
DPDispatcher

Deep Modeling

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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).

INSTALL DPDISPATCHER

DPDispatcher can installed by pip:

```
pip install dpdispatcher
```


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_DEVICES 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*.

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: Lebesgue, LSF, Torque, PBS, SlurmJobArray, DpCloudServer, DistributedShell, Slurm, Shell

local_root:

type: str
argument path: machine/local_root

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

remote_root:

type: 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: LazyLocalContext, LocalContext, LebesgueContext, HDFSContext, DpCloudServerContext, SSHContext

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

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 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 LebesgueContext (or its aliases lebesguecontext, Lebesgue, lebesgue):

remote_profile:

type: dict

argument path: machine[LebesgueContext]/remote_profile

The information used to maintain the connection with remote machine.

email:

type: str

argument path: machine[LebesgueContext]/remote_profile/email

Email

password:

type: str

argument path: machine[LebesgueContext]/remote_profile/password

Password

program_id:

type: int

argument path: machine[LebesgueContext]/remote_profile/program_id

Program ID

input_data:

type: dict
argument path: machine[LebesgueContext]/remote_profile/input_data
Configuration of job

When *context_type* is set to HDFSText (or its aliases hdfstext, HDFS, hdfs):

remote_profile:

type: dict, optional
argument path: machine[HDFSText]/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 DpCloudServerContext (or its aliases dpcloudservercontext, DpCloudServer, dpcloudserver):

remote_profile:

type: dict
argument path: machine[DpCloudServerContext]/remote_profile

The information used to maintain the connection with remote machine.

email:

type: str
argument path: machine[DpCloudServerContext]/remote_profile/email
Email

password:

type: str
argument path: machine[DpCloudServerContext]/remote_profile/password
Password

program_id:

type: int
argument path: machine[DpCloudServerContext]/remote_profile/program_id
Program ID

input_data:

type: dict
argument path: machine[DpCloudServerContext]/remote_profile/input_data
Configuration of job

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.

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
argument path: resources/number_node
The number of node need for each *job*

cpu_per_node:

type: int
argument path: resources/cpu_per_node
cpu numbers of each node assigned to each job.

gpu_per_node:

type: int
argument path: resources/gpu_per_node
gpu numbers of each node assigned to each job.

queue_name:

type: str
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

ratio_unfinished:

type: float, optional, default: 0.0

argument path: resources/strategy/ratio_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

wait_time:

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

The waiting 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: Torque, Shell, DpCloudServer, PBS, Lebesgue, DistributedShell, SlurmJobArray, Slurm, LSF

The batch job system type loaded from machine/*batch_type*.

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 Shell (or its alias `shell`):

kwargs:

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

This field is empty for this batch.

When *batch_type* is set to DpCloudServer (or its alias `dpcloudserver`):

kwargs:

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

This field is empty for this batch.

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 Lebesgue (or its alias `lebesgue`):

kwargs:

type: dict, optional
argument path: `resources[Lebesgue]/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 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 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 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

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 executed.

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

DPDISPATCHER API

6.1 dpdispatcher package

`dpdispatcher.info()`

6.1.1 Subpackages

`dpdispatcher.dpcloudserver` package

Submodules

`dpdispatcher.dpcloudserver.api` module

class `dpdispatcher.dpcloudserver.api.API(email, password)`

Bases: `object`

Methods

check_job_has_uploaded	
download	
download_from_url	
get	
get_job_result_url	
get_jobs	
get_tasks	
get_tasks_list	
job_create	
post	
refresh_token	
upload	

check_job_has_uploaded(*job_id*)

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

download_from_url(*url, save_file*)

```
get(url, params, retry=0)
get_job_result_url(job_id)
get_jobs(page=1, per_page=10)
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, params, retry=0)
refresh_token()
upload(oss_task_zip, zip_task_file, endpoint, bucket_name)
```

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=[])`

6.1.2 Submodules

6.1.3 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

6.1.4 dpdispatcher.base_context module

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

Bases: `object`

Methods

<code>machine_arginfo()</code>	Generate the machine arginfo.
<code>machine_subfields()</code>	Generate the machine subfields.

