argument path: run_jdata[fp_style=gaussian]/cluster_cutoff_hard

The hard cutoff radius of clusters if *use_clusters* is set to true. Outside the hard cutoff radius, atoms will not be taken even if they are in a molecule where some atoms are within the cutoff radius.

cluster_minify:

type: bool, optional, default: False
argument path: run_jdata[fp_style=gaussian]/cluster_minify

If enabled, when an atom within the soft cutoff radius connects a single bond with a non-hydrogen atom out of the soft cutoff radius, the outer atom will be replaced by a hydrogen atom. When the outer atom is a hydrogen atom, the outer atom will be kept. In this case, other atoms out of the soft cutoff radius will be removed.

fp_params:

type: dict
argument path: run_jdata[fp_style=gaussian]/fp_params

Parameters for Gaussian calculation.

keywords:

type: str | list[str]
argument path: run_jdata[fp_style=gaussian]/fp_params/keywords

Keywords for Gaussian input, e.g. force b3lyp/6-31g**. If a list, run multiple steps.

multiplicity:

type: str | int, optional, default: auto
argument path: run_jdata[fp_style=gaussian]/fp_params/multiplicity

Spin multiplicity for Gaussian input. If *auto*, multiplicity will be detected automatically, with the following rules: when fragment_guesses=True, multiplicity will +1 for each radical, and +2 for each oxygen molecule; when fragment_guesses=False, multiplicity will be 1 or 2, but +2 for each oxygen molecule.

nproc:

type: int
argument path: run_jdata[fp_style=gaussian]/fp_params/nproc

The number of processors for Gaussian input.

charge:

type: int, optional, default: 0
argument path: run_jdata[fp_style=gaussian]/fp_params/charge

Molecule charge. Only used when charge is not provided by the system.

fragment_guesses:

type: bool, optional, default: False
argument path: run_jdata[fp_style=gaussian]/fp_params/fragment_guesses

Initial guess generated from fragment guesses. If True, *multiplicity* should be *auto*.

basis_set:

type: str, optional
argument path: run_jdata[fp_style=gaussian]/fp_params/basis_set

Custom basis set.

keywords_high_multiplicity:

type: str, optional
argument path: run_jdata[fp_style=gaussian]/fp_params/keywords_high_multiplicity

Keywords for points with multiple raicals. *multiplicity* should be *auto*. If not set, fallback to normal keywords.

When fp_style is set to siesta:

use_clusters:

type: bool, optional
argument path: run_jdata[fp_style=siesta]/use_clusters

If set to true, clusters will be taken instead of the whole system. This option does not work with DeePMD-kit 0.x.

cluster_cutoff:

type: float, optional
argument path: run_jdata[fp_style=siesta]/cluster_cutoff

The cutoff radius of clusters if use_clusters is set to true.

fp_params:

type: dict
argument path: run_jdata[fp_style=siesta]/fp_params

Parameters for siesta calculation.

ecut:

type: int
argument path: run_jdata[fp_style=siesta]/fp_params/ecut

Define the plane wave cutoff for grid.

ediff:

type: float
argument path: run_jdata[fp_style=siesta]/fp_params/ediff

Tolerance of Density Matrix.

kspacing:

type: float
argument path: run_jdata[fp_style=siesta]/fp_params/kspacing

Sample factor in Brillouin zones.

mixingWeight:

type: float
argument path: run_jdata[fp_style=siesta]/fp_params/mixingWeight

Proportion a of output Density Matrix to be used for the input Density Matrix of next SCF cycle (linear mixing).

NumberPulay:

type: int
argument path: run_jdata[fp_style=siesta]/fp_params/NumberPulay

Controls the Pulay convergence accelerator.

fp_pp_path:

type: str
argument path: run_jdata[fp_style=siesta]/fp_pp_path

Directory of psuedo-potential or numerical orbital files to be used for 02.fp exists.

fp_pp_files:

type: list[str]
argument path: run_jdata[fp_style=siesta]/fp_pp_files

Psuedo-potential file to be used for 02.fp. Note that the order of elements should correspond to the order in type_map.

When fp_style is set to cp2k:

user_fp_params:

type: dict, optional, alias: *fp_params*

argument path: run_jdata[fp_style=cp2k]/user_fp_params

Parameters for cp2k calculation. find detail in manual.cp2k.org. only the kind section must be set before use. we assume that you have basic knowledge for cp2k input.

external_input_path:

type: str, optional

argument path: run_jdata[fp_style=cp2k]/external_input_path

Conflict with key:user_fp_params. enable the template input provided by user. some rules should be followed, read the following text in detail:

1. One must present a KEYWORD ABC in the section CELL so that the DP-GEN can replace the cell on-the-fly.
2. One need to add these lines under FORCE_EVAL section to print forces and stresses:

```
STRESS_TENSOR ANALYTICAL
  &PRINT
    &FORCES ON
    &END FORCES
    &STRESS_TENSOR ON
    &END STRESS_TENSOR
  &END PRINT
```

When fp_style is set to abacus:

fp_pp_path:

type: str

argument path: run_jdata[fp_style=abacus]/fp_pp_path

Directory of psuedo-potential or numerical orbital files to be used for 02.fp exists.

fp_pp_files:

type: list[str]

argument path: run_jdata[fp_style=abacus]/fp_pp_files

Psuedo-potential file to be used for 02.fp. Note that the order of elements should correspond to the order in type_map.

fp_orb_files:

type: list[str], optional

argument path: run_jdata[fp_style=abacus]/fp_orb_files

numerical orbital file to be used for 02.fp when using LCAO basis. Note that the order of elements should correspond to the order in type_map.

fp_incar:

type: str, optional

argument path: `run_jdata[fp_style=abacus]/fp_incar`

Input file for ABACUS. This is optinal but the priority is lower than user_fp_params, and you should not set user_fp_params if you want to use fp_incar.

fp_kpt_file:

type: `str`, optional

argument path: `run_jdata[fp_style=abacus]/fp_kpt_file`

KPT file for ABACUS.If the "kspacing" or "gamma_only=1" is defined in INPUT or "k_points" is defined, fp_kpt_file will be ignored.

fp_dpks_descriptor:

type: `str`, optional

argument path: `run_jdata[fp_style=abacus]/fp_dpks_descriptor`

DeePKS descriptor file name. The file should be in pseudopotential directory.

user_fp_params:

type: `dict`, optional

argument path: `run_jdata[fp_style=abacus]/user_fp_params`

Set the key and value of INPUT.

k_points:

type: `list[int]`, optional

argument path: `run_jdata[fp_style=abacus]/k_points`

Monkhorst-Pack k-grids setting for generating KPT file of ABACUS, such as: [1,1,1,0,0,0]. NB: if "kspacing" or "gamma_only=1" is defined in INPUT, k_points will be ignored.

When fp_style is set to `amber/diff`:

Amber/diff style for DPRc models. Note: this fp style only supports to be used with model_devi_engine *amber*, where some arguments are reused. The command argument in the machine file should be path to sander. One should also install dpamber and make it visible in the PATH.

high_level:

type: `str`

argument path: `run_jdata[fp_style=amber/diff]/high_level`

High level method. The value will be filled into mdin template as @qm_theory@.

fp_params:

type: `dict`

argument path: `run_jdata[fp_style=amber/diff]/fp_params`

Parameters for FP calculation.

high_level_mdin:

type: `str`

argument path: run_jdata[fp_style=amber/diff]/fp_params/high_level_mdin

Path to high-level AMBER mdin template file. %qm_theory%, %qm_region%, and %qm_charge% will be replaced.

low_level_mdin:

type: str
argument path: run_jdata[fp_style=amber/diff]/fp_params/low_level_mdin

Path to low-level AMBER mdin template file. %qm_theory%, %qm_region%, and %qm_charge% will be replaced.

When fp_style is set to pwmat:

TODO: add doc

When fp_style is set to pwscf:

fp_pp_path:

type: str
argument path: run_jdata[fp_style=pwscf]/fp_pp_path

Directory of psuedo-potential file to be used for 02.fp exists.

fp_pp_files:

type: list[str]
argument path: run_jdata[fp_style=pwscf]/fp_pp_files

Psuedo-potential file to be used for 02.fp. Note that the order of elements should correspond to the order in type_map.

fp_params:

type: dict, optional
argument path: run_jdata[fp_style=pwscf]/fp_params

Parameters for pwscf calculation. It has lower priority than user_fp_params.

ecut:

type: float
argument path: run_jdata[fp_style=pwscf]/fp_params/ecut

ecutwfc in pwscf.

ediff:

type: float
argument path: run_jdata[fp_style=pwscf]/fp_params/ediff

conv_thr and ts_vdw_econv_thr in pwscf.

smearing:

type: str

argument path:
`run_jdata[fp_style=pwscf]/fp_params/smearing`

smearing in pwscf.

sigma:

type: `float`
argument path:
`run_jdata[fp_style=pwscf]/fp_params/sigma`

degauss in pwscf.

kspacing:

type: `float`
argument path:
`run_jdata[fp_style=pwscf]/fp_params/kspacing`

The spacing between kpoints. Helps to determin KPOINTS in pwscf.

user_fp_params:

type: `dict`, optional
argument path: `run_jdata[fp_style=pwscf]/user_fp_params`

Parameters for pwscf calculation. Find details at https://www.quantum-espresso.org/Doc/INPUT_PW.html. When user_fp_params is set, the settings in fp_params will be ignored. If one wants to use user_fp_params, kspacing must be set in user_fp_params. kspacing is the spacing between kpoints, and helps to determin KPOINTS in pwscf.

When fp_style is set to `custom`:

Custom FP code. You need to provide the input and output file format and name. The command argument in the machine file should be the script to run custom FP codes. The extra forward and backward files can be defined in the machine file.

fp_params:

type: `dict`
argument path: `run_jdata[fp_style=custom]/fp_params`

Parameters for FP calculation.

input_fmt:

type: `str`
argument path:
`run_jdata[fp_style=custom]/fp_params/input_fmt`

Input dpdata format of the custom FP code. Such format should only need the first argument as the file name.

input_fn:

type: `str`
argument path:
`run_jdata[fp_style=custom]/fp_params/input_fn`

Input file name of the custom FP code.

output_fmt:

type: str
argument path: run_jdata[fp_style=custom]/fp_params/output_fmt

Output dpata format of the custom FP code. Such format should only need the first argument as the file name.

output_fn:

type: str
argument path: run_jdata[fp_style=custom]/fp_params/output_fn

Output file name of the custom FP code.

4.5 dpgen run machine parameters

Note: One can load, modify, and export the input file by using our effective web-based tool DP-GUI online or hosted using the *command line interface* `dpgen gui`. All parameters below can be set in DP-GUI. By clicking "SAVE JSON", one can download the input file.

run_mdata:

type: dict
argument path: run_mdata

machine.json file

api_version:

type: str, optional, default: 1.0
argument path: run_mdata/api_version

Please set to 1.0

deepmd_version:

type: str, optional, default: 2
argument path: run_mdata/deepmd_version

DeePMD-kit version, e.g. 2.1.3

train:

type: dict
argument path: run_mdata/train

Parameters of command, machine, and resources for train

command:

type: str
argument path: run_mdata/train/command

Command of a program.

machine:

type: dict

argument path: run_mdata/train/machine

batch_type:

type: str

argument path: run_mdata/train/machine/batch_type

The batch job system type. Option: Slurm, LSF, DistributedShell, SGE, Shell, SlurmJobArray, PBS, OpenAPI, Torque, Bohrium, Fugaku

local_root:

type: str | NoneType

argument path: run_mdata/train/machine/local_root

The dir where the tasks and relating files locate. Typically the project dir.

remote_root:

type: str | NoneType, optional

argument path: run_mdata/train/machine/remote_root

The dir where the tasks are executed on the remote machine. Only needed when context is not lazy-local.

clean_asynchronously:

type: bool, optional, default: False

argument path: run_mdata/train/machine/clean_asynchronously

Clean the remote directory asynchronously after the job finishes.

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

context_type:

type: str (flag key)

argument path: run_mdata/train/machine/context_type

possible choices: *LocalContext*, *LazyLocalContext*, *BohriumContext*, *HDFSContext*, *OpenAPIContext*, *SSHContext*

The connection used to remote machine. Option: LazyLocalContext, HDFSContext, BohriumContext, SSHContext, LocalContext, OpenAPIContext

When context_type is set to LocalContext (or its aliases localcontext, Local, local):

remote_profile:

type: dict, optional

argument path: run_mdata/train/machine[LocalContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to LazyLocalContext (or its aliases lazylocalcontext, LazyLocal, lazylocal):

remote_profile:

type: dict, optional

argument path: run_mdata/train/machine[LazyLocalContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to BohriumContext (or its aliases bohriumcontext, Bohrium, bohrium, DpCloudServerContext, dpcloudservercontext, DpCloudServer, dpcloudserver, LebesgueContext, lebesguecontext, Lebesgue, lebesgue):

remote_profile:

type: dict

argument path: run_mdata/train/machine[BohriumContext]/remote_profile

The information used to maintain the connection with remote machine.

email:

type: str, optional

argument path: run_mdata/train/machine[BohriumContext]/remote_profile/email

Email

password:

type: str, optional

argument path: run_mdata/train/machine[BohriumContext]/remote_profile/password

Password

program_id:

type: int, alias: *project_id*

argument path: run_mdata/train/machine[BohriumContext]/remote_profile/program_id

Program ID

retry_count:

type: NoneType | int, optional, default: 2

argument path: run_mdata/train/machine[BohriumContext]/remote_profile/retry_count

The retry count when a job is terminated

ignore_exit_code:

type: bool, optional, default: True

argument path: run_mdata/train/machine[BohriumContext]/remote_profile/ignore_exit_code

The job state will be marked as finished if the exit code is non-zero when set to True. Otherwise,
the job state will be designated as terminated.

keep_backup:

type: bool, optional

argument path: run_mdata/train/machine[BohriumContext]/remote_profile/keep_backup

keep download and upload zip

input_data:

type: dict

argument path: run_mdata/train/machine[BohriumContext]/remote_profile/input_data

Configuration of job

When context_type is set to HDFSContext (or its aliases hdfscontext, HDFS, hdfs):

remote_profile:

type: dict, optional

argument path: run_mdata/train/machine[HDFSContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to OpenAPIContext (or its aliases openapicontext, OpenAPI, openapi):

remote_profile:

type: dict, optional

argument path: run_mdata/train/machine[OpenAPIContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to SSHContext (or its aliases sshcontext, SSH, ssh):

remote_profile:

type: dict

argument path: run_mdata/train/machine[SSHContext]/remote_profile

The information used to maintain the connection with remote machine.

hostname:

type: str

argument path: run_mdata/train/machine[SSHContext]/remote_profile/hostname

hostname or ip of ssh connection.

username:

type: str

argument path: run_mdata/train/machine[SSHContext]/remote_profile/username

username of target linux system

password:

type: str, optional

argument path: run_mdata/train/machine[SSHContext]/remote_profile/password

(deprecated) password of linux system. Please use SSH keys instead to improve security.

port:

type: int, optional, default: 22

argument path: run_mdata/train/machine[SSHContext]/remote_profile/port

ssh connection port.

key_filename:

type: str | NoneType, optional, default: None

argument path: run_mdata/train/machine[SSHContext]/remote_profile/key_filename

key filename used by ssh connection. If left None, find key in ~/.ssh or use password for login

passphrase:

type: str | NoneType, optional, default: None

argument path: run_mdata/train/machine[SSHContext]/remote_profile/passphrase

passphrase of key used by ssh connection

timeout:

type: int, optional, default: 10

argument path: run_mdata/train/machine[SSHContext]/remote_profile/timeout

timeout of ssh connection

totp_secret:

type: str | NoneType, optional, default: None

argument path: run_mdata/train/machine[SSHContext]/remote_profile/totp_secret

Time-based one time password secret. It should be a base32-encoded string extracted from the 2D code.

tar_compress:

type: bool, optional, default: True

argument path: run_mdata/train/machine[SSHContext]/remote_profile/tar_compress

The archive will be compressed in upload and download if it is True. If not, compression will be skipped.

look_for_keys:

type: bool, optional, default: True

argument path: run_mdata/train/machine[SSHContext]/remote_profile/look_for_keys

enable searching for discoverable private key files in ~/.ssh/

resources:

type: dict

argument path: run_mdata/train/resources

number_node:

type: int, optional, default: 1

argument path: run_mdata/train/resources/number_node

The number of node need for each *job*

cpu_per_node:

type: int, optional, default: 1
argument path: run_mdata/train/resources/cpu_per_node

cpu numbers of each node assigned to each job.

gpu_per_node:

type: int, optional, default: 0
argument path: run_mdata/train/resources/gpu_per_node

gpu numbers of each node assigned to each job.

queue_name:

type: str, optional, default: (empty string)
argument path: run_mdata/train/resources/queue_name

The queue name of batch job scheduler system.

group_size:

type: int
argument path: run_mdata/train/resources/group_size

The number of *tasks* in a *job*. 0 means infinity.

custom_flags:

type: typing.List[str], optional
argument path: run_mdata/train/resources/custom_flags

The extra lines pass to job submitting script header

strategy:

type: dict, optional
argument path: run_mdata/train/resources/strategy

strategies we use to generation job submitting scripts.

if_cuda_multi_devices:

type: bool, optional, default: False
argument path: run_mdata/train/resources/strategy/if_cuda_multi_devices

If there are multiple nvidia GPUS on the node, and we want to assign the tasks to different GPUS.If true, dpdispatcher will manually export environment variable

CUDA_VISIBLE_DEVICES to different task.Usually, this option will be used with Task.task_need_resources variable simultaneously.

ratio_unfinished:

type: `float`, optional, default: `0.0`
argument path: `run_mdata/train/resources/strategy/ratio_unfinished`

The ratio of *tasks* that can be unfinished.

customized_script_header_template_file:

type: `str`, optional
argument path: `run_mdata/train/resources/strategy/customized_script_header_template_file`

The customized template file to generate job submitting script header, which overrides the default file.

para_deg:

type: `int`, optional, default: 1
argument path: `run_mdata/train/resources/para_deg`

Decide how many tasks will be run in parallel.

source_list:

type: `typing.List[str]`, optional, default: `[]`
argument path: `run_mdata/train/resources/source_list`

The env file to be sourced before the command execution.

module_purge:

type: `bool`, optional, default: `False`
argument path: `run_mdata/train/resources/module_purge`

Remove all modules on HPC system before module load (module_list)

module_unload_list:

type: `typing.List[str]`, optional, default: `[]`
argument path: `run_mdata/train/resources/module_unload_list`

The modules to be unloaded on HPC system before submitting jobs

module_list:

type: typing.List[str], optional, default: []
argument path: run_mdata/train/resources/module_list

The modules to be loaded on HPC system before submitting jobs

envs:

type: dict, optional, default: {}
argument path: run_mdata/train/resources/envs

The environment variables to be exported on before submitting jobs

prepend_script:

type: typing.List[str], optional, default: []
argument path: run_mdata/train/resources/prepend_script

Optional script run before jobs submitted.

append_script:

type: typing.List[str], optional, default: []
argument path: run_mdata/train/resources/append_script

Optional script run after jobs submitted.

wait_time:

type: float | int, optional, default: 0
argument path: run_mdata/train/resources/wait_time

The waitting time in second after a single *task* submitted

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

batch_type:

type: str (flag key)
argument path: run_mdata/train/resources/batch_type
possible choices: *Fugaku*, *Slurm*, *SlurmJobArray*, *Shell*, *LSF*, *PBS*, *SGE*, *Torque*, *OpenAPI*, *DistributedShell*, *Bohrium*

The batch job system type loaded from machine/batch_type.

When batch_type is set to Fugaku (or its alias fugaku):

kwargs:

type: dict, optional
argument path: run_mdata/train/resources[Fugaku]/kwargs

This field is empty for this batch.

When batch_type is set to Slurm (or its alias slurm):

kwargs:

type: dict, optional
argument path: run_mdata/train/resources[Slurm]/kwargs

Extra arguments.

custom_gpu_line:

type: str | NoneType, optional, default: None
argument path: run_mdata/train/resources[Slurm]/kwargs/custom_gpu_line

Custom GPU configuration, starting with #SBATCH

When batch_type is set to SlurmJobArray (or its alias slurmjobarray):

kwargs:

type: dict, optional
argument path: run_mdata/train/resources[SlurmJobArray]/kwargs

Extra arguments.

custom_gpu_line:

type: str | NoneType, optional, default: None
argument path: run_mdata/train/resources[SlurmJobArray]/kwargs/custom_gpu_line

Custom GPU configuration, starting with #SBATCH

slurm_job_size:

type: int, optional, default: 1
argument path: run_mdata/train/resources[SlurmJobArray]/kwargs/slurm_job_size

Number of tasks in a Slurm job

When batch_type is set to Shell (or its alias shell):

kwargs:

type: dict, optional
argument path: run_mdata/train/resources[Shell]/kwargs

This field is empty for this batch.

When batch_type is set to LSF (or its alias lsf):

kwargs:

type: dict
argument path: run_mdata/train/resources[LSF]/kwargs

Extra arguments.

gpu_usage:

type: bool, optional, default: False
argument path: run_mdata/train/resources[LSF]/kwargs/gpu_usage

Choosing if GPU is used in the calculation step.

gpu_new_syntax:

type: bool, optional, default: False
argument path: run_mdata/train/resources[LSF]/kwargs/gpu_new_syntax

For LFS >= 10.1.0.3, new option -gpu for #BSUB could be used. If False, and old syntax would be used.

gpu_exclusive:

type: bool, optional, default: True
argument path: run_mdata/train/resources[LSF]/kwargs/gpu_exclusive

Only take effect when new syntax enabled. Control whether submit tasks in exclusive way for GPU.

custom_gpu_line:

type: str | NoneType, optional, default: None
argument path: run_mdata/train/resources[LSF]/kwargs/custom_gpu_line

Custom GPU configuration, starting with #BSUB

When batch_type is set to PBS (or its alias pbs):

kwargs:

type: dict, optional
argument path: run_mdata/train/resources[PBS]/kwargs

This field is empty for this batch.

When batch_type is set to SGE (or its alias sge):

kwargs:

type: dict, optional
argument path: run_mdata/train/resources[SGE]/kwargs

This field is empty for this batch.

When batch_type is set to Torque (or its alias torque):

kwargs:

type: dict, optional
argument path: run_mdata/train/resources[Torque]/kwargs

This field is empty for this batch.

When batch_type is set to OpenAPI (or its alias openapi):

kwargs:

type: dict, optional
argument path: run_mdata/train/resources[OpenAPI]/kwargs

This field is empty for this batch.

When batch_type is set to DistributedShell (or its alias distributedshell):

kwargs:

type: dict, optional
argument path: run_mdata/train/resources[DistributedShell]/kwargs

This field is empty for this batch.

When batch_type is set to Bohrium (or its aliases bohrium, Lebesgue, lebesgue, DpCloudServer, dpcloudserver):

kwargs:

type: dict, optional
argument path: run_mdata/train/resources[Bohrium]/kwargs

This field is empty for this batch.

user_forward_files:

type: list, optional
argument path: run_mdata/train/user_forward_files

Files to be forwarded to the remote machine.

user_backward_files:

type: list, optional
argument path: run_mdata/train/user_backward_files

Files to be backwarded from the remote machine.

model_devi:

type: dict
argument path: run_mdata/model_devi

Parameters of command, machine, and resources for model_devi

command:

type: str
argument path: run_mdata/model_devi/command

Command of a program.

machine:

type: dict
argument path: run_mdata/model_devi/machine

batch_type:

type: str
argument path: run_mdata/model_devi/machine/batch_type

The batch job system type. Option: Slurm, LSF, DistributedShell, SGE, Shell, SlurmJobArray, PBS, OpenAPI, Torque, Bohrium, Fugaku

local_root:

type: str | NoneType
argument path: run_mdata/model_devi/machine/local_root

The dir where the tasks and relating files locate. Typically the project dir.

remote_root:

type: str | NoneType, optional
argument path: run_mdata/model_devi/machine/remote_root

The dir where the tasks are executed on the remote machine. Only needed when context is not lazy-local.

clean_asynchronously:

type: bool, optional, default: False
argument path: run_mdata/model_devi/machine/clean_asynchronously

Clean the remote directory asynchronously after the job finishes.

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

context_type:

type: str (flag key)
argument path: run_mdata/model_devi/machine/context_type
possible choices: *LocalContext*, *LazyLocalContext*, *BohriumContext*, *HDFSContext*, *OpenAPIContext*, *SSHContext*

The connection used to remote machine. Option: LazyLocalContext, HDFSContext, BohriumContext, SSHContext, LocalContext, OpenAPIContext

When context_type is set to LocalContext (or its aliases localcontext, Local, local):

remote_profile:

type: dict, optional
argument path: run_mdata/model_devi/machine[LocalContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to LazyLocalContext (or its aliases lazylocalcontext, LazyLocal, lazylocal):

remote_profile:

type: dict, optional
argument path: run_mdata/model_devi/machine[LazyLocalContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to BohriumContext (or its aliases bohriumcontext, Bohrium, bohrium, DpCloudServerContext, dpcloudservercontext, DpCloudServer, dpcloudserver, LebesgueContext, lebesguecontext, Lebesgue, lebesgue):

remote_profile:

type: dict

argument path: run_mdata/model_devi/machine[BohriumContext]/remote_profile

The information used to maintain the connection with remote machine.

email:

type: str, optional

argument path: run_mdata/model_devi/machine[BohriumContext]/remote_profile/email

Email

password:

type: str, optional

argument path: run_mdata/model_devi/machine[BohriumContext]/remote_profile/password

Password

program_id:

type: int, alias: *project_id*

argument path: run_mdata/model_devi/machine[BohriumContext]/remote_profile/program_id

Program ID

retry_count:

type: NoneType | int, optional, default: 2

argument path: run_mdata/model_devi/machine[BohriumContext]/remote_profile/retry_count

The retry count when a job is terminated

ignore_exit_code:

type: bool, optional, default: True

argument path: run_mdata/model_devi/machine[BohriumContext]/remote_profile/ignore_exit_code

The job state will be marked as finished if the exit code is non-zero when set to True. Otherwise,
the job state will be designated as terminated.

keep_backup:

type: bool, optional

argument path: run_mdata/model_devi/machine[BohriumContext]/remote_profile/keep_backup

keep download and upload zip

input_data:

type: dict

argument path: run_mdata/model_devi/machine[BohriumContext]/remote_profile/input_data

Configuration of job

When context_type is set to HDFSContext (or its aliases hdfscontext, HDFS, hdfs):

remote_profile:

type: dict, optional

argument path: run_mdata/model_devi/machine[HDFSContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to OpenAPIContext (or its aliases openapicontext, OpenAPI, openapi):

remote_profile:

type: dict, optional

argument path: run_mdata/model_devi/machine[OpenAPIContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to SSHContext (or its aliases sshcontext, SSH, ssh):

remote_profile:

type: dict

argument path: run_mdata/model_devi/machine[SSHContext]/remote_profile

The information used to maintain the connection with remote machine.

hostname:

type: str

argument path: run_mdata/model_devi/machine[SSHContext]/remote_profile/hostname

hostname or ip of ssh connection.

username:

type: str

argument path: run_mdata/model_devi/machine[SSHContext]/remote_profile/username

username of target linux system

password:

type: str, optional

argument path: run_mdata/model_devi/machine[SSHContext]/remote_profile/password

(deprecated) password of linux system. Please use SSH keys instead to improve security.

port:

type: int, optional, default: 22

argument path: run_mdata/model_devi/machine[SSHContext]/remote_profile/port

ssh connection port.

key_filename:

type: str | NoneType, optional, default: None

argument path: run_mdata/model_devi/machine[SSHContext]/remote_profile/key_filename

key filename used by ssh connection. If left None, find key in ~/.ssh or use password for login

passphrase:

type: str | NoneType, optional, default: None

argument path:
run_mdata/model_devi/
machine[SSHContext]/
remote_profile/passphrase

passphrase of key used by ssh connection

timeout:

type: int, optional, default: 10
argument path:
run_mdata/model_devi/
machine[SSHContext]/
remote_profile/timeout

timeout of ssh connection

totp_secret:

type: str | NoneType, optional, default: None
argument path:
run_mdata/model_devi/
machine[SSHContext]/
remote_profile/totp_secret

Time-based one time password secret. It should be a base32-encoded string extracted from the 2D code.

tar_compress:

type: bool, optional, default: True
argument path:
run_mdata/model_devi/
machine[SSHContext]/
remote_profile/tar_compress

The archive will be compressed in upload and download if it is True. If not, compression will be skipped.

look_for_keys:

type: bool, optional, default: True
argument path:
run_mdata/model_devi/
machine[SSHContext]/
remote_profile/look_for_keys

enable searching for discoverable private key files in ~/.ssh/

resources:

type: dict
argument path: run_mdata/model_devi/resources

number_node:

type: int, optional, default: 1

argument path: `run_mdata/model_devi/resources/number_node`

The number of node need for each *job*

cpu_per_node:

type: `int`, optional, default: `1`

argument path: `run_mdata/model_devi/resources/cpu_per_node`

cpu numbers of each node assigned to each job.

gpu_per_node:

type: `int`, optional, default: `0`

argument path: `run_mdata/model_devi/resources/gpu_per_node`

gpu numbers of each node assigned to each job.

queue_name:

type: `str`, optional, default: (empty string)

argument path: `run_mdata/model_devi/resources/queue_name`

The queue name of batch job scheduler system.

group_size:

type: `int`

argument path: `run_mdata/model_devi/resources/group_size`

The number of *tasks* in a *job*. 0 means infinity.

custom_flags:

type: `typing.List[str]`, optional

argument path: `run_mdata/model_devi/resources/custom_flags`

The extra lines pass to job submitting script header

strategy:

type: `dict`, optional

argument path: `run_mdata/model_devi/resources/strategy`

strategies we use to generation job submitting scripts.

if_cuda_multi_devices:

type: `bool`, optional, default: `False`

argument path: `run_mdata/model_devi/resources/strategy/if_cuda_multi_devices`

If there are multiple nvidia GPUS on the node, and we want to assign the tasks to different GPUS.If true, dpdispatcher will manually export environment variable CUDA_VISIBLE_DEVICES to different task.Usually, this option will be used with Task.task_need_resources variable simultaneously.

ratio_unfinished:

type: `float`, optional, default: `0.0`

argument path: `run_mdata/model_devi/resources/strategy/ratio_unfinished`

The ratio of *tasks* that can be unfinished.

customized_script_header_template_file:

type: `str`, optional

argument path: `run_mdata/model_devi/resources/strategy/customized_script_header_template_file`

The customized template file to generate job submitting script header, which overrides the default file.

para_deg:

type: `int`, optional, default: 1

argument path: `run_mdata/model_devi/resources/para_deg`

Decide how many tasks will be run in parallel.

source_list:

type: `typing.List[str]`, optional, default: `[]`

argument path: `run_mdata/model_devi/resources/source_list`

The env file to be sourced before the command execution.

module_purge:

type: `bool`, optional, default: `False`

argument path: `run_mdata/model_devi/resources/module_purge`

Remove all modules on HPC system before module load (module_list)

module_unload_list:

type: typing.List[str], optional, default: []
argument path: run_mdata/model_devi/resources/module_unload_list

The modules to be unloaded on HPC system before submitting jobs

module_list:

type: typing.List[str], optional, default: []
argument path: run_mdata/model_devi/resources/module_list

The modules to be loaded on HPC system before submitting jobs

envs:

type: dict, optional, default: {}
argument path: run_mdata/model_devi/resources/envs

The environment variables to be exported on before submitting jobs

prepend_script:

type: typing.List[str], optional, default: []
argument path: run_mdata/model_devi/resources/prepend_script

Optional script run before jobs submitted.

append_script:

type: typing.List[str], optional, default: []
argument path: run_mdata/model_devi/resources/append_script

Optional script run after jobs submitted.

wait_time:

type: float | int, optional, default: 0
argument path: run_mdata/model_devi/resources/wait_time

The waitting time in second after a single *task* submitted

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

batch_type:

type: str (flag key)
argument path: run_mdata/model_devi/resources/batch_type
possible choices: *Fugaku*, *Slurm*, *SlurmJobArray*, *Shell*, *LSF*, *PBS*, *SGE*, *Torque*, *OpenAPI*, *DistributedShell*, *Bohrium*

The batch job system type loaded from machine/batch_type.

When batch_type is set to Fugaku (or its alias fugaku):

kwargs:

type: dict, optional
argument path: run_mdata/model_devi/resources[Fugaku]/kwargs

This field is empty for this batch.

When batch_type is set to Slurm (or its alias slurm):

kwargs:

type: dict, optional
argument path: run_mdata/model_devi/resources[Slurm]/kwargs

Extra arguments.

custom_gpu_line:

type: str | NoneType, optional, default: None
argument path: run_mdata/model_devi/resources[Slurm]/kwargs/custom_gpu_line

Custom GPU configuration, starting with #SBATCH

When batch_type is set to SlurmJobArray (or its alias slurmjobarray):

kwargs:

type: dict, optional
argument path: run_mdata/model_devi/resources[SlurmJobArray]/kwargs

Extra arguments.

custom_gpu_line:

type: str | NoneType, optional, default: None

argument path: `run_mdata/model_devi/resources[SlurmJobArray]/kwargs/custom_gpu_line`

Custom GPU configuration, starting with #SBATCH

slurm_job_size:

type: `int`, optional, default: `1`

argument path: `run_mdata/model_devi/resources[SlurmJobArray]/kwargs/slurm_job_size`

Number of tasks in a Slurm job

When batch_type is set to `Shell` (or its alias `shell`):

kwargs:

type: `dict`, optional

argument path: `run_mdata/model_devi/resources[Shell]/kwargs`

This field is empty for this batch.

When batch_type is set to `LSF` (or its alias `lsf`):

kwargs:

type: `dict`

argument path: `run_mdata/model_devi/resources[LSF]/kwargs`

Extra arguments.

gpu_usage:

type: `bool`, optional, default: `False`

argument path: `run_mdata/model_devi/resources[LSF]/kwargs/gpu_usage`

Choosing if GPU is used in the calculation step.

gpu_new_syntax:

type: `bool`, optional, default: `False`

argument path: `run_mdata/model_devi/resources[LSF]/kwargs/gpu_new_syntax`

For LFS >= 10.1.0.3, new option -gpu for #BSUB could be used. If False, and old syntax would be used.

gpu_exclusive:

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

argument path: run_mdata/model_devi/resources[LSF]/kwargs/gpu_exclusive

Only take effect when new syntax enabled. Control whether submit tasks in exclusive way for GPU.

custom_gpu_line:

type: str | NoneType, optional, default: None

argument path: run_mdata/model_devi/resources[LSF]/kwargs/custom_gpu_line

Custom GPU configuration, starting with #BSUB

When batch_type is set to PBS (or its alias pbs):

kwargs:

type: dict, optional

argument path: run_mdata/model_devi/resources[PBS]/kwargs

This field is empty for this batch.

When batch_type is set to SGE (or its alias sge):

kwargs:

type: dict, optional

argument path: run_mdata/model_devi/resources[SGE]/kwargs

This field is empty for this batch.

When batch_type is set to Torque (or its alias torque):

kwargs:

type: dict, optional

argument path: run_mdata/model_devi/resources[Torque]/kwargs

This field is empty for this batch.

When batch_type is set to OpenAPI (or its alias openapi):

kwargs:

type: dict, optional

argument path: run_mdata/model_devi/resources[OpenAPI]/kwargs

This field is empty for this batch.

When batch_type is set to DistributedShell (or its alias distributedshell):

kwargs:

type: dict, optional
argument path: run_mdata/model_devi/resources[DistributedShell]/kwargs

This field is empty for this batch.

When batch_type is set to Bohrium (or its aliases bohrium, Lebesgue, lebesgue, DpCloudServer, dpcloudserver):

kwargs:

type: dict, optional
argument path: run_mdata/model_devi/resources[Bohrium]/kwargs

This field is empty for this batch.

user_forward_files:

type: list, optional
argument path: run_mdata/model_devi/user_forward_files

Files to be forwarded to the remote machine.

user_backward_files:

type: list, optional
argument path: run_mdata/model_devi/user_backward_files

Files to be backwarded from the remote machine.

fp:

type: dict
argument path: run_mdata/fp

Parameters of command, machine, and resources for fp

command:

type: str
argument path: run_mdata/fp/command

Command of a program.

machine:

type: dict
argument path: run_mdata/fp/machine

batch_type:

type: str
argument path: run_mdata/fp/machine/batch_type

The batch job system type. Option: Slurm, LSF, DistributedShell, SGE, Shell, SlurmJobArray, PBS, OpenAPI, Torque, Bohrium, Fugaku

local_root:

type: str | NoneType
argument path: run_mdata/fp/machine/local_root

The dir where the tasks and relating files locate. Typically the project dir.

remote_root:

type: str | NoneType, optional
argument path: run_mdata/fp/machine/remote_root

The dir where the tasks are executed on the remote machine. Only needed when context is not lazy-local.

clean_asynchronously:

type: bool, optional, default: False
argument path: run_mdata/fp/machine/clean_asynchronously

Clean the remote directory asynchronously after the job finishes.

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

context_type:

type: str (flag key)
argument path: run_mdata/fp/machine/context_type
possible choices: *LocalContext*, *LazyLocalContext*, *BohriumContext*, *HDFSContext*, *OpenAPIContext*, *SSHContext*

The connection used to remote machine. Option: LazyLocalContext, HDFSContext, BohriumContext, SSHContext, LocalContext, OpenAPIContext

When context_type is set to LocalContext (or its aliases localcontext, Local, local):

remote_profile:

type: dict, optional
argument path: run_mdata/fp/machine[LocalContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to LazyLocalContext (or its aliases lazylocalcontext, LazyLocal, lazylocal):

remote_profile:

type: dict, optional
argument path: run_mdata/fp/machine[LazyLocalContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to BohriumContext (or its aliases bohriumcontext, Bohrium, bohrium, DpCloudServerContext, dpcloudservercontext, DpCloudServer, dpcloudserver, LebesgueContext, lebesguecontext, Lebesgue, lebesgue):

remote_profile:

type: dict
argument path: run_mdata/fp/machine[BohriumContext]/remote_profile

The information used to maintain the connection with remote machine.

email:

type: str, optional
argument path: run_mdata/fp/machine[BohriumContext]/remote_profile/email

Email

password:

type: str, optional
argument path: run_mdata/fp/machine[BohriumContext]/remote_profile/password

Password

program_id:

type: int, alias: *project_id*
argument path: run_mdata/fp/machine[BohriumContext]/remote_profile/program_id

Program ID

retry_count:

type: NoneType | int, optional, default: 2

argument path: run_mdata/fp/machine[BohriumContext]/remote_profile/retry_count

The retry count when a job is terminated

ignore_exit_code:

type: bool, optional, default: True

argument path: run_mdata/fp/machine[BohriumContext]/remote_profile/ignore_exit_code

The job state will be marked as finished if the exit code is non-zero when set to True. Otherwise, the job state will be designated as terminated.

keep_backup:

type: bool, optional

argument path: run_mdata/fp/machine[BohriumContext]/remote_profile/keep_backup

keep download and upload zip

input_data:

type: dict

argument path: run_mdata/fp/machine[BohriumContext]/remote_profile/input_data

Configuration of job

When context_type is set to HDFSContext (or its aliases hdfscontext, HDFS, hdfs):

remote_profile:

type: dict, optional

argument path: run_mdata/fp/machine[HDFSContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to OpenAPIContext (or its aliases openapicontext, OpenAPI, openapi):

remote_profile:

type: dict, optional

argument path: run_mdata/fp/machine[OpenAPIContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to SSHContext (or its aliases sshcontext, SSH, ssh):

remote_profile:

type: dict

argument path: run_mdata/fp/machine[SSHContext]/remote_profile

The information used to maintain the connection with remote machine.

hostname:

type: str

argument path: run_mdata/fp/machine[SSHContext]/remote_profile/hostname

hostname or ip of ssh connection.

username:

type: str

argument path: run_mdata/fp/machine[SSHContext]/remote_profile/username

username of target linux system

password:

type: str, optional

argument path: run_mdata/fp/machine[SSHContext]/remote_profile/password

(deprecated) password of linux system. Please use SSH keys instead to improve security.

port:

type: int, optional, default: 22

argument path: run_mdata/fp/machine[SSHContext]/remote_profile/port

ssh connection port.

key_filename:

type: str | NoneType, optional, default: None

argument path: run_mdata/fp/machine[SSHContext]/remote_profile/key_filename

key filename used by ssh connection. If left None, find key in ~/.ssh or use password for login

passphrase:

type: str | NoneType, optional, default: None

argument path: run_mdata/fp/machine[SSHContext]/remote_profile/passphrase

passphrase of key used by ssh connection

timeout:

type: int, optional, default: 10

argument path: run_mdata/fp/machine[SSHContext]/remote_profile/timeout

timeout of ssh connection

totp_secret:

type: str | NoneType, optional, default: None

argument path: run_mdata/fp/machine[SSHContext]/remote_profile/totp_secret

Time-based one time password secret. It should be a base32-encoded string extracted from the 2D code.

tar_compress:

type: bool, optional, default: True

argument path: run_mdata/fp/machine[SSHContext]/remote_profile/tar_compress

The archive will be compressed in upload and download if it is True. If not, compression will be skipped.

look_for_keys:

type: bool, optional, default: True

argument path: run_mdata/fp/machine[SSHContext]/remote_profile/look_for_keys

enable searching for discoverable private key files in ~/.ssh/

resources:

type: dict
argument path: run_mdata/fp/resources

number_node:

type: int, optional, default: 1
argument path: run_mdata/fp/resources/number_node

The number of node need for each *job*

cpu_per_node:

type: int, optional, default: 1
argument path: run_mdata/fp/resources/cpu_per_node

cpu numbers of each node assigned to each job.

gpu_per_node:

type: int, optional, default: 0
argument path: run_mdata/fp/resources/gpu_per_node

gpu numbers of each node assigned to each job.

queue_name:

type: str, optional, default: (empty string)
argument path: run_mdata/fp/resources/queue_name

The queue name of batch job scheduler system.

group_size:

type: int
argument path: run_mdata/fp/resources/group_size

The number of *tasks* in a *job*. 0 means infinity.

custom_flags:

type: typing.List[str], optional
argument path: run_mdata/fp/resources/custom_flags

The extra lines pass to job submitting script header

strategy:

type: dict, optional
argument path: run_mdata/fp/resources/strategy

strategies we use to generation job submitting scripts.

if_cuda_multi_devices:

type: bool, optional, default: False
argument path: run_mdata/fp/resources/strategy/if_cuda_multi_devices

If there are multiple nvidia GPUS on the node, and we want to assign the tasks to different GPUS.If true, dpdispatcher will manually export environment variable CUDA_VISIBLE_DEVICES to different task.Usually, this option will be used with Task.task_need_resources variable simultaneously.

ratio_unfinished:

type: float, optional, default: 0.0
argument path: run_mdata/fp/resources/strategy/ratio_unfinished

The ratio of *tasks* that can be unfinished.

customized_script_header_template_file:

type: str, optional
argument path: run_mdata/fp/resources/strategy/customized_script_header_template_file

The customized template file to generate job submitting script header, which overrides the default file.

para_deg:

type: int, optional, default: 1
argument path: run_mdata/fp/resources/para_deg

Decide how many tasks will be run in parallel.

source_list:

type: typing.List[str], optional, default: []
argument path: run_mdata/fp/resources/source_list

The env file to be sourced before the command execution.

module_purge:

type: bool, optional, default: False
argument path: run_mdata/fp/resources/module_purge

Remove all modules on HPC system before module load (module_list)

module_unload_list:

type: typing.List[str], optional, default: []
argument path: run_mdata/fp/resources/module_unload_list

The modules to be unloaded on HPC system before submitting jobs

module_list:

type: typing.List[str], optional, default: []
argument path: run_mdata/fp/resources/module_list

The modules to be loaded on HPC system before submitting jobs

envs:

type: dict, optional, default: {}
argument path: run_mdata/fp/resources/envs

The environment variables to be exported on before submitting jobs

prepend_script:

type: typing.List[str], optional, default: []
argument path: run_mdata/fp/resources/prepend_script

Optional script run before jobs submitted.

append_script:

type: typing.List[str], optional, default: []
argument path: run_mdata/fp/resources/append_script

Optional script run after jobs submitted.

wait_time:

type: float | int, optional, default: 0
argument path: run_mdata/fp/resources/wait_time

The waitting time in second after a single *task* submitted

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

batch_type:

type: str (flag key)
argument path: run_mdata/fp/resources/batch_type
possible choices: *Fugaku*, *Slurm*, *SlurmJobArray*, *Shell*, *LSF*, *PBS*, *SGE*, *Torque*, *OpenAPI*, *DistributedShell*, *Bohrium*

The batch job system type loaded from machine/batch_type.

When batch_type is set to Fugaku (or its alias fugaku):

kwargs:

type: dict, optional
argument path: run_mdata/fp/resources[Fugaku]/kwargs

This field is empty for this batch.

When batch_type is set to Slurm (or its alias slurm):

kwargs:

type: dict, optional
argument path: run_mdata/fp/resources[Slurm]/kwargs

Extra arguments.

custom_gpu_line:

type: str | NoneType, optional, default: None
argument path: run_mdata/fp/resources[Slurm]/kwargs/custom_gpu_line

Custom GPU configuration, starting with #SBATCH

When batch_type is set to SlurmJobArray (or its alias slurmjobarray):

kwargs:

type: dict, optional
argument path: run_mdata/fp/resources[SlurmJobArray]/kwargs

Extra arguments.

custom_gpu_line:

type: str | NoneType, optional, default: None
argument path: run_mdata/fp/resources[SlurmJobArray]/kwargs/custom_gpu_line

Custom GPU configuration, starting with #SBATCH

slurm_job_size:

type: int, optional, default: 1
argument path: run_mdata/fp/resources[SlurmJobArray]/kwargs/slurm_job_size

Number of tasks in a Slurm job

When batch_type is set to Shell (or its alias shell):

kwargs:

type: dict, optional
argument path: run_mdata/fp/resources[Shell]/kwargs

This field is empty for this batch.

