DPDispatcher

Deep Modeling

Jan 05, 2023

CONTENTS:

DPDispatcher is a Python package used to generate HPC (High Performance Computing) scheduler systems (Slurm/PBS/LSF/dpcloudserver) jobs input scripts and submit these scripts to HPC systems and poke until they finish.

DPDispatcher will monitor (poke) until these jobs finish and download the results files (if these jobs is running on remote systems connected by SSH).

CHAPTER

ONE

INSTALL DPDISPATCHER

DPDispatcher can installed by `pip`:

```
pip install dpdispatcher
```

CHAPTER

TWO

GETTING STARTED

DPDispatcher provides the following classes:

- *Task* class, which represents a command to be run on batch job system, as well as the essential files need by the command.
- *Submission* class, which represents a collection of jobs defined by the HPC system. And there may be common files to be uploaded by them. DPDispatcher will create and submit these jobs when a `submission` instance execute *run_submission* method. This method will poke until the jobs finish and return.
- *Job* class, a class used by *Submission* class, which represents a job on the HPC system. *Submission* will generate jobs' submitting scripts used by HPC systems automatically with the *Task* and *Resources*
- *Resources* class, which represents the computing resources for each job within a `submission`.

You can use DPDispatcher in a Python script to submit five tasks:

```
from dpdispatcher import Machine, Resources, Task, Submission

machine = Machine.load_from_json('machine.json')
resources = Resources.load_from_json('resources.json')

task0 = Task.load_from_json('task.json')

task1 = Task(command='cat example.txt', task_work_path='dir1/', forward_files=['example.
↪txt'], backward_files=['out.txt'], outlog='out.txt')
task2 = Task(command='cat example.txt', task_work_path='dir2/', forward_files=['example.
↪txt'], backward_files=['out.txt'], outlog='out.txt')
task3 = Task(command='cat example.txt', task_work_path='dir3/', forward_files=['example.
↪txt'], backward_files=['out.txt'], outlog='out.txt')
task4 = Task(command='cat example.txt', task_work_path='dir4/', forward_files=['example.
↪txt'], backward_files=['out.txt'], outlog='out.txt')

task_list = [task0, task1, task2, task3, task4]

submission = Submission(work_base='lammps_md_300K_5GPa/',
    machine=machine,
    resources=resources,
    task_list=task_list,
    forward_common_files=['graph.pb'],
    backward_common_files=[]
)

submission.run_submission()
```

where `machine.json` is

```
{
    "batch_type": "Slurm",
    "context_type": "SSHContext",
    "local_root" : "/home/user123/workplace/22_new_project/",
    "remote_root": "/home/user123/dpdispatcher_work_dir/",
    "remote_profile":{
        "hostname": "39.106.xx.xxx",
        "username": "user123",
        "port": 22,
        "timeout": 10
    }
}
```

`resources.json` is

```
{
    "number_node": 1,
    "cpu_per_node": 4,
    "gpu_per_node": 1,
    "queue_name": "GPUV100",
    "group_size": 5
}
```

and `task.json` is

```
{
    "command": "lmp -i input.lammps",
    "task_work_path": "bct-0/",
    "forward_files": [
        "conf.lmp",
        "input.lammps"
    ],
    "backward_files": [
        "log.lammps"
    ],
    "outlog": "log",
    "errlog": "err",
}
```

You may also submit mutiple GPU jobs: complex resources example

```
resources = Resources(
    number_node=1,
    cpu_per_node=4,
    gpu_per_node=2,
    queue_name="GPU_2080Ti",
    group_size=4,
    custom_flags=[
        "#SBATCH --nice=100",
        "#SBATCH --time=24:00:00"
    ],
    strategy={
```

