
DPDispatcher

Deep Modeling

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CONTENTS:

1	Install DPDispatcher	3
2	Getting Started	5
3	Machine parameters	9
4	DPDispatcher API	11
5	Indices and tables	21
	Python Module Index	23
	Index	25

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(clean=False)
```

where `machine.json` is

```
{
  "machine_type": "Slurm",
  "context_type": "SSHContext",
  "local_root" : "/home/user123/workplace/22_new_project/",
  "remote_root": "~/dpdispatcher_work_dir/",
  "remote_profile":{
    "hostname": "39.106.xx.xxx",
    "username": "user1",
    "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:

```
resources = Resources(number_node=1,
  cpu_per_node=8,
  gpu_per_node=2,
  queue_name="GPU2080TI",
  group_size=12,
  custom_flags=[
    "#SBATCH --mem=32G",
  ],
  strategy={'if_cuda_multi_devices': true},
  para_deg=3,
  source_list=["~/deepmd.env"],
```

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)

The details of parameters can be found in *Machine 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

passphrase:

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

timeout:

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

DPDISPATCHER API

```
dpdispatcher.info()

class dpdispatcher.JobStatus.JobStatus(value)
    An enumeration.
    completing = 6
    finished = 5
    running = 3
    terminated = 4
    unknown = 100
    unsubmitted = 1
    waiting = 2

class dpdispatcher.base_context.BaseContext

    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 = {'LazyLocalContext': <class
'dpdispatcher.lazy_local_context.LazyLocalContext'>, 'LocalContext': <class
'dpdispatcher.local_context.LocalContext'>, 'SSHContext': <class
'dpdispatcher.ssh_context.SSHContext'>}}
    upload(submission)
    write_file(fname, write_str)

dpdispatcher.dpdisp.main()

class dpdispatcher.lazy_local_context.LazyLocalContext(local_root, remote_root=None,
                                                         remote_profile={})

    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)

    read()
    readlines()

class dpdispatcher.local_context.LocalContext(local_root, remote_root, remote_profile={})

    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)

    read()
    readlines()

class dpdispatcher.lsf.LSF(context)
    LSF batch
    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)

class dpdispatcher.machine.Machine(context)
    A machine is used to handle the connection with remote machines.

    context [SubClass derived fromBaseContext] The context is used to maintain the connection with remote machine.

    static arginfo()
    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 = {'LSF': <class 'dpdispatcher.lsf.LSF'>, 'PBS': <class 'dpdispatcher.pbs.PBS'>, 'Shell': <class 'dpdispatcher.shell.Shell'>, 'Slurm': <class 'dpdispatcher.slurm.Slurm'>}
```

```
class dpdispatcher.pbs.PBS(context)
```

```
    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.shell.Shell(context)
```

```
    check_finish_tag(job)
```

```
    check_status(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.slurm.Slurm(context)
```

```
    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)
```

```
class dpdispatcher.ssh_context.SSHContext(local_root, remote_root, remote_profile,  
                                           clean_asynchronously=False)
```

```
    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.
```

```
        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)

    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.

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

    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.
    classmethod deserialize(job_dict, machine=None)
        convert the job_dict to a Submission class object
        submission_dict [dict] path-like, the base directory of the local tasks

        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.

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.

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

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,  
                                     source_list=[], **kwargs)
```

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

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_resource 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.