When batch_type is set to LSF (or its alias lsf):

kwargs:

type: dict
argument path: run_mdata/fp/resources[LSF]/kwargs

Extra arguments.

gpu_usage:

type: bool, optional, default: False
argument path: run_mdata/fp/resources[LSF]/kwargs/gpu_usage

Choosing if GPU is used in the calculation step.

gpu_new_syntax:

type: bool, optional, default: False
argument path: run_mdata/fp/resources[LSF]/kwargs/gpu_new_syntax

For LFS >= 10.1.0.3, new option -gpu for #BSUB could be used. If False, and old syntax would be used.

gpu_exclusive:

type: bool, optional, default: True
argument path: run_mdata/fp/resources[LSF]/kwargs/gpu_exclusive

Only take effect when new syntax enabled. Control whether submit tasks in exclusive way for GPU.

custom_gpu_line:

type: str | NoneType, optional, default: None

argument path: run_mdata/fp/resources[LSF]/kwargs/custom_gpu_line

Custom GPU configuration, starting with #BSUB

When batch_type is set to PBS (or its alias pbs):

kwargs:

type: dict, optional

argument path: run_mdata/fp/resources[PBS]/kwargs

This field is empty for this batch.

When batch_type is set to SGE (or its alias sge):

kwargs:

type: dict, optional

argument path: run_mdata/fp/resources[SGE]/kwargs

This field is empty for this batch.

When batch_type is set to Torque (or its alias torque):

kwargs:

type: dict, optional

argument path: run_mdata/fp/resources[Torque]/kwargs

This field is empty for this batch.

When batch_type is set to OpenAPI (or its alias openapi):

kwargs:

type: dict, optional

argument path: run_mdata/fp/resources[OpenAPI]/kwargs

This field is empty for this batch.

When batch_type is set to DistributedShell (or its alias distributedshell):

kwargs:

type: dict, optional

argument path: run_mdata/fp/resources[DistributedShell]/kwargs

This field is empty for this batch.

When batch_type is set to Bohrium (or its aliases bohrium, Lebesgue, lebesgue, DpCloudServer, dpcloudserver):

kwargs:

type: dict, optional
argument path: run_mdata/fp/resources[Bohrium]/kwargs

This field is empty for this batch.

user_forward_files:

type: list, optional
argument path: run_mdata/fp/user_forward_files

Files to be forwarded to the remote machine.

user_backward_files:

type: list, optional
argument path: run_mdata/fp/user_backward_files

Files to be backwarded from the remote machine.

CHAPTER

FIVE

INIT

5.1 Init_bulk

You may prepare initial data for bulk systems with VASP by:

```
dpgen init_bulk PARAM [MACHINE]
```

The MACHINE configure file is optional. If this parameter exists, then the optimization tasks or MD tasks will be submitted automatically according to MACHINE.json.

Basically `init_bulk` can be divided into four parts , denoted as `stages` in `PARAM`:

1. Relax in folder `00.place_ele`
2. Perturb and scale in folder `01.scale_pert`
3. Run a short AIMD in folder `02.md`
4. Collect data in folder `02.md`.

All stages must be **in order**. One doesn't need to run all stages. For example, you may run stage 1 and 2, generating supercells as starting point of exploration in `dpgen run`.

If MACHINE is None, there should be only one stage in stages. Corresponding tasks will be generated, but user's intervention should be involved in, to manually run the scripts.

Following is an example for `PARAM`, which generates data from a typical structure hcp.

```
{
    "stages" : [1,2,3,4],
    "cell_type":    "hcp",
    "latt":     4.479,
    "super_cell":   [2, 2, 2],
    "elements":     ["Mg"],
    "potcars":      ["....../POTCAR"],
    "relax_incar": "....../INCAR_metal_rlx",
    "md_incar" : "....../INCAR_metal_md",
    "scale":        [1.00],
    "skip_relax":   false,
    "pert_numb":    2,
    "md_nstep" : 5,
    "pert_box":     0.03,
    "pert_atom":    0.01,
    "coll_ndata":   5000,
    "type_map" : [ "Mg", "Al"],
```

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```
    "_comment":     "that's all"
}
```

If you want to specify a structure as starting point for `init_bulk`, you may set in `PARAM` as follows.

```
"from_poscar":        true,
"from_poscar_path":        "....../C_mp-47_conventional.POSCAR",
```

`init_bulk` supports both VASP and ABACUS for first-principle calculation. You can choose the software by specifying the key *`init_fp_style`*. If *`init_fp_style`* is not specified, the default software will be VASP.

When using ABACUS for *`init_fp_style`*, the keys of the paths of `INPUT` files for relaxation and MD simulations are the same as `INCAR` for VASP, which are *`relax_incar`* and *`md_incar`* respectively. Use *`relax_kpt`* and *`md_kpt`* for the relative path for `KPT` files of relaxation and MD simulations. They two can be omitted if `kspacing` (in unit of 1/Bohr) or `gamma_only` has been set in corresponding INPUT files. If *`from_poscar`* is set to `false`, you have to specify *`atom_masses`* in the same order as `elements`.

5.2 dpgen init_bulk parameters

Note: One can load, modify, and export the input file by using our effective web-based tool DP-GUI online or hosted using the *command line interface* `dpgen gui`. All parameters below can be set in DP-GUI. By clicking "SAVE JSON", one can download the input file.

`init_bulk_jdata:`

type: `dict`
argument path: `init_bulk_jdata`

Generate initial data for bulk systems.

`stages:`

type: `list[int]`
argument path: `init_bulk_jdata/stages`

Stages for *init_bulk*.

`elements:`

type: `list[str]`
argument path: `init_bulk_jdata/elements`

Atom types.

`potcars:`

type: `list[str]`, optional
argument path: `init_bulk_jdata/potcars`

Path of POTCAR.

`cell_type:`

type: `str`, optional
argument path: `init_bulk_jdata/cell_type`

Specifying which typical structure to be generated. **Options** include fcc, hcp, bcc, sc, diamond.

super_cell:

type: list[int]
argument path: init_bulk_jdata/super_cell

Size of supercell.

from_poscar:

type: bool, optional, default: False
argument path: init_bulk_jdata/from_poscar

Deciding whether to use a given poscar as the beginning of relaxation. If it's true, keys (*cell_type*, *latt*) will be aborted. Otherwise, these two keys are **necessary**.

from_poscar_path:

type: str, optional
argument path: init_bulk_jdata/from_poscar_path

Path of POSCAR for VASP or STRU for ABACUS. **Necessary** if *from_poscar* is true.

relax_incar:

type: str, optional
argument path: init_bulk_jdata/relax_incar

Path of INCAR for VASP or INPUT for ABACUS for relaxation in VASP. **Necessary** if *stages* include 1.

md_incar:

type: str, optional
argument path: init_bulk_jdata/md_incar

Path of INCAR for VASP or INPUT for ABACUS for MD in VASP. **Necessary** if *stages* include 3.

scale:

type: list[float]
argument path: init_bulk_jdata/scale

Scales for isotropic transforming cells.

skip_relax:

type: bool
argument path: init_bulk_jdata/skip_relax

If it's true, you may directly run stage 2 (perturb and scale) using an unrelaxed POSCAR.

pert_numb:

type: int
argument path: init_bulk_jdata/pert_numb

Number of perturbations for each scaled (key *scale*) POSCAR.

pert_box:

type: float
argument path: init_bulk_jdata/pert_box

Anisotropic Perturbation for cells (independent changes of lengths of three box vectors as well as angel among) in decimal formats. 9 elements of the 3x3 perturbation matrix will be randomly sampled from a uniform distribution (default) in the range [-pert_box, pert_box]. Such a perturbation matrix adds the identity matrix gives the actual transformation matrix for this perturbation operation.

pert_atom:

type: `float`

argument path: `init_bulk_jdata/pert_atom`

Perturbation of atom coordinates (Angstrom). Random perturbations are performed on three coordinates of each atom by adding values randomly sampled from a uniform distribution in the range [-pert_atom, pert_atom].

md_nstep:

type: `int`

argument path: `init_bulk_jdata/md_nstep`

Steps of AIMD in stage 3. If it's not equal to settings via *NSW* in *md_incar*, DP-GEN will follow *NSW*.

coll_ndata:

type: `int`

argument path: `init_bulk_jdata/coll_ndata`

Maximal number of collected data.

type_map:

type: `list[str]`, optional

argument path: `init_bulk_jdata/type_map`

The indices of elements in deepmd formats will be set in this order.

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

init_fp_style:

type: `str` (flag key), default: `VASP`

argument path: `init_bulk_jdata/init_fp_style`

possible choices: *VASP*, *ABACUS*

First-principle software. If this key is absent.

When init_fp_style is set to `VASP`:

No more parameters is needed to be added.

When init_fp_style is set to `ABACUS`:

ABACUS

relax_kpt:

type: `str`, optional

argument path: `init_bulk_jdata[ABACUS]/relax_kpt`

Path of *KPT* file for relaxation in stage 1. Only useful if *init_fp_style* is "ABACUS".

md_kpt:

type: `str`, optional

argument path: `init_bulk_jdata[ABACUS]/md_kpt`

Path of *KPT* file for MD simulations in stage 3. Only useful if *init_fp_style* is "ABACUS".

atom_masses:

type: `list[float]`, optional

argument path: `init_bulk_jdata[ABACUS]/atom_masses`

List of atomic masses of elements. The order should be the same as *Elements*. Only useful if *init_fp_style* is "ABACUS".

5.3 dpgen init_bulk machine parameters

Note: One can load, modify, and export the input file by using our effective web-based tool DP-GUI online or hosted using the *command line interface* `dpgen gui`. All parameters below can be set in DP-GUI. By clicking "SAVE JSON", one can download the input file.

init_bulk_mdata:

type: `dict`

argument path: `init_bulk_mdata`

machine.json file

api_version:

type: `str`, optional, default: `1.0`

argument path: `init_bulk_mdata/api_version`

Please set to 1.0

deepmd_version:

type: `str`, optional, default: `2`

argument path: `init_bulk_mdata/deepmd_version`

DeePMD-kit version, e.g. 2.1.3

fp:

type: `dict`

argument path: `init_bulk_mdata/fp`

Parameters of command, machine, and resources for fp

command:

type: `str`

argument path: `init_bulk_mdata/fp/command`

Command of a program.

machine:

type: `dict`

argument path: `init_bulk_mdata/fp/machine`

batch_type:

type: str
argument path: init_bulk_mdata/fp/machine/batch_type

The batch job system type. Option: Slurm, LSF, DistributedShell, SGE, Shell, SlurmJobArray, PBS, OpenAPI, Torque, Bohrium, Fugaku

local_root:

type: str | NoneType
argument path: init_bulk_mdata/fp/machine/local_root

The dir where the tasks and relating files locate. Typically the project dir.

remote_root:

type: str | NoneType, optional
argument path: init_bulk_mdata/fp/machine/remote_root

The dir where the tasks are executed on the remote machine. Only needed when context is not lazy-local.

clean_asynchronously:

type: bool, optional, default: False
argument path: init_bulk_mdata/fp/machine/clean_asynchronously

Clean the remote directory asynchronously after the job finishes.

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

context_type:

type: str (flag key)
argument path: init_bulk_mdata/fp/machine/context_type
possible choices: *LocalContext*, *LazyLocalContext*, *BohriumContext*, *HDFSContext*, *OpenAPIContext*, *SSHContext*

The connection used to remote machine. Option: LazyLocalContext, HDFSContext, BohriumContext, SSHContext, LocalContext, OpenAPIContext

When context_type is set to LocalContext (or its aliases localcontext, Local, local):

remote_profile:

type: dict, optional
argument path: init_bulk_mdata/fp/machine[LocalContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to LazyLocalContext (or its aliases lazylocalcontext, LazyLocal, lazylocal):

remote_profile:

type: dict, optional
argument path: init_bulk_mdata/fp/machine[LazyLocalContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to BohriumContext (or its aliases bohriumcontext, Bohrium, bohrium, DpCloudServerContext, dpcloudservercontext, DpCloudServer, dpcloudserver, LebesgueContext, lebesguecontext, Lebesgue, lebesgue):

remote_profile:

type: dict
argument path: init_bulk_mdata/fp/machine[BohriumContext]/remote_profile

The information used to maintain the connection with remote machine.

email:

type: str, optional
argument path: init_bulk_mdata/fp/machine[BohriumContext]/remote_profile/email

Email

password:

type: str, optional
argument path: init_bulk_mdata/fp/machine[BohriumContext]/remote_profile/password

Password

program_id:

type: int, alias: *project_id*

argument path: init_bulk_mdata/fp/machine[BohriumContext]/remote_profile/program_id

Program ID

retry_count:

type: NoneType | int, optional, default: 2

argument path: init_bulk_mdata/fp/machine[BohriumContext]/remote_profile/retry_count

The retry count when a job is terminated

ignore_exit_code:

type: bool, optional, default: True

argument path: init_bulk_mdata/fp/machine[BohriumContext]/remote_profile/ignore_exit_code

The job state will be marked as finished if the exit code is non-zero when set to True. Otherwise,
the job state will be designated as terminated.

keep_backup:

type: bool, optional

argument path: init_bulk_mdata/fp/machine[BohriumContext]/remote_profile/keep_backup

keep download and upload zip

input_data:

type: dict

argument path: init_bulk_mdata/fp/machine[BohriumContext]/remote_profile/input_data

Configuration of job

When context_type is set to HDFSContext (or its aliases hdfscontext, HDFS, hdfs):

remote_profile:

type: dict, optional

argument path: init_bulk_mdata/fp/machine[HDFSContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to OpenAPIContext (or its aliases openapicontext, OpenAPI, openapi):

remote_profile:

type: dict, optional

argument path: init_bulk_mdata/fp/machine[OpenAPIContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to SSHContext (or its aliases sshcontext, SSH, ssh):

remote_profile:

type: dict

argument path: init_bulk_mdata/fp/machine[SSHContext]/remote_profile

The information used to maintain the connection with remote machine.

hostname:

type: str

argument path: init_bulk_mdata/fp/machine[SSHContext]/remote_profile/hostname

hostname or ip of ssh connection.

username:

type: str

argument path: init_bulk_mdata/fp/machine[SSHContext]/remote_profile/username

username of target linux system

password:

type: str, optional

argument path: init_bulk_mdata/fp/machine[SSHContext]/remote_profile/password

(deprecated) password of linux system. Please use SSH keys instead to improve security.

port:

type: int, optional, default: 22

argument path: init_bulk_mdata/fp/machine[SSHContext]/remote_profile/port

ssh connection port.

key_filename:

type: str | NoneType, optional, default: None

argument path: init_bulk_mdata/fp/machine[SSHContext]/remote_profile/key_filename

key filename used by ssh connection. If left None, find key in ~/.ssh or use password for login

passphrase:

type: str | NoneType, optional, default: None

argument path: init_bulk_mdata/fp/machine[SSHContext]/remote_profile/passphrase

passphrase of key used by ssh connection

timeout:

type: int, optional, default: 10

argument path: init_bulk_mdata/fp/machine[SSHContext]/remote_profile/timeout

timeout of ssh connection

totp_secret:

type: str | NoneType, optional, default: None

argument path: init_bulk_mdata/fp/machine[SSHContext]/remote_profile/totp_secret

Time-based one time password secret. It should be a base32-encoded string extracted from the 2D code.

tar_compress:

type: bool, optional, default: True

argument path: init_bulk_mdata/fp/machine[SSHContext]/remote_profile/tar_compress

The archive will be compressed in upload and download if it is True. If not, compression will be skipped.

look_for_keys:

type: bool, optional, default: True

argument path: init_bulk_mdata/fp/machine[SSHContext]/remote_profile/look_for_keys

enable searching for discoverable private key files in ~/.ssh/

resources:

type: dict
argument path: init_bulk_mdata/fp/resources

number_node:

type: int, optional, default: 1
argument path: init_bulk_mdata/fp/resources/number_node

The number of node need for each *job*

cpu_per_node:

type: int, optional, default: 1
argument path: init_bulk_mdata/fp/resources/cpu_per_node

cpu numbers of each node assigned to each job.

gpu_per_node:

type: int, optional, default: 0
argument path: init_bulk_mdata/fp/resources/gpu_per_node

gpu numbers of each node assigned to each job.

queue_name:

type: str, optional, default: (empty string)
argument path: init_bulk_mdata/fp/resources/queue_name

The queue name of batch job scheduler system.

group_size:

type: int
argument path: init_bulk_mdata/fp/resources/group_size

The number of *tasks* in a *job*. 0 means infinity.

custom_flags:

type: typing.List[str], optional
argument path: init_bulk_mdata/fp/resources/custom_flags

The extra lines pass to job submitting script header

strategy:

type: dict, optional

argument path: init_bulk_mdata/fp/resources/strategy

strategies we use to generation job submitting scripts.

if_cuda_multi_devices:

type: bool, optional, default: False
argument path: init_bulk_mdata/fp/resources/strategy/if_cuda_multi_devices

If there are multiple nvidia GPUS on the node, and we want to assign the tasks to different GPUS.If true, dpdispatcher will manually export environment variable CUDA_VISIBLE_DEVICES to different task.Usually, this option will be used with Task.task_need_resources variable simultaneously.

ratio_unfinished:

type: float, optional, default: 0.0
argument path: init_bulk_mdata/fp/resources/strategy/ratio_unfinished

The ratio of *tasks* that can be unfinished.

customized_script_header_template_file:

type: str, optional
argument path: init_bulk_mdata/fp/resources/strategy/customized_script_header_template_file

The customized template file to generate job submitting script header, which overrides the default file.

para_deg:

type: int, optional, default: 1
argument path: init_bulk_mdata/fp/resources/para_deg

Decide how many tasks will be run in parallel.

source_list:

type: typing.List[str], optional, default: []
argument path: init_bulk_mdata/fp/resources/source_list

The env file to be sourced before the command execution.

module_purge:

type: bool, optional, default: False
argument path: init_bulk_mdata/fp/resources/module_purge

Remove all modules on HPC system before module load (module_list)

module_unload_list:

type: typing.List[str], optional, default: []
argument path: init_bulk_mdata/fp/resources/module_unload_list

The modules to be unloaded on HPC system before submitting jobs

module_list:

type: typing.List[str], optional, default: []
argument path: init_bulk_mdata/fp/resources/module_list

The modules to be loaded on HPC system before submitting jobs

envs:

type: dict, optional, default: {}
argument path: init_bulk_mdata/fp/resources/envs

The environment variables to be exported on before submitting jobs

prepend_script:

type: typing.List[str], optional, default: []
argument path: init_bulk_mdata/fp/resources/prepend_script

Optional script run before jobs submitted.

append_script:

type: typing.List[str], optional, default: []
argument path: init_bulk_mdata/fp/resources/append_script

Optional script run after jobs submitted.

wait_time:

type: float | int, optional, default: 0

argument path: `init_bulk_mdata/fp/resources/wait_time`

The waitting time in second after a single *task* submitted

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

batch_type:

type: `str` (flag key)
argument path: `init_bulk_mdata/fp/resources/batch_type`
possible choices: *Fugaku*, *Slurm*, *SlurmJobArray*, *Shell*, *LSF*, *PBS*, *SGE*, *Torque*, *OpenAPI*, *DistributedShell*, *Bohrium*

The batch job system type loaded from machine/batch_type.

When batch_type is set to `Fugaku` (or its alias `fugaku`):

kwargs:

type: `dict`, optional
argument path: `init_bulk_mdata/fp/resources[Fugaku]/kwargs`

This field is empty for this batch.

When batch_type is set to `Slurm` (or its alias `slurm`):

kwargs:

type: `dict`, optional
argument path: `init_bulk_mdata/fp/resources[Slurm]/kwargs`

Extra arguments.

custom_gpu_line:

type: `str` | `NoneType`, optional, default: `None`
argument path: `init_bulk_mdata/fp/resources[Slurm]/kwargs/custom_gpu_line`

Custom GPU configuration, starting with #SBATCH

When batch_type is set to `SlurmJobArray` (or its alias `slurmjobarray`):

kwargs:

type: `dict`, optional
argument path: `init_bulk_mdata/fp/resources[SlurmJobArray]/kwargs`

Extra arguments.

custom_gpu_line:

type: str | NoneType, optional, default: None

argument path: init_bulk_mdata/fp/resources[SlurmJobArray]/kwargs/custom_gpu_line

Custom GPU configuration, starting with #SBATCH

slurm_job_size:

type: int, optional, default: 1

argument path: init_bulk_mdata/fp/resources[SlurmJobArray]/kwargs/slurm_job_size

Number of tasks in a Slurm job

When batch_type is set to Shell (or its alias shell):

kwargs:

type: dict, optional

argument path: init_bulk_mdata/fp/resources[Shell]/kwargs

This field is empty for this batch.

When batch_type is set to LSF (or its alias lsf):

kwargs:

type: dict

argument path: init_bulk_mdata/fp/resources[LSF]/kwargs

Extra arguments.

gpu_usage:

type: bool, optional, default: False

argument path: init_bulk_mdata/fp/resources[LSF]/kwargs/gpu_usage

Choosing if GPU is used in the calculation step.

gpu_new_syntax:

type: bool, optional, default: False

argument path: init_bulk_mdata/fp/resources[LSF]/kwargs/gpu_new_syntax

For LFS >= 10.1.0.3, new option -gpu for #BSUB could be used. If False, and old syntax would be used.

gpu_exclusive:

type: bool, optional, default: True

argument path: `init_bulk_mdata/fp/resources[LSF]/kwargs/gpu_exclusive`

Only take effect when new syntax enabled. Control whether submit tasks in exclusive way for GPU.

`custom_gpu_line:`

type: `str` | `NoneType`, optional, default: `None`

argument path: `init_bulk_mdata/fp/resources[LSF]/kwargs/custom_gpu_line`

Custom GPU configuration, starting with #BSUB

When batch_type is set to `PBS` (or its alias `pbs`):

`kwargs:`

type: `dict`, optional

argument path: `init_bulk_mdata/fp/resources[PBS]/kwargs`

This field is empty for this batch.

When batch_type is set to `SGE` (or its alias `sge`):

`kwargs:`

type: `dict`, optional

argument path: `init_bulk_mdata/fp/resources[SGE]/kwargs`

This field is empty for this batch.

When batch_type is set to `Torque` (or its alias `torque`):

`kwargs:`

type: `dict`, optional

argument path: `init_bulk_mdata/fp/resources[Torque]/kwargs`

This field is empty for this batch.

When batch_type is set to `OpenAPI` (or its alias `openapi`):

`kwargs:`

type: `dict`, optional

argument path: `init_bulk_mdata/fp/resources[OpenAPI]/kwargs`

This field is empty for this batch.

When batch_type is set to `DistributedShell` (or its alias `distributedshell`):

kwargs:

type: dict, optional
argument path: init_bulk_mdata/fp/resources[DistributedShell]/kwargs

This field is empty for this batch.

When batch_type is set to Bohrium (or its aliases bohrium, Lebesgue, lebesgue, DpCloudServer, dpcloudserver):

kwargs:

type: dict, optional
argument path: init_bulk_mdata/fp/resources[Bohrium]/kwargs

This field is empty for this batch.

user_forward_files:

type: list, optional
argument path: init_bulk_mdata/fp/user_forward_files

Files to be forwarded to the remote machine.

user_backward_files:

type: list, optional
argument path: init_bulk_mdata/fp/user_backward_files

Files to be backwarded from the remote machine.

5.4 Init_surf

You may prepare initial data for surface systems with VASP by:

```
dpgen init_surf PARAM [MACHINE]
```

The MACHINE configure file is optional. If this parameter exists, then the optimization tasks or MD tasks will be submitted automatically according to MACHINE.json. That is to say, if one only wants to prepare surf-xxx/sys-xxx folders for the second stage but wants to skip relaxation, dpgen init_surf PARAM should be used (without MACHINE). "stages" and "skip_relax" in PARAM should be set as:

```
  "stages": [1,2],
  "skip_relax": true,
```

Basically init_surf can be divided into two parts , denoted as *stages* in PARAM:

1. Build specific surface in folder 00.place_ele
2. Pertub and scale in folder 01.scale_pert

All stages must be **in order**.

Generally, init_surf does not run AIMD but only generates a lot of configurations. Compared with init_bulk, which runs DFT calculations twice, init_surf does once. Usually, we do init_bulk, run many rounds of DP-GEN

iterations, collect enough data for the bulk system, and do `init_surf` after that. At this point, the lattice constant has been determined, and the lattice constant required for the initial configuration of `init_surf` can be used directly. These configurations made by `init_surf` are prepared for `01.model_devi`. Candidates will do DFT calculation in `02.fp`.

- Generate vacuum layers

According to the source code of pert_scaled, init_surf will generate a series of surface structures with specified separations between the sample layer and its periodic image. There are two ways to specify the interval in generating the vacuum layers: 1) to set the interval value and 2) to set the number of intervals.

You can use *layer_numb* (the number of layers of the slab) or *z_min* (the total thickness) to specify the thickness of the atoms below. Then `vacuum_*` parameters specify the vacuum layers above. `dpgen init_surf` will make a series of structures with the thickness of vacuum layers from *vacuum_min* to *vacuum_max*. The number of vacuum layers is controlled by the parameter *vacuum_resol*.

The layers will be generated even when the size of *vacuum_resol* is 1. When the size of *vacuum_resol* is 2 or it is empty, the whole interval range is divided into the nearby region with denser intervals (head region) and the far-away region with sparser intervals (tail region), which are divided by *mid_point*.

When the size of *vacuum_resol* is 2, two elements respectively decide the number of intervals in head region and tail region.

When *vacuum_resol* is empty, the number of intervals in the head region = vacuum_num * head_ratio. *vacuum_num* and *head_ratio* are both keys in `param.json`.

- Attach files in the task path

One can use the machine parameter `forward_files` to upload other files besides POSCAR, INCAR, and POTCAR. For example, "vdw_kernal.bindat" for each task.

See the document of task parameters.

Following is an example for `PARAM`, which generates data from a typical structure fcc.

```
{
  "stages": [
    1,
    2
  ],
  "cell_type": "fcc",
  "latt": 4.034,
  "super_cell": [
    2,
    2,
    2
  ],
  "layer_numb": 3,
  "vacuum_max": 9.0,
  "vacuum_resol": [
    0.5,
    1
  ],
  "mid_point": 4.0,
  "millers": [
    [
      1,
      0,
```

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```
      0
    ],
    [
      1,
      1,
      0
    ],
    [
      1,
      1,
      1
    ]
  ],
  "elements": [
    "Al"
  ],
  "potcars": [
    "....../POTCAR"
  ],
  "relax_incar": "....../INCAR_metal_rlx_low",
  "scale": [
    1.0
  ],
  "skip_relax": true,
  "pert_numb": 2,
  "pert_box": 0.03,
  "pert_atom": 0.01,
  "_comment": "that's all"
}
```

Another example is `from_poscar` method. Here you need to specify the POSCAR file.

```
{
  "stages": [
    1,
    2
  ],
  "cell_type": "fcc",
  "from_poscar":        true,
  "from_poscar_path":        "POSCAR",
  "super_cell": [
    1,
    1,
    1
  ],
  "layer_numb": 3,
  "vacuum_max": 5.0,
  "vacuum_resol": [0.5,2],
  "mid_point": 2.0,
  "millers": [
    [
      1,
```

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```
      0,
      0
    ]
  ],
  "elements": [
    "Al"
  ],
  "potcars": [
    "./POTCAR"
  ],
  "relax_incar" : "INCAR_metal_rlx_low",
  "scale": [
    1.0
  ],
  "skip_relax": true,
  "pert_numb": 5,
  "pert_box": 0.03,
  "pert_atom": 0.01,
  "coll_ndata": 5000,
  "_comment": "that's all"
}
```

5.5 dpgen init_surf parameters

Note: One can load, modify, and export the input file by using our effective web-based tool DP-GUI online or hosted using the *command line interface* `dpgen gui`. All parameters below can be set in DP-GUI. By clicking "SAVE JSON", one can download the input file.

`init_surf_jdata:`

type: `dict`
argument path: `init_surf_jdata`

Generate initial data for surface systems.

`stages:`

type: `list[int]`
argument path: `init_surf_jdata/stages`

Stages for *init_surf*.

`elements:`

type: `list[str]`
argument path: `init_surf_jdata/elements`

Atom types.

`potcars:`

type: `list[str]`, optional
argument path: `init_surf_jdata/potcars`

Path of POTCAR.

cell_type:

type: str, optional

argument path: init_surf_jdata/cell_type

Specifying which typical structure to be generated. **Options** include fcc, hcp, bcc, sc, diamond.

super_cell:

type: list[int]

argument path: init_surf_jdata/super_cell

Size of supercell.

from_poscar:

type: bool, optional, default: False

argument path: init_surf_jdata/from_poscar

Deciding whether to use a given poscar as the beginning of relaxation. If it's true, keys (*cell_type*, *latt*) will be aborted. Otherwise, these two keys are **necessary**.

from_poscar_path:

type: str, optional

argument path: init_surf_jdata/from_poscar_path

Path of POSCAR for VASP or STRU for ABACUS. **Necessary** if *from_poscar* is true.

latt:

type: float

argument path: init_surf_jdata/latt

Lattice constant for single cell.

layer_numb:

type: int, optional

argument path: init_surf_jdata/layer_numb

Number of atom layers constructing the slab.

z_min:

type: int, optional

argument path: init_surf_jdata/z_min

Thickness of slab without vacuum (Angstrom). If *layer_numb* is set, *z_min* will be ignored.

vacuum_max:

type: float

argument path: init_surf_jdata/vacuum_max

Maximal thickness of vacuum (Angstrom).

vacuum_min:

type: float, optional

argument path: init_surf_jdata/vacuum_min

Minimal thickness of vacuum (Angstrom). Default value is 2 times atomic radius.

vacuum_resol:

type: list[float]

argument path: init_surf_jdata/vacuum_resol

Interval of thickness of vacuum. If size of *vacuum_resol* is 1, the interval is fixed to its value. If size of *vacuum_resol* is 2, the interval is *vacuum_resol[0]* before *mid_point*, otherwise *vacuum_resol[1]* after *mid_point*.

vacuum_numb:

type: int, optional

argument path: init_surf_jdata/vacuum_numb

The total number of vacuum layers **Necessary** if vacuum_resol is empty.

mid_point:

type: float, optional

argument path: init_surf_jdata/mid_point

The mid point separating head region and tail region. **Necessary** if the size of vacuum_resol is 2 or 0.

head_ratio:

type: float, optional

argument path: init_surf_jdata/head_ratio

Ratio of vacuum layers in the nearby region with denser intervals(head region). **Necessary** if vacuum_resol is empty.

millers:

type: list[list[int]]

argument path: init_surf_jdata/millers

Miller indices.

relax_incar:

type: str, optional

argument path: init_surf_jdata/relax_incar

Path of INCAR for relaxation in VASP. **Necessary** if *stages* include 1.

scale:

type: list[float]

argument path: init_surf_jdata/scale

Scales for isotropic transforming cells.

skip_relax:

type: bool

argument path: init_surf_jdata/skip_relax

If it's true, you may directly run stage 2 (perturb and scale) using an unrelaxed POSCAR.

pert_numb:

type: int

argument path: init_surf_jdata/pert_numb

Number of perturbations for each scaled (key *scale*) POSCAR.

pert_box:

type: `float`

argument path: `init_surf_jdata/pert_box`

Anisotropic Perturbation for cells (independent changes of lengths of three box vectors as well as angel among) in decimal formats. 9 elements of the 3x3 perturbation matrix will be randomly sampled from a uniform distribution (default) in the range [-pert_box, pert_box]. Such a perturbation matrix adds the identity matrix gives the actual transformation matrix for this perturbation operation.

pert_atom:

type: `float`

argument path: `init_surf_jdata/pert_atom`

Perturbation of atom coordinates (Angstrom). Random perturbations are performed on three coordinates of each atom by adding values randomly sampled from a uniform distribution in the range [-pert_atom, pert_atom].

coll_ndata:

type: `int`

argument path: `init_surf_jdata/coll_ndata`

Maximal number of collected data.

5.6 dpgen init_surf machine parameters

Note: One can load, modify, and export the input file by using our effective web-based tool DP-GUI online or hosted using the *command line interface* `dpgen gui`. All parameters below can be set in DP-GUI. By clicking "SAVE JSON", one can download the input file.

init_surf_mdata:

type: `dict`

argument path: `init_surf_mdata`

machine.json file

api_version:

type: `str`, optional, default: `1.0`

argument path: `init_surf_mdata/api_version`

Please set to 1.0

deepmd_version:

type: `str`, optional, default: `2`

argument path: `init_surf_mdata/deepmd_version`

DeePMD-kit version, e.g. 2.1.3

fp:

type: `dict`

argument path: `init_surf_mdata/fp`

Parameters of command, machine, and resources for fp

command:

type: str
argument path: init_surf_mdata/fp/command

Command of a program.

machine:

type: dict
argument path: init_surf_mdata/fp/machine

batch_type:

type: str
argument path: init_surf_mdata/fp/machine/batch_type

The batch job system type. Option: Slurm, LSF, DistributedShell, SGE, Shell, SlurmJobArray, PBS, OpenAPI, Torque, Bohrium, Fugaku

local_root:

type: str | NoneType
argument path: init_surf_mdata/fp/machine/local_root

The dir where the tasks and relating files locate. Typically the project dir.

remote_root:

type: str | NoneType, optional
argument path: init_surf_mdata/fp/machine/remote_root

The dir where the tasks are executed on the remote machine. Only needed when context is not lazy-local.

clean_asynchronously:

type: bool, optional, default: False
argument path: init_surf_mdata/fp/machine/clean_asynchronously

Clean the remote directory asynchronously after the job finishes.

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

context_type:

type: str (flag key)
argument path: init_surf_mdata/fp/machine/context_type

possible choices: *LocalContext*, *LazyLocalContext*, *BohriumContext*, *HDFSContext*, *OpenAPIContext*, *SSHContext*

The connection used to remote machine. Option: LazyLocalContext, HDFSContext, BohriumContext, SSHContext, LocalContext, OpenAPIContext

When context_type is set to `LocalContext` (or its aliases `localcontext`, `Local`, `local`):

remote_profile:

type: `dict`, optional

argument path: `init_surf_mdata/fp/machine[LocalContext]/remote_profile`

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to `LazyLocalContext` (or its aliases `lazylocalcontext`, `LazyLocal`, `lazylocal`):

remote_profile:

type: `dict`, optional

argument path: `init_surf_mdata/fp/machine[LazyLocalContext]/remote_profile`

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to `BohriumContext` (or its aliases `bohriumcontext`, `Bohrium`, `bohrium`, `DpCloudServerContext`, `dpcloudservercontext`, `DpCloudServer`, `dpcloudserver`, `LebesgueContext`, `lebesguecontext`, `Lebesgue`, `lebesgue`):

remote_profile:

type: `dict`

argument path: `init_surf_mdata/fp/machine[BohriumContext]/remote_profile`

The information used to maintain the connection with remote machine.

email:

type: `str`, optional

argument path: `init_surf_mdata/fp/machine[BohriumContext]/remote_profile/email`

Email

password:

type: str, optional

argument path: init_surf_mdata/fp/machine[BohriumContext]/remote_profile/password

Password

program_id:

type: int, alias: *project_id*

argument path: init_surf_mdata/fp/machine[BohriumContext]/remote_profile/program_id

Program ID

retry_count:

type: NoneType | int, optional, default: 2

argument path: init_surf_mdata/fp/machine[BohriumContext]/remote_profile/retry_count

The retry count when a job is terminated

ignore_exit_code:

type: bool, optional, default: True

argument path: init_surf_mdata/fp/machine[BohriumContext]/remote_profile/ignore_exit_code

The job state will be marked as finished if the exit code is non-zero when set to True. Otherwise,
the job state will be designated as terminated.

keep_backup:

type: bool, optional

argument path: init_surf_mdata/fp/machine[BohriumContext]/remote_profile/keep_backup

keep download and upload zip

input_data:

type: dict

argument path: init_surf_mdata/fp/machine[BohriumContext]/remote_profile/input_data

Configuration of job

When context_type is set to HDFSContext (or its aliases hdfscontext, HDFS, hdfs):

remote_profile:

type: dict, optional
argument path: init_surf_mdata/fp/machine[HDFSContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to OpenAPIContext (or its aliases openapicontext, OpenAPI, openapi):

remote_profile:

type: dict, optional
argument path: init_surf_mdata/fp/machine[OpenAPIContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to SSHContext (or its aliases sshcontext, SSH, ssh):

remote_profile:

type: dict
argument path: init_surf_mdata/fp/machine[SSHContext]/remote_profile

The information used to maintain the connection with remote machine.

hostname:

type: str
argument path: init_surf_mdata/fp/machine[SSHContext]/remote_profile/hostname

hostname or ip of ssh connection.

username:

type: str
argument path: init_surf_mdata/fp/machine[SSHContext]/remote_profile/username

username of target linux system

password:

type: str, optional
argument path: init_surf_mdata/fp/machine[SSHContext]/remote_profile/password

(deprecated) password of linux system. Please use SSH keys instead to improve security.

port:

type: int, optional, default: 22

argument path: init_surf_mdata/fp/machine[SSHContext]/remote_profile/port

ssh connection port.

key_filename:

type: str | NoneType, optional, default: None

argument path: init_surf_mdata/fp/machine[SSHContext]/remote_profile/key_filename

key filename used by ssh connection. If left None, find key in ~/.ssh or use password for login

passphrase:

type: str | NoneType, optional, default: None

argument path: init_surf_mdata/fp/machine[SSHContext]/remote_profile/passphrase

passphrase of key used by ssh connection

timeout:

type: int, optional, default: 10

argument path: init_surf_mdata/fp/machine[SSHContext]/remote_profile/timeout

timeout of ssh connection

totp_secret:

type: str | NoneType, optional, default: None

argument path: init_surf_mdata/fp/machine[SSHContext]/remote_profile/totp_secret

Time-based one time password secret. It should be a base32-encoded string extracted from the 2D code.

tar_compress:

type: bool, optional, default: True

argument path: init_surf_mdata/fp/machine[SSHContext]/remote_profile/tar_compress

The archive will be compressed in upload and download if it is True. If not, compression will be skipped.

look_for_keys:

type: bool, optional, default: True
argument path: init_surf_mdata/fp/machine[SSHContext]/remote_profile/look_for_keys

enable searching for discoverable private key files in ~/.ssh/

resources:

type: dict
argument path: init_surf_mdata/fp/resources

number_node:

type: int, optional, default: 1
argument path: init_surf_mdata/fp/resources/number_node

The number of node need for each *job*

cpu_per_node:

type: int, optional, default: 1
argument path: init_surf_mdata/fp/resources/cpu_per_node

cpu numbers of each node assigned to each job.

gpu_per_node:

type: int, optional, default: 0
argument path: init_surf_mdata/fp/resources/gpu_per_node

gpu numbers of each node assigned to each job.

queue_name:

type: str, optional, default: (empty string)
argument path: init_surf_mdata/fp/resources/queue_name

The queue name of batch job scheduler system.

group_size:

type: int
argument path: init_surf_mdata/fp/resources/group_size

The number of *tasks* in a *job*. 0 means infinity.

custom_flags:

type: typing.List[str], optional

argument path: init_surf_mdata/fp/resources/custom_flags

The extra lines pass to job submitting script header

strategy:

type: dict, optional
argument path: init_surf_mdata/fp/resources/strategy

strategies we use to generation job submitting scripts.

if_cuda_multi_devices:

type: bool, optional, default: False
argument path: init_surf_mdata/fp/resources/strategy/if_cuda_multi_devices

If there are multiple nvidia GPUS on the node, and we want to assign the tasks to different GPUS.If true, dpdispatcher will manually export environment variable CUDA_VISIBLE_DEVICES to different task.Usually, this option will be used with Task.task_need_resources variable simultaneously.

ratio_unfinished:

type: float, optional, default: 0.0
argument path: init_surf_mdata/fp/resources/strategy/ratio_unfinished

The ratio of *tasks* that can be unfinished.

customized_script_header_template_file:

type: str, optional
argument path: init_surf_mdata/fp/resources/strategy/customized_script_header_template_file

The customized template file to generate job submitting script header, which overrides the default file.

para_deg:

type: int, optional, default: 1
argument path: init_surf_mdata/fp/resources/para_deg

Decide how many tasks will be run in parallel.

source_list:

type: typing.List[str], optional, default: []
argument path: init_surf_mdata/fp/resources/source_list

The env file to be sourced before the command execution.

module_purge:

type: bool, optional, default: False
argument path: init_surf_mdata/fp/resources/module_purge

Remove all modules on HPC system before module load (module_list)

module_unload_list:

type: typing.List[str], optional, default: []
argument path: init_surf_mdata/fp/resources/module_unload_list

The modules to be unloaded on HPC system before submitting jobs

module_list:

type: typing.List[str], optional, default: []
argument path: init_surf_mdata/fp/resources/module_list

The modules to be loaded on HPC system before submitting jobs

envs:

type: dict, optional, default: {}
argument path: init_surf_mdata/fp/resources/envs

The environment variables to be exported on before submitting jobs

prepend_script:

type: typing.List[str], optional, default: []
argument path: init_surf_mdata/fp/resources/prepend_script

Optional script run before jobs submitted.

append_script:

type: typing.List[str], optional, default: []

argument path: `init_surf_mdata/fp/resources/append_script`

Optional script run after jobs submitted.

wait_time:

type: `float` | `int`, optional, default: `0`

argument path: `init_surf_mdata/fp/resources/wait_time`

The waitting time in second after a single *task* submitted

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

batch_type:

type: `str` (flag key)

argument path: `init_surf_mdata/fp/resources/batch_type`

possible choices: *Fugaku*, *Slurm*, *SlurmJobArray*, *Shell*, *LSF*, *PBS*, *SGE*, *Torque*, *OpenAPI*, *DistributedShell*, *Bohrium*

The batch job system type loaded from machine/batch_type.

When batch_type is set to `Fugaku` (or its alias `fugaku`):

kwargs:

type: `dict`, optional

argument path: `init_surf_mdata/fp/resources[Fugaku]/kwargs`

This field is empty for this batch.

When batch_type is set to `Slurm` (or its alias `slurm`):

kwargs:

type: `dict`, optional

argument path: `init_surf_mdata/fp/resources[Slurm]/kwargs`

Extra arguments.

custom_gpu_line:

type: `str` | `NoneType`, optional, default: `None`

argument path: `init_surf_mdata/fp/resources[Slurm]/kwargs/custom_gpu_line`

Custom GPU configuration, starting with #SBATCH

When batch_type is set to SlurmJobArray (or its alias slurmjobarray):

kwargs:

type: dict, optional

argument path: init_surf_mdata/fp/resources[SlurmJobArray]/kwargs

Extra arguments.

custom_gpu_line:

type: str | NoneType, optional, default: None

argument path: init_surf_mdata/fp/resources[SlurmJobArray]/kwargs/custom_gpu_line

Custom GPU configuration, starting with #SBATCH

slurm_job_size:

type: int, optional, default: 1

argument path: init_surf_mdata/fp/resources[SlurmJobArray]/kwargs/slurm_job_size

Number of tasks in a Slurm job

When batch_type is set to Shell (or its alias shell):

kwargs:

type: dict, optional

argument path: init_surf_mdata/fp/resources[Shell]/kwargs

This field is empty for this batch.

When batch_type is set to LSF (or its alias lsf):

kwargs:

type: dict

argument path: init_surf_mdata/fp/resources[LSF]/kwargs

Extra arguments.

gpu_usage:

type: bool, optional, default: False

argument path: init_surf_mdata/fp/resources[LSF]/kwargs/gpu_usage

Choosing if GPU is used in the calculation step.

gpu_new_syntax:

type: bool, optional, default: False

argument path: `init_surf_mdata/fp/resources[LSF]/kwargs/gpu_new_syntax`

For LFS >= 10.1.0.3, new option -gpu for #BSUB could be used. If False, and old syntax would be used.

gpu_exclusive:

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

argument path: `init_surf_mdata/fp/resources[LSF]/kwargs/gpu_exclusive`

Only take effect when new syntax enabled. Control whether submit tasks in exclusive way for GPU.

custom_gpu_line:

type: `str` | `NoneType`, optional, default: `None`

argument path: `init_surf_mdata/fp/resources[LSF]/kwargs/custom_gpu_line`

Custom GPU configuration, starting with #BSUB

When batch_type is set to `PBS` (or its alias `pbs`):

kwargs:

type: `dict`, optional

argument path: `init_surf_mdata/fp/resources[PBS]/kwargs`

This field is empty for this batch.

When batch_type is set to `SGE` (or its alias `sge`):

kwargs:

type: `dict`, optional

argument path: `init_surf_mdata/fp/resources[SGE]/kwargs`

This field is empty for this batch.

When batch_type is set to `Torque` (or its alias `torque`):

kwargs:

type: `dict`, optional

argument path: `init_surf_mdata/fp/resources[Torque]/kwargs`

This field is empty for this batch.

When batch_type is set to `OpenAPI` (or its alias `openapi`):

kwargs:

type: dict, optional
argument path: init_surf_mdata/fp/resources[OpenAPI]/kwargs

This field is empty for this batch.

When batch_type is set to DistributedShell (or its alias distributedshell):

kwargs:

type: dict, optional
argument path: init_surf_mdata/fp/resources[DistributedShell]/kwargs

This field is empty for this batch.

When batch_type is set to Bohrium (or its aliases bohrium, Lebesgue, lebesgue, DpCloudServer, dpcloudserver):

kwargs:

type: dict, optional
argument path: init_surf_mdata/fp/resources[Bohrium]/kwargs

This field is empty for this batch.

user_forward_files:

type: list, optional
argument path: init_surf_mdata/fp/user_forward_files

Files to be forwarded to the remote machine.

user_backward_files:

type: list, optional
argument path: init_surf_mdata/fp/user_backward_files

Files to be backwarded from the remote machine.

5.7 init_reaction

dpgen init_reaction is a workflow to initilize data for reactive systems of small gas-phase molecules. The workflow was introduced in the "Initialization" section of Energy & Fuels, 2021, 35 (1), 762–769.

To start the workflow, one needs a box containing reactive systems. The following packages are required for each of the step:

- Exploring: LAMMPS
- Sampling: MDDatasetBuilder
- Labeling: Gaussian

The Exploring step uses LAMMPS pair_style reaxff to run a short ReaxMD NVT MD simulation. In the Sampling step, molecular clusters are taken and k-means clustering algorithm is applied to remove the redundancy, which is described in Nature Communications, 11, 5713 (2020). The Labeling step calculates energies and forces using the Gaussian package.

An example of `reaction.json` is given below:

```
{
    "type_map": [
        "H",
        "O"
    ],
    "reaxff": {
        "data": "data.hydrogen",
        "ff": "ffield.reax.cho",
        "control": "lmp_control",
        "temp": 3000,
        "tau_t": 100,
        "dt": 0.1,
        "nstep": 10000,
        "dump_freq": 100
    },
    "cutoff": 3.5,
    "dataset_size": 100,
    "qmkeywords": "b3lyp/6-31g** force Geom=PrintInputOrient"
}
```

For detailed parameters, see *parametes* and *machine parameters*.

The genereated data can be used to continue DP-GEN concurrent learning workflow. Read Energy & Fuels, 2021, 35 (1), 762–769 for details.

5.8 dpgen init_reaction parameters

Note: One can load, modify, and export the input file by using our effective web-based tool DP-GUI online or hosted using the *command line interface* `dpgen gui`. All parameters below can be set in DP-GUI. By clicking "SAVE JSON", one can download the input file.

`init_reaction_jdata:`

type: `dict`

argument path: `init_reaction_jdata`

Generate initial data for reactive systems for small gas-phase molecules, from a ReaxFF NVT MD trajectory.

`type_map:`

type: `list[str]`

argument path: `init_reaction_jdata/type_map`

Type map, which should match types in the initial data. e.g. ["C", "H", "O"]

`reaxff:`

type: `dict`

argument path: `init_reaction_jdata/reaxff`

Parameters for ReaxFF NVT MD.

data:

type: `str`
argument path: `init_reaction_jdata/reaxff/data`

Path to initial LAMMPS data file. The atom_style should be charge.

ff:

type: `str`
argument path: `init_reaction_jdata/reaxff/ff`

Path to ReaxFF force field file. Available in the lammps/potentials directory.

control:

type: `str`
argument path: `init_reaction_jdata/reaxff/control`

Path to ReaxFF control file.

temp:

type: `int` | `float`
argument path: `init_reaction_jdata/reaxff/temp`

Target Temperature for the NVT MD simulation. Unit: K.

dt:

type: `int` | `float`
argument path: `init_reaction_jdata/reaxff/dt`

Real time for every time step. Unit: fs.

tau_t:

type: `int` | `float`
argument path: `init_reaction_jdata/reaxff/tau_t`

Time to determine how rapidly the temperature. Unit: fs.

dump_freq:

type: `int`
argument path:
`init_reaction_jdata/reaxff/dump_freq`

Frequency of time steps to collect trajectory.

nstep:

type: `int`
argument path: `init_reaction_jdata/reaxff/nstep`

Total steps to run the ReaxFF MD simulation.

cutoff:

type: float

argument path: init_reaction_jdata/cutoff

Cutoff radius to take clusters from the trajectory. Note that only a complete molecule or free radical will be taken.

dataset_size:

type: int

argument path: init_reaction_jdata/dataset_size

Collected dataset size for each bond type.

qmkeywords:

type: str

argument path: init_reaction_jdata/qmkeywords

Gaussian keywords for first-principle calculations. e.g. force mn15/6-31g** Geom=PrintInputOrient. Note that "force" job is necessary to collect data. Geom=PrintInputOrient should be used when there are more than 50 atoms in a cluster.

5.9 dpgen init_reaction machine parameters

Note: One can load, modify, and export the input file by using our effective web-based tool DP-GUI online or hosted using the *command line interface* `dpgen gui`. All parameters below can be set in DP-GUI. By clicking "SAVE JSON", one can download the input file.

init_reaction_mdata:

type: dict

argument path: init_reaction_mdata

machine.json file

api_version:

type: str, optional, default: 1.0

argument path: init_reaction_mdata/api_version

Please set to 1.0

deepmd_version:

type: str, optional, default: 2

argument path: init_reaction_mdata/deepmd_version

DeePMD-kit version, e.g. 2.1.3

reaxff:

type: dict

argument path: init_reaction_mdata/reaxff

Parameters of command, machine, and resources for reaxff

command:

type: str
argument path: init_reaction_mdata/reaxff/command

Command of a program.

machine:

type: dict
argument path: init_reaction_mdata/reaxff/machine

batch_type:

type: str
argument path: init_reaction_mdata/reaxff/machine/batch_type

The batch job system type. Option: Slurm, LSF, DistributedShell, SGE, Shell, SlurmJobArray, PBS, OpenAPI, Torque, Bohrium, Fugaku

local_root:

type: str | NoneType
argument path: init_reaction_mdata/reaxff/machine/local_root

The dir where the tasks and relating files locate. Typically the project dir.

remote_root:

type: str | NoneType, optional
argument path: init_reaction_mdata/reaxff/machine/remote_root

The dir where the tasks are executed on the remote machine. Only needed when context is not lazy-local.

clean_asynchronously:

type: bool, optional, default: False
argument path: init_reaction_mdata/reaxff/machine/clean_asynchronously

Clean the remote directory asynchronously after the job finishes.

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

context_type:

type: str (flag key)
argument path: init_reaction_mdata/reaxff/machine/context_type

possible choices: *LocalContext*, *LazyLocalContext*, *BohriumContext*, *HDFSContext*, *OpenAPIContext*, *SSHContext*

The connection used to remote machine. Option: LazyLocalContext, HDFSContext, BohriumContext, SSHContext, LocalContext, OpenAPIContext

When context_type is set to `LocalContext` (or its aliases `localcontext`, `Local`, `local`):

remote_profile:

type: `dict`, optional

argument path: `init_reaction_mdata/reaxff/machine[LocalContext]/remote_profile`

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to `LazyLocalContext` (or its aliases `lazylocalcontext`, `LazyLocal`, `lazylocal`):

remote_profile:

type: `dict`, optional

argument path: `init_reaction_mdata/reaxff/machine[LazyLocalContext]/remote_profile`

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to `BohriumContext` (or its aliases `bohriumcontext`, `Bohrium`, `bohrium`, `DpCloudServerContext`, `dpcloudservercontext`, `DpCloudServer`, `dpcloudserver`, `LebesgueContext`, `lebesguecontext`, `Lebesgue`, `lebesgue`):

remote_profile:

type: `dict`

argument path: `init_reaction_mdata/reaxff/machine[BohriumContext]/remote_profile`

The information used to maintain the connection with remote machine.

email:

type: `str`, optional

argument path: `init_reaction_mdata/reaxff/machine[BohriumContext]/remote_profile/email`

Email

password:

type: str, optional

argument path: init_reaction_mdata/reaxff/machine[BohriumContext]/remote_profile/password

Password

program_id:

type: int, alias: *project_id*

argument path: init_reaction_mdata/reaxff/machine[BohriumContext]/remote_profile/program_id

Program ID

retry_count:

type: NoneType | int, optional, default: 2

argument path: init_reaction_mdata/reaxff/machine[BohriumContext]/remote_profile/retry_count

The retry count when a job is terminated

ignore_exit_code:

type: bool, optional, default: True

argument path: init_reaction_mdata/reaxff/machine[BohriumContext]/remote_profile/ignore_exit_code

The job state will be marked as finished if the exit code is non-zero when set to True. Otherwise,
the job state will be designated as terminated.

keep_backup:

type: bool, optional

argument path: init_reaction_mdata/reaxff/machine[BohriumContext]/remote_profile/keep_backup

keep download and upload zip

input_data:

type: dict

argument path:
init_reaction_mdata/reaxff/
machine[BohriumContext]/
remote_profile/input_data

Configuration of job

When context_type is set to HDFSContext (or its aliases hdfscontext, HDFS, hdfs):

remote_profile:

type: dict, optional
argument path:
init_reaction_mdata/reaxff/
machine[HDFSContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to OpenAPIContext (or its aliases openapicontext, OpenAPI, openapi):

remote_profile:

type: dict, optional
argument path: init_reaction_mdata/
reaxff/machine[OpenAPIContext]/
remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to SSHContext (or its aliases sshcontext, SSH, ssh):

remote_profile:

type: dict
argument path:
init_reaction_mdata/reaxff/
machine[SSHContext]/remote_profile

The information used to maintain the connection with remote machine.

hostname:

type: str
argument path:
init_reaction_mdata/reaxff/
machine[SSHContext]/
remote_profile/hostname

hostname or ip of ssh connection.

username:

type: str

argument path: `init_reaction_mdata/reaxff/machine[SSHContext]/remote_profile/username`

username of target linux system

password:

type: `str`, optional

argument path: `init_reaction_mdata/reaxff/machine[SSHContext]/remote_profile/password`

(deprecated) password of linux system. Please use SSH keys instead to improve security.

port:

type: `int`, optional, default: `22`

argument path: `init_reaction_mdata/reaxff/machine[SSHContext]/remote_profile/port`

ssh connection port.

key_filename:

type: `str` | `NoneType`, optional, default: `None`

argument path: `init_reaction_mdata/reaxff/machine[SSHContext]/remote_profile/key_filename`

key filename used by ssh connection. If left None, find key in ~/.ssh or use password for login

passphrase:

type: `str` | `NoneType`, optional, default: `None`

argument path: `init_reaction_mdata/reaxff/machine[SSHContext]/remote_profile/passphrase`

passphrase of key used by ssh connection

timeout:

type: `int`, optional, default: `10`

argument path: `init_reaction_mdata/reaxff/machine[SSHContext]/remote_profile/timeout`

timeout of ssh connection

totp_secret:

type: str | NoneType, optional, default: None

argument path: init_reaction_mdata/reaxff/machine[SSHContext]/remote_profile/totp_secret

Time-based one time password secret. It should be a base32-encoded string extracted from the 2D code.

tar_compress:

type: bool, optional, default: True

argument path: init_reaction_mdata/reaxff/machine[SSHContext]/remote_profile/tar_compress

The archive will be compressed in upload and download if it is True. If not, compression will be skipped.

look_for_keys:

type: bool, optional, default: True

argument path: init_reaction_mdata/reaxff/machine[SSHContext]/remote_profile/look_for_keys

enable searching for discoverable private key files in ~/.ssh/

resources:

type: dict

argument path: init_reaction_mdata/reaxff/resources

number_node:

type: int, optional, default: 1

argument path: init_reaction_mdata/reaxff/resources/number_node

The number of node need for each *job*

cpu_per_node:

type: int, optional, default: 1

argument path: init_reaction_mdata/reaxff/resources/cpu_per_node

cpu numbers of each node assigned to each job.

gpu_per_node:

type: int, optional, default: 0

argument path: `init_reaction_mdata/reaxff/resources/gpu_per_node`

gpu numbers of each node assigned to each job.

queue_name:

type: `str`, optional, default: (empty string)

argument path: `init_reaction_mdata/reaxff/resources/queue_name`

The queue name of batch job scheduler system.

group_size:

type: `int`

argument path: `init_reaction_mdata/reaxff/resources/group_size`

The number of *tasks* in a *job*. 0 means infinity.

custom_flags:

type: `typing.List[str]`, optional

argument path: `init_reaction_mdata/reaxff/resources/custom_flags`

The extra lines pass to job submitting script header

strategy:

type: `dict`, optional

argument path: `init_reaction_mdata/reaxff/resources/strategy`

strategies we use to generation job submitting scripts.

if_cuda_multi_devices:

type: `bool`, optional, default: `False`

argument path: `init_reaction_mdata/reaxff/resources/strategy/if_cuda_multi_devices`

If there are multiple nvidia GPUS on the node, and we want to assign the tasks to different GPUS.If true, dpdispatcher will manually export environment variable CUDA_VISIBLE_DEVICES to different task.Usually, this option will be used with Task.task_need_resources variable simultaneously.

ratio_unfinished:

type: `float`, optional, default: `0.0`

argument path:
`init_reaction_mdata/reaxff/resources/strategy/ratio_unfinished`

The ratio of *tasks* that can be unfinished.

customized_script_header_template_file:

type: `str`, optional

argument path:
`init_reaction_mdata/reaxff/resources/strategy/customized_script_header_template_file`

The customized template file to generate job submitting script header, which overrides the default file.

para_deg:

type: `int`, optional, default: 1

argument path: `init_reaction_mdata/reaxff/resources/para_deg`

Decide how many tasks will be run in parallel.

source_list:

type: `typing.List[str]`, optional, default: `[]`

argument path: `init_reaction_mdata/reaxff/resources/source_list`

The env file to be sourced before the command execution.

module_purge:

type: `bool`, optional, default: `False`

argument path: `init_reaction_mdata/reaxff/resources/module_purge`

Remove all modules on HPC system before module load (module_list)

module_unload_list:

type: `typing.List[str]`, optional, default: `[]`

argument path: `init_reaction_mdata/reaxff/resources/module_unload_list`

The modules to be unloaded on HPC system before submitting jobs

module_list:

type: `typing.List[str]`, optional, default: `[]`

argument path: `init_reaction_mdata/reaxff/resources/module_list`

The modules to be loaded on HPC system before submitting jobs

envs:

type: `dict`, optional, default: `{}`

argument path: `init_reaction_mdata/reaxff/resources/envs`

The environment variables to be exported on before submitting jobs

prepend_script:

type: `typing.List[str]`, optional, default: `[]`

argument path: `init_reaction_mdata/reaxff/resources/prepend_script`

Optional script run before jobs submitted.

append_script:

type: `typing.List[str]`, optional, default: `[]`

argument path: `init_reaction_mdata/reaxff/resources/append_script`

Optional script run after jobs submitted.

wait_time:

type: `float | int`, optional, default: `0`

argument path: `init_reaction_mdata/reaxff/resources/wait_time`

The waitting time in second after a single *task* submitted

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

batch_type:

type: `str` (flag key)

argument path: `init_reaction_mdata/reaxff/resources/batch_type`

possible choices: *Fugaku*, *Slurm*, *SlurmJobArray*, *Shell*, *LSF*, *PBS*, *SGE*, *Torque*, *OpenAPI*, *DistributedShell*, *Bohrium*

The batch job system type loaded from machine/batch_type.

When batch_type is set to `Fugaku` (or its alias `fugaku`):

kwargs:

type: dict, optional
argument path: init_reaction_mdata/reaxff/resources[Fugaku]/kwargs

This field is empty for this batch.

When batch_type is set to Slurm (or its alias slurm):

kwargs:

type: dict, optional
argument path: init_reaction_mdata/reaxff/resources[Slurm]/kwargs

Extra arguments.

custom_gpu_line:

type: str | NoneType, optional, default: None
argument path: init_reaction_mdata/reaxff/resources[Slurm]/kwargs/custom_gpu_line

Custom GPU configuration, starting with #SBATCH

When batch_type is set to SlurmJobArray (or its alias slurmjobarray):

kwargs:

type: dict, optional
argument path: init_reaction_mdata/reaxff/resources[SlurmJobArray]/kwargs

Extra arguments.

custom_gpu_line:

type: str | NoneType, optional, default: None
argument path: init_reaction_mdata/reaxff/resources[SlurmJobArray]/kwargs/custom_gpu_line

Custom GPU configuration, starting with #SBATCH

slurm_job_size:

type: int, optional, default: 1
argument path: init_reaction_mdata/reaxff/resources[SlurmJobArray]/kwargs/slurm_job_size

Number of tasks in a Slurm job

When batch_type is set to `Shell` (or its alias `shell`):

kwargs:

type: `dict`, optional
argument path: `init_reaction_mdata/reaxff/resources[Shell]/kwargs`

This field is empty for this batch.

When batch_type is set to `LSF` (or its alias `lsf`):

kwargs:

type: `dict`
argument path: `init_reaction_mdata/reaxff/resources[LSF]/kwargs`

Extra arguments.

gpu_usage:

type: `bool`, optional, default: `False`
argument path: `init_reaction_mdata/reaxff/resources[LSF]/kwargs/gpu_usage`

Choosing if GPU is used in the calculation step.

gpu_new_syntax:

type: `bool`, optional, default: `False`
argument path: `init_reaction_mdata/reaxff/resources[LSF]/kwargs/gpu_new_syntax`

For LFS >= 10.1.0.3, new option -gpu for #BSUB could be used. If False, and old syntax would be used.

gpu_exclusive:

type: `bool`, optional, default: `True`
argument path: `init_reaction_mdata/reaxff/resources[LSF]/kwargs/gpu_exclusive`

Only take effect when new syntax enabled. Control whether submit tasks in exclusive way for GPU.

custom_gpu_line:

type: `str` | `NoneType`, optional, default: `None`
argument path: `init_reaction_mdata/reaxff/resources[LSF]/kwargs/custom_gpu_line`

Custom GPU configuration, starting with #BSUB

When batch_type is set to PBS (or its alias pbs):

kwargs:

type: dict, optional
argument path: init_reaction_mdata/reaxff/resources[PBS]/kwargs

This field is empty for this batch.

When batch_type is set to SGE (or its alias sge):

kwargs:

type: dict, optional
argument path: init_reaction_mdata/reaxff/resources[SGE]/kwargs

This field is empty for this batch.

When batch_type is set to Torque (or its alias torque):

kwargs:

type: dict, optional
argument path: init_reaction_mdata/reaxff/resources[Torque]/kwargs

This field is empty for this batch.

When batch_type is set to OpenAPI (or its alias openapi):

kwargs:

type: dict, optional
argument path: init_reaction_mdata/reaxff/resources[OpenAPI]/kwargs

This field is empty for this batch.

When batch_type is set to DistributedShell (or its alias distributedshell):

kwargs:

type: dict, optional
argument path: init_reaction_mdata/reaxff/resources[DistributedShell]/kwargs

This field is empty for this batch.

When batch_type is set to Bohrium (or its aliases bohrium, Lebesgue, lebesgue, DpCloudServer, dpcloudserver):

kwargs:

type: dict, optional

argument path: init_reaction_mdata/reaxff/resources[Bohrium]/kwargs

This field is empty for this batch.

user_forward_files:

type: list, optional
argument path: init_reaction_mdata/reaxff/user_forward_files

Files to be forwarded to the remote machine.

user_backward_files:

type: list, optional
argument path: init_reaction_mdata/reaxff/user_backward_files

Files to be backwarded from the remote machine.

build:

type: dict
argument path: init_reaction_mdata/build

Parameters of command, machine, and resources for build

command:

type: str
argument path: init_reaction_mdata/build/command

Command of a program.

machine:

type: dict
argument path: init_reaction_mdata/build/machine

batch_type:

type: str
argument path: init_reaction_mdata/build/machine/batch_type

The batch job system type. Option: Slurm, LSF, DistributedShell, SGE, Shell, SlurmJobArray, PBS, OpenAPI, Torque, Bohrium, Fugaku

local_root:

type: str | NoneType
argument path: init_reaction_mdata/build/machine/local_root

The dir where the tasks and relating files locate. Typically the project dir.

remote_root:

type: str | NoneType, optional

argument path: init_reaction_mdata/build/machine/remote_root

The dir where the tasks are executed on the remote machine. Only needed when context is not lazy-local.

clean_asynchronously:

type: bool, optional, default: False

argument path: init_reaction_mdata/build/machine/clean_asynchronously

Clean the remote directory asynchronously after the job finishes.

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

context_type:

type: str (flag key)

argument path: init_reaction_mdata/build/machine/context_type

possible choices: *LocalContext*, *LazyLocalContext*, *BohriumContext*, *HDFSContext*, *OpenAPIContext*, *SSHContext*

The connection used to remote machine. Option: LazyLocalContext, HDFSContext, BohriumContext, SSHContext, LocalContext, OpenAPIContext

When context_type is set to LocalContext (or its aliases localcontext, Local, local):

remote_profile:

type: dict, optional

argument path: init_reaction_mdata/build/machine[LocalContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to LazyLocalContext (or its aliases lazylocalcontext, LazyLocal, lazylocal):

remote_profile:

type: dict, optional

argument path: init_reaction_mdata/build/machine[LazyLocalContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to `BohriumContext` (or its aliases `bohriumcontext`, `Bohrium`, `bohrium`, `DpCloudServerContext`, `dpcloudservercontext`, `DpCloudServer`, `dpcloudserver`, `LebesgueContext`, `lebesguecontext`, `Lebesgue`, `lebesgue`):

remote_profile:

type: `dict`

argument path: `init_reaction_mdata/build/machine[BohriumContext]/remote_profile`

The information used to maintain the connection with remote machine.

email:

type: `str`, optional

argument path: `init_reaction_mdata/build/machine[BohriumContext]/remote_profile/email`

Email

password:

type: `str`, optional

argument path: `init_reaction_mdata/build/machine[BohriumContext]/remote_profile/password`

Password

program_id:

type: `int`, alias: *project_id*

argument path: `init_reaction_mdata/build/machine[BohriumContext]/remote_profile/program_id`

Program ID

retry_count:

type: `NoneType | int`, optional, default: `2`

argument path: `init_reaction_mdata/build/machine[BohriumContext]/remote_profile/retry_count`

The retry count when a job is terminated

ignore_exit_code:

type: bool, optional, default: True

argument path: init_reaction_mdata/build/machine[BohriumContext]/remote_profile/ignore_exit_code

The job state will be marked as finished if the exit code is non-zero when set to True. Otherwise, the job state will be designated as terminated.

keep_backup:

type: bool, optional

argument path: init_reaction_mdata/build/machine[BohriumContext]/remote_profile/keep_backup

keep download and upload zip

input_data:

type: dict

argument path: init_reaction_mdata/build/machine[BohriumContext]/remote_profile/input_data

Configuration of job

When context_type is set to HDFSContext (or its aliases hdfscontext, HDFS, hdfs):

remote_profile:

type: dict, optional

argument path: init_reaction_mdata/build/machine[HDFSContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to OpenAPIContext (or its aliases openapicontext, OpenAPI, openapi):

remote_profile:

type: dict, optional

argument path: init_reaction_mdata/build/machine[OpenAPIContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to SSHContext (or its aliases sshcontext, SSH, ssh):

remote_profile:

type: dict
argument path: init_reaction_mdata/build/machine[SSHContext]/remote_profile

The information used to maintain the connection with remote machine.

hostname:

type: str
argument path: init_reaction_mdata/build/machine[SSHContext]/remote_profile/hostname

hostname or ip of ssh connection.

username:

type: str
argument path: init_reaction_mdata/build/machine[SSHContext]/remote_profile/username

username of target linux system

password:

type: str, optional
argument path: init_reaction_mdata/build/machine[SSHContext]/remote_profile/password

(deprecated) password of linux system. Please use SSH keys instead to improve security.

port:

type: int, optional, default: 22
argument path: init_reaction_mdata/build/machine[SSHContext]/remote_profile/port

ssh connection port.

key_filename:

type: str | NoneType, optional, default: None
argument path: init_reaction_mdata/build/machine[SSHContext]/remote_profile/key_filename

key filename used by ssh connection. If left None, find key in ~/.ssh or use password for login

passphrase:

type: str | NoneType, optional, default: None

argument path: init_reaction_mdata/build/machine[SSHContext]/remote_profile/passphrase

passphrase of key used by ssh connection

timeout:

type: int, optional, default: 10

argument path: init_reaction_mdata/build/machine[SSHContext]/remote_profile/timeout

timeout of ssh connection

totp_secret:

type: str | NoneType, optional, default: None

argument path: init_reaction_mdata/build/machine[SSHContext]/remote_profile/totp_secret

Time-based one time password secret. It should be a base32-encoded string extracted from the 2D code.

tar_compress:

type: bool, optional, default: True

argument path: init_reaction_mdata/build/machine[SSHContext]/remote_profile/tar_compress

The archive will be compressed in upload and download if it is True. If not, compression will be skipped.

look_for_keys:

type: bool, optional, default: True

argument path: init_reaction_mdata/build/machine[SSHContext]/remote_profile/look_for_keys

enable searching for discoverable private key files in ~/.ssh/

resources:

type: dict
argument path: init_reaction_mdata/build/resources

number_node:

type: int, optional, default: 1
argument path: init_reaction_mdata/build/resources/number_node

The number of node need for each *job*

cpu_per_node:

type: int, optional, default: 1
argument path: init_reaction_mdata/build/resources/cpu_per_node

cpu numbers of each node assigned to each job.

gpu_per_node:

type: int, optional, default: 0
argument path: init_reaction_mdata/build/resources/gpu_per_node

gpu numbers of each node assigned to each job.

queue_name:

type: str, optional, default: (empty string)
argument path: init_reaction_mdata/build/resources/queue_name

The queue name of batch job scheduler system.

group_size:

type: int
argument path: init_reaction_mdata/build/resources/group_size

The number of *tasks* in a *job*. 0 means infinity.

custom_flags:

type: typing.List[str], optional
argument path: init_reaction_mdata/build/resources/custom_flags

The extra lines pass to job submitting script header

strategy:

type: dict, optional
argument path: init_reaction_mdata/build/resources/strategy

strategies we use to generation job submitting scripts.

if_cuda_multi_devices:

type: bool, optional, default: False

argument path: init_reaction_mdata/build/resources/strategy/if_cuda_multi_devices

If there are multiple nvidia GPUS on the node, and we want to assign the tasks to different GPUS.If true, dpdispatcher will manually export environment variable CUDA_VISIBLE_DEVICES to different task.Usually, this option will be used with Task.task_need_resources variable simultaneously.

ratio_unfinished:

type: float, optional, default: 0.0

argument path: init_reaction_mdata/build/resources/strategy/ratio_unfinished

The ratio of *tasks* that can be unfinished.

customized_script_header_template_file:

type: str, optional

argument path: init_reaction_mdata/build/resources/strategy/customized_script_header_template_file

The customized template file to generate job submitting script header, which overrides the default file.

para_deg:

type: int, optional, default: 1

argument path: init_reaction_mdata/build/resources/para_deg

Decide how many tasks will be run in parallel.

source_list:

type: typing.List[str], optional, default: []

argument path: init_reaction_mdata/build/resources/source_list

The env file to be sourced before the command execution.

module_purge:

type: bool, optional, default: False

argument path: init_reaction_mdata/build/resources/module_purge

Remove all modules on HPC system before module load (module_list)

module_unload_list:

type: typing.List[str], optional, default: []

argument path: init_reaction_mdata/build/resources/module_unload_list

The modules to be unloaded on HPC system before submitting jobs

module_list:

type: typing.List[str], optional, default: []

argument path: init_reaction_mdata/build/resources/module_list

The modules to be loaded on HPC system before submitting jobs

envs:

type: dict, optional, default: {}

argument path: init_reaction_mdata/build/resources/envs

The environment variables to be exported on before submitting jobs

prepend_script:

type: typing.List[str], optional, default: []

argument path: init_reaction_mdata/build/resources/prepend_script

Optional script run before jobs submitted.

append_script:

type: typing.List[str], optional, default: []

argument path: init_reaction_mdata/build/resources/append_script

Optional script run after jobs submitted.

wait_time:

type: float | int, optional, default: 0

argument path: `init_reaction_mdata/build/resources/wait_time`

The waitting time in second after a single *task* submitted

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

batch_type:

type: `str` (flag key)
argument path: `init_reaction_mdata/build/resources/batch_type`
possible choices: *Fugaku*, *Slurm*, *SlurmJobArray*, *Shell*, *LSF*, *PBS*, *SGE*, *Torque*, *OpenAPI*, *DistributedShell*, *Bohrium*

The batch job system type loaded from machine/batch_type.

When batch_type is set to `Fugaku` (or its alias `fugaku`):

kwargs:

type: `dict`, optional
argument path: `init_reaction_mdata/build/resources[Fugaku]/kwargs`

This field is empty for this batch.

When batch_type is set to `Slurm` (or its alias `slurm`):

kwargs:

type: `dict`, optional
argument path: `init_reaction_mdata/build/resources[Slurm]/kwargs`

Extra arguments.

custom_gpu_line:

type: `str` | `NoneType`, optional, default: `None`
argument path: `init_reaction_mdata/build/resources[Slurm]/kwargs/custom_gpu_line`

Custom GPU configuration, starting with #SBATCH

When batch_type is set to `SlurmJobArray` (or its alias `slurmjobarray`):

kwargs:

type: `dict`, optional

argument path: `init_reaction_mdata/build/resources[SlurmJobArray]/kwargs`

Extra arguments.

custom_gpu_line:

type: `str` | `NoneType`, optional, default: `None`

argument path: `init_reaction_mdata/build/resources[SlurmJobArray]/kwargs/custom_gpu_line`

Custom GPU configuration, starting with #SBATCH

slurm_job_size:

type: `int`, optional, default: `1`

argument path: `init_reaction_mdata/build/resources[SlurmJobArray]/kwargs/slurm_job_size`

Number of tasks in a Slurm job

When batch_type is set to `Shell` (or its alias `shell`):

kwargs:

type: `dict`, optional

argument path: `init_reaction_mdata/build/resources[Shell]/kwargs`

This field is empty for this batch.

When batch_type is set to `LSF` (or its alias `lsf`):

kwargs:

type: `dict`

argument path: `init_reaction_mdata/build/resources[LSF]/kwargs`

Extra arguments.

gpu_usage:

type: `bool`, optional, default: `False`

argument path: `init_reaction_mdata/build/resources[LSF]/kwargs/gpu_usage`

Choosing if GPU is used in the calculation step.

gpu_new_syntax:

type: `bool`, optional, default: `False`

argument path: `init_reaction_mdata/build/resources[LSF]/kwargs/gpu_new_syntax`

For LFS >= 10.1.0.3, new option -gpu for #BSUB could be used. If False, and old syntax would be used.

gpu_exclusive:

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

argument path: `init_reaction_mdata/build/resources[LSF]/kwargs/gpu_exclusive`

Only take effect when new syntax enabled. Control whether submit tasks in exclusive way for GPU.

custom_gpu_line:

type: `str` | `NoneType`, optional, default: `None`

argument path: `init_reaction_mdata/build/resources[LSF]/kwargs/custom_gpu_line`

Custom GPU configuration, starting with #BSUB

When batch_type is set to `PBS` (or its alias `pbs`):

kwargs:

type: `dict`, optional

argument path: `init_reaction_mdata/build/resources[PBS]/kwargs`

This field is empty for this batch.

When batch_type is set to `SGE` (or its alias `sge`):

kwargs:

type: `dict`, optional

argument path: `init_reaction_mdata/build/resources[SGE]/kwargs`

This field is empty for this batch.

When batch_type is set to `Torque` (or its alias `torque`):

kwargs:

type: `dict`, optional

argument path: `init_reaction_mdata/build/resources[Torque]/kwargs`

This field is empty for this batch.

When batch_type is set to OpenAPI (or its alias openapi):

kwargs:

type: dict, optional
argument path: init_reaction_mdata/build/resources[OpenAPI]/kwargs

This field is empty for this batch.

When batch_type is set to DistributedShell (or its alias distributedshell):

kwargs:

type: dict, optional
argument path: init_reaction_mdata/build/resources[DistributedShell]/kwargs

This field is empty for this batch.

When batch_type is set to Bohrium (or its aliases bohrium, Lebesgue, lebesgue, DpCloudServer, dpcloudserver):

kwargs:

type: dict, optional
argument path: init_reaction_mdata/build/resources[Bohrium]/kwargs

This field is empty for this batch.

user_forward_files:

type: list, optional
argument path: init_reaction_mdata/build/user_forward_files

Files to be forwarded to the remote machine.

user_backward_files:

type: list, optional
argument path: init_reaction_mdata/build/user_backward_files

Files to be backwarded from the remote machine.

fp:

type: dict
argument path: init_reaction_mdata/fp

Parameters of command, machine, and resources for fp

command:

type: str
argument path: init_reaction_mdata/fp/command

Command of a program.

machine:

type: dict
argument path: init_reaction_mdata/fp/machine

batch_type:

type: str
argument path: init_reaction_mdata/fp/machine/batch_type

The batch job system type. Option: Slurm, LSF, DistributedShell, SGE, Shell, SlurmJobArray, PBS, OpenAPI, Torque, Bohrium, Fugaku

local_root:

type: str | NoneType
argument path: init_reaction_mdata/fp/machine/local_root

The dir where the tasks and relating files locate. Typically the project dir.

remote_root:

type: str | NoneType, optional
argument path: init_reaction_mdata/fp/machine/remote_root

The dir where the tasks are executed on the remote machine. Only needed when context is not lazy-local.

clean_asynchronously:

type: bool, optional, default: False
argument path: init_reaction_mdata/fp/machine/clean_asynchronously

Clean the remote directory asynchronously after the job finishes.

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

context_type:

type: str (flag key)
argument path: init_reaction_mdata/fp/machine/context_type
possible choices: *LocalContext*, *LazyLocalContext*, *BohriumContext*, *HDFSContext*, *OpenAPIContext*, *SSHContext*

The connection used to remote machine. Option: LazyLocalContext, HDFSContext,

BohriumContext, SSHContext, LocalContext, OpenAPIContext

When context_type is set to `LocalContext` (or its aliases `localcontext`, `Local`, `local`):

remote_profile:

type: `dict`, optional

argument path: `init_reaction_mdata/fp/machine[LocalContext]/remote_profile`

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to `LazyLocalContext` (or its aliases `lazylocalcontext`, `LazyLocal`, `lazylocal`):

remote_profile:

type: `dict`, optional

argument path: `init_reaction_mdata/fp/machine[LazyLocalContext]/remote_profile`

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to `BohriumContext` (or its aliases `bohriumcontext`, `Bohrium`, `bohrium`, `DpCloudServerContext`, `dpcloudservercontext`, `DpCloudServer`, `dpcloudserver`, `LebesgueContext`, `lebesguecontext`, `Lebesgue`, `lebesgue`):

remote_profile:

type: `dict`

argument path: `init_reaction_mdata/fp/machine[BohriumContext]/remote_profile`

The information used to maintain the connection with remote machine.

email:

type: `str`, optional

argument path: `init_reaction_mdata/fp/machine[BohriumContext]/remote_profile/email`

Email

password:

type: `str`, optional

argument path:
`init_reaction_mdata/fp/`
`machine[BohriumContext]/`
`remote_profile/password`

Password

program_id:

type: `int`, alias: *project_id*

argument path:
`init_reaction_mdata/fp/`
`machine[BohriumContext]/`
`remote_profile/program_id`

Program ID

retry_count:

type: `NoneType | int`, optional, default: `2`

argument path:
`init_reaction_mdata/fp/`
`machine[BohriumContext]/`
`remote_profile/retry_count`

The retry count when a job is terminated

ignore_exit_code:

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

argument path:
`init_reaction_mdata/fp/`
`machine[BohriumContext]/`
`remote_profile/`
`ignore_exit_code`

The job state will be marked as finished if the exit code is non-zero when set to True. Otherwise,
the job state will be designated as terminated.

keep_backup:

type: `bool`, optional

argument path:
`init_reaction_mdata/fp/`
`machine[BohriumContext]/`
`remote_profile/keep_backup`

keep download and upload zip

input_data:

type: `dict`

argument path:
`init_reaction_mdata/fp/`
`machine[BohriumContext]/`
`remote_profile/input_data`

Configuration of job

When context_type is set to HDFSContext (or its aliases hdfscontext, HDFS, hdfs):

remote_profile:

type: dict, optional

argument path: init_reaction_mdata/fp/machine[HDFSContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to OpenAPIContext (or its aliases openapicontext, OpenAPI, openapi):

remote_profile:

type: dict, optional

argument path: init_reaction_mdata/fp/machine[OpenAPIContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to SSHContext (or its aliases sshcontext, SSH, ssh):

remote_profile:

type: dict

argument path: init_reaction_mdata/fp/machine[SSHContext]/remote_profile

The information used to maintain the connection with remote machine.

hostname:

type: str

argument path: init_reaction_mdata/fp/machine[SSHContext]/remote_profile/hostname

hostname or ip of ssh connection.

username:

type: str

argument path: init_reaction_mdata/fp/machine[SSHContext]/remote_profile/username

username of target linux system

password:

type: str, optional

argument path:
`init_reaction_mdata/fp/machine[SSHContext]/remote_profile/password`

(deprecated) password of linux system. Please use SSH keys instead to improve security.

port:

type: `int`, optional, default: `22`

argument path:
`init_reaction_mdata/fp/machine[SSHContext]/remote_profile/port`

ssh connection port.

key_filename:

type: `str` | `NoneType`, optional, default: `None`

argument path:
`init_reaction_mdata/fp/machine[SSHContext]/remote_profile/key_filename`

key filename used by ssh connection. If left None, find key in ~/.ssh or use password for login

passphrase:

type: `str` | `NoneType`, optional, default: `None`

argument path:
`init_reaction_mdata/fp/machine[SSHContext]/remote_profile/passphrase`

passphrase of key used by ssh connection

timeout:

type: `int`, optional, default: `10`

argument path:
`init_reaction_mdata/fp/machine[SSHContext]/remote_profile/timeout`

timeout of ssh connection

totp_secret:

type: `str` | `NoneType`, optional, default: `None`

argument path:
`init_reaction_mdata/fp/machine[SSHContext]/remote_profile/totp_secret`

Time-based one time password secret. It should be a base32-encoded string extracted from the 2D code.

tar_compress:

type: bool, optional, default: True

argument path: init_reaction_mdata/fp/machine[SSHContext]/remote_profile/tar_compress

The archive will be compressed in upload and download if it is True. If not, compression will be skipped.

look_for_keys:

type: bool, optional, default: True

argument path: init_reaction_mdata/fp/machine[SSHContext]/remote_profile/look_for_keys

enable searching for discoverable private key files in ~/.ssh/

resources:

type: dict

argument path: init_reaction_mdata/fp/resources

number_node:

type: int, optional, default: 1

argument path: init_reaction_mdata/fp/resources/number_node

The number of node need for each *job*

cpu_per_node:

type: int, optional, default: 1

argument path: init_reaction_mdata/fp/resources/cpu_per_node

cpu numbers of each node assigned to each job.

gpu_per_node:

type: int, optional, default: 0

argument path: init_reaction_mdata/fp/resources/gpu_per_node

gpu numbers of each node assigned to each job.

queue_name:

type: str, optional, default: (empty string)

argument path: init_reaction_mdata/fp/resources/queue_name

The queue name of batch job scheduler system.

group_size:

type: int

argument path: init_reaction_mdata/fp/resources/group_size

The number of *tasks* in a *job*. 0 means infinity.

custom_flags:

type: typing.List[str], optional

argument path: init_reaction_mdata/fp/resources/custom_flags

The extra lines pass to job submitting script header

strategy:

type: dict, optional

argument path: init_reaction_mdata/fp/resources/strategy

strategies we use to generation job submitting scripts.

if_cuda_multi_devices:

type: bool, optional, default: False

argument path: init_reaction_mdata/fp/resources/strategy/if_cuda_multi_devices

If there are multiple nvidia GPUS on the node, and we want to assign the tasks to different GPUS.If true, dpdispatcher will manually export environment variable CUDA_VISIBLE_DEVICES to different task.Usually, this option will be used with Task.task_need_resources variable simultaneously.

ratio_unfinished:

type: float, optional, default: 0.0

argument path: init_reaction_mdata/fp/resources/strategy/ratio_unfinished

The ratio of *tasks* that can be unfinished.

customized_script_header_template_file:

type: str, optional

argument path: init_reaction_mdata/fp/

resources/strategy/
customized_script_header_template_file

The customized template file to generate job submitting script header, which overrides the default file.

para_deg:

type: int, optional, default: 1
argument path: init_reaction_mdata/fp/
resources/para_deg

Decide how many tasks will be run in parallel.

source_list:

type: typing.List[str], optional, default:
[]
argument path: init_reaction_mdata/fp/
resources/source_list

The env file to be sourced before the command execution.

module_purge:

type: bool, optional, default: False
argument path: init_reaction_mdata/fp/
resources/module_purge

Remove all modules on HPC system before module load (module_list)

module_unload_list:

type: typing.List[str], optional, default:
[]
argument path: init_reaction_mdata/fp/
resources/module_unload_list

The modules to be unloaded on HPC system before submitting jobs

module_list:

type: typing.List[str], optional, default:
[]
argument path: init_reaction_mdata/fp/
resources/module_list

The modules to be loaded on HPC system before submitting jobs

envs:

type: dict, optional, default: {}
argument path: init_reaction_mdata/fp/
resources/envs

The environment variables to be exported on before submitting jobs

prepend_script:

type: `typing.List[str]`, optional, default: `[]`
argument path: `init_reaction_mdata/fp/resources/prepend_script`

Optional script run before jobs submitted.

append_script:

type: `typing.List[str]`, optional, default: `[]`
argument path: `init_reaction_mdata/fp/resources/append_script`

Optional script run after jobs submitted.

wait_time:

type: `float | int`, optional, default: `0`
argument path: `init_reaction_mdata/fp/resources/wait_time`

The waitting time in second after a single *task* submitted

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

batch_type:

type: `str` (flag key)
argument path: `init_reaction_mdata/fp/resources/batch_type`
possible choices: *Fugaku*, *Slurm*, *SlurmJobArray*, *Shell*, *LSF*, *PBS*, *SGE*, *Torque*, *OpenAPI*, *DistributedShell*, *Bohrium*

The batch job system type loaded from machine/batch_type.

When batch_type is set to `Fugaku` (or its alias `fugaku`):

kwargs:

type: `dict`, optional
argument path: `init_reaction_mdata/fp/resources[Fugaku]/kwargs`

This field is empty for this batch.

When batch_type is set to `Slurm` (or its alias `slurm`):

kwargs:

type: `dict`, optional

argument path: `init_reaction_mdata/fp/resources[Slurm]/kwargs`

Extra arguments.

custom_gpu_line:

type: `str` | `NoneType`, optional, default: `None`

argument path: `init_reaction_mdata/fp/resources[Slurm]/kwargs/custom_gpu_line`

Custom GPU configuration, starting with #SBATCH

When batch_type is set to `SlurmJobArray` (or its alias `slurmjobarray`):

kwargs:

type: `dict`, optional

argument path: `init_reaction_mdata/fp/resources[SlurmJobArray]/kwargs`

Extra arguments.

custom_gpu_line:

type: `str` | `NoneType`, optional, default: `None`

argument path: `init_reaction_mdata/fp/resources[SlurmJobArray]/kwargs/custom_gpu_line`

Custom GPU configuration, starting with #SBATCH

slurm_job_size:

type: `int`, optional, default: `1`

argument path: `init_reaction_mdata/fp/resources[SlurmJobArray]/kwargs/slurm_job_size`

Number of tasks in a Slurm job

When batch_type is set to `Shell` (or its alias `shell`):

kwargs:

type: `dict`, optional

argument path: `init_reaction_mdata/fp/resources[Shell]/kwargs`

This field is empty for this batch.

When batch_type is set to `LSF` (or its alias `lsf`):

kwargs:

type: dict
argument path: init_reaction_mdata/fp/resources[LSF]/kwargs

Extra arguments.

gpu_usage:

type: bool, optional, default: False
argument path: init_reaction_mdata/fp/resources[LSF]/kwargs/gpu_usage

Choosing if GPU is used in the calculation step.

gpu_new_syntax:

type: bool, optional, default: False
argument path: init_reaction_mdata/fp/resources[LSF]/kwargs/gpu_new_syntax

For LFS >= 10.1.0.3, new option -gpu for #BSUB could be used. If False, and old syntax would be used.

gpu_exclusive:

type: bool, optional, default: True
argument path: init_reaction_mdata/fp/resources[LSF]/kwargs/gpu_exclusive

Only take effect when new syntax enabled. Control whether submit tasks in exclusive way for GPU.

custom_gpu_line:

type: str | NoneType, optional, default: None
argument path: init_reaction_mdata/fp/resources[LSF]/kwargs/custom_gpu_line

Custom GPU configuration, starting with #BSUB

When batch_type is set to PBS (or its alias pbs):

kwargs:

type: dict, optional
argument path: init_reaction_mdata/fp/resources[PBS]/kwargs

This field is empty for this batch.

When batch_type is set to SGE (or its alias sge):

kwargs:

type: dict, optional
argument path: init_reaction_mdata/fp/resources[SGE]/kwargs

This field is empty for this batch.

When batch_type is set to Torque (or its alias torque):

kwargs:

type: dict, optional
argument path: init_reaction_mdata/fp/resources[Torque]/kwargs

This field is empty for this batch.

When batch_type is set to OpenAPI (or its alias openapi):

kwargs:

type: dict, optional
argument path: init_reaction_mdata/fp/resources[OpenAPI]/kwargs

This field is empty for this batch.

When batch_type is set to DistributedShell (or its alias distributedshell):

kwargs:

type: dict, optional
argument path: init_reaction_mdata/fp/resources[DistributedShell]/kwargs

This field is empty for this batch.

When batch_type is set to Bohrium (or its aliases bohrium, Lebesgue, lebesgue, DpCloudServer, dpcloudserver):

kwargs:

type: dict, optional
argument path: init_reaction_mdata/fp/resources[Bohrium]/kwargs

This field is empty for this batch.

user_forward_files:

type: list, optional
argument path: init_reaction_mdata/fp/user_forward_files

Files to be forwarded to the remote machine.

user_backward_files:

type: list, optional
argument path:
init_reaction_mdata/fp/user_backward_files

Files to be backwarded from the remote machine.

CHAPTER

SIX

SIMPLIFY

6.1 Simplify

When you have a dataset containing lots of repeated data, this step will help you simplify your dataset. The workflow contains three stages: train, model_devi, and fp. The train stage and the fp stage are as the same as the run step, and the model_devi stage will calculate model deviations of the rest data that has not been confirmed accurate. Data with small model deviations will be confirmed accurate, while the program will pick data from those with large model deviations to the new dataset.

Use the following script to start the workflow:

```
dpgen simplify param.json machine.json
```

Here is an example of `param.json` for QM7 dataset:

```
{
    "type_map": [
        "C",
        "H",
        "N",
        "O",
        "S"
    ],
    "mass_map": [
        12.011,
        1.008,
        14.007,
        15.999,
        32.065
    ],
    "pick_data": "/scratch/jz748/simplify/qm7",
    "init_data_prefix": "",
    "init_data_sys": [],
    "sys_batch_size": [
        "auto"
    ],
    "numb_models": 4,
    "default_training_param": {
        "model": {
            "type_map": [
                "C",
```

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```
            "H",
            "N",
            "O",
            "S"
        ],
        "descriptor": {
            "type": "se_a",
            "sel": [
                7,
                16,
                3,
                3,
                1
            ],
            "rcut_smth": 1.00,
            "rcut": 6.00,
            "neuron": [
                25,
                50,
                100
            ],
            "resnet_dt": false,
            "axis_neuron": 12
        },
        "fitting_net": {
            "neuron": [
                240,
                240,
                240
            ],
            "resnet_dt": true
        }
    },
    "learning_rate": {
        "type": "exp",
        "start_lr": 0.001,
        "stop_lr": 5e-8,
        "decay_rate": 0.99
    },
    "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,
        "start_pref_pf": 0,
        "limit_pref_pf": 0
    },
    "training": {
        "set_prefix": "set",
        "numb_steps": 10000,
```

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```
            "disp_file": "lcurve.out",
            "disp_freq": 1000,
            "numb_test": 1,
            "save_freq": 1000,
            "disp_training": true,
            "time_training": true,
            "profiling": false,
            "profiling_file": "timeline.json"
        },
        "_comment": "that's all"
    },
    "fp_style": "gaussian",
    "shuffle_poscar": false,
    "fp_task_max": 1000,
    "fp_task_min": 10,
    "fp_pp_path": "/home/jzzeng/",
    "fp_pp_files": [],
    "fp_params": {
        "keywords": "mn15/6-31g** force nosymm scf(maxcyc=512)",
        "nproc": 28,
        "multiplicity": 1,
        "_comment": " that's all "
    },
    "init_pick_number":100,
    "iter_pick_number":100,
    "model_devi_f_trust_lo":0.25,
    "model_devi_f_trust_hi":0.45,
    "_comment": " that's all "
}
```

Here *pick_data* is the directory to data to simplify where the program recursively detects systems `System` with `deepmd/npy` format. *init_pick_number* and *iter_pick_number* are the numbers of picked frames. *model_devi_f_trust_lo* and *model_devi_f_trust_hi* mean the range of the max deviation of atomic forces in a frame. *fp_style* can be either `gaussian` or `vasp` currently. Other parameters are as the same as those of generator.

6.2 dpgen simplify parameters

Note: One can load, modify, and export the input file by using our effective web-based tool DP-GUI online or hosted using the *command line interface* `dpgen gui`. All parameters below can be set in DP-GUI. By clicking "SAVE JSON", one can download the input file.

simplify_jdata:

type: `dict`
argument path: `simplify_jdata`

Parameters for simplify.json, the first argument of *dpgen simplify*.

type_map:

type: `list[str]`
argument path: `simplify_jdata/type_map`

Atom types. Reminder: The elements in param.json, type.raw and data.lmp(when using lammps) should be in the same order.

mass_map:

type: `str | list[float]`, optional, default: `auto`

argument path: `simplify_jdata/mass_map`

Standard atomic weights (default: "auto"). if one want to use isotopes, or non-standard element names, chemical symbols, or atomic number in the type_map list, please customize the mass_map list instead of using "auto".

use_ele_temp:

type: `int`, optional, default: `0`

argument path: `simplify_jdata/use_ele_temp`

Currently only support fp_style vasp.

- 0: no electron temperature.
- 1: eletron temperature as frame parameter.
- 2: electron temperature as atom parameter.

init_data_prefix:

type: `str`, optional

argument path: `simplify_jdata/init_data_prefix`

Prefix of initial data directories.

init_data_sys:

type: `list[str]`

argument path: `simplify_jdata/init_data_sys`

Paths of initial data. The path can be either a system diretory containing NumPy files or an HDF5 file. You may use either absolute or relative path here. Systems will be detected recursively in the directories or the HDF5 file.

sys_format:

type: `str`, optional, default: `vasp/poscar`

argument path: `simplify_jdata/sys_format`

Format of sys_configs.

init_batch_size:

type: `list[typing.Union[int, str]] | str`, optional

argument path: `simplify_jdata/init_batch_size`

Each number is the batch_size of corresponding system for training in init_data_sys. One recommended rule for setting the sys_batch_size and init_batch_size is that batch_size mutiply number of atoms ot the stucture should be larger than 32. If set to auto, batch size will be 32 divided by number of atoms. This argument will not override the mixed batch size in *default_training_param*.

sys_configs_prefix:

type: `str`, optional

argument path: `simplify_jdata/sys_configs_prefix`

Prefix of sys_configs.

sys_configs:

type: `list[list[str]]`

argument path: simplify_jdata/sys_configs

2D list. Containing directories of structures to be explored in iterations for each system. Wildcard characters are supported here.

sys_batch_size:

type: list[typing.Union[int, str]], optional

argument path: simplify_jdata/sys_batch_size

Each number is the batch_size for training of corresponding system in sys_configs. If set to auto, batch size will be 32 divided by number of atoms. This argument will not override the mixed batch size in *default_training_param*.

labeled:

type: bool, optional, default: False

argument path: simplify_jdata/labeled

If true, the initial data is labeled.

pick_data:

type: str | list[str]

argument path: simplify_jdata/pick_data

(List of) Path to the directory with the pick data with the deepmd/npy or the HDF5 file with deepmd/hdf5 format. Systems are detected recursively.

init_pick_number:

type: int

argument path: simplify_jdata/init_pick_number

The number of initial pick data.

iter_pick_number:

type: int

argument path: simplify_jdata/iter_pick_number

The number of pick data in each iteration.

model_devi_f_trust_lo:

type: float

argument path: simplify_jdata/model_devi_f_trust_lo

The lower bound of forces for the selection for the model deviation.

model_devi_f_trust_hi:

type: float

argument path: simplify_jdata/model_devi_f_trust_hi

The higher bound of forces for the selection for the model deviation.

model_devi_e_trust_lo:

type: float, optional, default: 10000000000.0

argument path: simplify_jdata/model_devi_e_trust_lo

The lower bound of energy per atom for the selection for the model deviation. Requires DeePMD-kit version >=2.2.2.

model_devi_e_trust_hi:

type: float, optional, default: 10000000000.0

argument path: simplify_jdata/model_devi_e_trust_hi

The higher bound of energy per atom for the selection for the model deviation. Requires DeePMD-kit version >=2.2.2.

true_error_f_trust_lo:

type: float, optional, default: 10000000000.0

argument path: simplify_jdata/true_error_f_trust_lo

The lower bound of forces for the selection for the true error. Requires DeePMD-kit version >=2.2.4.

true_error_f_trust_hi:

type: float, optional, default: 10000000000.0

argument path: simplify_jdata/true_error_f_trust_hi

The higher bound of forces for the selection for the true error. Requires DeePMD-kit version >=2.2.4.

true_error_e_trust_lo:

type: float, optional, default: 10000000000.0

argument path: simplify_jdata/true_error_e_trust_lo

The lower bound of energy per atom for the selection for the true error. Requires DeePMD-kit version >=2.2.4.

true_error_e_trust_hi:

type: float, optional, default: 10000000000.0

argument path: simplify_jdata/true_error_e_trust_hi

The higher bound of energy per atom for the selection for the true error. Requires DeePMD-kit version >=2.2.4.

numb_models:

type: int

argument path: simplify_jdata/numb_models

Number of models to be trained in 00.train. 4 is recommend.

training_iter0_model_path:

type: list[str], optional

argument path: simplify_jdata/training_iter0_model_path

The model used to init the first iter training. Number of element should be equal to numb_models.

training_init_model:

type: bool, optional

argument path: simplify_jdata/training_init_model

Iteration > 0, the model parameters will be initilized from the model trained at the previous iteration. Iteration == 0, the model parameters will be initialized from training_iter0_model_path.

default_training_param:

type: dict

argument path: simplify_jdata/default_training_param

Training parameters for deepmd-kit in 00.train. You can find instructions from DeePMD-kit documentation.

dp_train_skip_neighbor_stat:

type: bool, optional, default: False

argument path: simplify_jdata/dp_train_skip_neighbor_stat

Append –skip-neighbor-stat flag to dp train.

dp_compress:

type: bool, optional, default: False

argument path: simplify_jdata/dp_compress

Use dp compress to compress the model.

training_reuse_iter:

type: int | NoneType, optional

argument path: simplify_jdata/training_reuse_iter

The minimal index of iteration that continues training models from old models of last iteration.

training_reuse_old_ratio:

type: str | float, optional, default: auto

argument path: simplify_jdata/training_reuse_old_ratio

The probability proportion of old data during training. It can be:

- float: directly assign the probability of old data;
- *auto:f*: automatic probability, where f is the new-to-old ratio;
- *auto*: equivalent to *auto:10*.

  This option is only adopted when continuing training models from old models. This option will override default parameters.

training_reuse_numb_steps:

type: int | NoneType, optional, default: None, alias: *training_reuse_stop_batch*

argument path: simplify_jdata/training_reuse_numb_steps

Number of training batch. This option is only adopted when continuing training models from old models. This option will override default parameters.

training_reuse_start_lr:

type: float | NoneType, optional, default: None

argument path: simplify_jdata/training_reuse_start_lr

The learning rate the start of the training. This option is only adopted when continuing training models from old models. This option will override default parameters.

training_reuse_start_pref_e:

type: int | float | NoneType, optional, default: None

argument path: simplify_jdata/training_reuse_start_pref_e

The prefactor of energy loss at the start of the training. This option is only adopted when continuing training models from old models. This option will override default parameters.

training_reuse_start_pref_f:

type: int | float | NoneType, optional, default: None

argument path: simplify_jdata/training_reuse_start_pref_f

The prefactor of force loss at the start of the training. This option is only adopted when continuing training models from old models. This option will override default parameters.

model_devi_activation_func:

type: list[list[str]] | NoneType, optional

argument path: simplify_jdata/model_devi_activation_func

The activation function in the model. The shape of list should be (N_models, 2), where 2 represents the embedding and fitting network. This option will override default parameters.

srtab_file_path:

type: str, optional

argument path: simplify_jdata/srtab_file_path

The path of the table for the short-range pairwise interaction which is needed when using DP-ZBL potential

one_h5:

type: bool, optional, default: False

argument path: simplify_jdata/one_h5

When using DeePMD-kit, all of the input data will be merged into one HDF5 file.

training_init_frozen_model:

type: list[str], optional

argument path: simplify_jdata/training_init_frozen_model

At interation 0, initilize the model parameters from the given frozen models. Number of element should be equal to numb_models.

training_finetune_model:

type: list[str], optional

argument path: simplify_jdata/training_finetune_model

At interation 0, finetune the model parameters from the given frozen models. Number of element should be equal to numb_models.

fp_task_max:

type: int, optional

argument path: simplify_jdata/fp_task_max

Maximum of structures to be calculated in 02.fp of each iteration.

fp_task_min:

type: int, optional

argument path: simplify_jdata/fp_task_min

Minimum of structures to be calculated in 02.fp of each iteration.

fp_accurate_threshold:

type: float, optional

argument path: simplify_jdata/fp_accurate_threshold

If the accurate ratio is larger than this number, no fp calculation will be performed, i.e. fp_task_max = 0.

fp_accurate_soft_threshold:

type: `float`, optional

argument path: `simplify_jdata/fp_accurate_soft_threshold`

If the accurate ratio is between this number and fp_accurate_threshold, the fp_task_max linearly decays to zero.

ratio_failed:

type: `float`, optional

argument path: `simplify_jdata/ratio_failed`

Check the ratio of unsuccessfully terminated jobs. If too many FP tasks are not converged, RuntimeError will be raised.

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

fp_style:

type: `str` (flag key), default: `none`

argument path: `simplify_jdata/fp_style`

possible choices: *none*, *vasp*, *gaussian*, *siesta*, *cp2k*, *abacus*, *pwmat*, *pwscf*, *custom*

Software for First Principles, if *labeled* is false.

When fp_style is set to `none`:

No fp.

When fp_style is set to `vasp`:

VASP.

fp_pp_path:

type: `str`

argument path: `simplify_jdata[vasp]/fp_pp_path`

Directory of psuedo-potential file to be used for 02.fp exists.

fp_pp_files:

type: `list[str]`

argument path: `simplify_jdata[vasp]/fp_pp_files`

Psuedo-potential file to be used for 02.fp. Note that the order of elements should correspond to the order in type_map.

fp_incar:

type: `str`

argument path: `simplify_jdata[vasp]/fp_incar`

Input file for VASP. INCAR must specify KSPACING and KGAMMA.

fp_aniso_kspacing:

type: `list[float]`, optional

argument path: `simplify_jdata[vasp]/fp_aniso_kspacing`

Set anisotropic kspacing. Usually useful for 1-D or 2-D materials. Only support VASP. If it is setting the KSPACING key in INCAR will be ignored.

cvasp:

type: bool, optional
argument path: simplify_jdata[vasp]/cvasp

If cvasp is true, DP-GEN will use Custodian to help control VASP calculation.

fp_skip_bad_box:

type: str, optional
argument path: simplify_jdata[vasp]/fp_skip_bad_box

Skip the configurations that are obviously unreasonable before 02.fp

When fp_style is set to gaussian:

Gaussian. The command should be set as *g16 < input*.

use_clusters:

type: bool, optional, default: False
argument path: simplify_jdata[gaussian]/use_clusters

If set to true, clusters will be taken instead of the whole system.

cluster_cutoff:

type: float, optional
argument path: simplify_jdata[gaussian]/cluster_cutoff

The soft cutoff radius of clusters if *use_clusters* is set to true. Molecules will be taken as whole even if part of atoms is out of the cluster. Use *cluster_cutoff_hard* to only take atoms within the hard cutoff radius.

cluster_cutoff_hard:

type: float, optional
argument path: simplify_jdata[gaussian]/cluster_cutoff_hard

The hard cutoff radius of clusters if *use_clusters* is set to true. Outside the hard cutoff radius, atoms will not be taken even if they are in a molecule where some atoms are within the cutoff radius.

cluster_minify:

type: bool, optional, default: False
argument path: simplify_jdata[gaussian]/cluster_minify

If enabled, when an atom within the soft cutoff radius connects a single bond with a non-hydrogen atom out of the soft cutoff radius, the outer atom will be replaced by a hydrogen atom. When the outer atom is a hydrogen atom, the outer atom will be kept. In this case, other atoms out of the soft cutoff radius will be removed.

fp_params:

type: dict
argument path: simplify_jdata[gaussian]/fp_params

Parameters for Gaussian calculation.

keywords:

type: str | list[str]
argument path: simplify_jdata[gaussian]/fp_params/keywords

Keywords for Gaussian input, e.g. force b3lyp/6-31g**. If a list, run multiple steps.

multiplicity:

type: str | int, optional, default: auto

argument path: simplify_jdata[gaussian]/fp_params/multiplicity

Spin multiplicity for Gaussian input. If *auto*, multiplicity will be detected automatically, with the following rules: when fragment_guesses=True, multiplicity will +1 for each radical, and +2 for each oxygen molecule; when fragment_guesses=False, multiplicity will be 1 or 2, but +2 for each oxygen molecule.

nproc:

type: int

argument path: simplify_jdata[gaussian]/fp_params/nproc

The number of processors for Gaussian input.

charge:

type: int, optional, default: 0

argument path: simplify_jdata[gaussian]/fp_params/charge

Molecule charge. Only used when charge is not provided by the system.

fragment_guesses:

type: bool, optional, default: False

argument path: simplify_jdata[gaussian]/fp_params/fragment_guesses

Initial guess generated from fragment guesses. If True, *multiplicity* should be *auto*.

basis_set:

type: str, optional

argument path: simplify_jdata[gaussian]/fp_params/basis_set

Custom basis set.

keywords_high_multiplicity:

type: str, optional

argument path: simplify_jdata[gaussian]/fp_params/keywords_high_multiplicity

Keywords for points with multiple raicals. *multiplicity* should be *auto*. If not set, fallback to normal keywords.

When fp_style is set to siesta:

use_clusters:

type: bool, optional
argument path: simplify_jdata[siesta]/use_clusters

If set to true, clusters will be taken instead of the whole system. This option does not work with DeePMD-kit 0.x.

cluster_cutoff:

type: float, optional
argument path: simplify_jdata[siesta]/cluster_cutoff

The cutoff radius of clusters if use_clusters is set to true.

fp_params:

type: dict
argument path: simplify_jdata[siesta]/fp_params

Parameters for siesta calculation.

ecut:

type: int
argument path: simplify_jdata[siesta]/fp_params/ecut

Define the plane wave cutoff for grid.

ediff:

type: float
argument path: simplify_jdata[siesta]/fp_params/ediff

Tolerance of Density Matrix.

kspacing:

type: float
argument path: simplify_jdata[siesta]/fp_params/kspacing

Sample factor in Brillouin zones.

mixingWeight:

type: float
argument path: simplify_jdata[siesta]/fp_params/mixingWeight

Proportion a of output Density Matrix to be used for the input Density Matrix of next SCF cycle (linear mixing).

NumberPulay:

type: int
argument path: simplify_jdata[siesta]/fp_params/NumberPulay

Controls the Pulay convergence accelerator.

fp_pp_path:

type: str

argument path: simplify_jdata[siesta]/fp_pp_path

Directory of psuedo-potential or numerical orbital files to be used for 02.fp exists.

fp_pp_files:

type: list[str]

argument path: simplify_jdata[siesta]/fp_pp_files

Psuedo-potential file to be used for 02.fp. Note that the order of elements should correspond to the order in type_map.

When fp_style is set to cp2k:

user_fp_params:

type: dict, optional, alias: *fp_params*

argument path: simplify_jdata[cp2k]/user_fp_params

Parameters for cp2k calculation. find detail in manual.cp2k.org. only the kind section must be set before use. we assume that you have basic knowledge for cp2k input.

external_input_path:

type: str, optional

argument path: simplify_jdata[cp2k]/external_input_path

Conflict with key:user_fp_params. enable the template input provided by user. some rules should be followed, read the following text in detail:

1. One must present a KEYWORD ABC in the section CELL so that the DP-GEN can replace the cell on-the-fly.
2. One need to add these lines under FORCE_EVAL section to print forces and stresses:

```
STRESS_TENSOR ANALYTICAL
  &PRINT
    &FORCES ON
    &END FORCES
    &STRESS_TENSOR ON
    &END STRESS_TENSOR
  &END PRINT
```

When fp_style is set to abacus:

fp_pp_path:

type: str

argument path: simplify_jdata[abacus]/fp_pp_path

Directory of psuedo-potential or numerical orbital files to be used for 02.fp exists.

fp_pp_files:

type: list[str]

argument path: simplify_jdata[abacus]/fp_pp_files

Psuedo-potential file to be used for 02.fp. Note that the order of elements should correspond to the order in type_map.

fp_orb_files:

type: list[str], optional

argument path: simplify_jdata[abacus]/fp_orb_files

numerical orbital file to be used for 02.fp when using LCAO basis. Note that the order of elements should correspond to the order in type_map.

fp_incar:

type: str, optional

argument path: simplify_jdata[abacus]/fp_incar

Input file for ABACUS. This is optinal but the priority is lower than user_fp_params, and you should not set user_fp_params if you want to use fp_incar.

fp_kpt_file:

type: str, optional

argument path: simplify_jdata[abacus]/fp_kpt_file

KPT file for ABACUS.If the "kspacing" or "gamma_only=1" is defined in INPUT or "k_points" is defined, fp_kpt_file will be ignored.

fp_dpks_descriptor:

type: str, optional

argument path: simplify_jdata[abacus]/fp_dpks_descriptor

DeePKS descriptor file name. The file should be in pseudopotential directory.

user_fp_params:

type: dict, optional

argument path: simplify_jdata[abacus]/user_fp_params

Set the key and value of INPUT.

k_points:

type: list[int], optional

argument path: simplify_jdata[abacus]/k_points

Monkhorst-Pack k-grids setting for generating KPT file of ABACUS, such as: [1,1,1,0,0,0]. NB: if "kspacing" or "gamma_only=1" is defined in INPUT, k_points will be ignored.

When fp_style is set to pwmat:

TODO: add doc

When fp_style is set to pwscf:

pwscf (Quantum Espresso).

fp_pp_path:

type: str

argument path: simplify_jdata[pwscf]/fp_pp_path

Directory of psuedo-potential file to be used for 02.fp exists.

fp_pp_files:

type: list[str]

argument path: simplify_jdata[pwscf]/fp_pp_files

Psuedo-potential file to be used for 02.fp. Note that the order of elements should correspond to the order in type_map.

fp_params:

type: dict, optional
argument path: simplify_jdata[pwscf]/fp_params

Parameters for pwscf calculation. It has lower priority than user_fp_params.

ecut:

type: float
argument path: simplify_jdata[pwscf]/fp_params/ecut

ecutwfc in pwscf.

ediff:

type: float
argument path: simplify_jdata[pwscf]/fp_params/ediff

conv_thr and ts_vdw_econv_thr in pwscf.

smearing:

type: str
argument path: simplify_jdata[pwscf]/fp_params/smearing

smearing in pwscf.

sigma:

type: float
argument path: simplify_jdata[pwscf]/fp_params/sigma

degauss in pwscf.

kspacing:

type: float
argument path: simplify_jdata[pwscf]/fp_params/kspacing

The spacing between kpoints. Helps to determin KPOINTS in pwscf.

user_fp_params:

type: dict, optional
argument path: simplify_jdata[pwscf]/user_fp_params

Parameters for pwscf calculation. Find details at https://www.quantum-espresso.org/Doc/INPUT_PW.html. When user_fp_params is set, the settings in fp_params will be ignored. If one wants to use user_fp_params, kspacing must be set in user_fp_params. kspacing is the spacing between kpoints, and helps to determin KPOINTS in pwscf.

When fp_style is set to `custom`:

Custom FP code. You need to provide the input and output file format and name. The command argument in the machine file should be the script to run custom FP codes. The extra forward and backward files can be defined in the machine file.

fp_params:

type: `dict`
argument path: `simplify_jdata[custom]/fp_params`

Parameters for FP calculation.

input_fmt:

type: `str`
argument path: `simplify_jdata[custom]/fp_params/input_fmt`

Input dpdata format of the custom FP code. Such format should only need the first argument as the file name.

input_fn:

type: `str`
argument path: `simplify_jdata[custom]/fp_params/input_fn`

Input file name of the custom FP code.

output_fmt:

type: `str`
argument path: `simplify_jdata[custom]/fp_params/output_fmt`

Output dpata format of the custom FP code. Such format should only need the first argument as the file name.

output_fn:

type: `str`
argument path: `simplify_jdata[custom]/fp_params/output_fn`

Output file name of the custom FP code.

6.3 dpgen simplify machine parameters

Note: One can load, modify, and export the input file by using our effective web-based tool DP-GUI online or hosted using the *command line interface* `dpgen gui`. All parameters below can be set in DP-GUI. By clicking "SAVE JSON", one can download the input file.

simplify_mdata:

type: `dict`
argument path: `simplify_mdata`

machine.json file

api_version:

type: str, optional, default: 1.0
argument path: simplify_mdata/api_version

Please set to 1.0

deepmd_version:

type: str, optional, default: 2
argument path: simplify_mdata/deepmd_version

DeePMD-kit version, e.g. 2.1.3

train:

type: dict
argument path: simplify_mdata/train

Parameters of command, machine, and resources for train

command:

type: str
argument path: simplify_mdata/train/command

Command of a program.

machine:

type: dict
argument path: simplify_mdata/train/machine

batch_type:

type: str
argument path: simplify_mdata/train/machine/batch_type

The batch job system type. Option: Slurm, LSF, DistributedShell, SGE, Shell, SlurmJobArray, PBS, OpenAPI, Torque, Bohrium, Fugaku

local_root:

type: str | NoneType
argument path: simplify_mdata/train/machine/local_root

The dir where the tasks and relating files locate. Typically the project dir.

remote_root:

type: str | NoneType, optional
argument path: simplify_mdata/train/machine/remote_root

The dir where the tasks are executed on the remote machine. Only needed when context is not lazy-local.

clean_asynchronously:

type: bool, optional, default: False
argument path: simplify_mdata/train/machine/clean_asynchronously

Clean the remote directory asynchronously after the job finishes.

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

context_type:

type: str (flag key)
argument path: simplify_mdata/train/machine/context_type
possible choices: *LocalContext*, *LazyLocalContext*, *BohriumContext*, *HDFSContext*, *OpenAPIContext*, *SSHContext*

The connection used to remote machine. Option: LazyLocalContext, HDFSContext, BohriumContext, SSHContext, LocalContext, OpenAPIContext

When context_type is set to LocalContext (or its aliases localcontext, Local, local):

remote_profile:

type: dict, optional
argument path: simplify_mdata/train/machine[LocalContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to LazyLocalContext (or its aliases lazylocalcontext, LazyLocal, lazylocal):

remote_profile:

type: dict, optional
argument path: simplify_mdata/train/machine[LazyLocalContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to BohriumContext (or its aliases bohriumcontext, Bohrium, bohrium, DpCloudServerContext, dpcloudservercontext, DpCloudServer, dpcloudserver, LebesgueContext, lebesguecontext, Lebesgue, lebesgue):

remote_profile:

type: dict
argument path: simplify_mdata/train/machine[BohriumContext]/remote_profile

The information used to maintain the connection with remote machine.

email:

type: str, optional
argument path: simplify_mdata/train/machine[BohriumContext]/remote_profile/email

Email

password:

type: str, optional
argument path: simplify_mdata/train/machine[BohriumContext]/remote_profile/password

Password

program_id:

type: int, alias: *project_id*
argument path: simplify_mdata/train/machine[BohriumContext]/remote_profile/program_id

Program ID

retry_count:

type: NoneType | int, optional, default: 2
argument path: simplify_mdata/train/machine[BohriumContext]/remote_profile/retry_count

The retry count when a job is terminated

ignore_exit_code:

type: bool, optional, default: True
argument path: simplify_mdata/train/machine[BohriumContext]/remote_profile/ignore_exit_code

The job state will be marked as finished if the exit code is non-zero when set to True. Otherwise, the job state will be designated as terminated.

keep_backup:

type: bool, optional

argument path: simplify_mdata/train/machine[BohriumContext]/remote_profile/keep_backup

keep download and upload zip

input_data:

type: dict

argument path: simplify_mdata/train/machine[BohriumContext]/remote_profile/input_data

Configuration of job

When context_type is set to HDFSContext (or its aliases hdfscontext, HDFS, hdfs):

remote_profile:

type: dict, optional

argument path: simplify_mdata/train/machine[HDFSContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to OpenAPIContext (or its aliases openapicontext, OpenAPI, openapi):

remote_profile:

type: dict, optional

argument path: simplify_mdata/train/machine[OpenAPIContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to SSHContext (or its aliases sshcontext, SSH, ssh):

remote_profile:

type: dict

argument path: simplify_mdata/train/machine[SSHContext]/remote_profile

The information used to maintain the connection with remote machine.

hostname:

type: str

argument path: simplify_mdata/train/machine[SSHContext]/remote_profile/hostname

hostname or ip of ssh connection.

username:

type: str

argument path: simplify_mdata/train/machine[SSHContext]/remote_profile/username

username of target linux system

password:

type: str, optional

argument path: simplify_mdata/train/machine[SSHContext]/remote_profile/password

(deprecated) password of linux system. Please use SSH keys instead to improve security.

port:

type: int, optional, default: 22

argument path: simplify_mdata/train/machine[SSHContext]/remote_profile/port

ssh connection port.

key_filename:

type: str | NoneType, optional, default: None

argument path: simplify_mdata/train/machine[SSHContext]/remote_profile/key_filename

key filename used by ssh connection. If left None, find key in ~/.ssh or use password for login

passphrase:

type: str | NoneType, optional, default: None

argument path: simplify_mdata/train/machine[SSHContext]/remote_profile/passphrase

passphrase of key used by ssh connection

timeout:

type: int, optional, default: 10

argument path: simplify_mdata/train/machine[SSHContext]/remote_profile/timeout

timeout of ssh connection

totp_secret:

type: str | NoneType, optional, default: None

argument path: simplify_mdata/train/machine[SSHContext]/remote_profile/totp_secret

Time-based one time password secret. It should be a base32-encoded string extracted from the 2D code.

tar_compress:

type: bool, optional, default: True

argument path: simplify_mdata/train/machine[SSHContext]/remote_profile/tar_compress

The archive will be compressed in upload and download if it is True. If not, compression will be skipped.

look_for_keys:

type: bool, optional, default: True

argument path: simplify_mdata/train/machine[SSHContext]/remote_profile/look_for_keys

enable searching for discoverable private key files in ~/.ssh/

resources:

type: dict

argument path: simplify_mdata/train/resources

number_node:

type: int, optional, default: 1

argument path: simplify_mdata/train/resources/number_node

The number of node need for each *job*

cpu_per_node:

type: int, optional, default: 1

argument path: simplify_mdata/train/resources/cpu_per_node

cpu numbers of each node assigned to each job.

gpu_per_node:

type: int, optional, default: 0
argument path: simplify_mdata/train/resources/gpu_per_node

gpu numbers of each node assigned to each job.

queue_name:

type: str, optional, default: (empty string)
argument path: simplify_mdata/train/resources/queue_name

The queue name of batch job scheduler system.

group_size:

type: int
argument path: simplify_mdata/train/resources/group_size

The number of *tasks* in a *job*. 0 means infinity.

custom_flags:

type: typing.List[str], optional
argument path: simplify_mdata/train/resources/custom_flags

The extra lines pass to job submitting script header

strategy:

type: dict, optional
argument path: simplify_mdata/train/resources/strategy

strategies we use to generation job submitting scripts.

if_cuda_multi_devices:

type: bool, optional, default: False
argument path: simplify_mdata/train/resources/strategy/if_cuda_multi_devices

If there are multiple nvidia GPUS on the node, and we want to assign the tasks to different GPUS.If true, dpdispatcher will manually export environment variable CUDA_VISIBLE_DEVICES to different task.Usually, this option will be used with Task.task_need_resources variable simultaneously.

ratio_unfinished:

type: float, optional, default: 0.0

argument path: simplify_mdata/train/resources/strategy/ratio_unfinished

The ratio of *tasks* that can be unfinished.

customized_script_header_template_file:

type: str, optional

argument path: simplify_mdata/train/resources/strategy/customized_script_header_template_file

The customized template file to generate job submitting script header, which overrides the default file.

para_deg:

type: int, optional, default: 1

argument path: simplify_mdata/train/resources/para_deg

Decide how many tasks will be run in parallel.

source_list:

type: typing.List[str], optional, default: []

argument path: simplify_mdata/train/resources/source_list

The env file to be sourced before the command execution.

module_purge:

type: bool, optional, default: False

argument path: simplify_mdata/train/resources/module_purge

Remove all modules on HPC system before module load (module_list)

module_unload_list:

type: typing.List[str], optional, default: []

argument path: simplify_mdata/train/resources/module_unload_list

The modules to be unloaded on HPC system before submitting jobs

module_list:

type: typing.List[str], optional, default: []

argument path: simplify_mdata/train/resources/module_list

The modules to be loaded on HPC system before submitting jobs

envs:

type: dict, optional, default: {}

argument path: simplify_mdata/train/resources/envs

The environment variables to be exported on before submitting jobs

prepend_script:

type: typing.List[str], optional, default: []

argument path: simplify_mdata/train/resources/prepend_script

Optional script run before jobs submitted.

append_script:

type: typing.List[str], optional, default: []

argument path: simplify_mdata/train/resources/append_script

Optional script run after jobs submitted.

wait_time:

type: float | int, optional, default: 0

argument path: simplify_mdata/train/resources/wait_time

The waitting time in second after a single *task* submitted

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

batch_type:

type: str (flag key)

argument path: simplify_mdata/train/resources/batch_type

possible choices: *Fugaku*, *Slurm*, *SlurmJobArray*, *Shell*, *LSF*, *PBS*, *SGE*, *Torque*, *OpenAPI*, *DistributedShell*, *Bohrium*

The batch job system type loaded from machine/batch_type.

When batch_type is set to Fugaku (or its alias fugaku):

kwargs:

type: dict, optional
argument path: simplify_mdata/train/resources[Fugaku]/kwargs

This field is empty for this batch.

When batch_type is set to Slurm (or its alias slurm):

kwargs:

type: dict, optional
argument path: simplify_mdata/train/resources[Slurm]/kwargs

Extra arguments.

custom_gpu_line:

type: str | NoneType, optional, default: None
argument path: simplify_mdata/train/resources[Slurm]/kwargs/custom_gpu_line

Custom GPU configuration, starting with #SBATCH

When batch_type is set to SlurmJobArray (or its alias slurmjobarray):

kwargs:

type: dict, optional
argument path: simplify_mdata/train/resources[SlurmJobArray]/kwargs

Extra arguments.

custom_gpu_line:

type: str | NoneType, optional, default: None
argument path: simplify_mdata/train/resources[SlurmJobArray]/kwargs/custom_gpu_line

Custom GPU configuration, starting with #SBATCH

slurm_job_size:

type: int, optional, default: 1
argument path: simplify_mdata/train/resources[SlurmJobArray]/kwargs/slurm_job_size

Number of tasks in a Slurm job

When batch_type is set to Shell (or its alias shell):

kwargs:

type: dict, optional
argument path: simplify_mdata/train/resources[Shell]/kwargs

This field is empty for this batch.

When batch_type is set to LSF (or its alias lsf):

kwargs:

type: dict
argument path: simplify_mdata/train/resources[LSF]/kwargs

Extra arguments.

gpu_usage:

type: bool, optional, default: False
argument path: simplify_mdata/train/resources[LSF]/kwargs/gpu_usage

Choosing if GPU is used in the calculation step.

gpu_new_syntax:

type: bool, optional, default: False
argument path: simplify_mdata/train/resources[LSF]/kwargs/gpu_new_syntax

For LFS >= 10.1.0.3, new option -gpu for #BSUB could be used. If False, and old syntax would be used.

gpu_exclusive:

type: bool, optional, default: True
argument path: simplify_mdata/train/resources[LSF]/kwargs/gpu_exclusive

Only take effect when new syntax enabled. Control whether submit tasks in exclusive way for GPU.

custom_gpu_line:

type: str | NoneType, optional, default: None
argument path: simplify_mdata/train/resources[LSF]/kwargs/custom_gpu_line

Custom GPU configuration, starting with #BSUB

When batch_type is set to PBS (or its alias pbs):

kwargs:

type: dict, optional
argument path: simplify_mdata/train/resources[PBS]/kwargs

This field is empty for this batch.

When batch_type is set to SGE (or its alias sge):

kwargs:

type: dict, optional
argument path: simplify_mdata/train/resources[SGE]/kwargs

This field is empty for this batch.

When batch_type is set to Torque (or its alias torque):

kwargs:

type: dict, optional
argument path: simplify_mdata/train/resources[Torque]/kwargs

This field is empty for this batch.

When batch_type is set to OpenAPI (or its alias openapi):

kwargs:

type: dict, optional
argument path: simplify_mdata/train/resources[OpenAPI]/kwargs

This field is empty for this batch.

When batch_type is set to DistributedShell (or its alias distributedshell):

kwargs:

type: dict, optional
argument path: simplify_mdata/train/resources[DistributedShell]/kwargs

This field is empty for this batch.

When batch_type is set to Bohrium (or its aliases bohrium, Lebesgue, lebesgue, DpCloudServer, dpcloudserver):

kwargs:

type: dict, optional
argument path: simplify_mdata/train/resources[Bohrium]/kwargs

This field is empty for this batch.

user_forward_files:

type: list, optional
argument path: simplify_mdata/train/user_forward_files

Files to be forwarded to the remote machine.

user_backward_files:

type: list, optional
argument path: simplify_mdata/train/user_backward_files

Files to be backwarded from the remote machine.

model_devi:

type: dict
argument path: simplify_mdata/model_devi

Parameters of command, machine, and resources for model_devi

command:

type: str
argument path: simplify_mdata/model_devi/command

Command of a program.

machine:

type: dict
argument path: simplify_mdata/model_devi/machine

batch_type:

type: str
argument path: simplify_mdata/model_devi/machine/batch_type

The batch job system type. Option: Slurm, LSF, DistributedShell, SGE, Shell, SlurmJobArray, PBS, OpenAPI, Torque, Bohrium, Fugaku

local_root:

type: str | NoneType
argument path: simplify_mdata/model_devi/machine/local_root

The dir where the tasks and relating files locate. Typically the project dir.

remote_root:

type: str | NoneType, optional
argument path: simplify_mdata/model_devi/machine/remote_root

The dir where the tasks are executed on the remote machine. Only needed when context is not lazy-local.

clean_asynchronously:

type: bool, optional, default: False
argument path: simplify_mdata/model_devi/machine/clean_asynchronously

Clean the remote directory asynchronously after the job finishes.

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

context_type:

type: str (flag key)
argument path: simplify_mdata/model_devi/machine/context_type
possible choices: *LocalContext*, *LazyLocalContext*, *BohriumContext*, *HDFSContext*, *OpenAPIContext*, *SSHContext*

The connection used to remote machine. Option: LazyLocalContext, HDFSContext, BohriumContext, SSHContext, LocalContext, OpenAPIContext

When context_type is set to LocalContext (or its aliases localcontext, Local, local):

remote_profile:

type: dict, optional
argument path: simplify_mdata/model_devi/machine[LocalContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to LazyLocalContext (or its aliases lazylocalcontext, LazyLocal, lazylocal):

remote_profile:

type: dict, optional
argument path: simplify_mdata/model_devi/machine[LazyLocalContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to BohriumContext (or its aliases bohriumcontext, Bohrium, bohrium, DpCloudServerContext, dpcloudservercontext, DpCloudServer, dpcloudserver, LebesgueContext, lebesguecontext, Lebesgue, lebesgue):

remote_profile:

type: dict
argument path: simplify_mdata/model_devi/machine[BohriumContext]/remote_profile

The information used to maintain the connection with remote machine.

email:

type: str, optional
argument path: simplify_mdata/model_devi/machine[BohriumContext]/remote_profile/email

Email

password:

type: str, optional
argument path: simplify_mdata/model_devi/machine[BohriumContext]/remote_profile/password

Password

program_id:

type: int, alias: *project_id*
argument path: simplify_mdata/model_devi/machine[BohriumContext]/remote_profile/program_id

Program ID

retry_count:

type: NoneType | int, optional, default: 2
argument path: simplify_mdata/model_devi/machine[BohriumContext]/remote_profile/retry_count

The retry count when a job is terminated

ignore_exit_code:

type: bool, optional, default: True

argument path:
simplify_mdata/model_devi/
machine[BohriumContext]/
remote_profile/
ignore_exit_code

The job state will be marked as finished if the exit code is non-zero when set to True. Otherwise,
the job state will be designated as terminated.

keep_backup:

type: bool, optional

argument path:
simplify_mdata/model_devi/
machine[BohriumContext]/
remote_profile/keep_backup

keep download and upload zip

input_data:

type: dict

argument path:
simplify_mdata/model_devi/
machine[BohriumContext]/
remote_profile/input_data

Configuration of job

When context_type is set to HDFSContext (or its aliases hdfscontext, HDFS, hdfs):

remote_profile:

type: dict, optional

argument path:
simplify_mdata/model_devi/
machine[HDFSContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to OpenAPIContext (or its aliases openapicontext, OpenAPI, openapi):

remote_profile:

type: dict, optional

argument path: simplify_mdata/
model_devi/machine[OpenAPIContext]/
remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to SSHContext (or its aliases sshcontext, SSH, ssh):

remote_profile:

type: dict

argument path: simplify_mdata/model_devi/machine[SSHContext]/remote_profile

The information used to maintain the connection with remote machine.

hostname:

type: str

argument path: simplify_mdata/model_devi/machine[SSHContext]/remote_profile/hostname

hostname or ip of ssh connection.

username:

type: str

argument path: simplify_mdata/model_devi/machine[SSHContext]/remote_profile/username

username of target linux system

password:

type: str, optional

argument path: simplify_mdata/model_devi/machine[SSHContext]/remote_profile/password

(deprecated) password of linux system. Please use SSH keys instead to improve security.

port:

type: int, optional, default: 22

argument path: simplify_mdata/model_devi/machine[SSHContext]/remote_profile/port

ssh connection port.

key_filename:

type: str | NoneType, optional, default: None

argument path: simplify_mdata/model_devi/machine[SSHContext]/remote_profile/key_filename

key filename used by ssh connection. If left None, find key in ~/.ssh or use password for login

passphrase:

type: str | NoneType, optional, default: None

argument path: simplify_mdata/model_devi/machine[SSHContext]/remote_profile/passphrase

passphrase of key used by ssh connection

timeout:

type: int, optional, default: 10

argument path: simplify_mdata/model_devi/machine[SSHContext]/remote_profile/timeout

timeout of ssh connection

totp_secret:

type: str | NoneType, optional, default: None

argument path: simplify_mdata/model_devi/machine[SSHContext]/remote_profile/totp_secret

Time-based one time password secret. It should be a base32-encoded string extracted from the 2D code.

tar_compress:

type: bool, optional, default: True

argument path: simplify_mdata/model_devi/machine[SSHContext]/remote_profile/tar_compress

The archive will be compressed in upload and download if it is True. If not, compression will be skipped.

look_for_keys:

type: bool, optional, default: True

argument path: simplify_mdata/model_devi/machine[SSHContext]/remote_profile/look_for_keys

enable searching for discoverable private key files in ~/.ssh/

resources:

type: dict
argument path: simplify_mdata/model_devi/resources

number_node:

type: int, optional, default: 1
argument path: simplify_mdata/model_devi/resources/number_node

The number of node need for each *job*

cpu_per_node:

type: int, optional, default: 1
argument path: simplify_mdata/model_devi/resources/cpu_per_node

cpu numbers of each node assigned to each job.

gpu_per_node:

type: int, optional, default: 0
argument path: simplify_mdata/model_devi/resources/gpu_per_node

gpu numbers of each node assigned to each job.

queue_name:

type: str, optional, default: (empty string)
argument path: simplify_mdata/model_devi/resources/queue_name

The queue name of batch job scheduler system.

group_size:

type: int
argument path: simplify_mdata/model_devi/resources/group_size

The number of *tasks* in a *job*. 0 means infinity.

custom_flags:

type: typing.List[str], optional
argument path: simplify_mdata/model_devi/resources/custom_flags

The extra lines pass to job submitting script header

strategy:

type: dict, optional
argument path: simplify_mdata/model_devi/resources/strategy

strategies we use to generation job submitting scripts.

if_cuda_multi_devices:

type: bool, optional, default: False

argument path: simplify_mdata/model_devi/resources/strategy/if_cuda_multi_devices

If there are multiple nvidia GPUS on the node, and we want to assign the tasks to different GPUS.If true, dpdispatcher will manually export environment variable CUDA_VISIBLE_DEVICES to different task.Usually, this option will be used with Task.task_need_resources variable simultaneously.

ratio_unfinished:

type: float, optional, default: 0.0

argument path: simplify_mdata/model_devi/resources/strategy/ratio_unfinished

The ratio of *tasks* that can be unfinished.

customized_script_header_template_file:

type: str, optional

argument path: simplify_mdata/model_devi/resources/strategy/customized_script_header_template_file

The customized template file to generate job submitting script header, which overrides the default file.

para_deg:

type: int, optional, default: 1

argument path: simplify_mdata/model_devi/resources/para_deg

Decide how many tasks will be run in parallel.

source_list:

type: typing.List[str], optional, default: []

argument path: simplify_mdata/model_devi/resources/source_list

The env file to be sourced before the command execution.

module_purge:

type: bool, optional, default: False
argument path: simplify_mdata/model_devi/resources/module_purge

Remove all modules on HPC system before module load (module_list)

module_unload_list:

type: typing.List[str], optional, default: []
argument path: simplify_mdata/model_devi/resources/module_unload_list

The modules to be unloaded on HPC system before submitting jobs

module_list:

type: typing.List[str], optional, default: []
argument path: simplify_mdata/model_devi/resources/module_list

The modules to be loaded on HPC system before submitting jobs

envs:

type: dict, optional, default: {}
argument path: simplify_mdata/model_devi/resources/envs

The environment variables to be exported on before submitting jobs

prepend_script:

type: typing.List[str], optional, default: []
argument path: simplify_mdata/model_devi/resources/prepend_script

Optional script run before jobs submitted.

append_script:

type: typing.List[str], optional, default: []
argument path: simplify_mdata/model_devi/resources/append_script

Optional script run after jobs submitted.

wait_time:

type: float | int, optional, default: 0

argument path: simplify_mdata/model_devi/resources/wait_time

The waitting time in second after a single *task* submitted

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

batch_type:

type: str (flag key)
argument path: simplify_mdata/model_devi/resources/batch_type
possible choices: *Fugaku*, *Slurm*, *SlurmJobArray*, *Shell*, *LSF*, *PBS*, *SGE*, *Torque*, *OpenAPI*, *DistributedShell*, *Bohrium*

The batch job system type loaded from machine/batch_type.

When batch_type is set to Fugaku (or its alias fugaku):

kwargs:

type: dict, optional
argument path: simplify_mdata/model_devi/resources[Fugaku]/kwargs

This field is empty for this batch.

When batch_type is set to Slurm (or its alias slurm):

kwargs:

type: dict, optional
argument path: simplify_mdata/model_devi/resources[Slurm]/kwargs

Extra arguments.

custom_gpu_line:

type: str | NoneType, optional, default: None
argument path: simplify_mdata/model_devi/resources[Slurm]/kwargs/custom_gpu_line

Custom GPU configuration, starting with #SBATCH

When batch_type is set to SlurmJobArray (or its alias slurmjobarray):

kwargs:

type: dict, optional
argument path: simplify_mdata/model_devi/resources[SlurmJobArray]/kwargs

Extra arguments.

custom_gpu_line:

type: str | NoneType, optional, default: None

argument path: simplify_mdata/model_devi/resources[SlurmJobArray]/kwargs/custom_gpu_line

Custom GPU configuration, starting with #SBATCH

slurm_job_size:

type: int, optional, default: 1

argument path: simplify_mdata/model_devi/resources[SlurmJobArray]/kwargs/slurm_job_size

Number of tasks in a Slurm job

When batch_type is set to Shell (or its alias shell):

kwargs:

type: dict, optional

argument path: simplify_mdata/model_devi/resources[Shell]/kwargs

This field is empty for this batch.

When batch_type is set to LSF (or its alias lsf):

kwargs:

type: dict

argument path: simplify_mdata/model_devi/resources[LSF]/kwargs

Extra arguments.

gpu_usage:

type: bool, optional, default: False

argument path: simplify_mdata/model_devi/resources[LSF]/kwargs/gpu_usage

Choosing if GPU is used in the calculation step.

gpu_new_syntax:

type: bool, optional, default: False

argument path: simplify_mdata/model_devi/resources[LSF]/kwargs/gpu_new_syntax

For LFS >= 10.1.0.3, new option -gpu for #BSUB could be used. If False, and old syntax would be used.

gpu_exclusive:

type: bool, optional, default: True

argument path: simplify_mdata/model_devi/resources[LSF]/kwargs/gpu_exclusive

Only take effect when new syntax enabled. Control whether submit tasks in exclusive way for GPU.

custom_gpu_line:

type: str | NoneType, optional, default: None

argument path: simplify_mdata/model_devi/resources[LSF]/kwargs/custom_gpu_line

Custom GPU configuration, starting with #BSUB

When batch_type is set to PBS (or its alias pbs):

kwargs:

type: dict, optional

argument path: simplify_mdata/model_devi/resources[PBS]/kwargs

This field is empty for this batch.

When batch_type is set to SGE (or its alias sge):

kwargs:

type: dict, optional

argument path: simplify_mdata/model_devi/resources[SGE]/kwargs

This field is empty for this batch.

When batch_type is set to Torque (or its alias torque):

kwargs:

type: dict, optional

argument path: simplify_mdata/model_devi/resources[Torque]/kwargs

This field is empty for this batch.

When batch_type is set to OpenAPI (or its alias openapi):

kwargs:

type: dict, optional

argument path: simplify_mdata/model_devi/resources[OpenAPI]/kwargs

This field is empty for this batch.

When batch_type is set to `DistributedShell` (or its alias `distributedshell`):

kwargs:

type: `dict`, optional
argument path: `simplify_mdata/model_devi/resources[DistributedShell]/kwargs`

This field is empty for this batch.

When batch_type is set to `Bohrium` (or its aliases `bohrium`, `Lebesgue`, `lebesgue`, `DpCloudServer`, `dpcloudserver`):

kwargs:

type: `dict`, optional
argument path: `simplify_mdata/model_devi/resources[Bohrium]/kwargs`

This field is empty for this batch.

user_forward_files:

type: `list`, optional
argument path: `simplify_mdata/model_devi/user_forward_files`

Files to be forwarded to the remote machine.

user_backward_files:

type: `list`, optional
argument path: `simplify_mdata/model_devi/user_backward_files`

Files to be backwarded from the remote machine.

fp:

type: `dict`
argument path: `simplify_mdata/fp`

Parameters of command, machine, and resources for fp

command:

type: `str`
argument path: `simplify_mdata/fp/command`

Command of a program.

machine:

type: `dict`
argument path: `simplify_mdata/fp/machine`

batch_type:

type: `str`

argument path: simplify_mdata/fp/machine/batch_type

The batch job system type. Option: Slurm, LSF, DistributedShell, SGE, Shell, SlurmJobArray, PBS, OpenAPI, Torque, Bohrium, Fugaku

local_root:

type: str | NoneType
argument path: simplify_mdata/fp/machine/local_root

The dir where the tasks and relating files locate. Typically the project dir.

remote_root:

type: str | NoneType, optional
argument path: simplify_mdata/fp/machine/remote_root

The dir where the tasks are executed on the remote machine. Only needed when context is not lazy-local.

clean_asynchronously:

type: bool, optional, default: False
argument path: simplify_mdata/fp/machine/clean_asynchronously

Clean the remote directory asynchronously after the job finishes.

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

context_type:

type: str (flag key)
argument path: simplify_mdata/fp/machine/context_type
possible choices: *LocalContext*, *LazyLocalContext*, *BohriumContext*, *HDFSContext*, *OpenAPIContext*, *SSHContext*

The connection used to remote machine. Option: LazyLocalContext, HDFSContext, BohriumContext, SSHContext, LocalContext, OpenAPIContext

When context_type is set to LocalContext (or its aliases localcontext, Local, local):

remote_profile:

type: dict, optional

argument path: simplify_mdata/fp/machine[LocalContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to LazyLocalContext (or its aliases lazylocalcontext, LazyLocal, lazylocal):

remote_profile:

type: dict, optional

argument path: simplify_mdata/fp/machine[LazyLocalContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to BohriumContext (or its aliases bohriumcontext, Bohrium, bohrium, DpCloudServerContext, dpcloudservercontext, DpCloudServer, dpcloudserver, LebesgueContext, lebesguecontext, Lebesgue, lebesgue):

remote_profile:

type: dict

argument path: simplify_mdata/fp/machine[BohriumContext]/remote_profile

The information used to maintain the connection with remote machine.

email:

type: str, optional

argument path: simplify_mdata/fp/machine[BohriumContext]/remote_profile/email

Email

password:

type: str, optional

argument path: simplify_mdata/fp/machine[BohriumContext]/remote_profile/password

Password

program_id:

type: int, alias: *project_id*

argument path: simplify_mdata/fp/machine[BohriumContext]/remote_profile/program_id

Program ID

retry_count:

type: NoneType | int, optional, default: 2

argument path: simplify_mdata/fp/machine[BohriumContext]/remote_profile/retry_count

The retry count when a job is terminated

ignore_exit_code:

type: bool, optional, default: True

argument path: simplify_mdata/fp/machine[BohriumContext]/remote_profile/ignore_exit_code

The job state will be marked as finished if the exit code is non-zero when set to True. Otherwise, the job state will be designated as terminated.

keep_backup:

type: bool, optional

argument path: simplify_mdata/fp/machine[BohriumContext]/remote_profile/keep_backup

keep download and upload zip

input_data:

type: dict

argument path: simplify_mdata/fp/machine[BohriumContext]/remote_profile/input_data

Configuration of job

When context_type is set to HDFSContext (or its aliases hdfscontext, HDFS, hdfs):

remote_profile:

type: dict, optional

argument path: simplify_mdata/fp/machine[HDFSContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to OpenAPIContext (or its aliases openapicontext, OpenAPI, openapi):

remote_profile:

type: dict, optional

argument path: simplify_mdata/fp/machine[OpenAPIContext]/remote_profile

The information used to maintain the connection with remote machine. This field is empty for this context.

When context_type is set to SSHContext (or its aliases sshcontext, SSH, ssh):

remote_profile:

type: dict

argument path: simplify_mdata/fp/machine[SSHContext]/remote_profile

The information used to maintain the connection with remote machine.

hostname:

type: str

argument path: simplify_mdata/fp/machine[SSHContext]/remote_profile/hostname

hostname or ip of ssh connection.

username:

type: str

argument path: simplify_mdata/fp/machine[SSHContext]/remote_profile/username

username of target linux system

password:

type: str, optional

argument path: simplify_mdata/fp/machine[SSHContext]/remote_profile/password

(deprecated) password of linux system. Please use SSH keys instead to improve security.

port:

type: int, optional, default: 22

argument path: simplify_mdata/fp/machine[SSHContext]/remote_profile/port

ssh connection port.

key_filename:

type: str | NoneType, optional, default: None

argument path: simplify_mdata/fp/machine[SSHContext]/remote_profile/key_filename

key filename used by ssh connection. If left None, find key in ~/.ssh or use password for login

passphrase:

type: str | NoneType, optional, default: None

argument path: simplify_mdata/fp/machine[SSHContext]/remote_profile/passphrase

passphrase of key used by ssh connection

timeout:

type: int, optional, default: 10

argument path: simplify_mdata/fp/machine[SSHContext]/remote_profile/timeout

timeout of ssh connection

totp_secret:

type: str | NoneType, optional, default: None

argument path: simplify_mdata/fp/machine[SSHContext]/remote_profile/totp_secret

Time-based one time password secret. It should be a base32-encoded string extracted from the 2D code.

tar_compress:

type: bool, optional, default: True

argument path: simplify_mdata/fp/machine[SSHContext]/remote_profile/tar_compress

The archive will be compressed in upload and download if it is True. If not, compression will be skipped.

look_for_keys:

type: bool, optional, default: True

argument path: simplify_mdata/fp/machine[SSHContext]/remote_profile/look_for_keys

enable searching for discoverable private key files in ~/.ssh/

resources:

type: dict
argument path: simplify_mdata/fp/resources

number_node:

type: int, optional, default: 1
argument path: simplify_mdata/fp/resources/number_node

The number of node need for each *job*

cpu_per_node:

type: int, optional, default: 1
argument path: simplify_mdata/fp/resources/cpu_per_node

cpu numbers of each node assigned to each job.

gpu_per_node:

type: int, optional, default: 0
argument path: simplify_mdata/fp/resources/gpu_per_node

gpu numbers of each node assigned to each job.

queue_name:

type: str, optional, default: (empty string)
argument path: simplify_mdata/fp/resources/queue_name

The queue name of batch job scheduler system.

group_size:

type: int
argument path: simplify_mdata/fp/resources/group_size

The number of *tasks* in a *job*. 0 means infinity.

custom_flags:

type: typing.List[str], optional
argument path: simplify_mdata/fp/resources/custom_flags

The extra lines pass to job submitting script header

strategy:

type: dict, optional
argument path: simplify_mdata/fp/resources/strategy

strategies we use to generation job submitting scripts.

if_cuda_multi_devices:

type: bool, optional, default: False

argument path: simplify_mdata/fp/resources/strategy/if_cuda_multi_devices

If there are multiple nvidia GPUS on the node, and we want to assign the tasks to different GPUS.If true, dpdispatcher will manually export environment variable CUDA_VISIBLE_DEVICES to different task.Usually, this option will be used with Task.task_need_resources variable simultaneously.

ratio_unfinished:

type: float, optional, default: 0.0

argument path: simplify_mdata/fp/resources/strategy/ratio_unfinished

The ratio of *tasks* that can be unfinished.

customized_script_header_template_file:

type: str, optional

argument path: simplify_mdata/fp/resources/strategy/customized_script_header_template_file

The customized template file to generate job submitting script header, which overrides the default file.

para_deg:

type: int, optional, default: 1

argument path: simplify_mdata/fp/resources/para_deg

Decide how many tasks will be run in parallel.

source_list:

type: typing.List[str], optional, default: []

argument path: simplify_mdata/fp/resources/source_list

The env file to be sourced before the command execution.

module_purge:

type: bool, optional, default: False

argument path: simplify_mdata/fp/resources/module_purge

Remove all modules on HPC system before module load (module_list)

module_unload_list:

type: typing.List[str], optional, default: []
argument path: simplify_mdata/fp/resources/module_unload_list

The modules to be unloaded on HPC system before submitting jobs

module_list:

type: typing.List[str], optional, default: []
argument path: simplify_mdata/fp/resources/module_list

The modules to be loaded on HPC system before submitting jobs

envs:

type: dict, optional, default: {}
argument path: simplify_mdata/fp/resources/envs

The environment variables to be exported on before submitting jobs

prepend_script:

type: typing.List[str], optional, default: []
argument path: simplify_mdata/fp/resources/prepend_script

Optional script run before jobs submitted.

append_script:

type: typing.List[str], optional, default: []
argument path: simplify_mdata/fp/resources/append_script

Optional script run after jobs submitted.

wait_time:

type: float | int, optional, default: 0
argument path: simplify_mdata/fp/resources/wait_time

The waitting time in second after a single *task* submitted

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

batch_type:

type: str (flag key)
argument path: simplify_mdata/fp/resources/batch_type
possible choices: *Fugaku*, *Slurm*, *SlurmJobArray*, *Shell*, *LSF*, *PBS*, *SGE*, *Torque*, *OpenAPI*, *DistributedShell*, *Bohrium*

The batch job system type loaded from machine/batch_type.

When batch_type is set to Fugaku (or its alias fugaku):

kwargs:

type: dict, optional
argument path: simplify_mdata/fp/resources[Fugaku]/kwargs

This field is empty for this batch.

When batch_type is set to Slurm (or its alias slurm):

kwargs:

type: dict, optional
argument path: simplify_mdata/fp/resources[Slurm]/kwargs

Extra arguments.

custom_gpu_line:

type: str | NoneType, optional, default: None
argument path: simplify_mdata/fp/resources[Slurm]/kwargs/custom_gpu_line

Custom GPU configuration, starting with #SBATCH

When batch_type is set to SlurmJobArray (or its alias slurmjobarray):

kwargs:

type: dict, optional
argument path: simplify_mdata/fp/resources[SlurmJobArray]/kwargs

Extra arguments.

custom_gpu_line:

type: str | NoneType, optional, default: None
argument path: simplify_mdata/fp/resources[SlurmJobArray]/kwargs/custom_gpu_line

Custom GPU configuration, starting with #SBATCH

slurm_job_size:

type: int, optional, default: 1
argument path: simplify_mdata/fp/resources[SlurmJobArray]/kwargs/slurm_job_size

Number of tasks in a Slurm job

When batch_type is set to Shell (or its alias shell):

kwargs:

type: dict, optional
argument path: simplify_mdata/fp/resources[Shell]/kwargs

This field is empty for this batch.

When batch_type is set to LSF (or its alias lsf):

kwargs:

type: dict
argument path: simplify_mdata/fp/resources[LSF]/kwargs

Extra arguments.

gpu_usage:

type: bool, optional, default: False
argument path: simplify_mdata/fp/resources[LSF]/kwargs/gpu_usage

Choosing if GPU is used in the calculation step.

gpu_new_syntax:

type: bool, optional, default: False
argument path: simplify_mdata/fp/resources[LSF]/kwargs/gpu_new_syntax

For LFS >= 10.1.0.3, new option -gpu for #BSUB could be used. If False, and old syntax would be used.

gpu_exclusive:

type: bool, optional, default: True
argument path: simplify_mdata/fp/resources[LSF]/kwargs/gpu_exclusive

Only take effect when new syntax enabled. Control whether submit tasks in exclusive way for GPU.

custom_gpu_line:

type: str | NoneType, optional, default: None

argument path: simplify_mdata/fp/resources[LSF]/kwargs/custom_gpu_line

Custom GPU configuration, starting with #BSUB

When batch_type is set to PBS (or its alias pbs):

kwargs:

type: dict, optional

argument path: simplify_mdata/fp/resources[PBS]/kwargs

This field is empty for this batch.

When batch_type is set to SGE (or its alias sge):

kwargs:

type: dict, optional

argument path: simplify_mdata/fp/resources[SGE]/kwargs

This field is empty for this batch.

When batch_type is set to Torque (or its alias torque):

kwargs:

type: dict, optional

argument path: simplify_mdata/fp/resources[Torque]/kwargs

This field is empty for this batch.

When batch_type is set to OpenAPI (or its alias openapi):

kwargs:

type: dict, optional

argument path: simplify_mdata/fp/resources[OpenAPI]/kwargs

This field is empty for this batch.

When batch_type is set to DistributedShell (or its alias distributedshell):

kwargs:

type: dict, optional

argument path: simplify_mdata/fp/resources[DistributedShell]/kwargs

This field is empty for this batch.

When batch_type is set to Bohrium (or its aliases bohrium, Lebesgue, lebesgue, DpCloudServer, dpcloudserver):

kwargs:

type: dict, optional
argument path: simplify_mdata/fp/resources[Bohrium]/kwargs

This field is empty for this batch.

user_forward_files:

type: list, optional
argument path: simplify_mdata/fp/user_forward_files

Files to be forwarded to the remote machine.

user_backward_files:

type: list, optional
argument path: simplify_mdata/fp/user_backward_files

Files to be backwarded from the remote machine.

CHAPTER

SEVEN

AUTO TEST

7.1 Autotest Overview: Autotest for Deep Generator

Suppose that we have a potential (can be DFT, DP, MEAM . . .), `autotest` helps us automatically calculate M properties on N configurations. The folder where the `autotest` runs is called the working directory of `autotest`. Different potentials should be tested in different working directories.

A property is tested in three steps: `make`, `run` and `post`. `make` prepares all computational tasks that are needed to calculate the property. For example to calculate EOS, `make` prepares a series of tasks, each of which has a scaled configuration with certain volume, and all necessary input files necessary for starting a VASP, ABACUS, or LAMMPS calculations. `run` sends all the computational tasks to remote computational resources defined in a machine configuration file like `machine.json`, and automatically collects the results when remote calculations finish. `post` calculates the desired property from the collected results.

7.1.1 Relaxation

The relaxation of a structure should be carried out before calculating all other properties:

```
dpgen autotest make relax.json
dpgen autotest run relax.json machine.json
dpgen autotest post relax.json
```

If, for some reasons, the main program terminated at stage `run`, one can easily restart with the same command. `relax.json` is the parameter file. An example for `deepmd` relaxation is given as:

```
{
        "structures":   ["confs/mp-*"],
        "interaction": {
                "type":         "deepmd",
                "model":        "frozen_model.pb",
                "type_map":     {"Al": 0, "Mg": 1}
        },
        "relaxation": {}
}
```

where the key `structures` provides the structures to relax. `interaction` is provided with `deepmd`, and other options are `vasp`, `abacus`, `meam`. . .

7.1.2 Task type

There are now six task types implemented in the package: `vasp`, `abacus`, `deepmd`, `meam`, `eam_fs`, and `eam_alloy`. An `inter.json` file in json format containing the interaction parameters will be written in the directory of each task after `make`. We give input examples of the `interaction` part for each type below:

VASP:

The default of `potcar_prefix` is "".

```
        "interaction": {
                "type":                 "vasp",
                "incar":        "vasp_input/INCAR",
                "potcar_prefix":"vasp_input",
                "potcars":        {"Al": "POTCAR.al", "Mg": "POTCAR.mg"}
        }
```

ABACUS:

The default of `potcar_prefix` is "". The path of potcars/orb_files/deepks_desc is `potcar_prefix` + `potcars/orb_files/deepks_desc/deepks_model`.

```
        "interaction": {
                "type":                 "abacus",
                "incar":        "abacus_input/INPUT",
                "potcar_prefix":"abacus_input",
                "potcars":        {"Al": "pseudo_potential.al", "Mg": "pseudo_potential.
↪mg"},
                "orb_files": {"Al": "numerical_orb.al", "Mg": "numerical_orb.mg"},
                "atom_masses": {"Al": 26.9815, "Mg":24.305},
                "deepks_desc": "jle.orb",
                "deepks_model": "model.ptg"
        }
```

deepmd:

Only 1 model can be used in autotest in one working directory.

```
        "interaction": {
                "type":                 "deepmd",
                "model":          "frozen_model.pb",
                "type_map":       {"Al": 0, "Mg": 1}
        }
```

meam:

Please make sure the USER-MEAMC package has already been installed in LAMMPS.

```
        "interaction": {
                "type":                 "meam",
                "model":          ["meam.lib","AlMg.meam"],
                "type_map":       {"Al": 1, "Mg": 2}
        }
```

eam_fs & eam_alloy:

Please make sure the MANYBODY package has already been installed in LAMMPS

```
        "interaction": {
                "type":                 "eam_fs (eam_alloy)",
                "model":            "AlMg.eam.fs (AlMg.eam.alloy)",
                "type_map":         {"Al": 1, "Mg": 2}
        }
```

7.1.3 Property type

Now the supported property types are `eos`, `elastic`, `vacancy`, `interstitial`, `surface`, and `gamma`. Before property tests, `relaxation` should be done first or the relaxation results should be present in the corresponding directory `confs/mp-*/relaxation/relax_task`. A file named `task.json` in json format containing the property parameter will be written in the directory of each task after `make` step. Multiple property tests can be performed simultaneously.

7.2 Make run and post

There are three operations in auto test package, namely `make`, `run`, and `post`. Here we take `eos` property as an example for property type.

7.2.1 Make

The `INCAR`, `POSCAR`, `POTCAR` input files for VASP or `in.lammps`, `conf.lmp`, and the interatomic potential files for LAMMPS will be generated in the directory `confs/mp-*/relaxation/relax_task` for relaxation or `confs/mp-*/eos_00/task.[0-9]*[0-9]` for EOS. The `machine.json` file is not needed for `make`. Example:

```
dpgen autotest make relaxation.json
```

7.2.2 Run

The jobs would be dispatched according to the parameter in `machine.json` file and the calculation results would be sent back. Example:

```
dpgen autotest run relaxation.json machine.json
```

7.2.3 Post

The post process of calculation results would be performed. `result.json` in json format will be generated in `confs/mp-*/relaxation/relax_task` for relaxation and `result.json` in json format and `result.out` in txt format in `confs/mp-*/eos_00` for EOS. The `machine.json` file is also not needed for `post`. Example:

```
dpgen autotest post relaxation.json
```

7.3 Relaxation

7.3.1 Relaxation get started and input examples

The relaxation of a structure should be carried out before calculating all other properties.

First, we need input parameter file and we name it `relax.json` here. All the relaxation calculations should be taken either by `VASP`, `ABACUS`, or `LAMMPS`. Here are two input examples for `VASP` and `LAMMPS` respectively.

An example of the input file for relaxation by VASP:

```
{
    "structures":            ["confs/std-*"],
    "interaction": {
            "type":           "vasp",
            "incar":          "vasp_input/INCAR",
            "potcar_prefix":  "vasp_input",
            "potcars":       {"Al": "POTCAR.al"}
        },
    "relaxation": {
            "cal_type":       "relaxation",
            "cal_setting":   {"relax_pos":       true,
                              "relax_shape":     true,
                              "relax_vol":       true,
                              "ediff":           1e-6,
                              "ediffg":         -0.01,
                              "encut":           650,
                              "kspacing":        0.1,
                              "kgamma":          false}
        }
}
```

Key words	data structure	example	description
structures	List of String	["confs/std-*"]	path of different structures
interaction	Dict	See above	description of the task type and atomic interaction
type	String	"vasp"	task type
incar	String	"vasp_input/INCAR"	path for INCAR file in vasp
pot-car_prefix	String	"vasp_input"	prefix of path for POTCAR file in vasp, default = ""
potcars	Dict	{"Al": "POT-CAR.al"}	key is element type and value is potcar name
relaxation	Dict	See above	calculation type and setting for relaxation
cal_type	String	"relaxation" or "static"	calculation type
cal_setting	Dict	See above	calculation setting
relax_pos	Boolean	true	relax atomic position or not, default = true for relaxation
relax_shape	Boolean	true	relax box shape or not, default = true for relaxation
relax_vol	Boolean	true	relax box volume or not, default = true for relaxation
ediff	Float	1e-6	set `EDIFF` parameter in INCAR files
ediffg	Float	-0.01	set `EDIFFG` parameter in INCAR files
encut	Int	650	set `encut` parameter in INCAR files
kspacing	Float	0.1	set `KSPACING` parameter in INCAR files
kgamma	Boolean	false	set `KGAMMA` parameter in INCAR files

An example of the input file for relaxation by LAMMPS:

```
{
    "structures":          ["confs/std-*"],
    "interaction": {
            "type":         "deepmd",
            "model":        "frozen_model.pb",
            "in_lammps":    "lammps_input/in.lammps",
            "type_map":     {"Al": 0}
        },
    "relaxation": {
            "cal_setting":{"etol": 0,
                           "ftol": 1e-10,
                           "maxiter": 5000,
                           "maximal": 500000}
        }
}
```

Other key words different from vasp:

Key words	data structure	example	description
model	String or List of String	"frozen_model.pb"	model file for atomic interaction
in_lammp	String	"lammps_input/in.lan	input file for lammps commands
type_ma	Dict	{"Al": 0}	key is element type and value is type number. DP starts from 0, others starts from 1
etol	Float	0	stopping tolerance for energy
ftol	Float	1e-10	stopping tolerance for force
maxiter	Int	5000	max iterations of minimizer
maxeval	Int	500000	max number of force/energy evaluations

For LAMMPS relaxation and all the property calculations, **package will help to generate `in.lammps` file for user automatically** according to the property type. We can also make the final changes in the `minimize` setting (`minimize etol ftol maxiter maxeval`) in `in.lammps`. In addition, users can apply the input file for lammps commands in the `interaction` part. For further information of the LAMMPS relaxation, we refer users to minimize command.

7.3.2 Relaxation make

The list of the directories storing structures are `["confs/std-*"]` in the previous example. For single element system, if `POSCAR` doesn't exist in the directories: `std-fcc`, `std-hcp`, `std-dhcp`, `std-bcc`, `std-diamond`, and `std-sc`, the package will automatically generate the standard crystal structures **`fcc`**, **`hcp`**, **`dhcp`**, **`bcc`**, **`diamond`**, and **`sc`** in the corresponding directories, respectively. In other conditions and for multi-component system (more than 1), if `POSCAR` doesn't exist, the package will terminate and print the error **"no configuration for autotest"**.

VASP relaxation

Take the input example of Al in the previous section, when we do `make` as follows:

```
dpgen autotest make relaxation.json
```

the following files would be generated:

```
tree confs/std-fcc/relaxation/
```

```
confs/std-fcc/relaxation/
|-- INCAR
|-- POTCAR
`-- relax_task
    |-- INCAR -> ../INCAR
    |-- inter.json
    |-- KPOINTS
    |-- POSCAR -> ../../POSCAR
    |-- POTCAR -> ../POTCAR
    `-- task.json
```

`inter.json` records the information in the `interaction` dictionary and `task.json` records the information in the `relaxation` dictionary.

LAMMPS relaxation

```
dpgen autotest make relaxation.json
tree confs/std-fcc/
```

the output would be:

```
confs/std-fcc/
|-- POSCAR
`-- relaxation
    |-- frozen_model.pb -> ../../../frozen_model.pb
    |-- in.lammps
    `-- relax_task
        |-- conf.lmp
        |-- frozen_model.pb -> ../frozen_model.pb
        |-- in.lammps -> ../in.lammps
        |-- inter.json
        |-- POSCAR -> ../../POSCAR
        `-- task.json
```

the `conf.lmp` is the input configuration and `in.lammps` is the input command file for lammps.

in.lammps: the package would generate the file `confs/mp-*/relaxation/in.lammps` as follows and we refer the user to the further information of fix box/relax function in lammps:

```
clear
units                   metal
dimension          3
boundary           p p p
atom_style           atomic
box                tilt large
read_data          conf.lmp
mass               1 26.982
neigh_modify       every 1 delay 0 check no
pair_style deepmd frozen_model.pb
pair_coeff
compute            mype all pe
thermo             100
thermo_style       custom step pe pxx pyy pzz pxy pxz pyz lx ly lz vol c_mype
dump               1 all custom 100 dump.relax id type xs ys zs fx fy fz
min_style          cg
fix                1 all box/relax iso 0.0
minimize           0 1.000000e-10 5000 500000
fix                1 all box/relax aniso 0.0
minimize           0 1.000000e-10 5000 500000
variable           N equal count(all)
variable           V equal vol
variable           E equal "c_mype"
variable           tmplx equal lx
variable           tmply equal ly
variable           Pxx equal pxx
variable           Pyy equal pyy
variable           Pzz equal pzz
variable           Pxy equal pxy
```

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```
variable          Pxz equal pxz
variable          Pyz equal pyz
variable          Epa equal ${E}/${N}
variable          Vpa equal ${V}/${N}
variable          AA equal (${tmplx}*${tmply})
print "All done"
print "Total number of atoms = ${N}"
print "Final energy per atoms = ${Epa}"
print "Final volume per atoms = ${Vpa}"
print "Final Base area = ${AA}"
print "Final Stress (xx yy zz xy xz yz) = ${Pxx} ${Pyy} ${Pzz} ${Pxy} ${Pxz} ${Pyz}"
```

If user provides lammps input command file `in.lammps`, the `thermo_style` and `dump` commands should be the same as the above file.

interatomic potential model: the `frozen_model.pb` in `confs/mp-*/relaxation` would link to the `frozen_model.pb` file given in the input.

7.3.3 Relaxation run

The work path of each task should be in the form like `confs/mp-*/relaxation` and all task is in the form like `confs/mp-*/relaxation/relax_task`.

The `machine.json` file should be applied in this process and the machine parameters (eg. GPU or CPU) are determined according to the task type (VASP or LAMMPS). Then in each work path, the corresponding tasks would be submitted and the results would be sent back through make_dispatcher.

Take `deepmd` run for example:

```
nohup dpgen autotest run relaxation.json machine-ali.json > run.result 2>&1 &
tree confs/std-fcc/relaxation/
```

the output would be:

```
confs/std-fcc/relaxation/
|-- frozen_model.pb -> ../../../frozen_model.pb
|-- in.lammps
|-- jr.json
`-- relax_task
    |-- conf.lmp
    |-- dump.relax
    |-- frozen_model.pb -> ../frozen_model.pb
    |-- in.lammps -> ../in.lammps
    |-- inter.json
    |-- log.lammps
    |-- outlog
    |-- POSCAR -> ../../POSCAR
    `-- task.json
```

`dump.relax` is the file storing configurations and `log.lammps` is the output file for lammps.

7.3.4 Relaxation post

Take deepmd post for example:

```
dpgen autotest post relaxation.json
tree confs/std-fcc/relaxation/
```

the output will be:

```
confs/std-fcc/relaxation/
|-- frozen_model.pb -> ../../../frozen_model.pb
|-- in.lammps
|-- jr.json
`-- relax_task
    |-- conf.lmp
    |-- CONTCAR
    |-- dump.relax
    |-- frozen_model.pb -> ../frozen_model.pb
    |-- in.lammps -> ../in.lammps
    |-- inter.json
    |-- log.lammps
    |-- outlog
    |-- POSCAR -> ../../POSCAR
    |-- result.json
    `-- task.json
```

`result.json` stores the box cell, coordinates, energy, force, virial,... information of each frame in the relaxation trajectory and `CONTCAR` is the final equilibrium configuration.

`result.json`:


```
{
    "@module": "dpdata.system",
    "@class": "LabeledSystem",
    "data": {
        "atom_numbs": [
            1
        ],
        "atom_names": [
            "Al"
        ],
        "atom_types": {
            "@module": "numpy",
            "@class": "array",
            "dtype": "int64",
            "data": [
                0
            ]
        },
        "orig": {
            "@module": "numpy",
            "@class": "array",
            "dtype": "int64",
            "data": [
```


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```
                0,
                0,
                0
            ]
        },
        "cells": {
            "@module": "numpy",
            "@class": "array",
            "dtype": "float64",
            "data": [
                [
                    [
                        2.8637824638,
                        0.0,
                        0.0
                    ],
                    [
                        1.4318912319,
                        2.4801083646,
                        0.0
                    ],
                    [
                        1.4318912319,
                        0.8267027882,
                        2.3382685902
                    ]
                ],
                [
                    [
                        2.8549207998018438,
                        0.0,
                        0.0
                    ],
                    [
                        1.4274603999009239,
                        2.472433938457684,
                        0.0
                    ],
                    [
                        1.4274603999009212,
                        0.8241446461525599,
                        2.331033071844216
                    ]
                ],
                [
                    [
                        2.854920788303194,
                        0.0,
                        0.0
                    ],
                    [
                        1.427460394144466,
```


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```
                    2.472433928487206,
                    0.0
                ],
                [
                    1.427460394154763,
                    0.8241446428350139,
                    2.331033062460779
                ]
            ]
        ]
    },
    "coords": {
        "@module": "numpy",
        "@class": "array",
        "dtype": "float64",
        "data": [
            [
                [
                    0.0,
                    0.0,
                    0.0
                ]
            ],
            [
                [
                    5.709841595683707e-25,
                    -4.3367974740910857e-19,
                    0.0
                ]
            ],
            [
                [
                    -8.673606219968035e-19,
                    8.673619637565944e-19,
                    8.673610853102186e-19
                ]
            ]
        ]
    },
    "energies": {
        "@module": "numpy",
        "@class": "array",
        "dtype": "float64",
        "data": [
            -3.745029,
            -3.7453815,
            -3.7453815
        ]
    },
    "forces": {
        "@module": "numpy",
        "@class": "array",
```


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```
            "dtype": "float64",
            "data": [
                [
                    [
                        0.0,
                        -6.93889e-18,
                        -3.46945e-18
                    ]
                ],
                [
                    [
                        1.38778e-17,
                        6.93889e-18,
                        -1.73472e-17
                    ]
                ],
                [
                    [
                        1.38778e-17,
                        1.73472e-17,
                        -4.51028e-17
                    ]
                ]
            ]
        },
        "virials": {
            "@module": "numpy",
            "@class": "array",
            "dtype": "float64",
            "data": [
                [
                    [
                        -0.07534992071654338,
                        1.2156615579052586e-17,
                        1.3904892126132796e-17
                    ],
                    [
                        1.2156615579052586e-17,
                        -0.07534992071654338,
                        4.61571024026576e-12
                    ],
                    [
                        1.3904892126132796e-17,
                        4.61571024026576e-12,
                        -0.07534992071654338
                    ]
                ],
                [
                    [
                        -9.978994290457664e-08,
                        -3.396452753975288e-15,
                        8.785831629151552e-16
```


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```
                ],
                [
                    -3.396452753975288e-15,
                    -9.991375413666671e-08,
                    5.4790751628409565e-12
                ],
                [
                    8.785831629151552e-16,
                    5.4790751628409565e-12,
                    -9.973497959053003e-08
                ]
            ],
            [
                [
                    1.506940521266962e-11,
                    1.1152016233536118e-11,
                    -8.231900529157644e-12
                ],
                [
                    1.1152016233536118e-11,
                    -6.517665029355618e-11,
                    -6.33706710415926e-12
                ],
                [
                    -8.231900529157644e-12,
                    -6.33706710415926e-12,
                    5.0011471096530724e-11
                ]
            ]
        ]
    },
    "stress": {
        "@module": "numpy",
        "@class": "array",
        "dtype": "float64",
        "data": [
            [
                [
                    -7.2692250000000005,
                    1.1727839e-15,
                    1.3414452e-15
                ],
                [
                    1.1727839e-15,
                    -7.2692250000000005,
                    4.4529093000000003e-10
                ],
                [
                    1.3414452e-15,
                    4.4529093000000003e-10,
                    -7.2692250000000005
                ]
```


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```
                ],
                [
                    [
                        -9.71695e-06,
                        -3.3072633e-13,
                        8.5551193e-14
                    ],
                    [
                        -3.3072633e-13,
                        -9.729006000000001e-06,
                        5.3351969e-10
                    ],
                    [
                        8.5551193e-14,
                        5.3351969e-10,
                        -9.711598e-06
                    ]
                ],
                [
                    [
                        1.4673689e-09,
                        1.0859169e-09,
                        -8.0157343e-10
                    ],
                    [
                        1.0859169e-09,
                        -6.3465139e-09,
                        -6.1706584e-10
                    ],
                    [
                        -8.0157343e-10,
                        -6.1706584e-10,
                        4.8698191e-09
                    ]
                ]
            ]
        }
    }
}
```

7.4 Property

7.4.1 Property get started and input examples

Here we take deepmd for example and the input file for other task types is similar.

```
{
    "structures":       ["confs/std-*"],
    "interaction": {
        "type":          "deepmd",
```

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```
        "model":          "frozen_model.pb",
        "type_map":      {"Al": 0}
    },
    "properties": [
        {
         "type":          "eos",
         "vol_start":     0.9,
         "vol_end":       1.1,
         "vol_step":      0.01
        },
        {
         "type":          "elastic",
         "norm_deform":   1e-2,
         "shear_deform":  1e-2
        },
        {
         "type":              "vacancy",
         "supercell":         [3, 3, 3],
         "start_confs_path": "../vasp/confs"
        },
        {
         "type":          "interstitial",
         "supercell":    [3, 3, 3],
         "insert_ele":   ["Al"],
         "conf_filters":{"min_dist": 1.5},
         "cal_setting": {"input_prop": "lammps_input/lammps_high"}
        },
        {
         "type":            "surface",
         "min_slab_size":   10,
         "min_vacuum_size":11,
         "max_miller":      2,
         "cal_type":        "static"
        },
        {
         "type": "gamma",
         "lattice_type": "fcc",
         "miller_index": [1, 1, 1],
         "displace_direction": [1, 1, 0],
         "supercell_size": [1, 1, 10],
         "min_vacuum_size": 10,
         "add_fix": ["true", "true", "false"],
         "n_steps": 20
        }
        ]
}
```

Universal key words for properties

Key words	data structure	example	description
type	String	"eos"	property type
skip	Boolean	true	whether to skip current property or not
start_confs_path	String	"../vasp/confs"	start from the equilibrium configuration in other path only for the current property type
cal_setting["input_prop'	String	"lammps_input/lamr	input commands file
cal_setting["overwrite_i	Dict		overwrite the interaction in the `interaction` part only for the current property type

other parameters in `cal_setting` and `cal_type` in `relaxation` also apply in `property`.

Key words for **EOS**

Key words	data structure	example	description
vol_start	Float	0.9	the starting volume related to the equilibrium structure
vol_end	Float	1.1	the biggest volume related to the equilibrium structure
vol_step	Float	0.01	the volume increment related to the equilibrium structure
vol_abs	Boolean	false	whether to treat vol_start, vol_end and vol_step as absolute volume or not (as relative volume), default = false

Key words for **Elastic**

Key words	data structure	example	description
norm_deform	Float	1e-2	deformation in xx, yy, zz, default = 1e-2
shear_deform	Float	1e-2	deformation in other directions, default = 1e-2

Key words for **Vacancy**

Key words	data structure	example	description
supercell	List of Int	[3,3,3]	the supercell to be constructed, default = [1,1,1]

Key words for **Interstitial**

Key words	data structure	example	description
insert_ele	List of String	["Al"]	the element to be inserted
supercell	List of Int	[3,3,3]	the supercell to be constructed, default = [1,1,1]
conf_filters	Dict	"min_dist": 1.5	filter out the undesirable configuration
bcc_self	Boolean	false	whether to do the self-interstitial calculations for bcc structures, default = false

Key words for **Surface**

Key words	data structure	example	description
min_slab_size	Int	10	minimum size of slab thickness
min_vacuum_siz	Int	11	minimum size of vacuum width
pert_xz	Float	0.01	perturbation through xz direction used to compute surface energy, default = 0.01
max_miller	Int	2	the maximum miller index, default = 2

Key words for **Gamma**

Key words	data structure	example	description
lattice_type	String	"fcc"	"bcc" or "fcc" at this stage
miller_index	List of Int	[1,1,1]	slip plane for gamma-line calculation
dis-place_direction	List of Int	[1,1,0]	slip direction for gamma-line calculation
supercell_size	List of Int	[1,1,10]	the supercell to be constructed, default = [1,1,5]
min_vacuum_si	Int or Float	10	minimum size of vacuum width, default = 20
add_fix	List of String	['true','true','fal	whether to fix atoms in the direction, default = ['true','true','false'] (standard method)
n_steps	Int	20	Number of points for gamma-line calculation, default = 10

7.4.2 Property make

```
dpgen autotest make property.json
```

EOS output:

```
confs/std-fcc/eos_00/
|-- frozen_model.pb -> ../../../frozen_model.pb
|-- task.000000
|   |-- conf.lmp
|   |-- eos.json
|   |-- frozen_model.pb -> ../frozen_model.pb
|   |-- in.lammps
|   |-- inter.json
|   |-- POSCAR
|   |-- POSCAR.orig -> ../../relaxation/relax_task/CONTCAR
|   `-- task.json
|-- task.000001
|   |-- conf.lmp
|   |-- eos.json
|   |-- frozen_model.pb -> ../frozen_model.pb
|   |-- in.lammps
|   |-- inter.json
|   |-- POSCAR
|   |-- POSCAR.orig -> ../../relaxation/relax_task/CONTCAR
```

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```
|   `-- task.json
...
`-- task.000019
    |-- conf.lmp
    |-- eos.json
    |-- frozen_model.pb -> ../frozen_model.pb
    |-- in.lammps
    |-- inter.json
    |-- POSCAR
    |-- POSCAR.orig -> ../../relaxation/relax_task/CONTCAR
    `-- task.json
```

`eos.json` records the `volume` and `scale` of the corresponding task.

Elastic output:

```
confs/std-fcc/elastic_00/
|-- equi.stress.json
|-- frozen_model.pb -> ../../../frozen_model.pb
|-- in.lammps
|-- POSCAR -> ../relaxation/relax_task/CONTCAR
|-- task.000000
|   |-- conf.lmp
|   |-- frozen_model.pb -> ../frozen_model.pb
|   |-- in.lammps -> ../in.lammps
|   |-- inter.json
|   |-- POSCAR
|   |-- strain.json
|   `-- task.json
|-- task.000001
|   |-- conf.lmp
|   |-- frozen_model.pb -> ../frozen_model.pb
|   |-- in.lammps -> ../in.lammps
|   |-- inter.json
|   |-- POSCAR
|   |-- strain.json
|   `-- task.json
...
`-- task.000023
    |-- conf.lmp
    |-- frozen_model.pb -> ../frozen_model.pb
    |-- in.lammps -> ../in.lammps
    |-- inter.json
    |-- POSCAR
    |-- strain.json
    `-- task.json
```

`equi.stress.json` records the stress information of the equilibrium task and `strain.json` records the deformation information of the corresponding task.

Vacancy output:

```
confs/std-fcc/vacancy_00/
```

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```
|-- frozen_model.pb -> ../../../frozen_model.pb
|-- in.lammps
|-- POSCAR -> ../relaxation/relax_task/CONTCAR
`-- task.000000
    |-- conf.lmp
    |-- frozen_model.pb -> ../frozen_model.pb
    |-- in.lammps -> ../in.lammps
    |-- inter.json
    |-- POSCAR
    |-- supercell.json
    `-- task.json
```

`supercell.json` records the supercell size information of the corresponding task.

Interstitial output:

```
confs/std-fcc/interstitial_00/
|-- element.out
|-- frozen_model.pb -> ../../../frozen_model.pb
|-- in.lammps
|-- POSCAR -> ../relaxation/relax_task/CONTCAR
|-- task.000000
|   |-- conf.lmp
|   |-- frozen_model.pb -> ../frozen_model.pb
|   |-- in.lammps -> ../in.lammps
|   |-- inter.json
|   |-- POSCAR
|   |-- supercell.json
|   `-- task.json
`-- task.000001
    |-- conf.lmp
    |-- frozen_model.pb -> ../frozen_model.pb
    |-- in.lammps -> ../in.lammps
    |-- inter.json
    |-- POSCAR
    |-- supercell.json
    `-- task.json
```

`element.out` records the inserted element type of each task and `supercell.json` records the supercell size information of the corresponding task.

