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# Python Cluster Documentation

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Submit jobs to slurm or torque, or with multiprocessing.

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License	MIT License, property of Stanford, use as you wish
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Allows easy job submission with *dependency tracking and queue waiting* with either torque, slurm, or locally with the multiprocessing module. It uses simple techniques to avoid overwhelming the queue and to catch bugs (e.g. queue stalling) on the fly.

NOTE: While this software is extremely powerful for pure python-based cluster job submission, [snakemake](#) is possibly a better choice for very large workflows.

Contents:



## INSTALLATION

This module will work with Python 2.7+ on Linux systems.

To install, use the standard python method:

```
git clone https://github.com/MikeDacre/python-cluster
cd python-cluster
python ./setup.py install --user
```

In general you want user level install even if you have sudo access, as most cluster environments share /home/<user> across the cluster, making this module available everywhere.

*Note:* While the name is *python-cluster* you will import it just as *cluster*:

```
import cluster
```

### 1.1 Prerequisites

The only external module that I use in this software is *dill*. It isn't 100% required but it makes function submission much more stable.

If you choose to use *dill*, it must be installed cluster wide.

### 1.2 Function Submission

In order to submit functions to the cluster, this module must import them on the compute node. This means that all of your python modules must be available on every compute node. To avoid pain and debugging, you can do this manually by running this on your login node:

```
freeze --local | grep -v '^-\e' | cut -d = -f 1 > module_list.txt
```

And then on the compute nodes:

```
cat module_list.txt | xargs pip install --user
```

This will ensure that all of your modules are installed globally.

In general it is a good idea to install modules as *-user* with *pip* to avoid this issue.





## SIMPLE USAGE

### 2.1 Setting Environment

To set the environment, set `queue.MODE` to one of ['torque', 'slurm', 'local'], or run `get_cluster_environment()`.

### 2.2 Simple Job Submission

At its simplest, this module can be used by just executing `submit(<command>)`, where `command` is a function or system command/shell script. The module will autodetect the cluster, generate an intuitive name, run the job, and write all outputs to files in the current directory. These can be cleaned with `clean_dir()`.

To run with dependency tracking, run:

```
import cluster
job = cluster.submit(<command1>)
job2 = cluster.submit(<command2>, dependencies=job1)
exitcode, stdout, stderr = job2.get() # Will block until job completes
```

### 2.3 Functions

The `submit` function works well with python functions as well as with shell scripts and shell commands.

*However*, in order for this to work, `cluster` ends up importing your original script file on the nodes. This means that all code in your file will be executed, so anything that isn't a function or class must be protected with an:

```
if __name__ == '__main__':
```

protecting statement.

If you do not do this you can end up with multi-submission and infinite recursion, which could mess up your jobs or just crash the job, but either way, it won't be good.

### 2.4 File Submission

If you want to just submit a file, that can be done like this:

```
from cluster import submit_file
submit_file('/path/to/script', dependencies=[7, 9])
```

This will return the job number and will enter the job into the queue as dependant on jobs 007 and 009. The dependencies can be omitted.

## 2.5 The Job Class

The core of this submission system is a *Job* class, this class allows easy job handling and debugging. All of the above commands work well with the Job class also, but more fine grained control is possible. For example:

```
my_job = """#!/bin/bash
parallel /usr/bin/parser {} ::: folder/*.txt
for i in folder/*.txt; do
    echo $i >> my_output.txt
    echo job_$i done!
fi"""
job = cluster.Job(my_job, cores=16)
job.submit()
job.wait()
print(job.stdout)
if job.exitcode != 0:
    print(job.stderr)
```

More is also possible, for a full description, see the API documentation here: [Job Documentation](#)

## SCRIPTS

While this software is designed to be used as a python library, several scripts are provided to make life easier.

### 3.1 my-queue

Uses python-cluster to check the job queue for only one user's jobs. Produces a very simple display, for full job information, the regular tools can be used (e.g squeue):

```
Choose jobs to show, default is all:
-r, --running  Show running jobs only
-q, --queued   Show queued jobs only

Choose alternate output style:
-c, --count     Display count only
-l, --list      Print space separated list of job numbers
```

### 3.2 cluster-profile

This script allows the user to save cluster keyword arguments in a config file located at ~/.python-cluster.

Rather than edit that file directly, use this script to add profiles and options.

There are two classes of options: global options, and profiles.

Global options will be used in all profiles, but only if the option is not already present in the profile definition. Profiles must be called every time and allow bundled keyword arguments, they can also be overridden by providing keyword arguments at runtime.

Global options are great for saving a default queue.

Modes:

```
General:
: list:    Display all global options and profiles.

Profile Management:
: add:     Add a profile
           Usage: add profile_name keyword:arg [keyword:arg ...]
: edit:    Edit an existing profile
           Usage: edit profile_name keyword:arg [keyword:arg ...]
: remove:  Delete an existing profile (The default profile will be recreated
           if it does not exist when a job is submitted.
```

```
Usage: remove|del profile_name

Global Option Management:
: add-global:      Add a global keyword
                   Usage: add-global keyword:arg [keyword:arg ...]
: remove-global:   Remove a global keyword
                   Usage: remove-global|del-global keyword [keyword ...]

Dangerous:
: reset:          Completely reset your entire profile to the defaults.
```

## 3.3 monitor-jobs

Blocks until provided jobs complete. Allows to monitor by user, partition, or simple job list:

```
Arguments are cumulative except user. For example::
    auto_resubmit -p bob -j 172436 172437
user can be 'self'
This command will monitor all jobs in the bob partition as
well as the two jobs specified directly.
However::
    monitor_jobs -p bob -u fred
This command will only monitor fred's jobs in bob (the union).
```

## 3.4 clean-job-files

Uses the `cluster.job.clean_dir()` function to clean all job files in the current directory.