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=[])
```

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.

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.

bind_machine(*machine*)

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

machine [Machine] the machine to bind with

check_all_finished()

check whether all the jobs in the submission.

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

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

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()

get_submission_state()

check whether all the jobs in the submission.

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

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*)

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.

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

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

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

submission_to_json()

submit_submission()

submit the job belonging to the submission.

try_recover_from_json()

upload_jobs()

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

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

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

classmethod deserialize(*task_dict*)

convert the task_dict to a Task class object

task_dict [dict] the dictionary which contains the task information

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

get_hash()

serialize()

class dpdispatcher.dpcloudserver.retcode.RETCODE

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.zip_file.**is_selected**(*arcname, selected*)

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

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

dpdispatcher.dpcloudserver.zip_file.**zip_files**(*root_path, out_file, selected=[]*)

INDICES AND TABLES

- genindex
- modindex
- search

PYTHON MODULE INDEX

d

- `dpdispatcher`, 11
- `dpdispatcher.base_context`, 11
- `dpdispatcher.dpcloudserver`, 18
- `dpdispatcher.dpcloudserver.config`, 18
- `dpdispatcher.dpcloudserver.retcode`, 18
- `dpdispatcher.dpcloudserver.zip_file`, 19
- `dpdispatcher.dpdisp`, 11
- `dpdispatcher.JobStatus`, 11
- `dpdispatcher.lazy_local_context`, 11
- `dpdispatcher.local_context`, 12
- `dpdispatcher.lsf`, 13
- `dpdispatcher.machine`, 13
- `dpdispatcher.pbs`, 13
- `dpdispatcher.shell`, 14
- `dpdispatcher.slurm`, 14
- `dpdispatcher.ssh_context`, 14
- `dpdispatcher.submission`, 15

A

`arginfo()` (`dpdispatcher.machine.Machine` static method), 13
`arginfo()` (`dpdispatcher.ssh_context.SSHSession` static method), 15
`arginfo()` (`dpdispatcher.submission.Resources` static method), 16

B

`BaseContext` (class in `dpdispatcher.base_context`), 11
`bind_machine()` (`dpdispatcher.submission.Submission` method), 17
`bind_submission()` (`dpdispatcher.base_context.BaseContext` method), 11
`bind_submission()` (`dpdispatcher.lazy_local_context.LazyLocalContext` method), 11
`bind_submission()` (`dpdispatcher.local_context.LocalContext` method), 12
`bind_submission()` (`dpdispatcher.ssh_context.SSHContext` method), 14
`block_call()` (`dpdispatcher.lazy_local_context.LazyLocalContext` method), 11
`block_call()` (`dpdispatcher.local_context.LocalContext` method), 12
`block_call()` (`dpdispatcher.ssh_context.SSHContext` method), 14
`block_checkcall()` (`dpdispatcher.lazy_local_context.LazyLocalContext` method), 12
`block_checkcall()` (`dpdispatcher.local_context.LocalContext` method), 12
`block_checkcall()` (`dpdispatcher.ssh_context.SSHContext` method), 14

C

`call()` (`dpdispatcher.lazy_local_context.LazyLocalContext`

method), 12
`call()` (`dpdispatcher.local_context.LocalContext` method), 12
`call()` (`dpdispatcher.ssh_context.SSHContext` method), 14
`check_all_finished()` (`dpdispatcher.submission.Submission` method), 17
`check_file_exists()` (`dpdispatcher.lazy_local_context.LazyLocalContext` method), 12
`check_file_exists()` (`dpdispatcher.local_context.LocalContext` method), 12
`check_file_exists()` (`dpdispatcher.ssh_context.SSHContext` method), 14