bind_submission	
check_finish	
clean	
download	
kill	
load_from_dict	
read_file	
upload	
write_file	

```
bind_submission(submission)

check_finish(proc)

clean()

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 = {'DpCloudServerContext', 'HDFSContext', 'LazyLocalContext',
          'LebesgueContext', 'LocalContext', 'SSHContext'}

read_file(fname)

subclasses_dict = {'DpCloudServer': <class
'dpdispatcher.dp_cloud_server_context.DpCloudServerContext'>,
'DpCloudServerContext': <class
'dpdispatcher.dp_cloud_server_context.DpCloudServerContext'>, '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.LebesgueContext'>, 'LebesgueContext': <class
'dpdispatcher.dp_cloud_server_context.LebesgueContext'>, 'Local': <class
'dpdispatcher.local_context.LocalContext'>, 'LocalContext': <class
'dpdispatcher.local_context.LocalContext'>, 'SSH': <class
'dpdispatcher.ssh_context.SSHContext'>, 'SSHContext': <class
'dpdispatcher.ssh_context.SSHContext'>, 'dpcloudserver': <class
'dpdispatcher.dp_cloud_server_context.DpCloudServerContext'>,
'dpcloudservercontext': <class
'dpdispatcher.dp_cloud_server_context.DpCloudServerContext'>, '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.LebesgueContext'>, 'lebesguecontext': <class
'dpdispatcher.dp_cloud_server_context.LebesgueContext'>, 'local': <class
'dpdispatcher.local_context.LocalContext'>, 'localcontext': <class
'dpdispatcher.local_context.LocalContext'>, 'ssh': <class
'dpdispatcher.ssh_context.SSHContext'>, 'sshcontext': <class
'dpdispatcher.ssh_context.SSHContext'>}
```

```
upload(submission)

write_file(fname, write_str)
```

6.1.5 dpdispatcher.distributed_shell module

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

Bases: *Machine*

Methods

<code>do_submit(job)</code>	submit th job to yarn using distributed shell
<code>resources_arginfo()</code>	Generate the resources arginfo.
<code>resources_subfields()</code>	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)
```

6.1.6 dpdispatcher.dp_cloud_server module

```
class dpdispatcher.dp_cloud_server.DpCloudServer(*args, **kwargs)
```

Bases: *Machine*

Methods

<i>do_submit</i> (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	

```
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*)

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

Bases: [DpCloudServer](#)

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	

6.1.7 dpdispatcher.dp_cloud_server_context module

class `dpdispatcher.dp_cloud_server_context.DpCloudServerContext(*args, **kwargs)`

Bases: [`BaseContext`](#)

Methods

<code>machine_arginfo()</code>	Generate the machine arginfo.
<code>machine_subfields()</code>	Generate the machine subfields.

<code>bind_submission</code>	
<code>check_file_exists</code>	
<code>check_finish</code>	
<code>check_home_file_exists</code>	
<code>clean</code>	
<code>download</code>	
<code>kill</code>	
<code>load_from_dict</code>	
<code>read_file</code>	
<code>read_home_file</code>	
<code>upload</code>	
<code>write_file</code>	
<code>write_home_file</code>	
<code>write_local_file</code>	

`bind_submission(submission)`

`check_file_exists(fname)`

`check_home_file_exists(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)`

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

```
write_home_file(fname, write_str)
```

```
write_local_file(fname, write_str)
```

```
class dpdispatcher.dp_cloud_server_context.LebesgueContext(*args, **kwargs)
```

Bases: [*DpCloudServerContext*](#)

Methods

<code>machine_arginfo()</code>	Generate the machine arginfo.
<code>machine_subfields()</code>	Generate the machine subfields.

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

6.1.8 dpdispatcher.dpdisp module

```
dpdispatcher.dpdisp.main()
```

6.1.9 dpdispatcher.hdfs_cli module

```
class dpdispatcher.hdfs_cli.HDFS
```

Bases: [*object*](#)

Fundamental class for HDFS basic manipulation

Methods

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

<code>copy_to_local</code>	
<code>move</code>	
<code>read_hdfs_file</code>	

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

6.1.10 dpdispatcher.hdfs_context module

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

Bases: `BaseContext`

Methods

<code>download(submission[, check_exists, ...])</code>	download backward files from HDFS root dir
<code>machine_arginfo()</code>	Generate the machine arginfo.
<code>machine_subfields()</code>	Generate the machine subfields.
<code>upload(submission[, dereference])</code>	upload forward files and forward command files to HDFS root dir

bind_submission	
check_file_exists	
check_finish	
clean	
get_job_root	
kill	
load_from_dict	
read_file	
write_file	

bind_submission(*submission*)

check_file_exists(*fname*)