Surface output:

```
confs/std-fcc/surface_00/
|-- frozen_model.pb -> ../../../frozen_model.pb
|-- in.lammps
|-- POSCAR -> ../relaxation/relax_task/CONTCAR
|-- task.000000
|   |-- conf.lmp
|   |-- frozen_model.pb -> ../frozen_model.pb
|   |-- in.lammps -> ../in.lammps
|   |-- inter.json
|   |-- miller.json
```

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```
|   |-- POSCAR
|   |-- POSCAR.tmp
|   `-- task.json
|-- task.000001
|   |-- conf.lmp
|   |-- frozen_model.pb -> ../frozen_model.pb
|   |-- in.lammps -> ../in.lammps
|   |-- inter.json
|   |-- miller.json
|   |-- POSCAR
|   |-- POSCAR.tmp
|   `-- task.json
...
`-- task.000008
    |-- conf.lmp
    |-- frozen_model.pb -> ../frozen_model.pb
    |-- in.lammps -> ../in.lammps
    |-- inter.json
    |-- miller.json
    |-- POSCAR
    |-- POSCAR.tmp
    `-- task.json
```

`miller.json` records the miller index of the corresponding task.

7.4.3 Property run

```
nohup dpgen autotest run property.json machine-ali.json > run.result 2>&1 &
```

the result file `log.lammps`, `dump.relax`, and `outlog` would be sent back.

7.4.4 Property-post

Use command

```
dpgen autotest post property.json
```

to post results as `result.json` and `result.out` in each property's path.

7.4.5 Properties

EOS get started and input examples

Equation of State (EOS) here calculates the energies of the most stable structures as a function of volume. Users can refer to Figure 4 of the dpgen CPC paper for more information of EOS.

An example of the input file for EOS by VASP:

```
{
        "structures":         ["confs/mp-*","confs/std-*","confs/test-*"],
        "interaction": {
                "type":                 "vasp",
                "incar":          "vasp_input/INCAR",
                "potcar_prefix":"vasp_input",
                "potcars":          {"Al": "POTCAR.al", "Mg": "POTCAR.mg"}
        },
        "properties": [
        {
         "type":          "eos",
         "vol_start":     0.9,
         "vol_end":       1.1,
         "vol_step":      0.01
        }
        ]
}
```

`vol_start` is the starting volume relative to the equilibrium structure, `vol_step` is the volume increment step relative to the equilibrium structure, and the biggest relative volume is smaller than `vol_end`.

EOS make

Step 1. Before `make` in EOS, the equilibrium configuration `CONTCAR` must be present in `confs/mp-*/relaxation`.

Step 2. For the input example in the previous section, when we do `make`, 40 tasks would be generated as `confs/mp-*/eos_00/task.000000`, `confs/mp-*/eos_00/task.000001`, ... , `confs/mp-*/eos_00/task.000039`. The suffix `00` is used for possible `refine` later.

Step 3. If the task directory, for example `confs/mp-*/eos_00/task.000000` is not empty, the old input files in it including `INCAR`, `POSCAR`, `POTCAR`, `conf.lmp`, `in.lammps` would be deleted.

Step 4. In each task directory, `POSCAR.orig` would link to `confs/mp-*/relaxation/CONTCAR`. Then the `scale` parameter can be calculated as:

```
scale = (vol_current / vol_equi) ** (1. / 3.)
```

`vol_current` is the corresponding volume per atom of the current task and `vol_equi` is the volume per atom of the equilibrium configuration. Then the `poscar_scale` function in `dpgen.auto_test.lib.vasp` module would help to generate `POSCAR` file with `vol_current` in `confs/mp-*/eos_00/task.[0-9]*[0-9]`.

Step 5. According to the task type, the input file including `INCAR`, `POTCAR` or `conf.lmp`, `in.lammps` would be written in every `confs/mp-*/eos_00/task.[0-9]*[0-9]`.

EOS run

The work path of each task should be in the form like `confs/mp-*/eos_00` and all task is in the form like `confs/mp-*/eos_00/task.[0-9]*[0-9]`.

When we dispatch tasks, we would go through every individual work path in the list `confs/mp-*/eos_00`, and then submit `task.[0-9]*[0-9]` in each work path.

EOS post

The post processing of EOS would go to every directory in `confs/mp-*/eos_00` and do the post processing. Let's suppose we are now in `confs/mp-100/eos_00` and there are `task.000000, task.000001,..., task.000039` in this directory. By reading `inter.json` file in every task directory, the task type can be determined and the energy and force information of every task can further be obtained. By appending the `dict` of energy and force into a list, an example of the list with 1 atom is given as:

```
[
    {"energy": E1, "force": [fx1, fy1, fz1]},
    {"energy": E2, "force": [fx2, fy2, fz2]},
    ...
    {"energy": E40, "force": [fx40, fy40, fz40]}
]
```

Then the volume can be calculated from the task id and the corresponding energy can be obtained from the list above. Finally, there would be `result.json` in json format and `result.out` in txt format in `confs/mp-100/eos_00` containing the EOS results.

An example of `result.json` is give as:

```
{
    "14.808453313267595": -3.7194474,
    "14.972991683415014": -3.7242038,
        ...
    "17.934682346068534": -3.7087655
}
```

An example of `result.out` is given below:

```
onf_dir: /root/auto_test_example/deepmd/confs/std-fcc/eos_00
 VpA(A^3)  EpA(eV)
 14.808   -3.7194
 14.973   -3.7242
   ...      ...
 17.935   -3.7088
```

Elastic get started and input examples

Here we calculate the mechanical properties which include elastic constants (C11 to C66), bulk modulus Bv, shear modulus Gv, Youngs modulus Ev, and Poission ratio Uv of a certain crystal structure.

An example of the input file for Elastic by deepmd:

```
{
        "structures":        ["confs/mp-*","confs/std-*","confs/test-*"],
        "interaction": {
                "type": "deepmd",
        "model": "frozen_model.pb",
                "type_map":        {"Al": 0, "Mg": 1}
        },
        "properties": [
            {
                "type": "elastic",
                "norm_deform": 1e-2,
                    "shear_deform": 1e-2
                }
        ]
}
```

Here the default values of `norm_deform` and `shear_deform` are **1e-2** and **1e-2**, respectively. A list of `norm_strains` and `shear_strains` would be generated as below:

```
[-norm_def, -0.5 * norm_def, 0.5 * norm_def, norm_def]
[-shear_def, -0.5 * shear_def, 0.5 * shear_def, shear_def]
```

Elastic make

Step 1. The `DeformedStructureSet` module in pymatgen.analysis.elasticity.strain is used to generate a set of independently deformed structures. `equi.stress.out` file is written to record the equilibrium stress in the Elastic directory. For the example in the previous section, `equi.stress.out` should be in `confs/mp-*/elastic_00`.

Step 2. If there are `init_from_suffix` and `output_suffix` parameter in the `properties` part, the *refine process* follows. Else, the deformed structure (`POSCAR`) and strain information (`strain.out`) are written in the task directory, for example, in `confs/mp-*/elastic_00/task.000000`.

Step 3. When doing `elastic` by VASP, `ISIF=2`. When doing by LAMMPS, the following `in.lammps` would be written.

```
units         metal
dimension        3
boundary        p        p    p
atom_style        atomic
box             tilt large
read_data       conf.lmp
mass            1 1
mass            2 1
neigh_modify    every 1 delay 0 check no
pair_style deepmd frozen_model.pb
```

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```
pair_coeff
compute         mype all pe
thermo          100
thermo_style    custom step pe pxx pyy pzz pxy pxz pyz lx ly lz vol c_mype
dump            1 all custom 100 dump.relax id type xs ys zs fx fy fz
min_style       cg
minimize        0 1.000000e-10 5000 500000
variable        N equal count(all)
variable        V equal vol
variable        E equal "c_mype"
variable        Pxx equal pxx
variable        Pyy equal pyy
variable        Pzz equal pzz
variable        Pxy equal pxy
variable        Pxz equal pxz
variable        Pyz equal pyz
variable        Epa equal ${E}/${N}
variable        Vpa equal ${V}/${N}
print "All done"
print "Total number of atoms = ${N}"
print "Final energy per atoms = ${Epa}"
print "Final volume per atoms = ${Vpa}"
print "Final Stress (xx yy zz xy xz yz) = ${Pxx} ${Pyy} ${Pzz} ${Pxy} ${Pxz} ${Pyz}"
```

Elastic run

Very similar to the `run` operation of `EOS` except for in different directories. Now the work path of each task should be in the form like `confs/mp-*/elastic_00` and all task is in the form like `confs/mp-*/elastic_00/task.[0-9]*[0-9]`.

Elastic post

The `ElasticTensor` module in pymatgen.analysis.elasticity.elastic is used to get the elastic tensor, Bv, and Gv. The mechanical properties of a crystal structure would be written in `result.json` in json format and `result.out` in txt format. The example of the output file is give below.

result.json

```
{
    "elastic_tensor": [
        134.90955999999997,
        54.329958699999985,
        51.802386099999985,
        3.5745279599999993,
        -1.3886325999999648e-05,
        -1.9638233999999486e-05,
        54.55840299999999,
        134.59654699999996,
        51.7972336,
```

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```
        -3.53972684,
        1.839568799999963e-05,
        8.756799399999951e-05,
        51.91324859999999,
        51.913292199999994,
        137.01763799999998,
        -5.090339399999969e-05,
        6.99251629999996e-05,
        3.736478699999946e-05,
        3.8780564440000007,
        -3.770445632,
        -1.2766205999999956,
        35.41343199999999,
        2.2479590800000023e-05,
        1.3837692000000172e-06,
        -4.959999999495933e-06,
        2.5800000003918792e-06,
        1.4800000030874965e-06,
        2.9000000008417968e-06,
        35.375960199999994,
        3.8608356,
        0.0,
        0.0,
        0.0,
        0.0,
        4.02554856,
        38.375018399999995
    ],
    "BV": 80.3153630222222,
    "GV": 38.40582656,
    "EV": 99.37716395728943,
    "uV": 0.2937771799031088
}
```


The order of `elastic_tensor` is C11, C12, ..., C16, C21, C22, ..., C26, ..., C66 and the unit of Bv, Gv, Ev, and uv is GPa.

result.out

```
/root/auto_test_example/deepmd/confs/std-fcc/elastic_00
 134.91   54.33   51.80    3.57   -0.00   -0.00
  54.56  134.60   51.80   -3.54    0.00    0.00
  51.91   51.91  137.02   -0.00    0.00    0.00
   3.88   -3.77   -1.28   35.41    0.00    0.00
  -0.00    0.00    0.00    0.00   35.38    3.86
   0.00    0.00    0.00    0.00    4.03   38.38
# Bulk   Modulus BV = 80.32 GPa
# Shear  Modulus GV = 38.41 GPa
# Youngs Modulus EV = 99.38 GPa
# Poission Ratio uV = 0.29
```

Vacancy get started and input examples

Vacancy calculates the energy difference when removing an atom from the crystal structure. We only need to give the information of supercell to help calculate the vacancy energy and the default value of supercell is [1, 1, 1].

An example of the input file for Vacancy by deepmd:

```
{
        "structures":         "confs/mp-*",
        "interaction": {
                "type":                "deepmd",
                "model":         "frozen_model.pb",
                "type_map":         {"Al": 0, "Mg": 1}
        },
        "properties": [
            {
                "type":          "vacancy",
                "supercell":         [1, 1, 1]
            }
        ]
}
```

Vacancy make

Step 1. The VacancyGenerator module in pymatgen.analysis.defects.generators is used to generate a set of structures with vacancy.

Step 2. If there are init_from_suffix and output_suffix parameter in the properties part, the *refine process* follows. If reproduce is evoked, the *reproduce process* follows. Otherwise, the vacancy structure (POSCAR) and supercell information (supercell.out) are written in the task directory, for example, in confs/mp-*/vacancy_00/task.000000 with the check and possible removing of the old input files like before.

Step 3. When doing vacancy by VASP, ISIF = 3. When doing vacancy by LAMMPS, the same in.lammps as that in *EOS (change_box is True)* would be generated with scale set to one.

Vacancy run

Very similar to the run operation of EOS except for in different directories. Now the work path of each task should be in the form like confs/mp-*/vacancy_00 and all task is in the form like confs/mp-*/vacancy_00/task.[0-9]*[0-9].

Vacancy post

For Vacancy, we need to calculate the energy difference between a crystal structure with and without a vacancy. The examples of the output files result.json in json format and result.out in txt format are given below.

result.json

```
{
    "[3, 3, 3]-task.000000": [
        0.7352769999999964,
        -96.644642,
        -97.379919
    ]
}
```

result.out

```
/root/auto_test_example/deepmd/confs/std-fcc/vacancy_00
Structure:          Vac_E(eV)  E(eV) equi_E(eV)
[3, 3, 3]-task.000000:   0.735  -96.645 -97.380
```

Interstitial get started and input examples

`Interstitial` calculates the energy difference when adding an atom into the crystal structure. We need to give the information of `supercell` (default value is [1, 1, 1]) and `insert_ele` list for the element types of the atoms added in.

An example of the input file for Interstitial by deepmd:

```
{
        "structures":         "confs/mp-*",
        "interaction": {
                "type":                "deepmd",
                "model":         "frozen_model.pb",
                "type_map":        {"Al": 0, "Mg": 1}
        },
        "properties": [
            {
                "type":         "interstitial",
                "supercell":    [3, 3, 3],
                "insert_ele":   ["Al"],
                "conf_filters":{"min_dist": 1.5},
                "cal_setting": {"input_prop": "lammps_input/lammps_high"}
            }
        ]
}
```

We add a `conf_filters` parameter in `properties` part and this parameter can help to eliminate undesirable structure which can render rather difficult convergence in calculations. In the example above, **"min_dist": 1.5** means if the smallest atomic distance in the structure is less than 1.5 angstrom, the configuration would be eliminated and not used in calculations.

Interstitial make

Step 1. For each element in `insert_ele` list, `InterstitialGenerator` module in pymatgen.analysis.defects.generators would help to generate interstitial structure. The structure would be appended into a list if it can meet the requirements in `conf_filters`.

Step 2. If `refine` is `True`, we do *refine process*. If `reprod-opt` is `True` (the default is **False**), we do *reproduce process*. Else, the vacancy structure (`POSCAR`) and supercell information (`supercell.out`) are written in the task directory, for example, in `confs/mp-*/interstitial_00/task.000000` with the check and possible removing of the old input files like before.

Step 3. In `interstitial` by VASP, `ISIF = 3`. In `interstitial` by LAMMPS, the same `in.lammps` as that in *EOS (change_box is True)* would be generated with `scale` set to one.

Interstitial run

Very similar to the `run` operation of `EOS` except for in different directories. Now the work path of each task should be in the form like `confs/mp-*/interstitial_00` and all task is in the form like `confs/mp-*/interstitial_00/task.[0-9]*[0-9]`.

Interstitial post

For `Interstitial`, we need to calculate the energy difference between a crystal structure with and without atom added in. The examples of the output files `result.json` in json format and `result.out` in txt format are given below.

result.json

```
{
    "Al-[3, 3, 3]-task.000000": [
        4.022952000000004,
        -100.84773,
        -104.870682
    ],
    "Al-[3, 3, 3]-task.000001": [
        2.7829520000000088,
        -102.08773,
        -104.870682
    ]
}
```

result.out

```
/root/auto_test_example/deepmd/confs/std-fcc/interstitial_00
Insert_ele-Struct: Inter_E(eV)  E(eV) equi_E(eV)
Al-[3, 3, 3]-task.000000:   4.023  -100.848 -104.871
Al-[3, 3, 3]-task.000001:   2.783  -102.088 -104.871
```

Surface get started and input examples

`Surface` calculates the surface energy. We need to give the information of `min_slab_size`, `min_vacuum_size`, `max_miller` (default value is 2), and `pert_xz` which means perturbations in xz and will help work around vasp bug.

An example of the input file for Surface by deepmd:

```
{
        "structures":         "confs/mp-*",
        "interaction": {
                "type":                "deepmd",
                "model":         "frozen_model.pb",
                "type_map":        {"Al": 0, "Mg": 1}
        },
        "properties": [
            {
                "type":            "surface",
                "min_slab_size":   10,
                "min_vacuum_size":11,
                "max_miller":      2,
                "cal_type":        "static"
            }
        ]
}
```

Surface make

Step 1. Based on the equilibrium configuration, `generate_all_slabs` module in pymatgen.core.surface would help to generate surface structure list with using `max_miller`, `min_slab_size`, and `min_vacuum_size` parameters.

Step 2. If `refine` is True, we do *refine process*. If `reprod-opt` is True (the default is False), we do *reproduce process*. Otherwise, the surface structure (`POSCAR`) with perturbations in xz and miller index information (`miller.out`) are written in the task directory, for example, in `confs/mp-*/interstitial_00/task.000000` with the check and possible removing of the old input files like before.

Surface run

Very similar to the `run` operation of `EOS` except for in different directories. Now the work path of each task should be in the form like `confs/mp-*/surface_00` and all task is in the form like `confs/mp-*/surface_00/task.[0-9]*[0-9]`.

Surface post

For `Surface`, we need to calculate the energy difference between a crystal structure with and without a surface with a certain miller index divided by the surface area.

The examples of the output files `result.json` in json format and `result.out` in txt format are given below.

result.json


```
{
    "[1, 1, 1]-task.000000": [
        0.8051037974207992,
        -3.6035018,
        -3.7453815
    ],
    "[2, 2, 1]-task.000001": [
        0.9913881928811771,
        -3.5781115999999997,
        -3.7453815
    ],
    "[1, 1, 0]-task.000002": [
        0.9457333586026173,
        -3.5529366000000002,
        -3.7453815
    ],
    "[2, 2, -1]-task.000003": [
        0.9868013100872397,
        -3.5590607142857142,
        -3.7453815
    ],
    "[2, 1, 1]-task.000004": [
        1.0138239046484236,
        -3.563035875,
        -3.7453815
    ],
    "[2, 1, -1]-task.000005": [
        1.0661817319108005,
        -3.5432459166666668,
        -3.7453815
    ],
    "[2, 1, -2]-task.000006": [
        1.034003253044026,
        -3.550884125,
        -3.7453815
    ],
    "[2, 0, -1]-task.000007": [
```


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```
        0.9569958287615818,
        -3.5685403333333334,
        -3.7453815
    ],
    "[2, -1, -1]-task.000008": [
        0.9432935501134583,
        -3.5774615714285716,
        -3.7453815
    ]
}
```

result.out

```
/root/auto_test_example/deepmd/confs/std-fcc/surface_00
Miller_Indices:         Surf_E(J/m^2) EpA(eV) equi_EpA(eV)
[1, 1, 1]-task.000000:          0.805      -3.604   -3.745
[2, 2, 1]-task.000001:          0.991      -3.578   -3.745
[1, 1, 0]-task.000002:          0.946      -3.553   -3.745
[2, 2, -1]-task.000003:         0.987      -3.559   -3.745
[2, 1, 1]-task.000004:          1.014      -3.563   -3.745
[2, 1, -1]-task.000005:         1.066      -3.543   -3.745
[2, 1, -2]-task.000006:         1.034      -3.551   -3.745
[2, 0, -1]-task.000007:         0.957      -3.569   -3.745
[2, -1, -1]-task.000008:        0.943      -3.577   -3.745
```

7.5 Refine

7.5.1 Refine get started and input examples

Sometimes we want to refine the calculation of a property from previous results. For example, when higher convergence criteria `EDIFF` and `EDIFFG` are necessary in VASP, the new VASP calculation is desired to start from the previous output configuration, rather than starting from scratch.

An example of the input file `refine.json` is given below:

```
{
    "structures":       ["confs/std-*"],
    "interaction": {
        "type":          "deepmd",
        "model":         "frozen_model.pb",
        "type_map":     {"Al": 0}
    },
    "properties": [
        {
        "type":             "vacancy",
        "init_from_suffix": "00",
        "output_suffix":    "01",
        "cal_setting":     {"input_prop":  "lammps_input/lammps_high"}
```

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```
        }
        ]
}
```

In this example, `refine` would output the results to `vacancy_01` based on the previous results in `vacancy_00` by using a different input commands file for lammps.

7.5.2 Refine make

```
dpgen autotest make refine.json
tree confs/std-fcc/vacancy_01/
```

the output will be:

```
confs/std-fcc/vacancy_01/
|-- frozen_model.pb -> ../../../frozen_model.pb
|-- in.lammps
`-- task.000000
    |-- conf.lmp
    |-- frozen_model.pb -> ../frozen_model.pb
    |-- in.lammps -> ../in.lammps
    |-- inter.json
    |-- POSCAR -> ../../vacancy_00/task.000000/CONTCAR
    |-- supercell.json -> ../../vacancy_00/task.000000/supercell.json
    `-- task.json
```

an new directory `vacancy_01` would be established and the starting configuration links to previous results.

7.5.3 Refine run

```
nohup dpgen autotest run refine.json machine-ali.json > run.result 2>&1 &
```

the run process of `refine` is similar to before.

7.5.4 Refine post

```
dpgen autotest post refine.json
```

the post process of `refine` is similar to the corresponding property.

7.6 Reproduce

7.6.1 Reproduce get started and input examples

Sometimes we want to reproduce the initial results with the same configurations for cross validation. This version of autotest package can accomplish this successfully in all property types except for `Elastic`. An input example for using `deepmd` to reproduce the `VASP` Interstitial results is given below:

```
{
    "structures":       ["confs/std-*"],
    "interaction": {
        "type":           "deepmd",
        "model":          "frozen_model.pb",
        "type_map":     {"Al": 0}
    },
    "properties": [
        {
        "type":             "interstitial",
        "reproduce":        true,
        "init_from_suffix": "00",
        "init_data_path":   "../vasp/confs",
        "reprod_last_frame":       false
        }
        ]
}
```

`reproduce` denotes whether to do `reproduce` or not and the default value is False.

`init_data_path` is the path of VASP or LAMMPS initial data to be reproduced. `init_from_suffix` is the suffix of the initial data and the default value is "00". In this case, the VASP Interstitial results are stored in `../vasp/confs/std-*/interstitial_00` and the reproduced Interstitial results would be in `deepmd/confs/std-*/interstitial_reprod`.

`reprod_last_frame` denotes if only the last frame is used in reproduce. The default value is True for eos and surface, but is False for vacancy and interstitial.

7.6.2 Reproduce make

```
dpgen autotest make reproduce.json
tree confs/std-fcc/interstitial_reprod/
```

the output will be:

```
confs/std-fcc/interstitial_reprod/
|-- frozen_model.pb -> ../../../frozen_model.pb
|-- in.lammps
|-- task.000000
|   |-- conf.lmp
|   |-- frozen_model.pb -> ../frozen_model.pb
|   |-- in.lammps -> ../in.lammps
|   |-- inter.json
|   |-- POSCAR
```

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```
|   `-- task.json
|-- task.000001
|   |-- conf.lmp
|   |-- frozen_model.pb -> ../frozen_model.pb
|   |-- in.lammps -> ../in.lammps
|   |-- inter.json
|   |-- POSCAR
|   `-- task.json
...
`-- task.000038
    |-- conf.lmp
    |-- frozen_model.pb -> ../frozen_model.pb
    |-- in.lammps -> ../in.lammps
    |-- inter.json
    |-- POSCAR
    `-- task.json
```

every singe frame in the initial data is split into each task and the following `in.lammps` would help to do the `static` calculation:

```
clear
units                  metal
dimension          3
boundary           p p p
atom_style           atomic
box                tilt large
read_data          conf.lmp
mass               1 26.982
neigh_modify       every 1 delay 0 check no
pair_style deepmd frozen_model.pb
pair_coeff
compute            mype all pe
thermo             100
thermo_style       custom step pe pxx pyy pzz pxy pxz pyz lx ly lz vol c_mype
dump               1 all custom 100 dump.relax id type xs ys zs fx fy fz
run                0
variable           N equal count(all)
variable           V equal vol
variable           E equal "c_mype"
variable           tmplx equal lx
variable           tmply equal ly
variable           Pxx equal pxx
variable           Pyy equal pyy
variable           Pzz equal pzz
variable           Pxy equal pxy
variable           Pxz equal pxz
variable           Pyz equal pyz
variable           Epa equal ${E}/${N}
variable           Vpa equal ${V}/${N}
variable           AA equal (${tmplx}*${tmply})
print "All done"
print "Total number of atoms = ${N}"
```

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```
print "Final energy per atoms = ${Epa}"
print "Final volume per atoms = ${Vpa}"
print "Final Base area = ${AA}"
print "Final Stress (xx yy zz xy xz yz) = ${Pxx} ${Pyy} ${Pzz} ${Pxy} ${Pxz} ${Pyz}"
```

7.6.3 Reproduce run

```
nohup dpgen autotest run reproduce.json machine-ali.json > run.result 2>&1 &
```

the run process of `reproduce` is similar to before.

7.6.4 Reproduce post

```
dpgen autotest post reproduce.json
```

the output will be:

`result.out`:

```
/root/auto_test_example/deepmd/confs/std-fcc/interstitial_reprod
Reproduce: Initial_path Init_E(eV/atom)  Reprod_E(eV/atom)  Difference(eV/atom)
.../vasp/confs/std-fcc/interstitial_00/task.000000  -3.020   -3.240   -0.220
.../vasp/confs/std-fcc/interstitial_00/task.000000  -3.539   -3.541   -0.002
.../vasp/confs/std-fcc/interstitial_00/task.000000  -3.582   -3.582   -0.001
.../vasp/confs/std-fcc/interstitial_00/task.000000  -3.582   -3.581    0.001
.../vasp/confs/std-fcc/interstitial_00/task.000000  -3.594   -3.593    0.001
.../vasp/confs/std-fcc/interstitial_00/task.000000  -3.594   -3.594    0.001
.../vasp/confs/std-fcc/interstitial_00/task.000000  -3.598   -3.597    0.001
.../vasp/confs/std-fcc/interstitial_00/task.000000  -3.600   -3.600    0.001
.../vasp/confs/std-fcc/interstitial_00/task.000000  -3.600   -3.600    0.001
.../vasp/confs/std-fcc/interstitial_00/task.000000  -3.601   -3.600    0.001
.../vasp/confs/std-fcc/interstitial_00/task.000000  -3.602   -3.601    0.001
.../vasp/confs/std-fcc/interstitial_00/task.000000  -3.603   -3.602    0.001
.../vasp/confs/std-fcc/interstitial_00/task.000000  -3.603   -3.602    0.001
.../vasp/confs/std-fcc/interstitial_00/task.000000  -3.603   -3.602    0.001
.../vasp/confs/std-fcc/interstitial_00/task.000000  -3.603   -3.602    0.001
.../vasp/confs/std-fcc/interstitial_00/task.000000  -3.603   -3.602    0.001
.../vasp/confs/std-fcc/interstitial_00/task.000000  -3.603   -3.602    0.001
.../vasp/confs/std-fcc/interstitial_00/task.000000  -3.603   -3.602    0.001
.../vasp/confs/std-fcc/interstitial_00/task.000001  -3.345   -3.372   -0.027
.../vasp/confs/std-fcc/interstitial_00/task.000001  -3.546   -3.556   -0.009
.../vasp/confs/std-fcc/interstitial_00/task.000001  -3.587   -3.593   -0.007
.../vasp/confs/std-fcc/interstitial_00/task.000001  -3.593   -3.599   -0.006
.../vasp/confs/std-fcc/interstitial_00/task.000001  -3.600   -3.606   -0.006
.../vasp/confs/std-fcc/interstitial_00/task.000001  -3.600   -3.606   -0.006
.../vasp/confs/std-fcc/interstitial_00/task.000001  -3.624   -3.631   -0.006
.../vasp/confs/std-fcc/interstitial_00/task.000001  -3.634   -3.640   -0.007
.../vasp/confs/std-fcc/interstitial_00/task.000001  -3.637   -3.644   -0.007
.../vasp/confs/std-fcc/interstitial_00/task.000001  -3.637   -3.644   -0.007
.../vasp/confs/std-fcc/interstitial_00/task.000001  -3.638   -3.645   -0.007
```

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```
.../vasp/confs/std-fcc/interstitial_00/task.000001  -3.638   -3.645   -0.007
.../vasp/confs/std-fcc/interstitial_00/task.000001  -3.639   -3.646   -0.007
.../vasp/confs/std-fcc/interstitial_00/task.000001  -3.639   -3.646   -0.007
.../vasp/confs/std-fcc/interstitial_00/task.000001  -3.639   -3.646   -0.007
.../vasp/confs/std-fcc/interstitial_00/task.000001  -3.639   -3.646   -0.007
.../vasp/confs/std-fcc/interstitial_00/task.000001  -3.639   -3.646   -0.007
.../vasp/confs/std-fcc/interstitial_00/task.000001  -3.639   -3.646   -0.007
.../vasp/confs/std-fcc/interstitial_00/task.000001  -3.639   -3.646   -0.007
.../vasp/confs/std-fcc/interstitial_00/task.000001  -3.639   -3.646   -0.007
.../vasp/confs/std-fcc/interstitial_00/task.000001  -3.639   -3.646   -0.007
```

the comparison of the initial and reproduced results as well as the absolute path of the initial data is recorded.

`result.json`:

```
{
    "/root/auto_test_example/vasp/confs/std-fcc/interstitial_00/task.000000": {
        "nframes": 18,
        "error": 0.0009738182472213228
    },
    "/root/auto_test_example/vasp/confs/std-fcc/interstitial_00/task.000001": {
        "nframes": 21,
        "error": 0.0006417039154057605
    }
}
```

the error analysis corresponding to the initial data is recorded and the error of the first frame is disregarded when all the frames are considered in reproduce.

CHAPTER

EIGHT

USER GUIDE

This part aims to show you how to get the community's help. Some frequently asked questions are listed in troubleshooting, and the explanation of errors that often occur is listed in common errors. If other unexpected problems occur, you're welcome to contact us for help.

8.1 Discussions

Welcome everyone to participate in the discussion about DP-GEN in the discussion module. You can ask for help, share an idea or anything to discuss here. Note: before you raise a question, please check TUTORIAL/FAQs and search history discussions to find solutions.

8.2 Issue

If you want to make a bug report or a request for new features, you can make an issue in the issue module.

Here are the types you can choose. A proper type can help developer figure out what you need. Also, you can assign yourself to solve the issue. Your contribution is welcome!

Note: before you raise a question, please check TUTORIAL/FAQs and search history issues to find solutions.

8.3 Tutorials

Tutorials can be found here.

8.4 Example for parameters

If you have no idea how to prepare a `PARAM` for your task, you can find examples of PARAM for different tasks in examples.

For example, if you want to set specific template for LAMMPS, you can find an example here

If you want to learn more about Machine parameters, please check docs for dpdispatcher

8.5 Pull requests - How to contribute

8.6 Troubleshooting

1. The most common problem is whether two settings correspond with each other, including:
    - The order of elements in `type_map` and `mass_map` and **`fp_pp_files`**.
    - Size of `init_data_sys` and `init_batch_size`.
    - Size of `sys_configs` and `sys_batch_size`.
    - Size of `sel_a` and actual types of atoms in your system.
    - Index of `sys_configs` and `sys_idx`.
2. Please verify the directories of `sys_configs`. If there isn't any POSCAR for `01.model_devi` in one iteration, it may happen that you write the false path of `sys_configs`. Note that `init_data_sys` is a list, while `sys_configs` should be a two-dimensional list. The first dimension corresponds to `sys_idx`, and the second level are some poscars under each group. Refer to the sample file.
3. Correct format of JSON file.
4. The frames of one system should be larger than `batch_size` and `numb_test` in `default_training_param`. It happens that one iteration adds only a few structures and causes error in next iteration's training. In this condition, you may let `fp_task_min` be larger than `numb_test`.
5. If you found the dpgen with the same version on two machines behaves differently, you may have modified the code in one of them.

8.7 Common Errors

(Errors are sorted alphabetically)

8.7.1 Command not found: xxx.

There is no such software in the environment, or it is unavailable. It may be because 1. It is not installed; 2. The Conda environment is not activated; 3. You have chosen the wrong image in machine.json.

8.7.2 dargs.dargs.ArgumentKeyError: [at location xxx] undefined key xxx is not allowed in strict mode.

Strict format check has been applied since version 0.10.7. To avoid misleading users, some older-version keys that are already ignored or absorbed into default settings are not allowed to be present. And the expected structure of the dictionary in the param.json also differs from those before version 0.10.7. This error will occur when format check finds older-fashion keys in the json file. Please try deleting or annotating these keys, or correspondingly modulate the json file. Example files in the newest format could be found in examples.

8.7.3 dargs.dargs.ArgumentTypeError: [at root location] key `xxx` gets wrong value type, requires but gets

Please check your parameters with DPGEN's Document. Maybe youhave superfluous parentheses in your parameter file.

8.7.4 FileNotFoundError: [Errno 2] No such file or directory: '.../01.model_devi/graph.xxx.pb'

If you find this error occurs, please check your initial data. Your model will not be generated if the initial data is incorrect.

8.7.5 json.decoder.JSONDecodeError

Your `.json` file is incorrect. It may be a mistake in syntax or a missing comma.

8.7.6 OSError: [Error cannot find valid a data system] Please check your setting for data systems

Check if the path to the dataset in the parameter file is set correctly. Note that `init_data_sys` is a list, while `sys_configs` should be a two-dimensional list. The first dimension corresponds to `sys_idx`, and the second level are some poscars under each group. Refer to the sample file.

8.7.7 RuntimeError: job:xxxxxxx failed 3 times

```
RuntimeError: job:xxxxxxx failed 3 times

......

RuntimeError: Meet errors will handle unexpected submission state.
Debug information: remote_root==xxxxxx
Debug information: submission_hash==xxxxxx
Please check the dirs and scripts in remote_root. The job information mentioned above␣
↪may help.
```

If a user finds an error like this, he or she is advised to check the files on the remote server. It shows that your job has failed 3 times, but has not shown the reason.

To find the reason, you can check the log on the remote root. For example, you can check train.log, which is generated by DeePMD-kit. It can tell you more details. If it doesn't help, you can manually run the `.sub` script, whose path is shown in `Debug information: remote_root==xxxxxx`

Some common reasons are as follows:

1. Two or more jobs are submitted manually or automatically at the same time, and their hash value collide. This bug will be fixed in dpdispatcher.
2. You may have something wrong in your input files, which causes the process to fail.

8.7.8 RuntimeError: find too many unsuccessfully terminated jobs.

The ratio of failed jobs is larger than ratio_failure. You can set a high value for ratio_failure or check if there is something wrong with your input files.

8.7.9 ValueError: Cannot load file containing picked data when allow_picked=False

Please ensure that you write the correct path of the dataset with no excess files.

8.7.10 warnings.warn("Some Gromacs commands were NOT found; "

You can ignore this warning if you don't need Gromacs. It just show that Gromacs is not installed in you environment.

CHAPTER

NINE

CONTRIBUTING GUIDE

9.1 Contributing Guide

The way to make contributions is through making pull requests(PR for short). After your PR is merged, the changes you make can be applied by other users.

Firstly, fork in DP-GEN repository. Then you can clone the repository, build a new branch, make changes and then make a pull request.

9.1.1 How to contribute to DP-GEN

Welcome to the repository of DP-GEN

DP-GEN adopts the same convention as other software in DeepModeling Community.

You can first refer to DeePMD-kit's Contributing guide and Developer guide.

You can also read relative chapters on Github Docs.

If you have no idea how to fix your problem or where to find the relative source code, please check *Code Structure* of the DP-GEN repository on this website.

Use command line

You can use git with the command line, or open the repository on Github Desktop. Here is a video as a demo of making changes to DP-GEN and publishing it with command line.

> If you have never used Github before, remember to generate your ssh key and configure the public key in Github Settings. If you can't configure your username and password, please use token. The explanation from Github see Github Blog: token authentication requirements for git operations. A discussion on StaskOverflow can solve this problem.

Use Github Desktop

Also, you can use Github Desktop to make PR. The following shows the steps to clone the repository and add your doc to tutorials. If it is your first time using Github, Open with Github Desktop is recommended. Github Desktop is a software, which can make your operations on branches visually.

After you clone it to your PC, you can open it with Github Desktop.

Firstly, create your new branch based on devel branch.

Secondly, add your doc to the certain directory in your local repository, and add its name into index.

Here is an example. Remember to add the filename of your doc into index!

Thirdly, select the changes that you what to push, and commit to it. Press "Publish branch" to push your origin repository to the remote branch.

Finally, you can check it on github and make a pull request. Press "Compare & pull request" to make a PR.

(Note: please commit pr to the devel branch)

9.1.2 How to contribute to DP-GEN tutorials and documents

Welcome to the documents of DP-GEN

- If you want to add the documentation of a toy model, simply put your file in the directory doc/toymodels/ and push;
- If you want to add a new directory for a new category of instructions, make a new directory and add it in doc/index.rst.

Also welcome to Tutorials repository You can find the structure of tutorials and preparations before writing a document in Writing Tips.

The latest page of DP-GEN Docs

Examples of contributions

- Example 1
- Example 2 (a simple one for beginner)

1. Push your doc

2. Add the directory in index.rst

3. Build and check it

As mentioned in "How to build the website to check if the modification works".

4. Make pull request to dpgen

9.1.3 Find how a parameter is used in the code

It is strongly recommended that you use the `find in files` function of Visual Studio software, `Search` function of Visual Studio Code, or similar functions of other software. Type in the name of the parameter you are looking for, and you will see where it is read in and used in the procedure. Of course, you can also search for the relevant code according to the above guide.

9.1.4 Want to modify a function?

If you have special requirements, you can make personalized modifications in the code corresponding to the function. If you think your modification can benefit the public, and it does not conflict with the current DP-GEN function; or if you fix a bug, please make a pull request to contribute the optimization to the DP-GEN repository.

9.1.5 DP-GEN dependencies

dpdispatcher and dpdata are dependencies of DP-GEN. dpdispatcher is related to task submission, monitoring and recovery, and dpdata is related to data processing. If you encounter an error and want to find the reason, please judge whether the problem comes from DP-GEN, dpdispatcher or dpdata according to the last line of `Traceback`.

9.1.6 About the update of the parameter file

You may have noticed that there are arginfo.py files in many folders. This is a file used to generate parameter documentation. If you add or modify a parameter in DP-GEN and intend to export it to the main repository, please sync your changes in arginfo.

9.1.7 Tips

1. Please try to submit a PR after finishing all the changes
2. Please briefly describe what you do with `git commit -m "<conclude-the-change-you-make>"`! "No description provided." will make the maintainer feel confused.
3. It is not recommended to make changes directly in the `devel` branch. It is recommended to pull a branch from devel: `git checkout -b <new-branch-name>`
4. When switching branches, remember to check if you want to bring the changes to the next branch!
5. Please fix the errors reported by the unit test. You can firstly test on your local machine before pushing commits. Hint: The way to test the code is to go from the main directory to the tests directory, and use the command `python3 -m unittest`. You can watch the demo video for review. Sometimes you may fail unit tests due to your local circumstance. You can check whether the error reported is related to the part you modified to eliminate this problem. After submitting, as long as there is a green check mark after the PR title on the webpage, it means that the test has been passed.
6. Pay attention to whether there are comments under your PR. If there is a change request, you need to check and modify the code. If there are conflicts, you need to solve them manually.

After successfully making a PR, developers will check it and give comments. It will be merged after everything done. Then CONGRATULATIONS! You become a first-time contributor to DP-GEN!

How to get help from the community

CHAPTER

TEN

DP-GEN API

10.1 dpgen package

dpgen.**info**()

10.1.1 Subpackages

dpgen.auto_test package

Subpackages

dpgen.auto_test.lib package

Submodules

dpgen.auto_test.lib.abacus module

dpgen.auto_test.lib.abacus.**check_finished**(*fname*)

dpgen.auto_test.lib.abacus.**check_stru_fixed**(*struf*, *fixed*)

dpgen.auto_test.lib.abacus.**final_stru**(*abacus_path*)

dpgen.auto_test.lib.abacus.**make_kspacing_kpt**(*struf*, *kspacing*)

dpgen.auto_test.lib.abacus.**modify_stru_path**(*strucf*, *tpath*)

dpgen.auto_test.lib.abacus.**poscar2stru**(*poscar*, *inter_param*, *stru='STRU'*)

- poscar: POSCAR for input
- **inter_param: dictionary of 'interaction' from param.json**
  some key words for ABACUS are:
  - atom_masses: a dictionary of atoms' masses
  - orb_files: a dictionary of orbital files
  - deepks_desc: a string of deepks descriptor file
- stru: output filename, usally is 'STRU'.

dpgen.auto_test.lib.abacus.**stru2Structure**(*struf*)

dpgen.auto_test.lib.abacus.**stru_fix_atom**(*struf*, *fix_atom=[True, True, True]*)

… ATOMIC_POSITIONS Cartesian #Cartesian(Unit is LATTICE_CONSTANT) Si #Name of element 0.0 #Magnetic for this element. 2 #Number of atoms 0.00 0.00 0.00 0 0 0 #x,y,z, move_x, move_y, move_z 0.25 0.25 0.25 0 0 0.

dpgen.auto_test.lib.abacus.**stru_scale**(*stru_in*, *stru_out*, *scale*)

dpgen.auto_test.lib.abacus.**write_input**(*inputf*, *inputdict*)

dpgen.auto_test.lib.abacus.**write_kpt**(*kptf*, *kptlist*)

dpgen.auto_test.lib.crys module

dpgen.auto_test.lib.crys.**bcc**(*ele_name='ele'*, *a=3.2144871302356037*)

dpgen.auto_test.lib.crys.**dhcp**(*ele_name='ele'*, *a=2.863782463805517*, *c=9.353074360871936*)

dpgen.auto_test.lib.crys.**diamond**(*ele_name='ele'*, *a=2.551340126037118*)

dpgen.auto_test.lib.crys.**fcc**(*ele_name='ele'*, *a=4.05*)

dpgen.auto_test.lib.crys.**fcc1**(*ele_name='ele'*, *a=4.05*)

dpgen.auto_test.lib.crys.**hcp**(*ele_name='ele'*, *a=2.863782463805517*, *c=4.676537180435968*)

dpgen.auto_test.lib.crys.**sc**(*ele_name='ele'*, *a=2.551340126037118*)

dpgen.auto_test.lib.lammps module

dpgen.auto_test.lib.lammps.**apply_type_map**(*conf_file*, *deepmd_type_map*, *ptypes*)

Apply type map. conf_file: conf file converted from POSCAR deepmd_type_map: deepmd atom type map ptypes: atom types defined in POSCAR.

dpgen.auto_test.lib.lammps.**check_finished**(*fname*)

dpgen.auto_test.lib.lammps.**check_finished_new**(*fname*, *keyword*)

dpgen.auto_test.lib.lammps.**cvt_lammps_conf**(*fin*, *fout*, *type_map*, *ofmt='lammps/data'*)

Format convert from fin to fout, specify the output format by ofmt Imcomplete situation.

dpgen.auto_test.lib.lammps.**element_list**(*type_map*)

dpgen.auto_test.lib.lammps.**get_base_area**(*log*)

Get base area.

dpgen.auto_test.lib.lammps.**get_nev**(*log*)

Get natoms, energy_per_atom and volume_per_atom from lammps log.

dpgen.auto_test.lib.lammps.**get_stress**(*log*)

Get stress from lammps log.

dpgen.auto_test.lib.lammps.**inter_deepmd**(*param*)

dpgen.auto_test.lib.lammps.**inter_eam_alloy**(*param*)

dpgen.auto_test.lib.lammps.**inter_eam_fs**(*param*)

dpgen.auto_test.lib.lammps.**inter_meam**(*param*)

dpgen.auto_test.lib.lammps.**make_lammps_elastic**(*conf*, *type_map*, *interaction*, *param*, *etol=0*, *ftol=1e-10*, *maxiter=5000*, *maxeval=500000*)

dpgen.auto_test.lib.lammps.**make_lammps_equi**(*conf*, *type_map*, *interaction*, *param*, *etol=0*, *ftol=1e-10*, *maxiter=5000*, *maxeval=500000*, *change_box=True*)

dpgen.auto_test.lib.lammps.**make_lammps_eval**(*conf*, *type_map*, *interaction*, *param*)

dpgen.auto_test.lib.lammps.**make_lammps_phonon**(*conf*, *masses*, *interaction*, *param*, *etol=0*, *ftol=1e-10*, *maxiter=5000*, *maxeval=500000*)

Make lammps input for elastic calculation.

dpgen.auto_test.lib.lammps.**make_lammps_press_relax**(*conf*, *type_map*, *scale2equi*, *interaction*, *param*, *B0=70*, *bp=0*, *etol=0*, *ftol=1e-10*, *maxiter=5000*, *maxeval=500000*)

dpgen.auto_test.lib.lammps.**poscar_from_last_dump**(*dump*, *poscar_out*, *deepmd_type_map*)

Get poscar from the last frame of a lammps MD traj (dump format).

dpgen.auto_test.lib.lmp module

dpgen.auto_test.lib.lmp.**box2lmpbox**(*orig*, *box*)

dpgen.auto_test.lib.lmp.**from_system_data**(*system*)

dpgen.auto_test.lib.lmp.**get_atoms**(*lines*)

dpgen.auto_test.lib.lmp.**get_atype**(*lines*)

dpgen.auto_test.lib.lmp.**get_lmpbox**(*lines*)

dpgen.auto_test.lib.lmp.**get_natoms**(*lines*)

dpgen.auto_test.lib.lmp.**get_natoms_vec**(*lines*)

dpgen.auto_test.lib.lmp.**get_natomtypes**(*lines*)

dpgen.auto_test.lib.lmp.**get_posi**(*lines*)

dpgen.auto_test.lib.lmp.**lmpbox2box**(*lohi*, *tilt*)

dpgen.auto_test.lib.lmp.**system_data**(*lines*)

dpgen.auto_test.lib.lmp.**to_system_data**(*lines*)

dpgen.auto_test.lib.mfp_eosfit module

dpgen.auto_test.lib.mfp_eosfit.**BM4**(*vol*, *pars*)

Birch-Murnaghan 4 pars equation from PRB 70, 224107, 3-order.

dpgen.auto_test.lib.mfp_eosfit.**BM5**(*vol*, *pars*)

Birch-Murnaghan 5 pars equation from PRB 70, 224107, 4-Order.

dpgen.auto_test.lib.mfp_eosfit.**LOG4**(*vol*, *pars*)

Natrual strain (Poirier-Tarantola)EOS with 4 paramters Seems only work in near-equillibrium range.

dpgen.auto_test.lib.mfp_eosfit.**LOG5**(*vol*, *parameters*)

Natrual strain (Poirier-Tarantola)EOS with 5 paramters.

dpgen.auto_test.lib.mfp_eosfit.**Li4p**(*V*, *parameters*)

Li JH, APL, 87, 194111 (2005).

dpgen.auto_test.lib.mfp_eosfit.**SJX_5p**(*vol*, *par*)

SJX_5p's five parameters EOS, Physica B: Condens Mater, 2011, 406: 1276-1282.