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```
        # used when you want to add CUDA_VISIBLE_DIVECES automatically
        "if_cuda_multi_devices": True
    },
    para_deg=1,
    # will unload these modules before running tasks
    module_unload_list=["singularity"],
    # will load these modules before running tasks
    module_list=["singularity/3.0.0"],
    # will source the environment files before running tasks
    source_list=["./slurm_test.env"],
    # the envs option is used to export environment variables
    # And it will generate a line like below.
    # export DP_DISPATCHER_EXPORT=test_foo_bar_baz
    envs={"DP_DISPATCHER_EXPORT": "test_foo_bar_baz"},
)
```

The details of parameters can be found in *Machine Parameters*, *Resources Parameters*, and *Task Parameters*.

CHAPTER

THREE

SUPPORTED CONTEXTS

Context is the way to connect to the remote server. One needs to set *context_type* to one of the following values:

3.1 LazyLocal

context_type: `LazyLocal`

`LazyLocal` directly runs jobs in the local server and local directory.

3.2 Local

context_type: `Local`

`Local` runs jobs in the local server, but in a different directory. Files will be copied to the remote directory before jobs start and copied back after jobs finish.

3.3 SSH

context_type: `SSH`

`SSH` runs jobs in a remote server. Files will be copied to the remote directory via SSH channels before jobs start and copied back after jobs finish. To use SSH, one needs to provide necessary parameters in *remote_profile*, such as *username* and `hostname`.

It's suggested to generate SSH keys and transfer the public key to the remote server in advance, which is more secure than password authentication.

Note that `SSH` context is non-login, so `bash_profile` files will not be executed.

3.4 Bohrium

context_type: `Bohrium`

Bohrium is the cloud platform for scientific computing. Read Bohrium documentation for details. To use Bohrium, one needs to provide necessary parameters in *remote_profile*.

3.5 HDFS

context_type: HDFS

The Hadoop Distributed File System (HDFS) is a distributed file system. Read Support DPDispatcher on Yarn for details.

CHAPTER

FOUR

SUPPORTED BATCH JOB SYSTEMS

Batch job system is a system to process batch jobs. One needs to set *batch_type* to one of the following values:

4.1 Bash

batch_type: `Shell`

When *batch_type* is set to `Shell`, dpdispatcher will generate a bash script to process jobs. No extra packages are required for `Shell`.

Due to lack of scheduling system, `Shell` runs all jobs at the same time. To avoid running multiple jobs at the same time, one could set *group_size* to `0` (means infinity) to generate only one job with multiple tasks.

4.2 Slurm

batch_type: `Slurm`, `SlurmJobArray`

Slurm is a job scheduling system used by lots of HPCs. One needs to make sure slurm has been setup in the remote server and the related environment is activated.

When `SlurmJobArray` is used, dpdispatcher submits Slurm jobs with job arrays. In this way, a dpdispatcher *task* maps to a Slurm job and a dpdispatcher *job* maps to a Slurm job array. Millions of Slurm jobs can be submitted quickly and Slurm can execute all Slurm jobs at the same time. One can use *group_size* to control how many Slurm jobs are contained in a Slurm job array.

4.3 OpenPBS or PBSPro

batch_type: `PBS`

OpenPBS is an open-source job scheduling of the Linux Foundation and PBS Profession is its commercial solution. One needs to make sure OpenPBS has been setup in the remote server and the related environment is activated.

Note that do not use `PBS` for Torque.

4.4 TORQUE

batch_type: `Torque`

The Terascale Open-source Resource and QUEue Manager (TORQUE) is a distributed resource manager based on standard OpenPBS. However, not all OpenPBS flags are still supported in TORQUE. One needs to make sure TORQUE has been setup in the remote server and the related environment is activated.

4.5 LSF

batch_type: `LSF`

IBM Spectrum LSF Suites is a comprehensive workload management solution used by HPCs. One needs to make sure LSF has been setup in the remote server and the related environment is activated.

4.6 Bohrium

batch_type: `Bohrium`

Bohrium is the cloud platform for scientific computing. Read Bohrium documentation for details.

4.7 DistributedShell

batch_type: `DistributedShell`

`DistributedShell` is used to submit yarn jobs. Read Support DPDispatcher on Yarn for details.

CHAPTER

FIVE

MACHINE PARAMETERS

Note: One can load, modify, and export the input file by using our effective web-based tool DP-GUI. All parameters below can be set in DP-GUI. By clicking "SAVE JSON", one can download the input file.

machine:

type: dict
argument path: machine

batch_type:

type: str
argument path: machine/batch_type

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

local_root:

type: NoneType | str
argument path: machine/local_root

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

remote_root:

type: NoneType | str, optional
argument path: 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: 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: machine/context_type
possible choices: *SSHContext*, *LocalContext*, *LazyLocalContext*, *HDFSContext*, *BohriumContext*

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

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

remote_profile:

type: `dict`

argument path: `machine[SSHContext]/remote_profile`

The information used to maintain the connection with remote machine.

hostname:

type: `str`

argument path: `machine[SSHContext]/remote_profile/hostname`

hostname or ip of ssh connection.

username:

type: `str`

argument path: `machine[SSHContext]/remote_profile/username`

username of target linux system

password:

type: `str`, optional

argument path: `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: `machine[SSHContext]/remote_profile/port`

ssh connection port.

key_filename:

type: `NoneType` | `str`, optional, default: `None`

argument path: `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: `NoneType` | `str`, optional, default: `None`

argument path: `machine[SSHContext]/remote_profile/passphrase`

passphrase of key used by ssh connection

timeout:

type: `int`, optional, default: `10`

argument path: `machine[SSHContext]/remote_profile/timeout`

timeout of ssh connection

totp_secret:

type: `NoneType` | `str`, optional, default: `None`

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

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

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

remote_profile:

type: dict, optional

argument path: 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: 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 HDFSContext (or its aliases hdfscontext, HDFS, hdfs):

remote_profile:

type: dict, optional

argument path: 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 BohriumContext (or its aliases bohriumcontext, Bohrium, bohrium, DpCloudServerContext, dpcloudservercontext, DpCloudServer, dpcloudserver, LebesgueContext, lebesguecontext, Lebesgue, lebesgue):

remote_profile:

type: dict

argument path: machine[BohriumContext]/remote_profile

The information used to maintain the connection with remote machine.

email:

type: str
argument path: machine[BohriumContext]/remote_profile/email

Email

password:

type: str
argument path:
machine[BohriumContext]/remote_profile/password

Password

program_id:

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

Program ID

keep_backup:

type: bool, optional
argument path:
machine[BohriumContext]/remote_profile/keep_backup

keep download and upload zip

input_data:

type: dict
argument path:
machine[BohriumContext]/remote_profile/input_data

Configuration of job

CHAPTER

SIX

RESOURCES PARAMETERS

Note: One can load, modify, and export the input file by using our effective web-based tool DP-GUI. All parameters below can be set in DP-GUI. By clicking "SAVE JSON", one can download the input file for.

resources:

type: dict
argument path: resources

number_node:

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

The number of node need for each *job*

cpu_per_node:

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

cpu numbers of each node assigned to each job.

gpu_per_node:

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

gpu numbers of each node assigned to each job.

queue_name:

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

The queue name of batch job scheduler system.

group_size:

type: int
argument path: resources/group_size

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

custom_flags:

type: list, optional
argument path: resources/custom_flags

The extra lines pass to job submitting script header

strategy:

type: dict, optional
argument path: resources/strategy

strategies we use to generation job submitting scripts.

if_cuda_multi_devices:

type: bool, optional, default: False
argument path: 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: resources/strategy/ratio_unfinished

The ratio of *jobs* that can be unfinished.

para_deg:

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

Decide how many tasks will be run in parallel.

source_list:

type: list, optional, default: []
argument path: resources/source_list

The env file to be sourced before the command execution.

module_purge:

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

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

module_unload_list:

type: list, optional, default: []
argument path: resources/module_unload_list

The modules to be unloaded on HPC system before submitting jobs

module_list:

type: list, optional, default: []
argument path: resources/module_list

The modules to be loaded on HPC system before submitting jobs

envs:

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

The environment variables to be exported on before submitting jobs

prepend_script:

type: list, optional, default: []
argument path: resources/prepend_script

Optional script run before jobs submitted.

append_script:

type: list, optional, default: []
argument path: resources/append_script

Optional script run after jobs submitted.

wait_time:

type: int | float, optional, default: 0
argument path: 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: resources/batch_type
possible choices: *Bohrium*, *DistributedShell*, *LSF*, *Torque*, *Slurm*, *PBS*, *SlurmJobArray*, *Shell*

The batch job system type loaded from machine/batch_type.

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

kwargs:

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

This field is empty for this batch.

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

kwargs:

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

Extra arguments.

gpu_usage:

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

Choosing if GPU is used in the calculation step.

gpu_new_syntax:

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

Custom GPU configuration, starting with #BSUB

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

kwargs:

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

Extra arguments.

custom_gpu_line:

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

Custom GPU configuration, starting with #SBATCH

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

kwargs:

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

This field is empty for this batch.

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

kwargs:

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

Extra arguments.

custom_gpu_line:

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

Custom GPU configuration, starting with #SBATCH

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

kwargs:

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

This field is empty for this batch.

CHAPTER

SEVEN

TASK PARAMETERS