`check_finish()` (`dpdispatcher.base_context.BaseContext` method), 11
`check_finish()` (`dpdispatcher.lazy_local_context.LazyLocalContext` method), 12
`check_finish()` (`dpdispatcher.local_context.LocalContext` method), 12
`check_finish()` (`dpdispatcher.ssh_context.SSHContext` method), 15
`check_finish_tag()` (`dpdispatcher.lsf.LSF` method), 13
`check_finish_tag()` (`dpdispatcher.machine.Machine` method), 13
`check_finish_tag()` (`dpdispatcher.pbs.PBS` method), 14
`check_finish_tag()` (`dpdispatcher.shell.Shell` method), 14
`check_finish_tag()` (`dpdispatcher.slurm.Slurm` method), 14
`check_if_recover()` (`dpdispatcher.machine.Machine` method), 13
`check_status()` (`dpdispatcher.lsf.LSF` method), 13
`check_status()` (`dpdispatcher.machine.Machine`

method), 13
 check_status() (dpdispatcher.pbs.PBS method), 14
 check_status() (dpdispatcher.shell.Shell method), 14
 check_status() (dpdispatcher.slurm.Slurm method), 14
 check_status_() (dpdispatcher.shell.Shell method), 14
 clean() (dpdispatcher.base_context.BaseContext method), 11
 clean() (dpdispatcher.lazy_local_context.LazyLocalContext method), 12
 clean() (dpdispatcher.local_context.LocalContext method), 12
 clean() (dpdispatcher.ssh_context.SSHContext method), 15
 clean_jobs() (dpdispatcher.submission.Submission method), 17
 close() (dpdispatcher.ssh_context.SSHContext method), 15
 close() (dpdispatcher.ssh_context.SSHSession method), 15
 completing (dpdispatcher.JobStatus.JobStatus attribute), 11

D

DATAERR (dpdispatcher.dpcloudserver.retcode.RETCODE attribute), 18
 DBERR (dpdispatcher.dpcloudserver.retcode.RETCODE attribute), 18
 default_resources() (dpdispatcher.lsf.LSF method), 13
 default_resources() (dpdispatcher.machine.Machine method), 13
 default_resources() (dpdispatcher.pbs.PBS method), 14
 default_resources() (dpdispatcher.shell.Shell method), 14
 default_resources() (dpdispatcher.slurm.Slurm method), 14
 deserialize() (dpdispatcher.submission.Job class method), 15
 deserialize() (dpdispatcher.submission.Resources class method), 16
 deserialize() (dpdispatcher.submission.Submission class method), 17
 deserialize() (dpdispatcher.submission.Task class method), 18
 do_submit() (dpdispatcher.lsf.LSF method), 13
 do_submit() (dpdispatcher.machine.Machine method), 13
 do_submit() (dpdispatcher.pbs.PBS method), 14
 do_submit() (dpdispatcher.shell.Shell method), 14
 do_submit() (dpdispatcher.slurm.Slurm method), 14
 download() (dpdispatcher.base_context.BaseContext method), 11

download() (dpdispatcher.lazy_local_context.LazyLocalContext method), 12
 download() (dpdispatcher.local_context.LocalContext method), 12
 download() (dpdispatcher.ssh_context.SSHContext method), 15
 download_() (dpdispatcher.local_context.LocalContext method), 12
 download_jobs() (dpdispatcher.submission.Submission method), 17
 dpdispatcher
 module, 11
 dpdispatcher.base_context
 module, 11
 dpdispatcher.dpcloudserver
 module, 18
 dpdispatcher.dpcloudserver.config
 module, 18
 dpdispatcher.dpcloudserver.retcode
 module, 18
 dpdispatcher.dpcloudserver.zip_file
 module, 19
 dpdispatcher.dpdisp
 module, 11
 dpdispatcher.JobStatus
 module, 11
 dpdispatcher.lazy_local_context
 module, 11
 dpdispatcher.local_context
 module, 12
 dpdispatcher.lsf
 module, 13
 dpdispatcher.machine
 module, 13
 dpdispatcher.pbs
 module, 13
 dpdispatcher.shell
 module, 14
 dpdispatcher.slurm
 module, 14
 dpdispatcher.ssh_context
 module, 14
 dpdispatcher.submission
 module, 15

E

ensure_alive() (dpdispatcher.ssh_context.SSHSession method), 15
 exec_command() (dpdispatcher.ssh_context.SSHSession method), 15

F

finished (dpdispatcher.JobStatus.JobStatus attribute),

- 11
- ## G
- gen_command_env_cuda_devices() (dpdispatcher.machine.Machine method), 13
- gen_script() (dpdispatcher.lsf.LSF method), 13
- gen_script() (dpdispatcher.machine.Machine method), 13
- gen_script() (dpdispatcher.pbs.PBS method), 14
- gen_script() (dpdispatcher.shell.Shell method), 14
- gen_script() (dpdispatcher.slurm.Slurm method), 14
- gen_script_command() (dpdispatcher.machine.Machine method), 13