dpgen.auto_test.lib.mfp_eosfit.**SJX_v2**(*vol*, *par*)

Sun Jiuxun, et al. J phys Chem Solids, 2005, 66: 773-782. They said it is satified for the limiting condition at high pressure.

dpgen.auto_test.lib.mfp_eosfit.**TEOS**(*v*, *par*)

Holland, et al, Journal of Metamorphic Geology, 2011, 29(3): 333-383 Modified Tait equation of Huang & Chow.

dpgen.auto_test.lib.mfp_eosfit.**birch**(*v*, *parameters*)

From Intermetallic compounds: Principles and Practice, Vol. I: Princples Chapter 9 pages 195-210 by M. Mehl. B. Klein, D. Papaconstantopoulos paper downloaded from Web.

case where n=0

dpgen.auto_test.lib.mfp_eosfit.**calc_props_BM4**(*pars*)

dpgen.auto_test.lib.mfp_eosfit.**calc_props_LOG4**(*pars*)

dpgen.auto_test.lib.mfp_eosfit.**calc_props_SJX_5p**(*par*)

dpgen.auto_test.lib.mfp_eosfit.**calc_props_mBM4**(*pars*)

dpgen.auto_test.lib.mfp_eosfit.**calc_props_mBM4poly**(*pars*)

dpgen.auto_test.lib.mfp_eosfit.**calc_props_mBM5poly**(*pars*)

dpgen.auto_test.lib.mfp_eosfit.**calc_props_morse**(*pars*)

dpgen.auto_test.lib.mfp_eosfit.**calc_props_morse_6p**(*par*)

dpgen.auto_test.lib.mfp_eosfit.**calc_props_vinet**(*pars*)

dpgen.auto_test.lib.mfp_eosfit.**calc_v0_mBM4poly**(*x*, *pars*)

dpgen.auto_test.lib.mfp_eosfit.**calc_v0_mBM5poly**(*x*, *pars*)

dpgen.auto_test.lib.mfp_eosfit.**ext_splint**(*xp*, *yp*, *order=3*, *method='unispl'*)

dpgen.auto_test.lib.mfp_eosfit.**ext_vec**(*func*, *fin*, *p0*, *fs*, *fe*, *vols=None*, *vole=None*, *ndata=101*, *refit=0*, *show_fig=False*)

Extrapolate the data points for E-V based on the fitted parameters in small or very large volume range.

dpgen.auto_test.lib.mfp_eosfit.**ext_velp**(*fin*, *fstart*, *fend*, *vols*, *vole*, *ndata*, *order=3*, *method='unispl'*, *fout='ext_velp.dat'*, *show_fig=False*)

Extrapolate the lattice parameters based on input data.

dpgen.auto_test.lib.mfp_eosfit.**get_eos_list**()

dpgen.auto_test.lib.mfp_eosfit.**get_eos_list_3p**()

dpgen.auto_test.lib.mfp_eosfit.**get_eos_list_4p**()

dpgen.auto_test.lib.mfp_eosfit.**get_eos_list_5p**()

dpgen.auto_test.lib.mfp_eosfit.**get_eos_list_6p**()

dpgen.auto_test.lib.mfp_eosfit.**init_guess**(*fin*)

dpgen.auto_test.lib.mfp_eosfit.**lsqfit_eos**(*func*, *fin*, *par*, *fstart*, *fend*, *show_fig=False*, *fout='EoSfit.out'*, *refit=-1*)

dpgen.auto_test.lib.mfp_eosfit.**mBM4**(*vol*, *pars*)

Birch-Murnaghan 4 pars equation from PRB 70, 224107, 3-order BM.

dpgen.auto_test.lib.mfp_eosfit.**mBM4poly**(*vol*, *parameters*)

Modified BM5 EOS, Shang SL comput mater sci, 2010: 1040-1048, original expressions.

dpgen.auto_test.lib.mfp_eosfit.**mBM5**(*vol*, *pars*)

Modified BM5 EOS, Shang SL comput mater sci, 2010: 1040-1048.

dpgen.auto_test.lib.mfp_eosfit.**mBM5poly**(*vol*, *pars*)

Modified BM5 EOS, Shang SL comput mater sci, 2010: 1040-1048, original expressions.

dpgen.auto_test.lib.mfp_eosfit.**mie**(*v*, *p*)

Mie model for song's FVT.

dpgen.auto_test.lib.mfp_eosfit.**mie_simple**(*v*, *p*)

Mie_simple model for song's FVT.

dpgen.auto_test.lib.mfp_eosfit.**morse**(*v*, *pars*)

Reproduce from ShunliShang's matlab script.

dpgen.auto_test.lib.mfp_eosfit.**morse_3p**(*volume*, *p*)

morse_AB EOS formula from Song's FVT souces A= 0.5*B.

dpgen.auto_test.lib.mfp_eosfit.**morse_6p**(*vol*, *par*)

Generalized Morse EOS proposed by Qin, see: Qin et al. Phys Rev B, 2008, 78, 214108. Qin et al. Phys Rev B, 2008, 77, 220103(R).

dpgen.auto_test.lib.mfp_eosfit.**morse_AB**(*volume*, *p*)

morse_AB EOS formula from Song's FVT souces.

dpgen.auto_test.lib.mfp_eosfit.**murnaghan**(*vol*, *pars*)

Four-parameters murnaghan EOS. From PRB 28,5480 (1983).

dpgen.auto_test.lib.mfp_eosfit.**parse_argument**()

dpgen.auto_test.lib.mfp_eosfit.**rBM4**(*vol*, *pars*)

Implementions as Alberto Otero-de-la-Roza, i.e. rBM4 is used here Comput Physics Comm, 2011, 182: 1708-1720.

dpgen.auto_test.lib.mfp_eosfit.**rBM4_pv**(*vol*, *pars*)

Implementions as Alberto Otero-de-la-Roza, i.e. rBM4 is used here Comput Physics Comm, 2011, 182: 1708-1720 Fit for V-P relations.

dpgen.auto_test.lib.mfp_eosfit.**rBM5**(*vol*, *pars*)

Implementions as Alberto Otero-de-la-Roza, i.e. rBM5 is used here Comput Physics Comm, 2011, 182: 1708-1720.

dpgen.auto_test.lib.mfp_eosfit.**rBM5_pv**(*vol*, *pars*)

Implementions as Alberto Otero-de-la-Roza, i.e. rBM5 is used here Comput Physics Comm, 2011, 182: 1708-1720 Fit for V-P relations.

dpgen.auto_test.lib.mfp_eosfit.**rPT4**(*vol*, *pars*)

Natrual strain EOS with 4 paramters Seems only work in near-equillibrium range. Implementions as Alberto Otero-de-la-Roza, i.e. rPT4 is used here Comput Physics Comm, 2011, 182: 1708-1720, in their article, labeled as PT3 (3-order), however, we mention it as rPT4 for 4-parameters EOS.

dpgen.auto_test.lib.mfp_eosfit.**rPT4_pv**(*vol*, *pars*)

Natrual strain (Poirier-Tarantola)EOS with 4 paramters Seems only work in near-equillibrium range. Implementions as Alberto Otero-de-la-Roza, i.e. rPT4 is used here Comput Physics Comm, 2011, 182: 1708-1720, in their article, labeled as PT3 (3-order), however, we mention it as rPT4 for 4-parameters EOS.

dpgen.auto_test.lib.mfp_eosfit.**rPT5**(*vol*, *pars*)

Natrual strain EOS with 4 paramters Seems only work in near-equillibrium range. Implementions as Alberto Otero-de-la-Roza, i.e. rPT5 is used here Comput Physics Comm, 2011, 182: 1708-1720, in their article, labeled as PT3 (3-order), however, we mention it as rPT5 for 4-parameters EOS.

dpgen.auto_test.lib.mfp_eosfit.**rPT5_pv**(*vol*, *pars*)

Natrual strain (Poirier-Tarantola)EOS with 5 paramters Implementions as Alberto Otero-de-la-Roza, i.e. rPT5 is used here Comput Physics Comm, 2011, 182: 1708-1720, in their article, labeled as PT3 (3-order), however, we mention it as rPT5 for 4-parameters EOS.

dpgen.auto_test.lib.mfp_eosfit.**read_ve**(*fin*)

dpgen.auto_test.lib.mfp_eosfit.**read_velp**(*fin*, *fstart*, *fend*)

dpgen.auto_test.lib.mfp_eosfit.**read_vlp**(*fin*, *fstart*, *fend*)

dpgen.auto_test.lib.mfp_eosfit.**repro_ve**(*func*, *vol_i*, *p*)

dpgen.auto_test.lib.mfp_eosfit.**repro_vp**(*func*, *vol_i*, *pars*)

dpgen.auto_test.lib.mfp_eosfit.**res_BM4**(*pars*, *y*, *x*)

dpgen.auto_test.lib.mfp_eosfit.**res_BM5**(*pars*, *y*, *x*)

dpgen.auto_test.lib.mfp_eosfit.**res_LOG4**(*pars*, *y*, *x*)

dpgen.auto_test.lib.mfp_eosfit.**res_LOG5**(*pars*, *y*, *x*)

dpgen.auto_test.lib.mfp_eosfit.**res_Li4p**(*p*, *y*, *x*)

dpgen.auto_test.lib.mfp_eosfit.**res_SJX_5p**(*p*, *e*, *v*)

dpgen.auto_test.lib.mfp_eosfit.**res_SJX_v2**(*p*, *e*, *v*)

dpgen.auto_test.lib.mfp_eosfit.**res_TEOS**(*p*, *e*, *v*)

dpgen.auto_test.lib.mfp_eosfit.**res_birch**(*pars*, *y*, *x*)

dpgen.auto_test.lib.mfp_eosfit.**res_mBM4**(*pars*, *y*, *x*)

dpgen.auto_test.lib.mfp_eosfit.**res_mBM4poly**(*pars*, *y*, *x*)

dpgen.auto_test.lib.mfp_eosfit.**res_mBM5**(*pars*, *y*, *x*)

dpgen.auto_test.lib.mfp_eosfit.**res_mBM5poly**(*pars*, *y*, *x*)

dpgen.auto_test.lib.mfp_eosfit.**res_mie**(*p*, *e*, *v*)

dpgen.auto_test.lib.mfp_eosfit.**res_mie_simple**(*p*, *e*, *v*)

dpgen.auto_test.lib.mfp_eosfit.**res_morse**(*p*, *en*, *volume*)

dpgen.auto_test.lib.mfp_eosfit.**res_morse_3p**(*p*, *en*, *volume*)

dpgen.auto_test.lib.mfp_eosfit.**res_morse_6p**(*p*, *en*, *volume*)

dpgen.auto_test.lib.mfp_eosfit.**res_morse_AB**(*p*, *en*, *volume*)

dpgen.auto_test.lib.mfp_eosfit.**res_murnaghan**(*pars*, *y*, *x*)

dpgen.auto_test.lib.mfp_eosfit.**res_rBM4**(*pars*, *y*, *x*)

dpgen.auto_test.lib.mfp_eosfit.**res_rBM4_pv**(*pars*, *y*, *x*)

dpgen.auto_test.lib.mfp_eosfit.**res_rBM5**(*pars*, *y*, *x*)

dpgen.auto_test.lib.mfp_eosfit.**res_rBM5_pv**(*pars*, *y*, *x*)

dpgen.auto_test.lib.mfp_eosfit.**res_rPT4**(*pars*, *y*, *x*)

dpgen.auto_test.lib.mfp_eosfit.**res_rPT4_pv**(*pars*, *y*, *x*)

dpgen.auto_test.lib.mfp_eosfit.**res_rPT5**(*pars*, *y*, *x*)

dpgen.auto_test.lib.mfp_eosfit.**res_rPT5_pv**(*pars*, *y*, *x*)

dpgen.auto_test.lib.mfp_eosfit.**res_universal**(*pars*, *y*, *x*)

dpgen.auto_test.lib.mfp_eosfit.**res_vinet**(*pars*, *y*, *x*)

dpgen.auto_test.lib.mfp_eosfit.**res_vinet_pv**(*pars*, *y*, *x*)

dpgen.auto_test.lib.mfp_eosfit.**universal**(*vol*, *parameters*)

Universal equation of state(Vinet P et al., J. Phys.: Condens. Matter 1, p1941 (1989)).

dpgen.auto_test.lib.mfp_eosfit.**vinet**(*vol*, *pars*)

Vinet equation from PRB 70, 224107 Following, Shang Shunli et al., comput mater sci, 2010: 1040-1048, original expressions.

dpgen.auto_test.lib.mfp_eosfit.**vinet_pv**(*vol*, *pars*)

dpgen.auto_test.lib.pwscf module

dpgen.auto_test.lib.pwscf.**make_pwscf_input**(*sys_data*, *fp_pp_files*, *fp_params*)

dpgen.auto_test.lib.siesta module

dpgen.auto_test.lib.siesta.**make_siesta_input**(*sys_data*, *fp_pp_files*, *fp_params*)

dpgen.auto_test.lib.util module

dpgen.auto_test.lib.util.**collect_task**(*all_task*, *task_type*)

dpgen.auto_test.lib.util.**get_machine_info**(*mdata*, *task_type*)

dpgen.auto_test.lib.util.**insert_data**(*task*, *task_type*, *username*, *file_name*)

dpgen.auto_test.lib.util.**make_work_path**(*jdata*, *task*, *reprod_opt*, *static*, *user*)

dpgen.auto_test.lib.util.**voigt_to_stress**(*inpt*)

dpgen.auto_test.lib.utils module

dpgen.auto_test.lib.utils.**cmd_append_log**(*cmd*, *log_file*)

dpgen.auto_test.lib.utils.**copy_file_list**(*file_list*, *from_path*, *to_path*)

dpgen.auto_test.lib.utils.**create_path**(*path*)

dpgen.auto_test.lib.utils.**log_iter**(*task*, *ii*, *jj*)

dpgen.auto_test.lib.utils.**log_task**(*message*)

dpgen.auto_test.lib.utils.**make_iter_name**(*iter_index*)

dpgen.auto_test.lib.utils.**record_iter**(*record*, *confs*, *ii*, *jj*)

dpgen.auto_test.lib.utils.**repeat_to_length**(*string_to_expand*, *length*)

dpgen.auto_test.lib.utils.**replace**(*file_name*, *pattern*, *subst*)

dpgen.auto_test.lib.vasp module

exception dpgen.auto_test.lib.vasp.**OutcarItemError**

Bases: Exception

dpgen.auto_test.lib.vasp.**check_finished**(*fname*)

dpgen.auto_test.lib.vasp.**get_boxes**(*fname*)

dpgen.auto_test.lib.vasp.**get_energies**(*fname*)

dpgen.auto_test.lib.vasp.**get_nev**(*fname*)

dpgen.auto_test.lib.vasp.**get_poscar_natoms**(*fname*)

dpgen.auto_test.lib.vasp.**get_poscar_types**(*fname*)

dpgen.auto_test.lib.vasp.**get_stress**(*fname*)

dpgen.auto_test.lib.vasp.**make_kspacing_kpoints**(*poscar*, *kspacing*, *kgamma*)

dpgen.auto_test.lib.vasp.**make_vasp_kpoints**(*kpoints*, *kgamma=False*)

dpgen.auto_test.lib.vasp.**make_vasp_kpoints_from_incar**(*work_dir*, *jdata*)

dpgen.auto_test.lib.vasp.**make_vasp_phonon_incar**(*ecut*, *ediff*, *npar*, *kpar*, *kspacing=0.5*, *kgamma=True*, *ismear=1*, *sigma=0.2*)

dpgen.auto_test.lib.vasp.**make_vasp_relax_incar**(*ecut*, *ediff*, *relax_ion*, *relax_shape*, *relax_volume*, *npar*, *kpar*, *kspacing=0.5*, *kgamma=True*, *ismear=1*, *sigma=0.22*)

dpgen.auto_test.lib.vasp.**make_vasp_static_incar**(*ecut*, *ediff*, *npar*, *kpar*, *kspacing=0.5*, *kgamma=True*, *ismear=1*, *sigma=0.2*)

dpgen.auto_test.lib.vasp.**perturb_xz**(*poscar_in*, *poscar_out*, *pert=0.01*)

dpgen.auto_test.lib.vasp.**poscar_natoms**(*poscar_in*)

dpgen.auto_test.lib.vasp.**poscar_scale**(*poscar_in*, *poscar_out*, *scale*)

dpgen.auto_test.lib.vasp.**poscar_vol**(*poscar_in*)

dpgen.auto_test.lib.vasp.**reciprocal_box**(*box*)

dpgen.auto_test.lib.vasp.**regulate_poscar**(*poscar_in*, *poscar_out*)

dpgen.auto_test.lib.vasp.**sort_poscar**(*poscar_in*, *poscar_out*, *new_names*)

Submodules

dpgen.auto_test.ABACUS module

class dpgen.auto_test.ABACUS.**ABACUS**(*inter_parameter*, *path_to_poscar*)

Bases: *Task*

Methods

backward_files([property_type])	Return backward files.
compute(output_dir)	Compute output of the task.
forward_common_files([property_type])	Return forward common files.
forward_files([property_type])	Return forward files.
make_input_file(output_dir, task_type, ...)	Prepare input files for a computational task For example, the VASP prepares INCAR.
make_potential_files(output_dir)	Prepare potential files for a computational task.

modify_input

backward_files(*property_type='relaxation'*)

Return backward files.

compute(*output_dir*)

Compute output of the task. IMPORTANT: The output configuration should be converted and stored in a CONTCAR file.

Parameters

output_dir

[str] The directory storing the input and output files.

Returns

result_dict: dict

A dict that storing the result. For example: { "energy": xxx, "force": [xxx] }

Notes

The following files are generated: CONTCAR: output file

The output configuration is converted to CONTCAR and stored in the *output_dir*

forward_common_files(*property_type='relaxation'*)

Return forward common files.

forward_files(*property_type='relaxation'*)

Return forward files.

make_input_file(*output_dir*, *task_type*, *task_param*)

Prepare input files for a computational task For example, the VASP prepares INCAR. LAMMPS (including DeePMD, MEAM...) prepares in.lammps.

Parameters

output_dir

[str] The directory storing the input files.

task_type

[str] Can be - "relaxation:": structure relaxation - "static": static computation calculates the energy, force... of a strcture

task_param

[dict] The parameters of the task. For example the VASP interaction can be provided with { "ediff": 1e-6, "ediffg": 1e-5 }

make_potential_files(*output_dir*)

Prepare potential files for a computational task. For example, the VASP prepares POTCAR. DeePMD prepares frozen model(s). IMPORTANT: Interaction should be stored in output_dir/inter.json.

Parameters

output_dir

[str] The directory storing the potential files.

Notes

The following files are generated:

inter.json: output file

The task information is stored in *output_dir/inter.json*

modify_input(*incar*, *x*, *y*)

dpgen.auto_test.EOS module

class dpgen.auto_test.EOS.**EOS**(*parameter*, *inter_param=None*)

Bases: *Property*

Methods

compute(output_file, print_file, path_to_work)	Postprocess the finished tasks to compute the property.
make_confs(path_to_work, path_to_equi[, refine])	Make configurations needed to compute the property.
post_process(task_list)	post_process the KPOINTS file in elastic.
task_param()	Return the parameter of each computational task, for example, {'ediffg': 1e-4}.
task_type()	Return the type of each computational task, for example, 'relaxation', 'static'....

make_confs(*path_to_work*, *path_to_equi*, *refine=False*)

Make configurations needed to compute the property. The tasks directory will be named as path_to_work/task.xxxxxx IMPORTANT: handel the case when the directory exists.

Parameters

path_to_work

[str] The path where the tasks for the property are located

path_to_equi

[str] -refine == False: The path to the directory that equilibrated the configuration. -refine == True: The path to the directory that has property confs.

refine

[str] To refine existing property confs or generate property confs from a equilibrated conf

Returns

task_list: list of str

The list of task directories.

post_process(*task_list*)

post_process the KPOINTS file in elastic.

task_param()

Return the parameter of each computational task, for example, {'ediffg': 1e-4}.

task_type()

Return the type of each computational task, for example, 'relaxation', 'static'....

dpgen.auto_test.Elastic module

class dpgen.auto_test.Elastic.**Elastic**(*parameter*, *inter_param=None*)

Bases: *Property*

Methods

compute(output_file, print_file, path_to_work)	Postprocess the finished tasks to compute the property.
make_confs(path_to_work, path_to_equi[, refine])	Make configurations needed to compute the property.
post_process(task_list)	post_process the KPOINTS file in elastic.
task_param()	Return the parameter of each computational task, for example, {'ediffg': 1e-4}.
task_type()	Return the type of each computational task, for example, 'relaxation', 'static'....

make_confs(*path_to_work*, *path_to_equi*, *refine=False*)

Make configurations needed to compute the property. The tasks directory will be named as path_to_work/task.xxxxxx IMPORTANT: handel the case when the directory exists.

Parameters

path_to_work

[str] The path where the tasks for the property are located

path_to_equi

[str] -refine == False: The path to the directory that equilibrated the configuration. -refine == True: The path to the directory that has property confs.

refine

[str] To refine existing property confs or generate property confs from a equilibrated conf

Returns

task_list: list of str

The list of task directories.

post_process(*task_list*)

post_process the KPOINTS file in elastic.

task_param()

Return the parameter of each computational task, for example, {'ediffg': 1e-4}.

task_type()

Return the type of each computational task, for example, 'relaxation', 'static'....

dpgen.auto_test.Gamma module

class dpgen.auto_test.Gamma.**Gamma**(*parameter*, *inter_param=None*)

Bases: *Property*

Calculation of common gamma lines for bcc and fcc.

Methods

compute(output_file, print_file, path_to_work)	Postprocess the finished tasks to compute the property.
make_confs(path_to_work, path_to_equi[, refine])	Make configurations needed to compute the property.
post_process(task_list)	post_process the KPOINTS file in elastic.
task_param()	Return the parameter of each computational task, for example, {'ediffg': 1e-4}.
task_type()	Return the type of each computational task, for example, 'relaxation', 'static'....

centralize_slab
return_direction

static centralize_slab(*slab*) → None

make_confs(*path_to_work*, *path_to_equi*, *refine=False*)

Make configurations needed to compute the property. The tasks directory will be named as path_to_work/task.xxxxxx IMPORTANT: handel the case when the directory exists.

Parameters

path_to_work

[str] The path where the tasks for the property are located

path_to_equi

[str] -refine == False: The path to the directory that equilibrated the configuration. -refine == True: The path to the directory that has property confs.

refine

[str] To refine existing property confs or generate property confs from a equilibrated conf

Returns

task_list: list of str

The list of task directories.

post_process(*task_list*)

post_process the KPOINTS file in elastic.

return_direction()

task_param()

Return the parameter of each computational task, for example, {'ediffg': 1e-4}.

task_type()

Return the type of each computational task, for example, 'relaxation', 'static'....

dpgen.auto_test.Interstitial module

class dpgen.auto_test.Interstitial.**Interstitial**(*parameter*, *inter_param=None*)

Bases: *Property*

Methods

compute(output_file, print_file, path_to_work)	Postprocess the finished tasks to compute the property.
make_confs(path_to_work, path_to_equi[, refine])	Make configurations needed to compute the property.
post_process(task_list)	post_process the KPOINTS file in elastic.
task_param()	Return the parameter of each computational task, for example, {'ediffg': 1e-4}.
task_type()	Return the type of each computational task, for example, 'relaxation', 'static'....

make_confs(*path_to_work*, *path_to_equi*, *refine=False*)

Make configurations needed to compute the property. The tasks directory will be named as path_to_work/task.xxxxxx IMPORTANT: handel the case when the directory exists.

Parameters

path_to_work

[str] The path where the tasks for the property are located

path_to_equi

[str] -refine == False: The path to the directory that equilibrated the configuration. -refine == True: The path to the directory that has property confs.

refine

[str] To refine existing property confs or generate property confs from a equilibrated conf

Returns

task_list: list of str

The list of task directories.

post_process(*task_list*)

post_process the KPOINTS file in elastic.

task_param()

Return the parameter of each computational task, for example, {'ediffg': 1e-4}.

task_type()

Return the type of each computational task, for example, 'relaxation', 'static'....

dpgen.auto_test.Lammps module

class dpgen.auto_test.Lammps.**Lammps**(*inter_parameter*, *path_to_poscar*)

Bases: *Task*

Methods

backward_files([property_type])	Return backward files.
compute(output_dir)	Compute output of the task.
forward_common_files([property_type])	Return forward common files.
forward_files([property_type])	Return forward files.
make_input_file(output_dir, task_type, ...)	Prepare input files for a computational task For example, the VASP prepares INCAR.
make_potential_files(output_dir)	Prepare potential files for a computational task.

set_inter_type_func
set_model_param

backward_files(*property_type='relaxation'*)

Return backward files.

compute(*output_dir*)

Compute output of the task. IMPORTANT: The output configuration should be converted and stored in a CONTCAR file.

Parameters

output_dir

[str] The directory storing the input and output files.

Returns

result_dict: dict

A dict that storing the result. For example: { "energy": xxx, "force": [xxx] }

Notes

The following files are generated: CONTCAR: output file

The output configuration is converted to CONTCAR and stored in the *output_dir*

forward_common_files(*property_type='relaxation'*)

Return forward common files.

forward_files(*property_type='relaxation'*)

Return forward files.

make_input_file(*output_dir*, *task_type*, *task_param*)

Prepare input files for a computational task For example, the VASP prepares INCAR. LAMMPS (including DeePMD, MEAM...) prepares in.lammps.

Parameters

output_dir

[str] The directory storing the input files.

task_type

[str] Can be - "relaxation:": structure relaxation - "static": static computation calculates the energy, force... of a strcture

task_param

[dict] The parameters of the task. For example the VASP interaction can be provided with { "ediff": 1e-6, "ediffg": 1e-5 }

make_potential_files(*output_dir*)

Prepare potential files for a computational task. For example, the VASP prepares POTCAR. DeePMD prepares frozen model(s). IMPORTANT: Interaction should be stored in output_dir/inter.json.

Parameters

output_dir

[str] The directory storing the potential files.

Notes

The following files are generated:

inter.json: output file

The task information is stored in *output_dir/inter.json*

set_inter_type_func()

set_model_param()

dpgen.auto_test.Property module

class dpgen.auto_test.Property.**Property**(*parameter*)

Bases: ABC

Attributes

task_param

Return the parameter of each computational task, for example, {'ediffg': 1e-4}.

task_type

Return the type of each computational task, for example, 'relaxation', 'static'....

Methods

compute(output_file, print_file, path_to_work)	Postprocess the finished tasks to compute the property.
make_confs(path_to_work, path_to_equi[, refine])	Make configurations needed to compute the property.
post_process(task_list)	post_process the KPOINTS file in elastic.

compute(*output_file*, *print_file*, *path_to_work*)

Postprocess the finished tasks to compute the property. Output the result to a json database.

Parameters

output_file:

The file to output the property in json format

print_file:

The file to output the property in txt format

path_to_work:

The working directory where the computational tasks locate.

abstract make_confs(*path_to_work*, *path_to_equi*, *refine=False*)

Make configurations needed to compute the property. The tasks directory will be named as path_to_work/task.xxxxxx IMPORTANT: handel the case when the directory exists.

Parameters

path_to_work

[str] The path where the tasks for the property are located

path_to_equi
[str] -refine == False: The path to the directory that equilibrated the configuration. -refine == True: The path to the directory that has property confs.
refine
[str] To refine existing property confs or generate property confs from a equilibrated conf
Returns
task_list: list of str
The list of task directories.

abstract post_process(*task_list*)
post_process the KPOINTS file in elastic.

abstract property task_param
Return the parameter of each computational task, for example, {'ediffg': 1e-4}.

abstract property task_type
Return the type of each computational task, for example, 'relaxation', 'static'....

dpgen.auto_test.Surface module

class dpgen.auto_test.Surface.**Surface**(*parameter*, *inter_param=None*)
Bases: *Property*

Methods

compute(output_file, print_file, path_to_work)	Postprocess the finished tasks to compute the property.
make_confs(path_to_work, path_to_equi[, refine])	Make configurations needed to compute the property.
post_process(task_list)	post_process the KPOINTS file in elastic.
task_param()	Return the parameter of each computational task, for example, {'ediffg': 1e-4}.
task_type()	Return the type of each computational task, for example, 'relaxation', 'static'....

make_confs(*path_to_work*, *path_to_equi*, *refine=False*)
Make configurations needed to compute the property. The tasks directory will be named as path_to_work/task.xxxxxx IMPORTANT: handel the case when the directory exists.
Parameters
path_to_work
[str] The path where the tasks for the property are located
path_to_equi
[str] -refine == False: The path to the directory that equilibrated the configuration. -refine == True: The path to the directory that has property confs.
refine
[str] To refine existing property confs or generate property confs from a equilibrated conf
Returns
task_list: list of str
The list of task directories.

post_process(*task_list*)

post_process the KPOINTS file in elastic.

task_param()

Return the parameter of each computational task, for example, {'ediffg': 1e-4}.

task_type()

Return the type of each computational task, for example, 'relaxation', 'static'....

dpgen.auto_test.Task module

class dpgen.auto_test.Task.**Task**(*inter_parameter*, *path_to_poscar*)

Bases: ABC

Attributes

backward_files

Return backward files.

forward_common_files

Return forward common files.

forward_files

Return forward files.

Methods

compute(output_dir)	Compute output of the task.
make_input_file(output_dir, task_type, ...)	Prepare input files for a computational task For example, the VASP prepares INCAR.
make_potential_files(output_dir)	Prepare potential files for a computational task.

abstract property backward_files

Return backward files.

abstract compute(*output_dir*)

Compute output of the task. IMPORTANT: The output configuration should be converted and stored in a CONTCAR file.

Parameters

output_dir

[str] The directory storing the input and output files.

Returns

result_dict: dict

A dict that storing the result. For example: { "energy": xxx, "force": [xxx] }

Notes

The following files are generated: CONTCAR: output file
The output configuration is converted to CONTCAR and stored in the *output_dir*

abstract property forward_common_files

Return forward common files.

abstract property forward_files

Return forward files.

abstract make_input_file(*output_dir*, *task_type*, *task_param*)

Prepare input files for a computational task For example, the VASP prepares INCAR. LAMMPS (including DeePMD, MEAM...) prepares in.lammps.

Parameters

output_dir
[str] The directory storing the input files.

task_type
[str] Can be - "relaxation:": structure relaxation - "static": static computation calculates the energy, force... of a strcture

task_param
[dict] The parameters of the task. For example the VASP interaction can be provided with { "ediff": 1e-6, "ediffg": 1e-5 }

abstract make_potential_files(*output_dir*)

Prepare potential files for a computational task. For example, the VASP prepares POTCAR. DeePMD prepares frozen model(s). IMPORTANT: Interaction should be stored in output_dir/inter.json.

Parameters

output_dir
[str] The directory storing the potential files.

Notes

The following files are generated:
inter.json: output file
The task information is stored in *output_dir/inter.json*

dpgen.auto_test.VASP module

class dpgen.auto_test.VASP.**VASP**(*inter_parameter*, *path_to_poscar*)

Bases: *Task*

Methods

backward_files([property_type])	Return backward files.
compute(output_dir)	Compute output of the task.
forward_common_files([property_type])	Return forward common files.
forward_files([property_type])	Return forward files.
make_input_file(output_dir, task_type, ...)	Prepare input files for a computational task For example, the VASP prepares INCAR.
make_potential_files(output_dir)	Prepare potential files for a computational task.

`backward_files`(*property_type='relaxation'*)

Return backward files.

`compute`(*output_dir*)

Compute output of the task. IMPORTANT: The output configuration should be converted and stored in a CONTCAR file.

Parameters

output_dir

[str] The directory storing the input and output files.

Returns

result_dict: dict

A dict that storing the result. For example: { "energy": xxx, "force": [xxx] }

Notes

The following files are generated: CONTCAR: output file

The output configuration is converted to CONTCAR and stored in the *output_dir*

`forward_common_files`(*property_type='relaxation'*)

Return forward common files.

`forward_files`(*property_type='relaxation'*)

Return forward files.

`make_input_file`(*output_dir*, *task_type*, *task_param*)

Prepare input files for a computational task For example, the VASP prepares INCAR. LAMMPS (including DeePMD, MEAM...) prepares in.lammps.

Parameters

output_dir

[str] The directory storing the input files.

task_type

[str] Can be - "relaxation:": structure relaxation - "static": static computation calculates the energy, force... of a strcture

task_param

[dict] The parameters of the task. For example the VASP interaction can be provided with { "ediff": 1e-6, "ediffg": 1e-5 }

`make_potential_files`(*output_dir*)

Prepare potential files for a computational task. For example, the VASP prepares POTCAR. DeePMD prepares frozen model(s). IMPORTANT: Interaction should be stored in output_dir/inter.json.

Parameters

output_dir

[str] The directory storing the potential files.

Notes

The following files are generated:

inter.json: output file

The task information is stored in *output_dir/inter.json*

dpgen.auto_test.Vacancy module

class dpgen.auto_test.Vacancy.**Vacancy**(*parameter*, *inter_param=None*)

Bases: *Property*

Methods

compute(output_file, print_file, path_to_work)	Postprocess the finished tasks to compute the property.
make_confs(path_to_work, path_to_equi[, refine])	Make configurations needed to compute the property.
post_process(task_list)	post_process the KPOINTS file in elastic.
task_param()	Return the parameter of each computational task, for example, {'ediffg': 1e-4}.
task_type()	Return the type of each computational task, for example, 'relaxation', 'static'....

make_confs(*path_to_work*, *path_to_equi*, *refine=False*)

Make configurations needed to compute the property. The tasks directory will be named as path_to_work/task.xxxxxx IMPORTANT: handel the case when the directory exists.

Parameters

path_to_work

[str] The path where the tasks for the property are located

path_to_equi

[str] -refine == False: The path to the directory that equilibrated the configuration.
-refine == True: The path to the directory that has property confs.

refine

[str] To refine existing property confs or generate property confs from a equilibrated conf

Returns

task_list: list of str

The list of task directories.

post_process(*task_list*)

post_process the KPOINTS file in elastic.

task_param()

Return the parameter of each computational task, for example, {'ediffg': 1e-4}.

task_type()

Return the type of each computational task, for example, 'relaxation', 'static'....

dpgen.auto_test.calculator module

dpgen.auto_test.calculator.**make_calculator**(*inter_parameter*, *path_to_poscar*)

Make an instance of Task.

dpgen.auto_test.common_equi module

dpgen.auto_test.common_equi.**make_equi**(*confs*, *inter_param*, *relax_param*)

dpgen.auto_test.common_equi.**post_equi**(*confs*, *inter_param*)

dpgen.auto_test.common_equi.**run_equi**(*confs*, *inter_param*, *mdata*)

dpgen.auto_test.common_prop module

dpgen.auto_test.common_prop.**make_property**(*confs*, *inter_param*, *property_list*)

dpgen.auto_test.common_prop.**make_property_instance**(*parameters*, *inter_param*)

Make an instance of Property.

dpgen.auto_test.common_prop.**post_property**(*confs*, *inter_param*, *property_list*)

dpgen.auto_test.common_prop.**run_property**(*confs*, *inter_param*, *property_list*, *mdata*)

dpgen.auto_test.common_prop.**worker**(*work_path*, *all_task*, *forward_common_files*, *forward_files*, *backward_files*, *mdata*, *inter_type*)

dpgen.auto_test.gen_confs module

dpgen.auto_test.gen_confs.**gen_alloy**(*eles*, *key*)

dpgen.auto_test.gen_confs.**gen_ele_std**(*ele_name*, *ctype*)

dpgen.auto_test.gen_confs.**gen_element**(*ele_name*, *key*)

dpgen.auto_test.gen_confs.**gen_element_std**(*ele_name*)

dpgen.auto_test.gen_confs.**make_path_mp**(*ii*)

dpgen.auto_test.gen_confs.**test_fit**(*struct*, *data*)

dpgen.auto_test.mpdb module

dpgen.auto_test.mpdb.**check_apikey**()

dpgen.auto_test.mpdb.**get_structure**(*mp_id*)

dpgen.auto_test.refine module

dpgen.auto_test.refine.**make_refine**(*init_from_suffix*, *output_suffix*, *path_to_work*)

dpgen.auto_test.reproduce module

dpgen.auto_test.reproduce.**make_repro**(*inter_param*, *init_data_path*, *init_from_suffix*, *path_to_work*, *reprod_last_frame=True*)

dpgen.auto_test.reproduce.**post_repro**(*init_data_path*, *init_from_suffix*, *all_tasks*, *ptr_data*, *reprod_last_frame=True*)

dpgen.auto_test.run module

dpgen.auto_test.run.**gen_test**(*args*)

dpgen.auto_test.run.**run_task**(*step*, *param_file*, *machine_file=None*)

dpgen.collect package

Submodules

dpgen.collect.collect module

dpgen.collect.collect.**collect_data**(*target_folder*, *param_file*, *output*, *verbose=True*, *shuffle=True*, *merge=True*)

dpgen.collect.collect.**gen_collect**(*args*)

dpgen.data package

Subpackages

dpgen.data.tools package

Submodules

dpgen.data.tools.bcc module

dpgen.data.tools.bcc.**gen_box**()

dpgen.data.tools.bcc.**numb_atoms**()

dpgen.data.tools.bcc.**poscar_unit**(*latt*)

dpgen.data.tools.cessp2force_lin module

dpgen.data.tools.cessp2force_lin.**Parser**()

dpgen.data.tools.cessp2force_lin.**get_outcar_files**(*directory*, *recursive*)

dpgen.data.tools.cessp2force_lin.**process_outcar_file_v5_dev**(*outcars*, *data*, *numbers*, *types*, *max_types*, *elements=None*, *windex=None*, *fout='potfit.configs'*)

dpgen.data.tools.cessp2force_lin.**scan_outcar_file**(*file_handle*)

dpgen.data.tools.cessp2force_lin.**uniq**(*seq*)

dpgen.data.tools.create_random_disturb module

dpgen.data.tools.create_random_disturb.**RandomDisturbParser**()

dpgen.data.tools.create_random_disturb.**create_disturbs_abacus_dev**(*fin*, *nfile*, *dmax=1.0*, *etmax=0.1*, *ofmt='abacus'*, *dstyle='uniform'*, *write_d=False*, *diag=0*)

dpgen.data.tools.create_random_disturb.**create_disturbs_ase**(*fin*, *nfile*, *dmax=1.0*, *ofmt='lmp'*, *dstyle='uniform'*, *write_d=False*)

dpgen.data.tools.create_random_disturb.**create_disturbs_ase_dev**(*fin*, *nfile*, *dmax=1.0*, *etmax=0.1*, *ofmt='lmp'*, *dstyle='uniform'*, *write_d=False*, *diag=0*)

dpgen.data.tools.create_random_disturb.**create_disturbs_atomsk**(*fin*, *nfile*, *dmax=1.0*, *ofmt='lmp'*)

dpgen.data.tools.create_random_disturb.**create_random_alloys**(*fin*, *alloy_dist*, *ifmt='vasp'*, *ofmt='vasp'*)

In fact, atomsk also gives us the convinient tool to do this.

dpgen.data.tools.create_random_disturb.**gen_random_disturb**(*dmax*, *a*, *b*, *dstyle='uniform'*)

dpgen.data.tools.create_random_disturb.**gen_random_emat**(*etmax*, *diag=0*)

dpgen.data.tools.create_random_disturb.**random_range**(*a*, *b*, *ndata=1*)

dpgen.data.tools.diamond module

dpgen.data.tools.diamond.**gen_box**()

dpgen.data.tools.diamond.**numb_atoms**()

dpgen.data.tools.diamond.**poscar_unit**(*latt*)

dpgen.data.tools.fcc module

dpgen.data.tools.fcc.**gen_box**()

dpgen.data.tools.fcc.**numb_atoms**()

dpgen.data.tools.fcc.**poscar_unit**(*latt*)

dpgen.data.tools.hcp module

dpgen.data.tools.hcp.**gen_box**()

dpgen.data.tools.hcp.**numb_atoms**()

dpgen.data.tools.hcp.**poscar_unit**(*latt*)

dpgen.data.tools.io_lammps module

ASE Atoms convert to LAMMPS configuration Some functions are adapted from ASE lammpsrun.py.

dpgen.data.tools.io_lammps.**ase2lammpsdata**(*atoms*, *typeids=None*, *fout='out.lmp'*)

dpgen.data.tools.io_lammps.**car2dir**(*v*, *Ainv*)

Cartesian to direct coordinates.

dpgen.data.tools.io_lammps.**convert_cell**(*ase_cell*)

Convert a parallel piped (forming right hand basis) to lower triangular matrix LAMMPS can accept. This function transposes cell matrix so the bases are column vectors.

dpgen.data.tools.io_lammps.**convert_forces**(*forces0*, *cell0*, *cell_new*)

dpgen.data.tools.io_lammps.**convert_positions**(*pos0*, *cell0*, *cell_new*, *direct=False*)

dpgen.data.tools.io_lammps.**convert_stress**(*s6_0*, *cell0*, *cell_new*)

dpgen.data.tools.io_lammps.**dir2car**(*v*, *A*)

Direct to cartesian coordinates.

dpgen.data.tools.io_lammps.**get_atoms_ntypes**(*atoms*)

dpgen.data.tools.io_lammps.**get_typeid**(*typeids*, *csymbol*)

dpgen.data.tools.io_lammps.**is_upper_triangular**(*mat*)

Test if 3x3 matrix is upper triangular LAMMPS has a rule for cell matrix definition.

dpgen.data.tools.io_lammps.**set_atoms_typeids**(*atoms*)

dpgen.data.tools.io_lammps.**set_atoms_typeids_with_atomic_numbers**(*atoms*)

dpgen.data.tools.io_lammps.**stress6_to_stress9**(*s6*)

dpgen.data.tools.io_lammps.**stress9_to_stress6**(*s9*)

dpgen.data.tools.ovito_file_convert module

dpgen.data.tools.poscar_copy module

dpgen.data.tools.sc module

dpgen.data.tools.sc.**gen_box**()

dpgen.data.tools.sc.**numb_atoms**()

dpgen.data.tools.sc.**poscar_unit**(*latt*)

Submodules

dpgen.data.arginfo module

dpgen.data.arginfo.**init_bulk_abacus_args**() → list[Argument]

dpgen.data.arginfo.**init_bulk_jdata_arginfo**() → Argument

Generate arginfo for dpgen init_bulk jdata.

Returns

Argument

dpgen init_bulk jdata arginfo

dpgen.data.arginfo.**init_bulk_mdata_arginfo**() → Argument

Generate arginfo for dpgen init_bulk mdata.

Returns

Argument

arginfo

dpgen.data.arginfo.**init_bulk_variant_type_args**() → list[Variant]

dpgen.data.arginfo.**init_bulk_vasp_args**() → list[Argument]

dpgen.data.arginfo.**init_reaction_jdata_arginfo**() → Argument

Generate arginfo for dpgen init_reaction jdata.

Returns

Argument

dpgen init_reaction jdata arginfo

dpgen.data.arginfo.**init_reaction_mdata_arginfo**() → Argument

Generate arginfo for dpgen init_reaction mdata.

Returns

Argument

arginfo

dpgen.data.arginfo.**init_surf_jdata_arginfo**() → Argument

Generate arginfo for dpgen init_surf jdata.

Returns

Argument

dpgen init_surf jdata arginfo

dpgen.data.arginfo.**init_surf_mdata_arginfo**() → Argument

Generate arginfo for dpgen init_surf mdata.