Note: One can load, modify, and export the input file by using our effective web-based tool DP-GUI. All parameters below can be set in DP-GUI. By clicking "SAVE JSON", one can download the input file.

task:

type: dict
argument path: task

command:

type: str
argument path: task/command

A command to be executed of this task. The expected return code is 0.

task_work_path:

type: str
argument path: task/task_work_path

The dir where the command to be executed.

forward_files:

type: list
argument path: task/forward_files

The files to be uploaded in task_work_path before the task exectued.

backward_files:

type: list
argument path: task/backward_files

The files to be download to local_root in task_work_path after the task finished

outlog:

type: NoneType | str
argument path: task/outlog

The out log file name. redirect from stdout

errlog:

type: NoneType | str
argument path: task/errlog

The err log file name. redirect from stderr

CHAPTER

EIGHT

DPDISPATCHER API

8.1 dpdispatcher package

dpdispatcher.**info**()

Show basic information about dpdispatcher, its location and version.

8.1.1 Subpackages

dpdispatcher.dpcloudserver package

Submodules

dpdispatcher.dpcloudserver.client module

class dpdispatcher.dpcloudserver.client.**Client**(*email=None*, *password=None*, *debug=False*, *base_url='https://bohrium.dp.tech/'*)

Bases: object

Methods

download	
download_from_url	
get	
get_job_result_url	
get_log	
get_tasks	
get_tasks_list	
job_create	
post	
refresh_token	
upload	

download(*oss_file*, *save_file*, *endpoint*, *bucket_name*)

download_from_url(*url*, *save_file*)

get(*url*, *header=None*, *params=None*, *retry=5*)

get_job_result_url(*job_id*)

get_log(*job_id*)

get_tasks(*job_id*, *group_id*, *page=1*, *per_page=10*)

get_tasks_list(*group_id*, *per_page=30*)

job_create(*job_type*, *oss_path*, *input_data*, *program_id=None*, *group_id=None*)

post(*url*, *data=None*, *header=None*, *params=None*, *retry=5*)

refresh_token()

upload(*oss_task_zip*, *zip_task_file*, *endpoint*, *bucket_name*)

exception dpdispatcher.dpcloudserver.client.**RequestInfoException**

Bases: Exception

dpdispatcher.dpcloudserver.config module

dpdispatcher.dpcloudserver.retcode module

class dpdispatcher.dpcloudserver.retcode.**RETCODE**

Bases: object

DATAERR = '2002'

DBERR = '2000'

IOERR = '2003'

NODATA = '2300'

OK = '0000'

PARAMERR = '2101'

PWDERR = '2104'

REQERR = '2200'

ROLEERR = '2103'

THIRDERR = '2001'

TOKENINVALID = '2100'

UNDERDEBUG = '2301'

UNKOWNERR = '2400'

USERERR = '2102'

VERIFYERR = '2105'

dpdispatcher.dpcloudserver.temp_test module

dpdispatcher.dpcloudserver.zip_file module

dpdispatcher.dpcloudserver.zip_file.**unzip_file**(*zip_file*, *out_dir='./'*)

dpdispatcher.dpcloudserver.zip_file.**zip_file_list**(*root_path*, *zip_filename*, *file_list=[]*)

8.1.2 Submodules

8.1.3 dpdispatcher.JobStatus module

class dpdispatcher.JobStatus.**JobStatus**(*value*)

Bases: IntEnum

An enumeration.

completing = 6

finished = 5

running = 3

terminated = 4

unknown = 100

unsubmitted = 1

waiting = 2

8.1.4 dpdispatcher.arginfo module

8.1.5 dpdispatcher.base_context module

class dpdispatcher.base_context.**BaseContext**(**args*, ***kwargs*)

Bases: object

Methods

machine_arginfo()	Generate the machine arginfo.
machine_subfields()	Generate the machine subfields.

bind_submission	
check_finish	
clean	
download	
kill	
load_from_dict	
read_file	
upload	
write_file	

alias: Tuple[str, ...] = ()

bind_submission(*submission*)

check_finish(*proc*)

abstract clean()

abstract download(*submission*, *check_exists=False*, *mark_failure=True*, *back_error=False*)

kill(*proc*)

classmethod load_from_dict(*context_dict*)

classmethod machine_arginfo() → Argument

Generate the machine arginfo.

Returns

Argument
machine arginfo

classmethod machine_subfields() → List[Argument]

Generate the machine subfields.

Returns

list[Argument]
machine subfields

options = {'BohriumContext', 'HDFSContext', 'LazyLocalContext', 'LocalContext', 'SSHContext'}

abstract read_file(*fname*)

subclasses_dict = {'Bohrium': <class 'dpdispatcher.dp_cloud_server_context.BohriumContext'>, 'BohriumContext': <class 'dpdispatcher.dp_cloud_server_context.BohriumContext'>, 'DpCloudServer': <class 'dpdispatcher.dp_cloud_server_context.BohriumContext'>, 'DpCloudServerContext': <class 'dpdispatcher.dp_cloud_server_context.BohriumContext'>, 'HDFS': <class 'dpdispatcher.hdfs_context.HDFSContext'>, 'HDFSContext': <class 'dpdispatcher.hdfs_context.HDFSContext'>, 'LazyLocal': <class 'dpdispatcher.lazy_local_context.LazyLocalContext'>, 'LazyLocalContext': <class 'dpdispatcher.lazy_local_context.LazyLocalContext'>, 'Lebesgue': <class 'dpdispatcher.dp_cloud_server_context.BohriumContext'>, 'LebesgueContext': <class 'dpdispatcher.dp_cloud_server_context.BohriumContext'>, 'Local': <class 'dpdispatcher.local_context.LocalContext'>, 'LocalContext': <class 'dpdispatcher.local_context.LocalContext'>, 'SSH': <class 'dpdispatcher.ssh_context.SSHContext'>, 'SSHContext': <class 'dpdispatcher.ssh_context.SSHContext'>, 'bohrium': <class 'dpdispatcher.dp_cloud_server_context.BohriumContext'>, 'bohriumcontext': <class 'dpdispatcher.dp_cloud_server_context.BohriumContext'>, 'dpcloudserver': <class 'dpdispatcher.dp_cloud_server_context.BohriumContext'>, 'dpcloudservercontext': <class 'dpdispatcher.dp_cloud_server_context.BohriumContext'>, 'hdfs': <class 'dpdispatcher.hdfs_context.HDFSContext'>, 'hdfscontext': <class 'dpdispatcher.hdfs_context.HDFSContext'>, 'lazylocal': <class 'dpdispatcher.lazy_local_context.LazyLocalContext'>, 'lazylocalcontext': <class 'dpdispatcher.lazy_local_context.LazyLocalContext'>, 'lebesgue': <class 'dpdispatcher.dp_cloud_server_context.BohriumContext'>, 'lebesguecontext': <class 'dpdispatcher.dp_cloud_server_context.BohriumContext'>, 'local': <class 'dpdispatcher.local_context.LocalContext'>, 'localcontext': <class 'dpdispatcher.local_context.LocalContext'>, 'ssh': <class 'dpdispatcher.ssh_context.SSHContext'>, 'sshcontext': <class 'dpdispatcher.ssh_context.SSHContext'>}

abstract upload(*submission*)

abstract write_file(*fname*, *write_str*)

8.1.6 dpdispatcher.distributed_shell module

class dpdispatcher.distributed_shell.**DistributedShell**(**args*, ***kwargs*)

Bases: *Machine*

Methods

do_submit(job)	submit th job to yarn using distributed shell
resources_arginfo()	Generate the resources arginfo.
resources_subfields()	Generate the resources subfields.

arginfo	
bind_context	
check_finish_tag	
check_if_recover	
check_status	
default_resources	
deserialize	
gen_command_env_cuda_devices	
gen_script	
gen_script_command	
gen_script_custom_flags_lines	
gen_script_end	
gen_script_env	
gen_script_header	
gen_script_wait	
load_from_dict	
load_from_json	
serialize	
sub_script_cmd	
sub_script_head	

check_finish_tag(*job*)

check_status(*job*)

do_submit(*job*)

submit th job to yarn using distributed shell

Parameters

job
[Job class instance] job to be submitted

Returns

job_id: string
submit process id

gen_script_end(*job*)

gen_script_env(*job*)

gen_script_header(*job*)

8.1.7 dpdispatcher.dp_cloud_server module

class dpdispatcher.dp_cloud_server.**Bohrium**(**args*, ***kwargs*)

Bases: *Machine*

Methods

do_submit(job)	submit a single job, assuming that no job is running there.
resources_arginfo()	Generate the resources arginfo.
resources_subfields()	Generate the resources subfields.

arginfo	
bind_context	
check_finish_tag	
check_if_recover	
check_status	
default_resources	
deserialize	
gen_command_env_cuda_devices	
gen_local_script	
gen_script	
gen_script_command	
gen_script_custom_flags_lines	
gen_script_end	
gen_script_env	
gen_script_header	
gen_script_wait	
load_from_dict	
load_from_json	
map_dp_job_state	
serialize	
sub_script_cmd	
sub_script_head	

alias: Tuple[str, ...] = ('Lebesgue', 'DpCloudServer')

check_finish_tag(*job*)

check_if_recover(*submission*)

check_status(*job*)

do_submit(*job*)

submit a single job, assuming that no job is running there.

gen_local_script(*job*)

gen_script(*job*)

gen_script_header(*job*)

static map_dp_job_state(*status*)

dpdispatcher.dp_cloud_server.**DpCloudServer**

alias of *Bohrium*

dpdispatcher.dp_cloud_server.**Lebesgue**

alias of *Bohrium*

8.1.8 dpdispatcher.dp_cloud_server_context module

class dpdispatcher.dp_cloud_server_context.**BohriumContext**(**args*, ***kwargs*)

Bases: *BaseContext*

Methods

machine_arginfo()	Generate the machine arginfo.
machine_subfields()	Generate the machine subfields.

bind_submission
check_file_exists
check_finish
check_home_file_exits
clean
download
kill
load_from_dict
read_file
read_home_file
upload
upload_job
write_file
write_home_file
write_local_file

alias: Tuple[str, ...] = ('DpCloudServerContext', 'LebesgueContext')

bind_submission(*submission*)

check_file_exists(*fname*)

check_home_file_exits(*fname*)

clean()

download(*submission*)

kill(*cmd_pipes*)

classmethod **load_from_dict**(*context_dict*)

classmethod **machine_subfields**() → List[Argument]

Generate the machine subfields.

Returns

list[Argument]
machine subfields

read_file(*fname*)

read_home_file(*fname*)

upload(*submission*)

upload_job(*job*, *common_files=None*)

write_file(*fname*, *write_str*)

write_home_file(*fname*, *write_str*)

write_local_file(*fname*, *write_str*)

dpdispatcher.dp_cloud_server_context.**DpCloudServerContext**
alias of *BohriumContext*

dpdispatcher.dp_cloud_server_context.**LebesgueContext**
alias of *BohriumContext*

8.1.9 dpdispatcher.dpdisp module

dpdispatcher.dpdisp.**main**()

8.1.10 dpdispatcher.hdfs_cli module

class dpdispatcher.hdfs_cli.**HDFS**
Bases: object

Fundamental class for HDFS basic manipulation

Methods

copy_from_local(local_path, to_uri)	Returns: True on success Raises: on unexpected error
exists(uri)	Check existence of hdfs uri Returns: True on exists Raises: RuntimeError
mkdir(uri)	Make new hdfs directory Returns: True on success Raises: RuntimeError
remove(uri)	Check existence of hdfs uri Returns: True on exists Raises: RuntimeError

copy_to_local	
move	
read_hdfs_file	

static copy_from_local(*local_path*, *to_uri*)
Returns: True on success Raises: on unexpected error

static copy_to_local(*from_uri*, *local_path*)

static exists(*uri*)
Check existence of hdfs uri Returns: True on exists Raises: RuntimeError

static mkdir(*uri*)
Make new hdfs directory Returns: True on success Raises: RuntimeError

static move(*from_uri*, *to_uri*)

static read_hdfs_file(*uri*)

static remove(*uri*)

Check existence of hdfs uri Returns: True on exists Raises: RuntimeError

8.1.11 dpdispatcher.hdfs_context module

class dpdispatcher.hdfs_context.**HDFSContext**(**args*, ***kwargs*)

Bases: *BaseContext*

Methods

check_file_exists(fname)	check whether the given file exists, often used in checking whether the belonging job has finished
download(submission[, check_exists, ...])	download backward files from HDFS root dir
machine_arginfo()	Generate the machine arginfo.
machine_subfields()	Generate the machine subfields.
upload(submission[, dereference])	upload forward files and forward command files to HDFS root dir

bind_submission	
check_finish	
clean	
get_job_root	
kill	
load_from_dict	
read_file	
write_file	

bind_submission(*submission*)

check_file_exists(*fname*)

check whether the given file exists, often used in checking whether the belonging job has finished

Parameters

fname

[string] file name to be checked

Returns

status: boolean

clean()

download(*submission*, *check_exists=False*, *mark_failure=True*, *back_error=False*)

download backward files from HDFS root dir

Parameters

submission
[Submission class instance] represents a collection of tasks, such as backward file names

Returns

none

`get_job_root`()

`kill`(*job_id*)

`classmethod load_from_dict`(*context_dict*)

`read_file`(*fname*)

`upload`(*submission*, *dereference=True*)
upload forward files and forward command files to HDFS root dir

Parameters

submission
[Submission class instance] represents a collection of tasks, such as forward file names