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*)

6.1.11 dpdispatcher.lazy_local_context module

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

Bases: `BaseContext`

Methods

<code>machine_arginfo()</code>	Generate the machine arginfo.
<code>machine_subfields()</code>	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()

6.1.12 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()
```

6.1.13 dpdispatcher.lsf module

```
class dpdispatcher.lsf.LSF(*args, **kwargs)
    Bases: Machine
    LSF batch
```


Methods

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

arginfo	
bind_context	
check_finish_tag	
check_if_recover	
check_status	
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*)

classmethod resources_subfields() → [List\[Argument\]](#)

Generate the resources subfields.

Returns

list[Argument]

resources subfields

sub_script_cmd(*res*)

sub_script_head(*res*)

6.1.14 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 maintain the connection with remote machine.

Methods

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

classmethod `arginfo()`

bind_context(*context*)

check_finish_tag(***kwargs*)

check_if_recover(*submission*)

check_status(*job*)

default_resources(*res*)

```

classmethod deserialize(machine_dict)

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)

gen_script_header(job)

gen_script_wait(resources)

classmethod load_from_dict(machine_dict)

classmethod load_from_json(json_path)

options = {'DistributedShell', 'DpCloudServer', 'LSF', 'Lebesgue', '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 = {'DistributedShell': <class
'dpdispatcher.distributed_shell.DistributedShell'>, 'DpCloudServer': <class
'dpdispatcher.dp_cloud_server.DpCloudServer'>, 'LSF': <class
'dpdispatcher.lsf.LSF'>, 'Lebesgue': <class
'dpdispatcher.dp_cloud_server.Lebesgue'>, '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'>,
'distributedshell': <class 'dpdispatcher.distributed_shell.DistributedShell'>,
'dpcloudserver': <class 'dpdispatcher.dp_cloud_server.DpCloudServer'>, 'lebesgue':
<class 'dpdispatcher.dp_cloud_server.Lebesgue'>, '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'>}
```

6.1.15 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 (<i>job</i>)	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*)

6.1.16 dpdispatcher.shell module

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

Bases: *Machine*

Methods

<i>do_submit</i> (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)

6.1.17 dpdispatcher.slurm module

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

Bases: [Machine](#)

Methods

<code>do_submit</code> (job[, retry, max_retry])	submit a single job, assuming that no job is running there.
<code>resources_arginfo</code> ()	Generate the resources arginfo.
<code>resources_subfields</code> ()	Generate the resources subfields.

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

`check_finish_tag`(job)

`check_status`(job, retry=0, max_retry=3)

`default_resources`(resources)

`do_submit`(job, retry=0, max_retry=3)

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

<code>do_submit(job[, retry, max_retry])</code>	submit a single job, assuming that no job is running there.
<code>resources_arginfo()</code>	Generate the resources arginfo.
<code>resources_subfields()</code>	Generate the resources subfields.

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

```
check_finish_tag(job)
```

```
check_status(job, retry=0, max_retry=3)
```

```
gen_script_command(job)
```

```
gen_script_end(job)
```

```
gen_script_header(job)
```


6.1.18 dpdispatcher.ssh_context module

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

Bases: *BaseContext*

Attributes

sftp
ssh

Methods

<i>block_checkcall</i> (cmd[, asynchronously, ...])	Run command with arguments.
<i>machine_arginfo</i> ()	Generate the machine arginfo.
<i>machine_subfields</i> ()	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)

Bases: [object](#)

Attributes

remote
rsync_available
[sftp](#)
Returns sftp.

Methods

exec_command (<i>cmd</i> [, <i>retry</i>])	Calling self.ssh.exec_command but has an exception check.
--	---

arginfo	
close	
ensure_alive	
get	
get_ssh_client	
put	

```

static arginfo()

close()

ensure_alive(max_check=10, sleep_time=10)

exec_command(cmd, retry=0)
    Calling self.ssh.exec_command but has an exception check.