Returns

Argument

arginfo

dpgen.data.gen module

dpgen.data.gen.**class_cell_type**(*jdata*)

dpgen.data.gen.**coll_abacus_md**(*jdata*)

dpgen.data.gen.**coll_vasp_md**(*jdata*)

dpgen.data.gen.**create_path**(*path*, *back=False*)

dpgen.data.gen.**gen_init_bulk**(*args*)

dpgen.data.gen.**make_abacus_md**(*jdata*, *mdata*)

dpgen.data.gen.**make_abacus_relax**(*jdata*, *mdata*)

dpgen.data.gen.**make_combines**(*dim*, *natoms*)

dpgen.data.gen.**make_scale**(*jdata*)

dpgen.data.gen.**make_scale_ABACUS**(*jdata*)

dpgen.data.gen.**make_super_cell**(*jdata*)

dpgen.data.gen.**make_super_cell_ABACUS**(*jdata*, *stru_data*)

dpgen.data.gen.**make_super_cell_STRU**(*jdata*)

dpgen.data.gen.**make_super_cell_poscar**(*jdata*)

dpgen.data.gen.**make_unit_cell**(*jdata*)

dpgen.data.gen.**make_unit_cell_ABACUS**(*jdata*)

dpgen.data.gen.**make_vasp_md**(*jdata*, *mdata*)

dpgen.data.gen.**make_vasp_relax**(*jdata*, *mdata*)

dpgen.data.gen.**out_dir_name**(*jdata*)

dpgen.data.gen.**pert_scaled**(*jdata*)

dpgen.data.gen.**place_element**(*jdata*)

dpgen.data.gen.**place_element_ABACUS**(*jdata*, *supercell_stru*)

dpgen.data.gen.**poscar_ele**(*poscar_in*, *poscar_out*, *eles*, *natoms*)

dpgen.data.gen.**poscar_natoms**(*lines*)

dpgen.data.gen.**poscar_scale**(*poscar_in*, *poscar_out*, *scale*)

dpgen.data.gen.**poscar_scale_abacus**(*poscar_in*, *poscar_out*, *scale*, *jdata*)

dpgen.data.gen.**poscar_scale_cartesian**(*str_in*, *scale*)

dpgen.data.gen.**poscar_scale_direct**(*str_in*, *scale*)

dpgen.data.gen.**poscar_shuffle**(*poscar_in*, *poscar_out*)

dpgen.data.gen.**replace**(*file_name*, *pattern*, *subst*)

dpgen.data.gen.**run_abacus_md**(*jdata*, *mdata*)

dpgen.data.gen.**run_abacus_relax**(*jdata*, *mdata*)

dpgen.data.gen.**run_vasp_md**(*jdata*, *mdata*)

dpgen.data.gen.**run_vasp_relax**(*jdata*, *mdata*)

dpgen.data.gen.**shuffle_stru_data**(*supercell_stru*)

dpgen.data.gen.**stru_ele**(*supercell_stru*, *stru_out*, *eles*, *natoms*, *jdata*, *path_work*)

dpgen.data.reaction module

input: trajectory 00: ReaxFF MD (lammps) 01: build dataset (mddatasetbuilder) 02: fp (gaussian) 03: convert to deepmd data output: data.

dpgen.data.reaction.**convert_data**(*jdata*)

dpgen.data.reaction.**gen_init_reaction**(*args*)

dpgen.data.reaction.**link_fp_input**()

dpgen.data.reaction.**link_reaxff**(*jdata*)

dpgen.data.reaction.**link_trj**(*jdata*)

Link lammpstrj.

dpgen.data.reaction.**make_lmp**(*jdata*)

dpgen.data.reaction.**run_build_dataset**(*jdata*, *mdata*, *log_file='build_log'*)

dpgen.data.reaction.**run_fp**(*jdata*, *mdata*, *log_file='output'*, *forward_common_files=[]*)

dpgen.data.reaction.**run_reaxff**(*jdata*, *mdata*, *log_file='reaxff_log'*)

dpgen.data.surf module

dpgen.data.surf.**class_cell_type**(*jdata*)

dpgen.data.surf.**create_path**(*path*)

dpgen.data.surf.**gen_init_surf**(*args*)

dpgen.data.surf.**make_combines**(*dim*, *natoms*)

dpgen.data.surf.**make_scale**(*jdata*)

dpgen.data.surf.**make_super_cell_pymatgen**(*jdata*)

dpgen.data.surf.**make_unit_cell**(*jdata*)

dpgen.data.surf.**make_vasp_relax**(*jdata*)

dpgen.data.surf.**out_dir_name**(*jdata*)

dpgen.data.surf.**pert_scaled**(*jdata*)

dpgen.data.surf.**place_element**(*jdata*)

dpgen.data.surf.**poscar_ele**(*poscar_in*, *poscar_out*, *eles*, *natoms*)

dpgen.data.surf.**poscar_elong**(*poscar_in*, *poscar_out*, *elong*, *shift_center=True*)

dpgen.data.surf.**poscar_natoms**(*poscar_in*)

dpgen.data.surf.**poscar_scale**(*poscar_in*, *poscar_out*, *scale*)

dpgen.data.surf.**poscar_scale_cartesian**(*str_in*, *scale*)

dpgen.data.surf.**poscar_scale_direct**(*str_in*, *scale*)

dpgen.data.surf.**poscar_shuffle**(*poscar_in*, *poscar_out*)

dpgen.data.surf.**replace**(*file_name*, *pattern*, *subst*)

dpgen.data.surf.**run_vasp_relax**(*jdata*, *mdata*)

dpgen.database package

class dpgen.database.**DPPotcar**(*symbols=None*, *functional='PBE'*, *pp_file=None*, *pp_lists=None*)

Bases: MSONable

Methods

as_dict()	A JSON serializable dict representation of an object.
from_dict(d)	**param d** Dict representation.
to_json()	Returns a json string representation of the MSONable object.
unsafe_hash()	Returns an hash of the current object.
validate_monty_v1(_MSONable__input_value)	Pydantic validator with correct signature for pydantic v1.x
validate_monty_v2(_MSONable__input_value, _)	Pydantic validator with correct signature for pydantic v2.x

from_file
write_file

as_dict()

A JSON serializable dict representation of an object.

classmethod from_dict(*d*)

Parameters
d – Dict representation.
Returns
MSONable class.

classmethod from_file(*filename*)

write_file(*filename*)

class dpgen.database.Entry(*composition*, *calculator*, *inputs*, *data*, *entry_id=None*, *attribute=None*, *tag=None*)

Bases: MSONable

An lightweight Entry object containing key computed data for storing purpose.

Parameters
composition
[Composition] Composition of the entry. For flexibility, this can take the form of all the typical input taken by a Composition, including a {symbol: amt} dict, a string formula, and others.
inputs
[dict] An dict of parameters associated with the entry. Defaults to None.
data
[dict] An dict of any additional data associated with the entry. Defaults to None.
entry_id
[obj] An optional id to uniquely identify the entry.
attribute
Optional attribute of the entry. This can be used to specify that the entry is a newly found compound, or to specify a particular label for the entry, or else … Used for further analysis and plotting purposes. An attribute can be anything but must be MSONable.
Attributes
number_element

Methods

as_dict()	A JSON serializable dict representation of an object.
from_dict(d)	**param d** Dict representation.
to_json()	Returns a json string representation of the MSONable object.
unsafe_hash()	Returns an hash of the current object.
validate_monty_v1(_MSONable__input_value)	Pydantic validator with correct signature for pydantic v1.x
validate_monty_v2(_MSONable__input_value, _)	Pydantic validator with correct signature for pydantic v2.x

as_dict()

A JSON serializable dict representation of an object.

classmethod from_dict(*d*)

Parameters
d – Dict representation.

Returns
MSONable class.

property number_element

class dpgen.database.**VaspInput**(*incar*, *poscar*, *potcar*, *kpoints=None*, *optional_files=None*, ***kwargs*)

Bases: dict, MSONable

Class to contain a set of vasp input objects corresponding to a run.

Args:

incar: Incar object. kpoints: Kpoints object. poscar: Poscar object. potcar: Potcar object. optional_files: Other input files supplied as a dict of {
filename: object}. The object should follow standard pymatgen conventions in implementing a as_dict() and from_dict method.

Methods

as_dict()	A JSON serializable dict representation of an object.
clear()	
copy()	
from_dict(d)	**param d** Dict representation.
from_directory(input_dir[, optional_files])	Read in a set of VASP input from a directory.
fromkeys(iterable[, value])	Create a new dictionary with keys from iterable and values set to value.
get(key[, default])	Return the value for key if key is in the dictionary, else default.
items()	
keys()	
pop(key[, default])	If the key is not found, return the default if given; otherwise, raise a KeyError.
popitem(/)	Remove and return a (key, value) pair as a 2-tuple.
setdefault(key[, default])	Insert key with a value of default if key is not in the dictionary.
to_json()	Returns a json string representation of the MSONable object.
unsafe_hash()	Returns an hash of the current object.
update([E,]**F)	If E is present and has a .keys() method, then does: for k in E: D[k] = E[k] If E is present and lacks a .keys() method, then does: for k, v in E: D[k] = v In either case, this is followed by: for k in F: D[k] = F[k]
validate_monty_v1(_MSONable__input_value)	Pydantic validator with correct signature for pydantic v1.x
validate_monty_v2(_MSONable__input_value, _)	Pydantic validator with correct signature for pydantic v2.x
values()	
write_input([output_dir, ...])	Write VASP input to a directory.

as_dict()

A JSON serializable dict representation of an object.

classmethod from_dict(*d*)

Parameters
d – Dict representation.
Returns
MSONable class.

static from_directory(*input_dir*, *optional_files=None*)

Read in a set of VASP input from a directory. Note that only the standard INCAR, POSCAR, POTCAR and KPOINTS files are read unless optional_filenames is specified.

Parameters

input_dir
[str] Directory to read VASP input from.
optional_files
[dict] Optional files to read in as well as a dict of {filename: Object type}. Object type must have a static method from_file.

`write_input`(*output_dir='.'*, *make_dir_if_not_present=True*)

Write VASP input to a directory.

Parameters
output_dir
[str] Directory to write to. Defaults to current directory (".").
make_dir_if_not_present
[bool] Create the directory if not present. Defaults to True.

Submodules

dpgen.database.entry module

`class dpgen.database.entry.Entry`(*composition*, *calculator*, *inputs*, *data*, *entry_id=None*, *attribute=None*, *tag=None*)

Bases: `MSONable`

An lightweight Entry object containing key computed data for storing purpose.

Parameters
composition
[Composition] Composition of the entry. For flexibility, this can take the form of all the typical input taken by a Composition, including a {symbol: amt} dict, a string formula, and others.
inputs
[dict] An dict of parameters associated with the entry. Defaults to None.
data
[dict] An dict of any additional data associated with the entry. Defaults to None.
entry_id
[obj] An optional id to uniquely identify the entry.
attribute
Optional attribute of the entry. This can be used to specify that the entry is a newly found compound, or to specify a particular label for the entry, or else … Used for further analysis and plotting purposes. An attribute can be anything but must be MSONable.

Attributes
number_element

Methods

as_dict()	A JSON serializable dict representation of an object.
from_dict(d)	**param d** Dict representation.
to_json()	Returns a json string representation of the MSONable object.
unsafe_hash()	Returns an hash of the current object.
validate_monty_v1(_MSONable__input_value)	Pydantic validator with correct signature for pydantic v1.x
validate_monty_v2(_MSONable__input_value, _)	Pydantic validator with correct signature for pydantic v2.x

as_dict()

A JSON serializable dict representation of an object.

classmethod from_dict(*d*)

Parameters
d – Dict representation.
Returns
MSONable class.

property number_element

dpgen.database.run module

dpgen.database.run.**db_run**(*args*)

dpgen.database.run.**parsing_gaussian**(*path*, *output='dpgen_db.json'*)

dpgen.database.run.**parsing_pwscf**(*path*, *output='dpgen_db.json'*)

dpgen.database.run.**parsing_vasp**(*path*, *config_info_dict*, *skip_init*, *output='dpgen_db.json'*, *id_prefix=None*)

dpgen.database.vasp module

class dpgen.database.vasp.**DPPotcar**(*symbols=None*, *functional='PBE'*, *pp_file=None*, *pp_lists=None*)

Bases: MSONable

Methods

as_dict()	A JSON serializable dict representation of an object.
from_dict(d)	**param d** Dict representation.
to_json()	Returns a json string representation of the MSONable object.
unsafe_hash()	Returns an hash of the current object.
validate_monty_v1(_MSONable__input_value)	Pydantic validator with correct signature for pydantic v1.x
validate_monty_v2(_MSONable__input_value, _)	Pydantic validator with correct signature for pydantic v2.x

from_file
write_file

as_dict()

A JSON serializable dict representation of an object.

classmethod from_dict(*d*)

Parameters
d – Dict representation.
Returns
MSONable class.

classmethod from_file(*filename*)

write_file(*filename*)

class dpgen.database.vasp.**VaspInput**(*incar*, *poscar*, *potcar*, *kpoints=None*, *optional_files=None*, ***kwargs*)

Bases: dict, MSONable

Class to contain a set of vasp input objects corresponding to a run.

Args:

incar: Incar object. kpoints: Kpoints object. poscar: Poscar object. potcar: Potcar object. optional_files: Other input files supplied as a dict of {
filename: object}. The object should follow standard pymatgen conventions in implementing a as_dict() and from_dict method.

Methods

as_dict()	A JSON serializable dict representation of an object.
clear()	
copy()	
from_dict(d)	**param d** Dict representation.
from_directory(input_dir[, optional_files])	Read in a set of VASP input from a directory.
fromkeys(iterable[, value])	Create a new dictionary with keys from iterable and values set to value.
get(key[, default])	Return the value for key if key is in the dictionary, else default.
items()	
keys()	
pop(key[, default])	If the key is not found, return the default if given; otherwise, raise a KeyError.
popitem(/)	Remove and return a (key, value) pair as a 2-tuple.
setdefault(key[, default])	Insert key with a value of default if key is not in the dictionary.
to_json()	Returns a json string representation of the MSONable object.
unsafe_hash()	Returns an hash of the current object.
update([E,]**F)	If E is present and has a .keys() method, then does: for k in E: D[k] = E[k] If E is present and lacks a .keys() method, then does: for k, v in E: D[k] = v In either case, this is followed by: for k in F: D[k] = F[k]
validate_monty_v1(_MSONable__input_value)	Pydantic validator with correct signature for pydantic v1.x
validate_monty_v2(_MSONable__input_value, _)	Pydantic validator with correct signature for pydantic v2.x
values()	
write_input([output_dir, ...])	Write VASP input to a directory.

as_dict()

A JSON serializable dict representation of an object.

classmethod from_dict(*d*)

Parameters
d – Dict representation.
Returns
MSONable class.

static from_directory(*input_dir*, *optional_files=None*)

Read in a set of VASP input from a directory. Note that only the standard INCAR, POSCAR, POTCAR and KPOINTS files are read unless optional_filenames is specified.

Parameters

input_dir
[str] Directory to read VASP input from.
optional_files
[dict] Optional files to read in as well as a dict of {filename: Object type}. Object type must have a static method from_file.

`write_input`(*output_dir='.'*, *make_dir_if_not_present=True*)

Write VASP input to a directory.

Parameters
output_dir
[str] Directory to write to. Defaults to current directory (".").
make_dir_if_not_present
[bool] Create the directory if not present. Defaults to True.

dpgen.dispatcher package

Submodules

dpgen.dispatcher.Dispatcher module

dpgen.dispatcher.Dispatcher.`make_submission`(*mdata_machine*, *mdata_resources*, *commands*, *work_path*, *run_tasks*, *group_size*, *forward_common_files*, *forward_files*, *backward_files*, *outlog*, *errlog*)

dpgen.dispatcher.Dispatcher.`make_submission_compat`(*machine: dict*, *resources: dict*, *commands: list[str]*, *work_path: str*, *run_tasks: list[str]*, *group_size: int*, *forward_common_files: list[str]*, *forward_files: list[str]*, *backward_files: list[str]*, *outlog: str = 'log'*, *errlog: str = 'err'*, *api_version: str = '1.0'*) → None

Make submission with compatibility of both dispatcher API v0 and v1.

If *api_version* is less than 1.0, raise RuntimeError. If *api_version* is large than 1.0, use *make_submission*.

Parameters
machine
[dict] machine dict
resources
[dict] resource dict
commands
[list[str]] list of commands
work_path
[str] working directory
run_tasks
[list[str]] list of paths to running tasks
group_size
[int] group size
forward_common_files
[list[str]] forwarded common files shared for all tasks
forward_files
[list[str]] forwarded files for each task
backward_files
[list[str]] backwarded files for each task

outlog
[str, default=log] path to log from stdout
errlog
[str, default=err] path to log from stderr
api_version
[str, default=1.0] API version. 1.0 is required

dpgen.dispatcher.Dispatcher.**mdata_arginfo**() → list[Argument]

This method generates arginfo for a single mdata.

A submission requires the following keys: command, machine, and resources.

Returns
list[Argument]
arginfo

dpgen.generator package

Subpackages

dpgen.generator.lib package

Submodules

dpgen.generator.lib.abacus_scf module

dpgen.generator.lib.abacus_scf.**get_abacus_STRU**(*STRU*, *INPUT=None*, *n_ele=None*)

dpgen.generator.lib.abacus_scf.**get_abacus_input_parameters**(*INPUT*)

dpgen.generator.lib.abacus_scf.**get_additional_from_STRU**(*geometry_inlines*, *nele*)

dpgen.generator.lib.abacus_scf.**get_mass_from_STRU**(*geometry_inlines*, *atom_names*)

dpgen.generator.lib.abacus_scf.**get_natoms_from_stru**(*geometry_inlines*)

dpgen.generator.lib.abacus_scf.**make_abacus_scf_input**(*fp_params*, *extra_file_path=''*)

dpgen.generator.lib.abacus_scf.**make_abacus_scf_kpt**(*fp_params*)

dpgen.generator.lib.abacus_scf.**make_abacus_scf_stru**(*sys_data*, *fp_pp_files*, *fp_orb_files=None*, *fp_dpks_descriptor=None*, *fp_params=None*, *type_map=None*, *pporb=''*)

dpgen.generator.lib.abacus_scf.**make_kspacing_kpoints_stru**(*stru*, *kspacing*)

dpgen.generator.lib.abacus_scf.**make_supercell_abacus**(*from_struct*, *super_cell*)

dpgen.generator.lib.calypso_check_outcar module

dpgen.generator.lib.calypso_run_model_devi module

dpgen.generator.lib.calypso_run_opt module

dpgen.generator.lib.cp2k module

dpgen.generator.lib.cp2k.**iterdict**(*d*, *out_list*, *flag=None*, *indent=0*)

Doc
: a recursive expansion of dictionary into cp2k input

K
: current key

V
: current value

D
: current dictionary under expansion

Flag
: used to record dictionary state. if flag is None,

it means we are in top level dict. flag is a string. :indent: intent for current section.

dpgen.generator.lib.cp2k.**make_cp2k_input**(*sys_data*, *fp_params*)

dpgen.generator.lib.cp2k.**make_cp2k_input_from_external**(*sys_data*, *exinput_path*)

dpgen.generator.lib.cp2k.**make_cp2k_xyz**(*sys_data*)

dpgen.generator.lib.cp2k.**update_dict**(*old_d*, *update_d*)

A method to recursive update dict :old_d: old dictionary :update_d: some update value written in dictionary form.

dpgen.generator.lib.cvasp module

dpgen.generator.lib.cvasp.**runvasp**(*cmd*, *opt=False*, *max_errors=3*, *backup=False*, *auto_gamma=False*, *auto_npar=False*, *ediffg=-0.05*)

Cmd example: cmd=[‘mpirun’, ‘-np’, ‘32’ , ‘-machinefile’, ‘hosts’,’vasp_std’].

dpgen.generator.lib.ele_temp module

class dpgen.generator.lib.ele_temp.**NBandsEsti**(*test_list*)

Bases: `object`

Methods

predict
save

predict(*target_dir*, *tolerance=0.5*)

save(*fname*)

dpgen.generator.lib.gaussian module

dpgen.generator.lib.gaussian.**detect_multiplicity**(*symbols*)

dpgen.generator.lib.gaussian.**make_gaussian_input**(*sys_data*, *fp_params*)

dpgen.generator.lib.gaussian.**take_cluster**(*old_conf_name*, *type_map*, *idx*, *jdata*)

dpgen.generator.lib.lammps module

dpgen.generator.lib.lammps.**get_all_dumped_forces**(*file_name*)

dpgen.generator.lib.lammps.**get_dumped_forces**(*file_name*)

dpgen.generator.lib.lammps.**make_lammps_input**(*ensemble*, *conf_file*, *graphs*, *nsteps*, *dt*, *neidelay*, *trj_freq*, *mass_map*, *temp*, *jdata*, *tau_t=0.1*, *pres=None*, *tau_p=0.5*, *pka_e=None*, *ele_temp_f=None*, *ele_temp_a=None*, *max_seed=1000000*, *nopbc=False*, *deepmd_version='0.1'*, *nbeads=None*)

dpgen.generator.lib.make_calypso module

dpgen.generator.lib.make_calypso.**make_calypso_input**(*nameofatoms*, *numberofatoms*, *numberofformula*, *volume*, *distanceofion*, *psoratio*, *popsize*, *maxstep*, *icode*, *split*, *vsc*, *maxnumatom*, *ctrlrange*, *pstress*, *fmax*)

dpgen.generator.lib.make_calypso.**write_model_devi_out**(*devi*, *fname*)

dpgen.generator.lib.parse_calypso module

dpgen.generator.lib.pwmat module

dpgen.generator.lib.pwmat.**input_upper**(*dinput*)

dpgen.generator.lib.pwmat.**make_pwmat_input_dict**(*node1*, *node2*, *atom_config*, *ecut*, *e_error*, *rho_error*, *icmix=None*, *smearing=None*, *sigma=None*, *kspacing=0.5*, *flag_symm=None*)

dpgen.generator.lib.pwmat.**make_pwmat_input_user_dict**(*fp_params*)

dpgen.generator.lib.pwmat.**write_input_dict**(*input_dict*)

dpgen.generator.lib.pwscf module

dpgen.generator.lib.pwscf.**cvt_1frame**(*fin*, *fout*)

dpgen.generator.lib.pwscf.**get_atom_types**(*lines*)

dpgen.generator.lib.pwscf.**get_block**(*lines*, *keyword*, *skip=0*)

dpgen.generator.lib.pwscf.**get_cell**(*lines*)

dpgen.generator.lib.pwscf.**get_coords**(*lines*)

dpgen.generator.lib.pwscf.**get_energy**(*lines*)

dpgen.generator.lib.pwscf.**get_force**(*lines*)

dpgen.generator.lib.pwscf.**get_natoms**(*lines*)

dpgen.generator.lib.pwscf.**get_stress**(*lines*, *cells*)

dpgen.generator.lib.pwscf.**get_types**(*lines*)

dpgen.generator.lib.pwscf.**make_pwscf_01_runctrl_dict**(*sys_data*, *idict*)

dpgen.generator.lib.pwscf.**make_pwscf_input**(*sys_data*, *fp_pp_files*, *fp_params*, *user_input=True*)

dpgen.generator.lib.run_calypso module

calypso as model devi engine: 1. gen_structures 2. analysis 3. model devi.

dpgen.generator.lib.run_calypso.**analysis**(*iter_index*, *jdata*, *calypso_model_devi_path*)

dpgen.generator.lib.run_calypso.**gen_main**(*iter_index*, *jdata*, *mdata*, *caly_run_opt_list*, *gen_idx*)

dpgen.generator.lib.run_calypso.**gen_structures**(*iter_index*, *jdata*, *mdata*, *caly_run_path*, *current_idx*, *length_of_caly_runopt_list*)

dpgen.generator.lib.run_calypso.**run_calypso_model_devi**(*iter_index*, *jdata*, *mdata*)

dpgen.generator.lib.siesta module

dpgen.generator.lib.siesta.**make_siesta_input**(*sys_data*, *fp_pp_files*, *fp_params*)

dpgen.generator.lib.utils module

dpgen.generator.lib.utils.**cmd_append_log**(*cmd*, *log_file*)

dpgen.generator.lib.utils.**copy_file_list**(*file_list*, *from_path*, *to_path*)

dpgen.generator.lib.utils.**create_path**(*path*)

dpgen.generator.lib.utils.**log_iter**(*task*, *ii*, *jj*)

dpgen.generator.lib.utils.**log_task**(*message*)

dpgen.generator.lib.utils.**make_iter_name**(*iter_index*)

dpgen.generator.lib.utils.**record_iter**(*record*, *ii*, *jj*)

dpgen.generator.lib.utils.**repeat_to_length**(*string_to_expand*, *length*)

dpgen.generator.lib.utils.**replace**(*file_name*, *pattern*, *subst*)

dpgen.generator.lib.utils.**symlink_user_forward_files**(*mdata*, *task_type*, *work_path*, *task_format=None*)

Symlink user-defined forward_common_files Current path should be work_path, such as 00.train.

Parameters

mdata
: [dict] machine parameters

task_type
: [str] task_type, such as "train"

work_path
: [str] work_path, such as "iter.000001/00.train"

task_format
: [dict] formats of tasks

Returns

None

dpgen.generator.lib.vasp module

dpgen.generator.lib.vasp.**incar_upper**(*dincar*)

dpgen.generator.lib.vasp.**make_vasp_incar_user_dict**(*fp_params*)

dpgen.generator.lib.vasp.**write_incar_dict**(*incar_dict*)

Submodules

dpgen.generator.arginfo module

dpgen.generator.arginfo.**basic_args**() → list[Argument]

dpgen.generator.arginfo.**data_args**() → list[Argument]

dpgen.generator.arginfo.**fp_args**() → list[Argument]

dpgen.generator.arginfo.**fp_style_abacus_args**() → list[Argument]

dpgen.generator.arginfo.**fp_style_amber_diff_args**() → list[Argument]

Arguments for FP style amber/diff.

Returns

list[dargs.Argument]

list of amber/diff fp style arguments

dpgen.generator.arginfo.**fp_style_cp2k_args**() → list[Argument]

dpgen.generator.arginfo.**fp_style_custom_args**() → list[Argument]

Arguments for FP style custom.

Returns

list[dargs.Argument]

list of custom fp style arguments

dpgen.generator.arginfo.**fp_style_gaussian_args**() → list[Argument]

Gaussian fp style arguments.

Returns

list[dargs.Argument]

list of Gaussian fp style arguments

dpgen.generator.arginfo.**fp_style_pwscf_args**() → list[Argument]

Arguments for FP style pwscf (Quantum Espresso).

Returns

list[dargs.Argument]

list of pwscf fp style arguments

dpgen.generator.arginfo.**fp_style_siesta_args**() → list[Argument]

dpgen.generator.arginfo.**fp_style_variant_type_args**() → Variant

dpgen.generator.arginfo.**fp_style_vasp_args**() → list[Argument]

dpgen.generator.arginfo.**model_devi_amber_args**() → list[Argument]

Amber engine arguments.

dpgen.generator.arginfo.**model_devi_args**() → list[Variant]

dpgen.generator.arginfo.**model_devi_jobs_args**() → list[Argument]

dpgen.generator.arginfo.**model_devi_jobs_rev_mat_args**() → Argument

dpgen.generator.arginfo.**model_devi_jobs_template_args**() → Argument

dpgen.generator.arginfo.**model_devi_lmp_args**() → list[Argument]

dpgen.generator.arginfo.**run_jdata_arginfo**() → Argument

Argument information for dpgen run mdata.

Returns

Argument

argument information

dpgen.generator.arginfo.**run_mdata_arginfo**() → Argument

Generate arginfo for dpgen run mdata.

Returns

Argument

arginfo

dpgen.generator.arginfo.**training_args**() → list[Argument]

Traning arguments.

Returns

list[dargs.Argument]

List of training arguments.

dpgen.generator.run module

init: data iter:

00.train 01.model_devi 02.vasp 03.data.

dpgen.generator.run.**check_bad_box**(*conf_name*, *criteria*, *fmt='lammps/dump'*)

dpgen.generator.run.**check_cluster**(*conf_name*, *fp_cluster_vacuum*, *fmt='lammps/dump'*)

dpgen.generator.run.**copy_model**(*numb_model*, *prv_iter_index*, *cur_iter_index*)

dpgen.generator.run.**detect_batch_size**(*batch_size*, *system=None*)

dpgen.generator.run.**dump_to_deepmd_raw**(*dump*, *deepmd_raw*, *type_map*, *fmt='gromacs/gro'*, *charge=None*)

dpgen.generator.run.**expand_idx**(*in_list*)

dpgen.generator.run.**expand_matrix_values**(*target_list*, *cur_idx=0*)

dpgen.generator.run.**find_only_one_key**(*lmp_lines*, *key*)

dpgen.generator.run.**gen_run**(*args*)

dpgen.generator.run.**get_atomic_masses**(*atom*)

dpgen.generator.run.**get_job_names**(*jdata*)

dpgen.generator.run.**get_nframes**(*system*)

dpgen.generator.run.**get_sys_index**(*task*)

dpgen.generator.run.**make_fp**(*iter_index*, *jdata*, *mdata*)

Select the candidate strutures and make the input file of FP calculation.

Parameters

iter_index

[int] iter index

jdata

[dict] Run parameters.

mdata

[dict] Machine parameters.

dpgen.generator.run.**make_fp_abacus_scf**(*iter_index*, *jdata*)

dpgen.generator.run.**make_fp_amber_diff**(*iter_index: int*, *jdata: dict*)

Run amber twice to calculate high-level and low-level potential, and then generate difference between them.

Besides AMBER, one needs to install *dpamber* package, which is avaiable at https://github.com/njzjz/dpamber

Currently, it should be used with the AMBER model_devi driver.

Parameters

iter_index
[int] iter index
jdata
[dict]
Run parameters. The following parameters are used in this method:

mdin_prefix
[str] The path prefix to AMBER mdin files

qm_region
[list[str]] AMBER mask of the QM region. Each mask maps to a system.

qm_charge
[list[int]] Charge of the QM region. Each charge maps to a system.

high_level
[str] high level method

low_level
[str] low level method

fp_params
[dict]

This parameters includes:

high_level_mdin
[str] High-level AMBER mdin file. %qm_theory%, %qm_region%, and %qm_charge% will be replace.

low_level_mdin
[str] Low-level AMBER mdin file. %qm_theory%, %qm_region%, and %qm_charge% will be replace.

parm7_prefix
[str] The path prefix to AMBER PARM7 files

parm7
[list[str]] List of paths to AMBER PARM7 files. Each file maps to a system.

References

[1]

dpgen.generator.run.**make_fp_calculation**(*iter_index*, *jdata*, *mdata*)

Make the input file of FP calculation.

Parameters
iter_index
[int] iter index
jdata
[dict] Run parameters.
mdata
[dict] Machine parameters.

dpgen.generator.run.**make_fp_cp2k**(*iter_index*, *jdata*)

dpgen.generator.run.**make_fp_custom**(*iter_index*, *jdata*)

Make input file for customized FP style.

Convert the POSCAR file to custom format.

Parameters

iter_index

[int] iter index

jdata

[dict] Run parameters.

dpgen.generator.run.**make_fp_gaussian**(*iter_index*, *jdata*)

dpgen.generator.run.**make_fp_pwmat**(*iter_index*, *jdata*)

dpgen.generator.run.**make_fp_pwscf**(*iter_index*, *jdata*)

dpgen.generator.run.**make_fp_siesta**(*iter_index*, *jdata*)

dpgen.generator.run.**make_fp_task_name**(*sys_idx*, *counter*)

dpgen.generator.run.**make_fp_vasp**(*iter_index*, *jdata*)

dpgen.generator.run.**make_fp_vasp_cp_cvasp**(*iter_index*, *jdata*)

dpgen.generator.run.**make_fp_vasp_incar**(*iter_index*, *jdata*, *nbands_esti=None*)

dpgen.generator.run.**make_fp_vasp_kp**(*iter_index*, *jdata*)

dpgen.generator.run.**make_model_devi**(*iter_index*, *jdata*, *mdata*)

dpgen.generator.run.**make_model_devi_conf_name**(*sys_idx*, *conf_idx*)

dpgen.generator.run.**make_model_devi_task_name**(*sys_idx*, *task_idx*)

dpgen.generator.run.**make_pwmat_input**(*jdata*, *filename*)

dpgen.generator.run.**make_train**(*iter_index*, *jdata*, *mdata*)

dpgen.generator.run.**make_vasp_incar**(*jdata*, *filename*)

dpgen.generator.run.**make_vasp_incar_ele_temp**(*jdata*, *filename*, *ele_temp*, *nbands_esti=None*)

dpgen.generator.run.**parse_cur_job**(*cur_job*)

dpgen.generator.run.**parse_cur_job_revmat**(*cur_job*, *use_plm=False*)

dpgen.generator.run.**parse_cur_job_sys_revmat**(*cur_job*, *sys_idx*, *use_plm=False*)

dpgen.generator.run.**poscar_natoms**(*lines*)

dpgen.generator.run.**poscar_shuffle**(*poscar_in*, *poscar_out*)

dpgen.generator.run.**poscar_to_conf**(*poscar*, *conf*)

dpgen.generator.run.**post_fp**(*iter_index*, *jdata*)

dpgen.generator.run.**post_fp_abacus_scf**(*iter_index*, *jdata*)

dpgen.generator.run.**post_fp_amber_diff**(*iter_index*, *jdata*)

dpgen.generator.run.**post_fp_check_fail**(*iter_index*, *jdata*, *rfailed=None*)

dpgen.generator.run.**post_fp_cp2k**(*iter_index*, *jdata*, *rfailed=None*)

dpgen.generator.run.**post_fp_custom**(*iter_index*, *jdata*)

Post fp for custom fp. Collect data from user-defined *output_fn*.

Parameters

iter_index

[int] The index of the current iteration.

jdata

[dict] The parameter data.

dpgen.generator.run.**post_fp_gaussian**(*iter_index*, *jdata*)

dpgen.generator.run.**post_fp_pwmat**(*iter_index*, *jdata*, *rfailed=None*)

dpgen.generator.run.**post_fp_pwscf**(*iter_index*, *jdata*)

dpgen.generator.run.**post_fp_siesta**(*iter_index*, *jdata*)

dpgen.generator.run.**post_fp_vasp**(*iter_index*, *jdata*, *rfailed=None*)

dpgen.generator.run.**post_model_devi**(*iter_index*, *jdata*, *mdata*)

dpgen.generator.run.**post_train**(*iter_index*, *jdata*, *mdata*)

dpgen.generator.run.**revise_by_keys**(*lmp_lines*, *keys*, *values*)

dpgen.generator.run.**revise_lmp_input_dump**(*lmp_lines*, *trj_freq*, *model_devi_merge_traj=False*)

dpgen.generator.run.**revise_lmp_input_model**(*lmp_lines*, *task_model_list*, *trj_freq*, *deepmd_version='1'*)

dpgen.generator.run.**revise_lmp_input_plm**(*lmp_lines*, *in_plm*, *out_plm='output.plumed'*)

dpgen.generator.run.**run_fp**(*iter_index*, *jdata*, *mdata*)

dpgen.generator.run.**run_fp_inner**(*iter_index*, *jdata*, *mdata*, *forward_files*, *backward_files*, *check_fin*, *log_file='fp.log'*, *forward_common_files=[]*)

dpgen.generator.run.**run_iter**(*param_file*, *machine_file*)

dpgen.generator.run.**run_md_model_devi**(*iter_index*, *jdata*, *mdata*)

dpgen.generator.run.**run_model_devi**(*iter_index*, *jdata*, *mdata*)

dpgen.generator.run.**run_train**(*iter_index*, *jdata*, *mdata*)

dpgen.generator.run.**set_version**(*mdata*)

dpgen.generator.run.**sys_link_fp_vasp_pp**(*iter_index*, *jdata*)

dpgen.generator.run.**update_mass_map**(*jdata*)

dpgen.remote package

Submodules

dpgen.remote.decide_machine module

dpgen.remote.decide_machine.**convert_mdata**(*mdata*, *task_types=['train', 'model_devi', 'fp']*)

Convert mdata for DP-GEN main process. New convension is like mdata[“fp”][“machine”], DP-GEN needs mdata[“fp_machine”].

Notice that we deprecate the function which can automatically select one most avalaible machine, since this function was only used by Angus, and only supports for Slurm. In the future this can be implemented.

Parameters

mdata

[dict] Machine parameters to be converted.

task_types

[list of string] Type of tasks, default is [“train”, “model_devi”, “fp”]

Returns

dict

mdata converted

dpgen.simplify package

Submodules

dpgen.simplify.arginfo module

dpgen.simplify.arginfo.**fp_args**() → list[Argument]

Generate arginfo for fp.

Returns

List[Argument]

arginfo

dpgen.simplify.arginfo.**fp_style_variant_type_args**() → Variant

Generate variant for fp style variant type.

Returns

Variant

variant for fp style

dpgen.simplify.arginfo.**general_simplify_arginfo**() → Argument

General simplify arginfo.

Returns

Argument

arginfo

dpgen.simplify.arginfo.**simplify_jdata_arginfo**() → Argument

Generate arginfo for dpgen simplify jdata.

Returns

Argument

arginfo

dpgen.simplify.arginfo.**simplify_mdata_arginfo**() → Argument

Generate arginfo for dpgen simplify mdata.

Returns

Argument

arginfo

dpgen.simplify.simplify module

Simplify dataset (minimize the dataset size).

Init: pick up init data from dataset randomly

Iter: 00: train models (same as generator) 01: calculate model deviations of the rest dataset, pick up data with proper model deviaiton 02: fp (optional, if the original dataset do not have fp data, same as generator)

dpgen.simplify.simplify.**gen_simplify**(*args*)

dpgen.simplify.simplify.**get_multi_system**(*path: str | list[str]*, *jdata: dict*) → MultiSystems

Get MultiSystems from a path or list of paths.

Both NumPy and HDF5 formats are supported. For details of two formats, refer to DeePMD-kit documentation.

If *labeled* in jdata is True, returns MultiSystems with LabeledSystem. Otherwise, returns MultiSystems with System.

Parameters

path

[str or list of str] path or list of paths to the dataset

jdata

[dict] parameters which may contain *labeled* key

Returns

dpdata.MultiSystems

MultiSystems with LabeledSystem or System

dpgen.simplify.simplify.**get_system_cls**(*jdata*)

dpgen.simplify.simplify.**init_model**(*iter_index*, *jdata*, *mdata*)

dpgen.simplify.simplify.**init_pick**(*iter_index*, *jdata*, *mdata*)

Pick up init data from dataset randomly.

dpgen.simplify.simplify.**make_fp**(*iter_index*, *jdata*, *mdata*)

dpgen.simplify.simplify.**make_fp_configs**(*iter_index*, *jdata*)

dpgen.simplify.simplify.**make_fp_labeled**(*iter_index*, *jdata*)

dpgen.simplify.simplify.**make_model_devi**(*iter_index*, *jdata*, *mdata*)

Calculate the model deviation of the rest idx.

dpgen.simplify.simplify.**post_model_devi**(*iter_index*, *jdata*, *mdata*)

Calculate the model deviation.

dpgen.simplify.simplify.**run_iter**(*param_file*, *machine_file*)

Init (iter 0): init_pick.

tasks (iter > 0): 00 make_train (same as generator) 01 run_train (same as generator) 02 post_train (same as generator) 03 make_model_devi 04 run_model_devi 05 post_model_devi 06 make_fp 07 run_fp (same as generator) 08 post_fp (same as generator)

dpgen.simplify.simplify.**run_model_devi**(*iter_index*, *jdata*, *mdata*)

Submit dp test tasks.

dpgen.tools package

Submodules

dpgen.tools.auto_gen_param module

class dpgen.tools.auto_gen_param.**Iteration**(*temps*, *nsteps_list=[500, 500, 1000, 1000, 3000, 3000, 6000, 6000]*, *sub_iteration_num=8*, *ensemble='npt'*, *press=[1.0, 10.0, 100.0, 1000.0, 5000.0, 10000.0, 20000.0, 50000.0]*, *trj_freq=10*)

Bases: object

Attributes

index_iteration

Methods

gen_sub_iter
register_iteration
register_sub_iteartion

current_num_of_itearation = 0

current_num_of_sub_itearation = 0

gen_sub_iter(*system_list*)

property index_iteration

classmethod register_iteration()

classmethod register_sub_iteartion()

class dpgen.tools.auto_gen_param.**System**(*system_prefix=''*)

Bases: object

Attributes

index_system

Methods

add_sub_system
get_sub_system
register_sub_system
register_system

add_sub_system(*idx2*, *files_list*)

current_num_of_sub_systems = 0

current_num_of_system = 0

get_sub_system()

property index_system

classmethod register_sub_system()

classmethod register_system()

dpgen.tools.auto_gen_param.**auto_gen_param**(*args*)

dpgen.tools.auto_gen_param.**default_map_generator**(*map_list=[1, 1, 2, 2, 2, 4, 4, 4]*, *data_list=None*)

dpgen.tools.auto_gen_param.**default_temps_generator**(*melt_point*, *temps_intervel=0.1*, *num_temps=5*)

dpgen.tools.auto_gen_param.**get_basic_param_json**(*melt_point*, *out_param_filename='param_basic.json'*, *scan_dir='./'*, *file_name='POSCAR'*, *init_file_name='type.raw'*, *min_allow_files_num=16*, *map_list=[1, 1, 2, 2, 2, 4, 4, 4]*, *meta_iter_num=4*, *sub_iteration_num=8*, *map_iterator=None*, *nsteps_list=[500, 500, 1000, 1000, 3000, 3000, 6000, 6000]*, *press=[1.0, 10.0, 100.0, 1000.0, 5000.0, 10000.0, 20000.0, 50000.0]*, *temps_iterator=None*, *ensemble='npt'*, *trj_freq=10*, *temps_intervel=0.1*, *num_temps=5*)

dpgen.tools.auto_gen_param.**get_init_data_sys**(*scan_dir='./'*, *init_file_name='type.raw'*)

dpgen.tools.auto_gen_param.**get_model_devi_jobs**(*melt_point*, *system_list*, *nsteps_list=[500, 500, 1000, 1000, 3000, 3000, 6000, 6000]*, *press=[1.0, 10.0, 100.0, 1000.0, 5000.0, 10000.0, 20000.0, 50000.0]*, *meta_iter_num=4*, *sub_iteration_num=8*, *temps_iterator=None*, *ensemble='npt'*, *trj_freq=10*, *temps_intervel=0.1*, *num_temps=5*)

dpgen.tools.auto_gen_param.**get_sys_configs**(*system_list*)

dpgen.tools.auto_gen_param.**get_system_list**(*system_dict*, *map_list=[1, 1, 2, 2, 2, 4, 4, 4]*, *meta_iter_num=4*, *sub_iteration_num=8*, *map_iterator=None*, *file_name='POSCAR'*)

:Exmaple [[‘000000’, ‘000001’,], [‘00000[2-9]’,], [‘00001?’, ‘000020’,],]

dpgen.tools.auto_gen_param.**scan_files**(*scan_dir='./'*, *file_name='POSCAR'*, *min_allow_files_num=20*)

dpgen.tools.collect_data module

dpgen.tools.collect_data.**collect_data**(*target_folder*, *param_file*, *output*, *verbose=True*)

dpgen.tools.collect_data.**file_len**(*fname*)

dpgen.tools.relabel module

dpgen.tools.relabel.**copy_pp_files**(*tdir*, *fp_pp_path*, *fp_pp_files*)

dpgen.tools.relabel.**create_init_tasks**(*target_folder*, *param_file*, *output*, *fp_json*, *verbose=True*)

dpgen.tools.relabel.**create_tasks**(*target_folder*, *param_file*, *output*, *fp_json*, *verbose=True*, *numb_iter=-1*)

dpgen.tools.relabel.**get_lmp_info**(*input_file*)

dpgen.tools.relabel.**link_pp_files**(*tdir*, *fp_pp_path*, *fp_pp_files*)

dpgen.tools.relabel.**make_pwscf**(*tdir*, *fp_params*, *mass_map*, *fp_pp_path*, *fp_pp_files*, *user_input*)

dpgen.tools.relabel.**make_siesta**(*tdir*, *fp_params*, *fp_pp_path*, *fp_pp_files*)

dpgen.tools.relabel.**make_vasp**(*tdir*, *fp_params*)

dpgen.tools.relabel.**make_vasp_incar**(*tdir*, *fp_incar*)

dpgen.tools.run_report module

dpgen.tools.run_report.**run_report**(*args*)

dpgen.tools.stat_iter module

dpgen.tools.stat_iter.**stat_iter**(*target_folder*, *param_file='param.json'*, *verbose=True*, *mute=False*)

dpgen.tools.stat_sys module

dpgen.tools.stat_sys.**ascii_hist**(*count*)

dpgen.tools.stat_sys.**run_report**(*args*)

dpgen.tools.stat_sys.**stat_sys**(*target_folder*, *param_file='param.json'*, *verbose=True*, *mute=False*)

dpgen.tools.stat_time module

dpgen.tools.stat_time.**stat_time**(*target_folder*, *param_file='param.json'*, *verbose=True*, *mute=False*)

10.1.2 Submodules

10.1.3 dpgen.arginfo module

dpgen.arginfo.**general_mdata_arginfo**(*name: str*, *tasks: tuple[str]*) → Argument

Generate arginfo for general mdata.

Parameters

name

[str] mdata name

tasks
[tuple[str]] tuple of task keys, e.g. ("train", "model_devi", "fp")
Returns
Argument
arginfo

10.1.4 dpgen.gui module

DP-GUI entrypoint.

dpgen.gui.**start_dpgui**(*args: Namespace*)

Host DP-GUI server.
Parameters
args
[argparse.Namespace] Arguments from argparse.
Raises
ModuleNotFoundError
The dpgui package is not installed

10.1.5 dpgen.main module

dpgen.main.**main**()

dpgen.main.**main_parser**() → ArgumentParser

Returns parser for *dpgen* command.
Returns
argparse.ArgumentParser
parser for *dpgen* command

10.1.6 dpgen.util module

dpgen.util.**box_center**(*ch=''*, *fill=' '*, *sp='|'*)

Put the string at the center of | |.

dpgen.util.**convert_training_data_to_hdf5**(*input_files: list[str]*, *h5_file: str*)

Convert training data to HDF5 format and update the input files.
Parameters
input_files
[list of str] DeePMD-kit input file names
h5_file
[str] HDF5 file name

dpgen.util.**expand_sys_str**(*root_dir: str | Path*) → list[str]

Recursively iterate over directories taking those that contain *type.raw* file.

If root_dir is a file but not a directory, it will be assumed as an HDF5 file.
Parameters
root_dir
[Union[str, Path]] starting directory
Returns
List[str]
list of string pointing to system directories

Raises

RuntimeError

No system was found in the directory

dpgen.util.**load_file**(*filename: str | PathLike*) → dict

Load data from a JSON or YAML file.

Parameters

filename

[str or os.PathLike] The filename to load data from, whose suffix should be .json, .yaml, or .yml

Returns

dict

The data loaded from the file

Raises

ValueError

If the file format is not supported

dpgen.util.**normalize**(*arginfo: Argument*, *data: dict*, *strict_check: bool = True*) → dict

Normalize and check input data.

Parameters

arginfo

[dargs.Argument] argument information

data

[dict] input data

strict_check

[bool, default=True] strict check data or not

Returns

dict

normalized data

dpgen.util.**sepline**(*ch='-'*, *sp='-'*, *screen=False*)

Seperate the output by '-'.

dpgen.util.**set_directory**(*path: Path*)

Sets the current working path within the context.

Parameters

path

[Path] The path to the cwd

Yields

None

Examples

```
>>> with set_directory("some_path"):
...     do_something()
```

dpgen.util.**setup_ele_temp**(*atomic: bool*)

Set electronic temperature as required input data.

Parameters

atomic

[bool] Whether to use atomic temperature or frame temperature

CHAPTER

ELEVEN

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