Returns

none

`write_file`(*fname*, *write_str*)

8.1.12 dpdispatcher.lazy_local_context module

`class` dpdispatcher.lazy_local_context.`LazyLocalContext`(**args*, ***kwargs*)
Bases: *BaseContext*

Methods

machine_arginfo()	Generate the machine arginfo.
machine_subfields()	Generate the machine subfields.

bind_submission
block_call
block_checkcall
call
check_file_exists
check_finish
clean
download
get_job_root
get_return
kill
load_from_dict
read_file
upload
write_file

bind_submission(*submission*)

block_call(*cmd*)

block_checkcall(*cmd*)

call(*cmd*)

check_file_exists(*fname*)

check_finish(*proc*)

clean()

download(*jobs*, *check_exists=False*, *mark_failure=True*, *back_error=False*)

get_job_root()

get_return(*proc*)

kill(*job_id*)

classmethod load_from_dict(*context_dict*)

read_file(*fname*)

upload(*jobs*, *dereference=True*)

write_file(*fname*, *write_str*)

class dpdispatcher.lazy_local_context.**SPRetObj**(*ret*)

Bases: object

Methods

read	
readlines	

read()

readlines()

8.1.13 dpdispatcher.local_context module

class dpdispatcher.local_context.**LocalContext**(**args*, ***kwargs*)

Bases: *BaseContext*

Methods

machine_arginfo()	Generate the machine arginfo.
machine_subfields()	Generate the machine subfields.

bind_submission
block_call
block_checkcall
call
check_file_exists
check_finish
clean
download
download_
get_job_root
get_return
kill
load_from_dict
read_file
upload
upload_
write_file

bind_submission(*submission*)

block_call(*cmd*)

block_checkcall(*cmd*)

call(*cmd*)

check_file_exists(*fname*)

check_finish(*proc*)

clean()

download(*submission*, *check_exists=False*, *mark_failure=True*, *back_error=False*)

download_(*job_dirs*, *remote_down_files*, *check_exists=False*, *mark_failure=True*, *back_error=False*)

get_job_root()

get_return(*proc*)

kill(*job_id*)

classmethod load_from_dict(*context_dict*)

read_file(*fname*)

upload(*submission*)

upload_(*job_dirs*, *local_up_files*, *dereference=True*)

write_file(*fname*, *write_str*)

class dpdispatcher.local_context.**SPRetObj**(*ret*)

Bases: object

Methods

read	
readlines	

read()

readlines()

8.1.14 dpdispatcher.lsf module

class dpdispatcher.lsf.**LSF**(**args*, ***kwargs*)

Bases: *Machine*

LSF batch

Methods

default_resources(resources)	
resources_arginfo()	Generate the resources arginfo.
resources_subfields()	Generate the resources subfields.

arginfo	
bind_context	
check_finish_tag	
check_if_recover	
check_status	
deserialize	
do_submit	
gen_command_env_cuda_devices	
gen_script	
gen_script_command	
gen_script_custom_flags_lines	
gen_script_end	
gen_script_env	
gen_script_header	
gen_script_wait	
load_from_dict	
load_from_json	
serialize	
sub_script_cmd	
sub_script_head	

check_finish_tag(*job*)

check_status(***kwargs*)

default_resources(*resources*)

do_submit(***kwargs*)

submit a single job, assuming that no job is running there.

gen_script(*job*)

gen_script_header(*job*)

classmethod resources_subfields() → List[Argument]

Generate the resources subfields.

Returns

list[Argument]
resources subfields

sub_script_cmd(*res*)

sub_script_head(*res*)

8.1.15 dpdispatcher.machine module

class dpdispatcher.machine.**Machine**(**args*, ***kwargs*)

Bases: object

A machine is used to handle the connection with remote machines.

Parameters

context
[SubClass derived from BaseContext] The context is used to mainatin the connection with remote machine.

Methods

do_submit(job)	submit a single job, assuming that no job is running there.
resources_arginfo()	Generate the resources arginfo.
resources_subfields()	Generate the resources subfields.

arginfo	
bind_context	
check_finish_tag	
check_if_recover	
check_status	
default_resources	
deserialize	
gen_command_env_cuda_devices	
gen_script	
gen_script_command	
gen_script_custom_flags_lines	
gen_script_end	
gen_script_env	
gen_script_header	
gen_script_wait	
load_from_dict	
load_from_json	
serialize	
sub_script_cmd	
sub_script_head	

alias: Tuple[str, ...] = ()

classmethod arginfo()

bind_context(*context*)

abstract check_finish_tag(***kwargs*)

check_if_recover(*submission*)

abstract check_status(*job*)

default_resources(*res*)

classmethod deserialize(*machine_dict*)

abstract do_submit(*job*)

submit a single job, assuming that no job is running there.

gen_command_env_cuda_devices(*resources*)

gen_script(*job*)

gen_script_command(*job*)

gen_script_custom_flags_lines(*job*)

gen_script_end(*job*)

gen_script_env(*job*)

abstract gen_script_header(*job*)

gen_script_wait(*resources*)

classmethod load_from_dict(*machine_dict*)

classmethod load_from_json(*json_path*)

options = {'Bohrium', 'DistributedShell', 'LSF', 'PBS', 'Shell', 'Slurm', 'SlurmJobArray', 'Torque'}

classmethod resources_arginfo() → Argument

Generate the resources arginfo.

Returns

Argument
resources arginfo

classmethod resources_subfields() → List[Argument]

Generate the resources subfields.

Returns

list[Argument]
resources subfields

serialize(*if_empty_remote_profile=False*)

sub_script_cmd(*res*)

sub_script_head(*res*)

subclasses_dict = {'Bohrium': <class 'dpdispatcher.dp_cloud_server.Bohrium'>, 'DistributedShell': <class 'dpdispatcher.distributed_shell.DistributedShell'>, 'DpCloudServer': <class 'dpdispatcher.dp_cloud_server.Bohrium'>, 'LSF': <class 'dpdispatcher.lsf.LSF'>, 'Lebesgue': <class 'dpdispatcher.dp_cloud_server.Bohrium'>, 'PBS': <class 'dpdispatcher.pbs.PBS'>, 'Shell': <class 'dpdispatcher.shell.Shell'>, 'Slurm': <class 'dpdispatcher.slurm.Slurm'>, 'SlurmJobArray': <class 'dpdispatcher.slurm.SlurmJobArray'>, 'Torque': <class 'dpdispatcher.pbs.Torque'>, 'bohrium': <class 'dpdispatcher.dp_cloud_server.Bohrium'>, 'distributedshell': <class 'dpdispatcher.distributed_shell.DistributedShell'>, 'dpcloudserver': <class 'dpdispatcher.dp_cloud_server.Bohrium'>, 'lebesgue': <class 'dpdispatcher.dp_cloud_server.Bohrium'>, 'lsf': <class 'dpdispatcher.lsf.LSF'>, 'pbs': <class 'dpdispatcher.pbs.PBS'>, 'shell': <class 'dpdispatcher.shell.Shell'>, 'slurm': <class 'dpdispatcher.slurm.Slurm'>, 'slurmjobarray': <class 'dpdispatcher.slurm.SlurmJobArray'>, 'torque': <class 'dpdispatcher.pbs.Torque'>}

8.1.16 dpdispatcher.pbs module

class dpdispatcher.pbs.**PBS**(**args*, ***kwargs*)

Bases: *Machine*

Methods

do_submit(job)	submit a single job, assuming that no job is running there.
resources_arginfo()	Generate the resources arginfo.
resources_subfields()	Generate the resources subfields.

arginfo
bind_context
check_finish_tag
check_if_recover
check_status
default_resources
deserialize
gen_command_env_cuda_devices
gen_script
gen_script_command
gen_script_custom_flags_lines
gen_script_end
gen_script_env
gen_script_header
gen_script_wait
load_from_dict
load_from_json
serialize
sub_script_cmd
sub_script_head

check_finish_tag(*job*)

check_status(*job*)

default_resources(*resources*)

do_submit(*job*)

submit a single job, assuming that no job is running there.

gen_script(*job*)

gen_script_header(*job*)

class dpdispatcher.pbs.**Torque**(**args*, ***kwargs*)

Bases: *PBS*

Methods

do_submit(job)	submit a single job, assuming that no job is running there.
resources_arginfo()	Generate the resources arginfo.
resources_subfields()	Generate the resources subfields.

arginfo
bind_context
check_finish_tag
check_if_recover
check_status
default_resources
deserialize
gen_command_env_cuda_devices
gen_script
gen_script_command
gen_script_custom_flags_lines
gen_script_end
gen_script_env
gen_script_header
gen_script_wait
load_from_dict
load_from_json
serialize
sub_script_cmd
sub_script_head

check_status(*job*)

gen_script_header(*job*)

8.1.17 dpdispatcher.shell module

class dpdispatcher.shell.**Shell**(**args*, ***kwargs*)

Bases: *Machine*

Methods

do_submit(job)	submit a single job, assuming that no job is running there.
resources_arginfo()	Generate the resources arginfo.
resources_subfields()	Generate the resources subfields.

arginfo	
bind_context	
check_finish_tag	
check_if_recover	
check_status	
default_resources	
deserialize	
gen_command_env_cuda_devices	
gen_script	
gen_script_command	
gen_script_custom_flags_lines	
gen_script_end	
gen_script_env	
gen_script_header	
gen_script_wait	
load_from_dict	
load_from_json	
serialize	
sub_script_cmd	
sub_script_head	

check_finish_tag(*job*)

check_status(*job*)

default_resources(*resources*)

do_submit(*job*)

submit a single job, assuming that no job is running there.

gen_script(*job*)

gen_script_header(*job*)

8.1.18 dpdispatcher.slurm module

class dpdispatcher.slurm.**Slurm**(**args*, ***kwargs*)

Bases: *Machine*

Methods

resources_arginfo()	Generate the resources arginfo.
resources_subfields()	Generate the resources subfields.

arginfo	
bind_context	
check_finish_tag	
check_if_recover	
check_status	
default_resources	
deserialize	
do_submit	
gen_command_env_cuda_devices	
gen_script	
gen_script_command	
gen_script_custom_flags_lines	
gen_script_end	
gen_script_env	
gen_script_header	
gen_script_wait	
load_from_dict	
load_from_json	
serialize	
sub_script_cmd	
sub_script_head	

check_finish_tag(*job*)

check_status(***kwargs*)

default_resources(*resources*)

do_submit(***kwargs*)

submit a single job, assuming that no job is running there.

gen_script(*job*)

gen_script_header(*job*)

classmethod resources_subfields() → List[Argument]

Generate the resources subfields.

Returns

list[Argument]
resources subfields

class dpdispatcher.slurm.**SlurmJobArray**(**args*, ***kwargs*)

Bases: *Slurm*

Slurm with job array enabled for multiple tasks in a job

Methods

resources_arginfo()	Generate the resources arginfo.
resources_subfields()	Generate the resources subfields.

arginfo
bind_context
check_finish_tag
check_if_recover
check_status
default_resources
deserialize
do_submit
gen_command_env_cuda_devices
gen_script
gen_script_command
gen_script_custom_flags_lines
gen_script_end
gen_script_env
gen_script_header
gen_script_wait
load_from_dict
load_from_json
serialize
sub_script_cmd
sub_script_head

check_finish_tag(*job*)

check_status(***kwargs*)

gen_script_command(*job*)

gen_script_end(*job*)

gen_script_header(*job*)

8.1.19 dpdispatcher.ssh_context module

class dpdispatcher.ssh_context.**SSHContext**(**args*, ***kwargs*)

Bases: *BaseContext*

Attributes

sftp
ssh

Methods

block_checkcall(cmd[, asynchronously, ...])	Run command with arguments.
machine_arginfo()	Generate the machine arginfo.
machine_subfields()	Generate the machine subfields.

bind_submission
block_call
call
check_file_exists
check_finish
clean
close
download
get_job_root
get_return
kill
load_from_dict
read_file
upload
write_file

bind_submission(*submission*)

block_call(*cmd*)

block_checkcall(*cmd*, *asynchronously=False*, *stderr_whitelist=None*)

Run command with arguments. Wait for command to complete. If the return code was zero then return, otherwise raise RuntimeError.

Parameters

cmd: str
The command to run.

asynchronously: bool, optional, default=False
Run command asynchronously. If True, *nohup* will be used to run the command.

call(*cmd*)

check_file_exists(*fname*)

check_finish(*cmd_pipes*)

clean()

close()

download(*submission*, *check_exists=False*, *mark_failure=True*, *back_error=False*)

get_job_root()

get_return(*cmd_pipes*)

kill(*cmd_pipes*)

classmethod load_from_dict(*context_dict*)

classmethod machine_subfields() → List[Argument]

Generate the machine subfields.

Returns

list[Argument]
machine subfields

read_file(*fname*)

property sftp

property ssh

upload(*submission*, *dereference=True*)

write_file(*fname*, *write_str*)

class dpdispatcher.ssh_context.**SSHSession**(*hostname*, *username*, *password=None*, *port=22*, *key_filename=None*, *passphrase=None*, *timeout=10*, *totp_secret=None*, *tar_compress=True*, *look_for_keys=True*)

Bases: object

Attributes

remote
rsync_available
sftp
Returns sftp.

Methods

inter_handler(title, instructions, prompt_list)	inter_handler: the callback for paramiko.transport.auth_interactive

