
DPDispatcher

Deep Modeling

Sep 09, 2021

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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=reasources,
    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

machine:

type: dict

argument path: machine

batch_type:

type: str

argument path: machine/batch_type

The batch job system type. Option: Slurm, PBS, LSF, Shell, DpCloudServer

context_type:

type: str

argument path: machine/context_type

The connection used to remote machine. Option: LocalContext, LazyLocalContext, SSHContext DpCloud-ServerContext

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.

remote_profile:

type: dict

argument path: machine/remote_profile

The information used to maintain the connection with remote machine. Only needed when context is ssh.

hostname:

type: str

argument path: machine/remote_profile/hostname

hostname or ip of ssh connection.

username:

type: str
argument path: machine/remote_profile/username
username of target linux system

password:

type: str, optional
argument path: machine/remote_profile/password
password of linux system

port:

type: int, optional, default: 22
argument path: machine/remote_profile/port
ssh connection port.

key_filename:

type: str | NoneType, optional, default: None
argument path: machine/remote_profile/key_filename
key filename used by ssh connection. If left None, find key in ~/.ssh or use password for login

passphrase:

type: str | NoneType, optional, default: None
argument path: machine/remote_profile/passphrase
passphrase of key used by ssh connection

timeout:

type: int, optional, default: 10
argument path: machine/remote_profile/timeout
timeout of ssh connection

totp_secret:

type: str | NoneType, optional, default: None
argument path: machine/remote_profile/totp_secret
Time-based one time password secret. It should be a base32-encoded string extracted from the 2D code.

clean_asynchronously:

type: bool, optional, default: False
argument path: machine/clean_asynchronously
Clean the remote directory asynchronously after the job finishes.

RESOURCES PARAMETERS

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*.

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: `True`

argument path: `resources/strategy/if_cuda_multi_devices`

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_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

TASK PARAMETERS

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: str | NoneType

argument path: task/outlog

The out log file name. redirect from stdout

errlog:

type: str | NoneType

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

`dpdispatcher.dpcloudserver.api.download(oss_file, save_file, endpoint, bucket_name)`

`dpdispatcher.dpcloudserver.api.get(url, params)`

`dpdispatcher.dpcloudserver.api.get_jobs(page=1, per_page=10)`

`dpdispatcher.dpcloudserver.api.get_tasks(job_id, page=1, per_page=10)`

`dpdispatcher.dpcloudserver.api.job_create(job_type, oss_path, input_data, program_id=None)`

`dpdispatcher.dpcloudserver.api.login(password, email=None, username=None)`

`dpdispatcher.dpcloudserver.api.post(url, params)`

`dpdispatcher.dpcloudserver.api.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'
    LOGINERR = '2100'
    NODATA = '2300'
    OK = '0000'
    PARAMERR = '2101'
    PWDERR = '2104'
    REQERR = '2200'
    ROLEERR = '2103'
    THIRDERR = '2001'
    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: enum.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

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)
```

```
read_file(fname)
```

```
subclasses_dict = {'DpCloudServer': <class
'dpdispatcher.dp_cloud_server_context.DpCloudServerContext'>,
'DpCloudServerContext': <class
'dpdispatcher.dp_cloud_server_context.DpCloudServerContext'>, 'LazyLocal': <class
'dpdispatcher.lazy_local_context.LazyLocalContext'>, 'LazyLocalContext': <class
'dpdispatcher.lazy_local_context.LazyLocalContext'>, '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'>, 'lazylocal': <class
'dpdispatcher.lazy_local_context.LazyLocalContext'>, 'lazylocalcontext': <class
'dpdispatcher.lazy_local_context.LazyLocalContext'>, '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.dp_cloud_server module

```
class dpdispatcher.dp_cloud_server.DpCloudServer(*args, **kwargs)
    Bases: dpdispatcher.machine.Machine
```

Methods

<i>do_submit</i> (job)	submit a single job, assuming that no job is running there.
------------------------	---

<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>gen_command_env_cuda_devices</code>	
<code>gen_local_script</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>map_dp_job_state</code>	
<code>sub_script_cmd</code>	
<code>sub_script_head</code>	

`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)`

6.1.6 dpdispatcher.dp_cloud_server_context module

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

Bases: `dpdispatcher.base_context.BaseContext`

Methods

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	

bind_submission(*submission*)

check_file_exists(*fname*)

check_home_file_exists(*fname*)

clean()

download(*submission*)

kill(*cmd_pipes*)

classmethod load_from_dict(*context_dict*)

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*)

6.1.7 dpdispatcher.dpdisp module

`dpdispatcher.dpdisp.main()`

6.1.8 dpdispatcher.lazy_local_context module

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

Methods

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(*proc*)

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()