- gen_script_custom_flags_lines() (dpdispatcher.machine.Machine method), 13
- gen_script_end() (dpdispatcher.machine.Machine method), 13
- gen_script_env() (dpdispatcher.machine.Machine method), 13
- gen_script_header() (dpdispatcher.machine.Machine method), 13
- gen_script_header() (dpdispatcher.pbs.PBS method), 14
- gen_script_header() (dpdispatcher.shell.Shell method), 14
- gen_script_header() (dpdispatcher.slurm.Slurm method), 14
- gen_script_wait() (dpdispatcher.machine.Machine method), 13
- generate_jobs() (dpdispatcher.submission.Submission method), 17
- get_hash() (dpdispatcher.submission.Job method), 15
- get_hash() (dpdispatcher.submission.Submission method), 17
- get_hash() (dpdispatcher.submission.Task method), 18
- get_job_root() (dpdispatcher.lazy_local_context.LazyLocalContext method), 12
- get_job_root() (dpdispatcher.local_context.LocalContext method), 12
- get_job_root() (dpdispatcher.ssh_context.SSHContext method), 15
- get_job_state() (dpdispatcher.submission.Job method), 15
- get_return() (dpdispatcher.lazy_local_context.LazyLocalContext method), 12
- get_return() (dpdispatcher.local_context.LocalContext method), 12
- get_return() (dpdispatcher.ssh_context.SSHContext method), 15
- get_ssh_client() (dpdispatcher.ssh_context.SSHSession method), 15
- get_submission_state() (dpdispatcher.submission.Submission method), 17
- ## H
- handle_unexpected_job_state() (dpdispatcher.submission.Job method), 16
- handle_unexpected_submission_state() (dpdispatcher.submission.Submission method), 17
- ## I
- info() (in module dpdispatcher), 11
- IOERR (dpdispatcher.dpcloudserver.retcode.RETCODE attribute), 18
- is_selected() (in module dpdispatcher.dpcloudserver.zip_file), 19
- ## J
- Job (class in dpdispatcher.submission), 15
- job_to_json() (dpdispatcher.submission.Job method), 16
- JobStatus (class in dpdispatcher.JobStatus), 11
- ## K
- kill() (dpdispatcher.base_context.BaseContext method), 11
- kill() (dpdispatcher.lazy_local_context.LazyLocalContext method), 12
- kill() (dpdispatcher.local_context.LocalContext method), 12
- kill() (dpdispatcher.ssh_context.SSHContext method), 15
- ## L
- LazyLocalContext (class in dpdispatcher.lazy_local_context), 11
- load_from_dict() (dpdispatcher.base_context.BaseContext class method), 11
- load_from_dict() (dpdispatcher.lazy_local_context.LazyLocalContext class method), 12
- load_from_dict() (dpdispatcher.local_context.LocalContext class method), 12
- load_from_dict() (dpdispatcher.machine.Machine class method), 13
- load_from_dict() (dpdispatcher.ssh_context.SSHContext class method), 15
- load_from_dict() (dpdispatcher.submission.Resources class method), 16

- `load_from_json()` (*dpdispatcher.machine.Machine* class method), 13
- `load_from_json()` (*dpdispatcher.submission.Resources* class method), 16
- `LocalContext` (class in *dpdispatcher.local_context*), 12
- `LOGINERR` (*dpdispatcher.dpcloudserver.retcode.RETCODE* attribute), 18
- `LSF` (class in *dpdispatcher.lsf*), 13
- M**
- `Machine` (class in *dpdispatcher.machine*), 13
- `main()` (in module *dpdispatcher.dpdisp*), 11
- module
 - dpdispatcher*, 11
 - dpdispatcher.base_context*, 11
 - dpdispatcher.dpcloudserver*, 18
 - dpdispatcher.dpcloudserver.config*, 18
 - dpdispatcher.dpcloudserver.retcode*, 18
 - dpdispatcher.dpcloudserver.zip_file*, 19
 - dpdispatcher.dpdisp*, 11
 - dpdispatcher.JobStatus*, 11
 - dpdispatcher.lazy_local_context*, 11
 - dpdispatcher.local_context*, 12
 - dpdispatcher.lsf*, 13
 - dpdispatcher.machine*, 13
 - dpdispatcher.pbs*, 13
 - dpdispatcher.shell*, 14
 - dpdispatcher.slurm*, 14
 - dpdispatcher.ssh_context*, 14
 - dpdispatcher.submission*, 15
- N**
- `NODATA` (*dpdispatcher.dpcloudserver.retcode.RETCODE* attribute), 18
- O**
- `OK` (*dpdispatcher.dpcloudserver.retcode.RETCODE* attribute), 18
- P**
- `PARAMERR` (*dpdispatcher.dpcloudserver.retcode.RETCODE* attribute), 18
- `PBS` (class in *dpdispatcher.pbs*), 13
- `PWDERR` (*dpdispatcher.dpcloudserver.retcode.RETCODE* attribute), 18
- R**
- `read()` (*dpdispatcher.lazy_local_context.SPRetObj* method), 12