arginfo
close
ensure_alive
exec_command
get
get_ssh_client
put

static arginfo()

close()

ensure_alive(*max_check=10*, *sleep_time=10*)

exec_command(***kwargs*)

get(*from_f*, *to_f*)

get_ssh_client()

inter_handler(*title*, *instructions*, *prompt_list*)

inter_handler: the callback for paramiko.transport.auth_interactive

The prototype for this function is defined by Paramiko, so all of the arguments need to be there, even though we don't use 'title' or 'instructions'.

The function is expected to return a tuple of data containing the responses to the provided prompts. Experimental results suggests that there will be one call of this function per prompt, but the mechanism allows for multiple prompts to be sent at once, so it's best to assume that that can happen.

Since tuples can't really be built on the fly, the responses are collected in a list which is then converted to a tuple when it's time to return a value.

Experiments suggest that the username prompt never happens. This makes sense, but the Username prompt is included here just in case.

put(*from_f*, *to_f*)

property remote: str

property rsync_available: bool

property sftp

Returns sftp. Open a new one if not existing.

8.1.20 dpdispatcher.submission module

class dpdispatcher.submission.**Job**(*job_task_list*, *, *resources*, *machine=None*)

Bases: object

Job is generated by Submission automatically. A job ususally has many tasks and it may request computing resources from job scheduler systems. Each Job can generate a script file to be submitted to the job scheduler system or executed locally.

Parameters

job_task_list
[list of Task] the tasks belonging to the job

resources
[Resources] the machine resources. Passed from Submission when it constructs jobs.

machine
[machine] machine object to execute the job. Passed from Submission when it constructs jobs.

Methods

deserialize(job_dict[, machine])	convert the job_dict to a Submission class object
get_job_state()	get the jobs.
serialize([if_static])	convert the Task class instance to a dictionary.

get_hash	
handle_unexpected_job_state	
job_to_json	
register_job_id	
submit_job	

classmethod deserialize(*job_dict*, *machine=None*)

convert the job_dict to a Submission class object

Parameters

submission_dict
[dict] path-like, the base directory of the local tasks

Returns

submission
[Job] the Job class instance converted from the job_dict

get_hash()

get_job_state()

get the jobs. Usually, this method will query the database of slurm or pbs job scheduler system and get the results.

Notes

this method will not submit or resubmit the jobs if the job is unsubmitted.

handle_unexpected_job_state()

job_to_json()

register_job_id(*job_id*)

serialize(*if_static=False*)

convert the Task class instance to a dictionary.

Parameters

if_static
[bool] whether dump the job runtime infomation (job_id, job_state, fail_count, job_uuid etc.) to the dictionary.

Returns

task_dict
[dict] the dictionary converted from the Task class instance

submit_job()

class dpdispatcher.submission.**Resources**(*number_node*, *cpu_per_node*, *gpu_per_node*, *queue_name*, *group_size*, ***, *custom_flags=[]*, *strategy={'if_cuda_multi_devices': False, 'ratio_unfinished': 0.0}*, *para_deg=1*, *module_unload_list=[]*, *module_purge=False*, *module_list=[]*, *source_list=[]*, *envs={}*, *prepend_script=[]*, *append_script=[]*, *wait_time=0*, ***kwargs*)

Bases: `object`

Resources is used to describe the machine resources we need to do calculations.

Parameters

number_node
[int] The number of node need for each *job*.

cpu_per_node
[int] cpu numbers of each node.

gpu_per_node
[int] gpu numbers of each node.

queue_name
[str] The queue name of batch job scheduler system.

group_size
[int] The number of *tasks* in a *job*.

custom_flags
[list of Str] The extra lines pass to job submitting script header

strategy
[dict] strategies we use to generation job submitting scripts. if_cuda_multi_devices : bool

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
[float] The ratio of *jobs* that can be unfinished.

para_deg
[int] Decide how many tasks will be run in parallel. Usually run with *strategy['if_cuda_multi_devices']*

source_list
[list of Path] The env file to be sourced before the command execution.

wait_time
[int] The waitting time in second after a single task submitted. Default: 0.

Methods

arginfo	
deserialize	
load_from_dict	
load_from_json	
serialize	

`static arginfo`(*detail_kwargs=True*)

`classmethod deserialize`(*resources_dict*)

classmethod load_from_dict(*resources_dict*)

classmethod load_from_json(*json_file*)

serialize()

class dpdispatcher.submission.**Submission**(*work_base*, *machine=None*, *resources=None*, *forward_common_files=[]*, *backward_common_files=[]*, ***, *task_list=[]*)

Bases: object

A submission represents a collection of tasks. These tasks usually locate at a common directory. And these Tasks may share common files to be uploaded and downloaded.

Parameters

work_base
[Path] the base directory of the local tasks. It is usually the dir name of project .

machine
[Machine] machine class object (for example, PBS, Slurm, Shell) to execute the jobs. The machine can still be bound after the instantiation with the bind_submission method.

resources
[Resources] the machine resources (cpu or gpu) used to generate the slurm/pbs script

forward_common_files
[list] the common files to be uploaded to other computers before the jobs begin

backward_common_files
[list] the common files to be downloaded from other computers after the jobs finish

task_list
[list of Task] a list of tasks to be run.

Methods

bind_machine(machine)	bind this submission to a machine.
check_all_finished()	check whether all the jobs in the submission.
deserialize(submission_dict[, machine])	convert the submission_dict to a Submission class object
generate_jobs()	After tasks register to the self.belonging_tasks, This method generate the jobs and add these jobs to self.belonging_jobs.
handle_unexpected_submission_state()	handle unexpected job state of the submission.
run_submission(*[, exit_on_submit, clean])	main method to execute the submission.
serialize([if_static])	convert the Submission class instance to a dictionary.
update_submission_state()	check whether all the jobs in the submission.

check_ratio_unfinished	
clean_jobs	
download_jobs	
get_hash	
register_task	
register_task_list	
remove_unfinished_jobs	
submission_from_json	
submission_to_json	
try_recover_from_json	
upload_jobs	

`bind_machine`(*machine*)

bind this submission to a machine. update the machine's context remote_root and local_root.

Parameters

machine
[Machine] the machine to bind with

`check_all_finished`()

check whether all the jobs in the submission.

Notes

This method will not handle unexpected job state in the submission.

`check_ratio_unfinished`(*ratio_unfinished*)

`clean_jobs`()

`classmethod deserialize`(*submission_dict*, *machine=None*)

convert the submission_dict to a Submission class object

Parameters

submission_dict
[dict] path-like, the base directory of the local tasks

Returns

submission
[Submission] the Submission class instance converted from the submission_dict

`download_jobs`()

`generate_jobs`()

After tasks register to the self.belonging_tasks, This method generate the jobs and add these jobs to self.belonging_jobs. The jobs are generated by the tasks randomly, and there are self.resources.group_size tasks in a task. Why we randomly shuffle the tasks is under the consideration of load balance. The random seed is a constant (to be concrete, 42). And this insures that the jobs are equal when we re-run the program.

`get_hash`()

`handle_unexpected_submission_state`()

handle unexpected job state of the submission. If the job state is unsubmitted, submit the job. If the job state is terminated (killed unexpectly), resubmit the job. If the job state is unknown, raise an error.

register_task(*task*)

register_task_list(*task_list*)

remove_unfinished_jobs()

run_submission(*, *exit_on_submit=False*, *clean=True*)

main method to execute the submission. First, check whether old Submission exists on the remote machine, and try to recover from it. Second, upload the local files to the remote machine where the tasks to be executed. Third, run the submission defined previously. Forth, wait until the tasks in the submission finished and download the result file to local directory. if exit_on_submit is True, submission will exit.

serialize(*if_static=False*)

convert the Submission class instance to a dictionary.

Parameters

if_static
[bool] whether dump the job runtime infomation (like job_id, job_state, fail_count) to the dictionary.

Returns

submission_dict
[dict] the dictionary converted from the Submission class instance

classmethod submission_from_json(*json_file_name='submission.json'*)

submission_to_json()

try_recover_from_json()

update_submission_state()

check whether all the jobs in the submission.

Notes

this method will not handle unexpected (like resubmit terminated) job state in the submission.

upload_jobs()

class dpdispatcher.submission.**Task**(*command*, *task_work_path*, *forward_files=[]*, *backward_files=[]*, *outlog='log'*, *errlog='err'*)

Bases: `object`

A task is a sequential command to be executed, as well as the files it depends on to transmit forward and backward.

Parameters

command
[Str] the command to be executed.

task_work_path
[Path] the directory of each file where the files are dependent on.

forward_files
[list of Path] the files to be transmitted to remote machine before the command execute.

backward_files
[list of Path] the files to be transmitted from remote machine after the comand finished.

outlog
[Str] the filename to which command redirect stdout

errlog
[Str] the filename to which command redirect stderr

Methods

deserialize(task_dict)	convert the task_dict to a Task class object

arginfo	
get_hash	
load_from_dict	
load_from_json	
serialize	

static arginfo()

classmethod deserialize(*task_dict*)
convert the task_dict to a Task class object

Parameters

task_dict
[dict] the dictionary which contains the task information

Returns

task
[Task] the Task class instance converted from the task_dict

get_hash()

classmethod load_from_dict(*task_dict: dict*) → *Task*

classmethod load_from_json(*json_file*)

serialize()

8.1.21 dpdispatcher.utils module

exception dpdispatcher.utils.**RetrySignal**
Bases: Exception

Exception to give a signal to retry the function.

dpdispatcher.utils.**generate_totp**(*secret: str*, *period: int = 30*, *token_length: int = 6*) → str
Generate time-based one time password (TOTP) from the secret.

Some HPCs use TOTP for two-factor authentication for safety.

Parameters

secret: str
The encoded secret provided by the HPC. It's usually extracted from a 2D code and base32 encoded.

period: int, default=30
Time period where the code is valid in seconds.

token_length: int, default=6
The token length.

Returns

token: str
The generated token.

References

https://github.com/lepture/otpauth/blob/49914d83d36dbcd33c9e26f65002b21ce09a6303/otpauth.py#L143-L160

dpdispatcher.utils.**get_sha256**(*filename*)

Get sha256 of a file.

Parameters

filename: str
The filename.

Returns

sha256: str
The sha256.

dpdispatcher.utils.**hotp**(*key: str*, *period: int*, *token_length: int = 6*, *digest='sha1'*)

dpdispatcher.utils.**retry**(*max_retry: int = 3*, *sleep: ~typing.Union[int, float] = 60*, *catch_exception: ~typing.Type[BaseException] = <class 'dpdispatcher.utils.RetrySignal'>*) → Callable

Retry the function until it succeeds or fails for certain times.

Parameters

max_retry: int, default=3
The maximum retry times. If None, it will retry forever.

sleep: int or float, default=60
The sleep time in seconds.

catch_exception: Exception, default=Exception
The exception to catch.

Returns

decorator: Callable
The decorator.

Examples