6.1.9 dpdispatcher.local_context module

class `dpdispatcher.local_context.LocalContext`(*args, **kwargs)
 Bases: `dpdispatcher.base_context.BaseContext`

Methods

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(*proc*)

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()

6.1.10 dpdispatcher.lsf module

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

Methods

default_resources(resources)

<i>do_submit</i> (job)	submit a single job, assuming that no job is running there.
------------------------	---

arginfo	
bind_context	
check_finish_tag	
check_if_recover	
check_status	
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	
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*)

sub_script_cmd(*res*)

sub_script_head(*res*)

6.1.11 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>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>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>sub_script_cmd</code>	
<code>sub_script_head</code>	

`static arginfo()`

`bind_context(context)`

`check_finish_tag(**kwargs)`

`check_if_recover(submission)`

`check_status(job)`

`default_resources(res)`

`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)
```

```
sub_script_cmd(res)
```

```
sub_script_head(res)
```

```
subclasses_dict = {'DpCloudServer': <class  
'dpdispatcher.dp_cloud_server.DpCloudServer'>, 'LSF': <class  
'dpdispatcher.lsf.LSF'>, 'PBS': <class 'dpdispatcher.pbs.PBS'>, 'Shell': <class  
'dpdispatcher.shell.Shell'>, 'Slurm': <class 'dpdispatcher.slurm.Slurm'>, 'Torque':  
<class 'dpdispatcher.pbs.Torque'>, 'dpcloudserver': <class  
'dpdispatcher.dp_cloud_server.DpCloudServer'>, 'lsf': <class  
'dpdispatcher.lsf.LSF'>, 'pbs': <class 'dpdispatcher.pbs.PBS'>, 'shell': <class  
'dpdispatcher.shell.Shell'>, 'slurm': <class 'dpdispatcher.slurm.Slurm'>, 'torque':  
<class 'dpdispatcher.pbs.Torque'>}
```

6.1.12 dpdispatcher.pbs module

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

Bases: [dpdispatcher.machine.Machine](#)

Methods

```
do\_submit(job)
```

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

arginfo	
bind_context	
check_finish_tag	
check_if_recover	
check_status	
default_resources	
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	
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: `dpdispatcher.pbs.PBS`

Methods

<code>do_submit(job)</code>	submit a single job, assuming that no job is running there.
-----------------------------	---

<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>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>sub_script_cmd</code>	
<code>sub_script_head</code>	

`check_status(job)`

6.1.13 dpdispatcher.shell module

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

Bases: `dpdispatcher.machine.Machine`

Methods

<code>do_submit(job)</code>	submit a single job, assuming that no job is running there.
-----------------------------	---

<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>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>sub_script_cmd</code>	
<code>sub_script_head</code>	

`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)`

6.1.14 dpdispatcher.slurm module

`class dpdispatcher.slurm.Slurm(*args, **kwargs)`
Bases: `dpdispatcher.machine.Machine`

Methods

<code>do_submit(job[, retry, max_retry])</code>	submit a single job, assuming that no job is running there.
---	---

arginfo	
bind_context	
check_finish_tag	
check_if_recover	
check_status	
default_resources	
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	
sub_script_cmd	
sub_script_head	

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*)

6.1.15 dpdispatcher.ssh_context module

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

Bases: *dpdispatcher.base_context.BaseContext*

Attributes

sftp

ssh

Methods

<code>block_checkcall(cmd[, asynchronously, ...])</code>	Run command with arguments.
--	-----------------------------

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)
```

```
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

`sftp` Returns sftp.

Methods

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

arginfo	
close	
ensure_alive	
get_ssh_client	

```
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_ssh_client()
```

```
property sftp
```

Returns sftp. Open a new one if not existing.

6.1.16 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}, para_deg=1,
                                       module_unload_list=[], module_list=[], source_list=[],
                                       envs={}, **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.

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.

Methods

arginfo	
deserialize	
load_from_dict	
load_from_json	
serialize	

static `arginfo()`

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] path-like, the base directory of the local tasks

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.

continues on next page

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<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, if_none_local_root])</code>	convert the Submission class instance to a dictionary.
<code>update_submission_state()</code>	check whether all the jobs in the submission.

<code>clean_jobs</code>	
<code>download_jobs</code>	
<code>get_hash</code>	
<code>register_task</code>	
<code>register_task_list</code>	
<code>submission_from_json</code>	
<code>submission_to_json</code>	
<code>try_recover_from_json</code>	
<code>upload_jobs</code>	

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.

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 unexpectedly), resubmit the job. If the job state is unknown, raise an error.

register_task(task)**register_task_list(task_list)****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, if_none_local_root=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 comand 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	
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()

serialize()

6.1.17 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.

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