- `read()` (*dpdispatcher.local_context.SPRetObj* method), 13
- `read_file()` (*dpdispatcher.base_context.BaseContext* method), 11
- `read_file()` (*dpdispatcher.lazy_local_context.LazyLocalContext* method), 12
- `read_file()` (*dpdispatcher.local_context.LocalContext* method), 12
- `read_file()` (*dpdispatcher.ssh_context.SSHContext* method), 15
- `readlines()` (*dpdispatcher.lazy_local_context.SPRetObj* method), 12
- `readlines()` (*dpdispatcher.local_context.SPRetObj* method), 13
- `register_job_id()` (*dpdispatcher.submission.Job* method), 16
- `register_task()` (*dpdispatcher.submission.Submission* method), 17
- `register_task_list()` (*dpdispatcher.submission.Submission* method), 17
- `REQERR` (*dpdispatcher.dpcloudserver.retcode.RETCODE* attribute), 19
- `Resources` (class in *dpdispatcher.submission*), 16
- `RETCODE` (class in *dpdispatcher.dpcloudserver.retcode*), 18
- `ROLEERR` (*dpdispatcher.dpcloudserver.retcode.RETCODE* attribute), 19
- `run_submission()` (*dpdispatcher.submission.Submission* method), 17
- `running` (*dpdispatcher.JobStatus.JobStatus* attribute), 11
- S**
- `serialize()` (*dpdispatcher.submission.Job* method), 16
- `serialize()` (*dpdispatcher.submission.Resources* method), 16
- `serialize()` (*dpdispatcher.submission.Submission* method), 18
- `serialize()` (*dpdispatcher.submission.Task* method), 18
- `sftp` (*dpdispatcher.ssh_context.SSHContext* property), 15
- `sftp` (*dpdispatcher.ssh_context.SSHSession* property), 15
- `Shell` (class in *dpdispatcher.shell*), 14
- `Slurm` (class in *dpdispatcher.slurm*), 14
- `SPRetObj` (class in *dpdispatcher.lazy_local_context*), 12
- `SPRetObj` (class in *dpdispatcher.local_context*), 12
- `ssh` (*dpdispatcher.ssh_context.SSHContext* property), 15
- `SSHContext` (class in *dpdispatcher.ssh_context*), 14
- `SSHSession` (class in *dpdispatcher.ssh_context*), 15
- `sub_script_cmd()` (*dpdispatcher.machine.Machine* method), 13
- `sub_script_head()` (*dpdispatcher.machine.Machine* method), 13

subclasses_dict (dpdispatcher.base_context.BaseContext attribute), 11
 subclasses_dict (dpdispatcher.machine.Machine attribute), 13
 Submission (class in dpdispatcher.submission), 16
 submission_from_json() (dpdispatcher.submission.Submission class method), 18
 submission_to_json() (dpdispatcher.submission.Submission method), 18
 submit_job() (dpdispatcher.submission.Job method), 16
 submit_submission() (dpdispatcher.submission.Submission method), 18

T

Task (class in dpdispatcher.submission), 18
 terminated (dpdispatcher.JobStatus.JobStatus attribute), 11
 THIRDERR (dpdispatcher.dpcloudserver.retcode.RETCODE attribute), 19
 try_recover_from_json() (dpdispatcher.submission.Submission method), 18

U

UNDERDEBUG (dpdispatcher.dpcloudserver.retcode.RETCODE attribute), 19
 unknown (dpdispatcher.JobStatus.JobStatus attribute), 11
 UNKOWNERR (dpdispatcher.dpcloudserver.retcode.RETCODE attribute), 19
 unsubmitted (dpdispatcher.JobStatus.JobStatus attribute), 11
 unzip_file() (in module dpdispatcher.dpcloudserver.zip_file), 19
 upload() (dpdispatcher.base_context.BaseContext method), 11
 upload() (dpdispatcher.lazy_local_context.LazyLocalContext method), 12
 upload() (dpdispatcher.local_context.LocalContext method), 12
 upload() (dpdispatcher.ssh_context.SSHContext method), 15
 upload_() (dpdispatcher.local_context.LocalContext method), 12
 upload_jobs() (dpdispatcher.submission.Submission method), 18
 USERERR (dpdispatcher.dpcloudserver.retcode.RETCODE attribute), 19

V

VERIFYERR (dpdispatcher.dpcloudserver.retcode.RETCODE attribute), 19

W

waiting (dpdispatcher.JobStatus.JobStatus attribute), 11
 write_file() (dpdispatcher.base_context.BaseContext method), 11
 write_file() (dpdispatcher.lazy_local_context.LazyLocalContext method), 12
 write_file() (dpdispatcher.local_context.LocalContext method), 12
 write_file() (dpdispatcher.ssh_context.SSHContext method), 15

Z

zip_file_list() (in module dpdispatcher.dpcloudserver.zip_file), 19
 zip_files() (in module dpdispatcher.dpcloudserver.zip_file), 19