```
>>> @retry(max_retry=3, sleep=60, catch_exception=RetrySignal)
... def func():
...     raise RetrySignal("Failed")
```

dpdispatcher.utils.**rsync**(*from_file: str*, *to_file: str*, *port: int = 22*, *key_filename: Optional[str] = None*, *timeout: Union[int, float] = 10*)

Call rsync to transfer files.

Parameters

from_file: str
SRC

to_file: str
DEST

port
[int, default=22] port for ssh

key_filename
[str, optional] identity file name

timeout
[int, default=10] timeout for ssh

Raises

RuntimeError
when return code is not 0

dpdispatcher.utils.**run_cmd_with_all_output**(*cmd*, *shell=True*)

CHAPTER

NINE

RUNNING THE DEEPMD-KIT ON THE EXPANSE CLUSTER

Expanse is a cluster operated by the San Diego Supercomputer Center. Here we provide an example to run jobs on the expanse.

The machine parameters are provided below. Expanse uses the SLURM workload manager for job scheduling. *remote_root* has been created in advance. It's worth metioned that we do not recommend to use the password, so SSH keys are used instead to improve security.

```
{
  "batch_type": "Slurm",
  "local_root": "./",
  "remote_root": "/expanse/lustre/scratch/njzjz/temp_project/dpgen_workdir",
  "clean_asynchronously": true,
  "context_type": "SSHContext",
  "remote_profile": {
    "hostname": "login.expanse.sdsc.edu",
    "username": "njzjz",
    "port": 22
  }
}
```

Expanse's standard compute nodes are each powered by two 64-core AMD EPYC 7742 processors and contain 256 GB of DDR4 memory. Here, we request one node with 32 cores and 16 GB memory from the `shared` partition. Expanse does not support `--gres=gpu:0` command, so we use *custom_gpu_line* to customize the statement.