get(from_f, to_f)

get_ssh_client()

put(from_f, to_f)

property remote: str

property rsync_available: bool

property sftp
    Returns sftp. Open a new one if not existing.

```

6.1.19 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

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

<code>get_hash</code>	
<code>handle_unexpected_job_state</code>	
<code>job_to_json</code>	
<code>register_job_id</code>	
<code>submit_job</code>	

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 information (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={},
                                     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 waiting 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

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

outlog

[Str] the filename to which command redirect stdout

errlog

[Str] the filename to which command redirect stderr

Methods

<code>deserialize(task_dict)</code>	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()`

6.1.20 dpdispatcher.utils module

`dpdispatcher.utils.generate_totp(secret: str, period: int = 30, token_length: int = 6) → int`

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: int

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.rsync(from_file: str, to_file: str)`

Call rsync to transfer files.

Parameters

from_file: str
SRC

to_file: str
DEST

Raises

RuntimeError
when return code is not 0

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

RUNNING THE DEEPM-DKIT 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 mentioned that we do not recommend to use the password, so SSH keys are used instead to improve security.

```
1 {
2   "batch_type": "Slurm",
3   "local_root": "./",
4   "remote_root": "/expansE/lustre/scratch/njzjz/temp_project/dpgen_workdir",
5   "clean_asynchronously": true,
6   "context_type": "SSHContext",
7   "remote_profile": {
8     "hostname": "login.expansE.sdsc.edu",
9     "username": "njzjz",
10    "port": 22
11  }
12 }
```

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.

```
1 {
2   "number_node": 1,
3   "cpu_per_node": 1,
4   "gpu_per_node": 0,
5   "queue_name": "shared",
6   "group_size": 1,
7   "custom_flags": [
8     "#SBATCH -c 32",
9     "#SBATCH --mem=16G",
10    "#SBATCH --time=48:00:00",
11    "#SBATCH --account=rut149",
12    "#SBATCH --requeue"
13  ],
14   "source_list": [
15     "activate /home/njzjz/deepmd-kit"
16  ],
17   "envs": {
```

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```
18     "OMP_NUM_THREADS": 4,  
19     "TF_INTRA_OP_PARALLELISM_THREADS": 4,  
20     "TF_INTER_OP_PARALLELISM_THREADS": 8,  
21     "DP_AUTO_PARALLELIZATION": 1  
22 },  
23 "batch_type": "Slurm",  
24 "kwargs": {  
25     "custom_gpu_line": "#SBATCH --gpus=0"  
26 }  
27 }
```

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`.

```
1 {  
2     "command": "dp train input.json && dp freeze && dp compress",  
3     "task_work_path": "model1/",  
4     "forward_files": [  
5         "input.json"  
6     ],  
7     "backward_files": [  
8         "frozen_model.pb",  
9         "frozen_model_compressed.pb"  
10    ],  
11     "outlog": "log",  
12     "errlog": "err"  
13 }
```

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:

```
1 {  
2   "command": "g16 < input > output ||:",  
3   "task_work_path": "p1/",  
4   "forward_files": [  
5     "input"  
6   ],  
7   "backward_files": [  
8     "output"  
9   ]  
10 }
```

This command ensures the task will always provide zero code.

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`.

```
1 {
2   "batch_type": "Shell",
3   "local_root": "./",
4   "remote_root": "/data2/jinzhe/dpgen_workdir",
5   "clean_asynchronously": true,
6   "context_type": "SSHContext",
7   "remote_profile": {
8     "hostname": "mandu.iqb.rutgers.edu",
9     "username": "jz748",
10    "port": 22
11  }
12 }
```

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.

```
1 {
2   "number_node": 1,
3   "cpu_per_node": 48,
4   "gpu_per_node": 8,
5   "queue_name": "shell",
6   "group_size": 0,
7   "strategy": {
8     "if_cuda_multi_devices": true
9   },
10  "source_list": [
11    "activate /home/jz748/deepmd-kit"
12  ],
13  "envs": {
14    "OMP_NUM_THREADS": 1,
15    "TF_INTRA_OP_PARALLELISM_THREADS": 1,
16    "TF_INTER_OP_PARALLELISM_THREADS": 1
17  },
18  "para_deg": 6
19 }
```

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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