```
{
  "number_node": 1,
  "cpu_per_node": 1,
  "gpu_per_node": 0,
  "queue_name": "shared",
  "group_size": 1,
  "custom_flags": [
    "#SBATCH -c 32",
    "#SBATCH --mem=16G",
    "#SBATCH --time=48:00:00",
    "#SBATCH --account=rut149",
    "#SBATCH --requeue"
  ],
  "source_list": [
    "activate /home/njzjz/deepmd-kit"
  ],
  "envs": {
```

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```
    "OMP_NUM_THREADS": 4,
    "TF_INTRA_OP_PARALLELISM_THREADS": 4,
    "TF_INTER_OP_PARALLELISM_THREADS": 8,
    "DP_AUTO_PARALLELIZATION": 1
  },
  "batch_type": "Slurm",
  "kwargs": {
    "custom_gpu_line": "#SBATCH --gpus=0"
  }
}
```

The following task parameter runs a DeePMD-kit task, forwarding an input file and backwarding graph files. Here, the data set will be used among all the tasks, so it is not included in the *forward_files*. Instead, it should be included in the submission's forward_common_files.

```
{
    "command": "dp train input.json && dp freeze && dp compress",
    "task_work_path": "model1/",
    "forward_files": [
      "input.json"
    ],
    "backward_files": [
      "frozen_model.pb",
      "frozen_model_compressed.pb"
    ],
    "outlog": "log",
    "errlog": "err"
}
```

CHAPTER

TEN

RUNNING GAUSSIAN 16 WITH FAILURE ALLOWED

Typically, a task will retry three times if the exit code is not zero. Sometimes, one may allow non-zero code. For example, when running large amounts of Gaussian 16 single-point calculation tasks, some of the Gaussian 16 tasks may throw SCF errors and return a non-zero code. One can append `||:` to the command:

```
{
    "command": "g16 < input > output ||:",
    "task_work_path": "p1/",
    "forward_files": [
      "input"
    ],
    "backward_files": [
      "output"
    ]
}
```

This command ensures the task will always provide zero code.

CHAPTER

ELEVEN

RUNNING MULTIPLE MD TASKS ON A GPU WORKSTATION

In this example, we are going to show how to run multiple MD tasks on a GPU workstation. This workstation does not install any job scheduling packages installed, so we will use `Shell` as *batch_type*.

```
{
  "batch_type": "Shell",
  "local_root": "./",
  "remote_root": "/data2/jinzhe/dpgen_workdir",
  "clean_asynchronously": true,
  "context_type": "SSHContext",
  "remote_profile": {
    "hostname": "mandu.iqb.rutgers.edu",
    "username": "jz748",
    "port": 22
  }
}
```

The workstation has 48 cores of CPUs and 8 RTX3090 cards. Here we hope each card runs 6 tasks at the same time, as each task does not consume too many GPU resources. Thus, *strategy/if_cuda_multi_devices* is set to `true` and *para_deg* is set to 6.

```
{
  "number_node": 1,
  "cpu_per_node": 48,
  "gpu_per_node": 8,
  "queue_name": "shell",
  "group_size": 0,
  "strategy": {
    "if_cuda_multi_devices": true
  },
  "source_list": [
    "activate /home/jz748/deepmd-kit"
  ],
  "envs": {
    "OMP_NUM_THREADS": 1,
    "TF_INTRA_OP_PARALLELISM_THREADS": 1,
    "TF_INTER_OP_PARALLELISM_THREADS": 1
  },
  "para_deg": 6
}
```

Note that *group_size* should be set to `0` (means infinity) to ensure there is only one job and avoid running multiple jobs

at the same time.

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TWELVE

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