Caution: The `clean()` function will delete **EVERY** file with extensions matching those these:

```
.<suffix>.err
.<suffix>.out
.<suffix>.sbatch & .cluster.script for slurm mode
.<suffix>.qsub for torque mode
.<suffix> for local mode
_func.<suffix>.py
_func.<suffix>.py.pickle.in
_func.<suffix>.py.pickle.out
```

Usage:

```
Will work with no commands.

optional arguments:
  -h, --help                show this help message and exit
  -d DIR, --dir DIR         Directory to clean
  -s, --suffix SUFFIX       Directory to clean
  -q, --qtype {torque,slurm,local} Limit deletions to this qtype
  -n, --no-confirm          Do not confirm before deleting (for scripts)
  -v, --verbose             Show debug information
```

## 3.5 cluster-keywords

Prints simple help information on the available keyword arguments. It calls the `cluster_help()` function, which means that keyword information is always up to date.



## QUEUE MANAGEMENT

This module provides simple queue management functions

To generate a queue object, do the following:

```
import cluster
q = cluster.Queue(user='self')
```

This will give you a simple queue object containing a list of jobs that belong to you. If you do not provide user, all jobs are included for all users. You can provide *qtype* to explicitly force the queue object to contain jobs from one queuing system (e.g. local or torque).

To get a dictionary of all jobs, running jobs, queued jobs, and complete jobs, use:

```
q.jobs
q.running
q.complete
q.queued
```

Every job has a number of attributes, including owner, nodes, cores, memory.





## ADVANCED USAGE

### 5.1 Keyword Arguments

To make submission easier, this module defines a number of keyword arguments in the options.py file that can be used for all submission and Job() functions. These include things like ‘cores’ and ‘nodes’ and ‘mem’.

The following is a complete list of arguments that can be used in this version:

```
Used in every mode::
cores:      Number of cores to use for the job
             Type: int; Default: 1
modules:    Modules to load with the `module load` command
             Type: list; Default: None
filedir:    Folder to write cluster files to, must be accessible to the compute
             nodes.
             Type: str; Default: .
dir:        The working directory for the job
             Type: str; Default: path argument
suffix:     A suffix to append to job files (e.g. job.suffix.qsub)
             Type: str; Default: cluster
outfile:    File to write STDOUT to
             Type: str; Default: None
errfile:    File to write STDERR to
             Type: str; Default: None

Used for function calls::
imports:     Imports to be used in function calls (e.g. sys, os) if not provided,
             defaults to all current imports, which may not work if you use complex
             imports. The list can include the import call, or just be a name, e.g.
             ['from os import path', 'sys']
             Type: list; Default: None

Used only in local mode::
threads:     Number of threads to use on the local machine
             Type: int; Default: 8

Options that work in both slurm and torque::
nodes:      Number of nodes to request
             Type: int; Default: 1
features:    A comma-separated list of node features to require
             Type: list; Default: None
time:       Walltime in HH:MM:SS
             Type: str; Default: 12:00:00
mem:        Memory to use in MB (e.g. 4000)
             Type: ['int', 'str']; Default: 4000
```

```
partition: The partition/queue to run in (e.g. local/batch)
            Type: str; Default: None
account:   Account to be charged
            Type: str; Default: None
export:    Comma separated list of environmental variables to export
            Type: str; Default: None

Used for slurm only::
begin:     Start after this much time
            Type: str; Default: None
```

In addition some synonyms are allowed:

```
cpus:      cores
memory:    mem
queue:     partition
depend, dependencies, dependency: depends
```

*Note:* Type is enforced, any provided argument must match that python type (automatic conversion is attempted), the default is just a recommendation and is not currently used. These arguments are passed like regular arguments to the submission and Job() functions, eg:

```
Job(nodes=1, cores=4, mem='20MB')
```

This will be interpreted correctly on any system. If torque or slurm are not available, any cluster arguments will be ignored. The module will attempt to honor the cores request, but if it exceeds the maximum number of cores on the local machine, then the request will be trimmed accordingly (i.e. a 50 core request will become 8 cores on an 8 core machine).

### Adding your own keywords

There are many more options available for torque and slurm, to add your own, edit the options.py file, and look for CLUSTER\_OPTS (or TORQUE/SLURM if your keyword option is only available on one system). Add your option using the same format as is present in that file. The format is:

```
('name', {'slurm': '--option-str={}', 'torque': '--torque-option={}',
          'help': 'This is an option!', 'type': str, 'default': None})
```

You can also add list options, but they must include 'sjoin' and 'tjoin' keys to define how to merge the list for slurm and torque, or you must write custom option handling code in cluster.options.options\_to\_string(). For an excellent example of both approaches included in a single option, see the 'features' keyword above.

I happily accept pull requests for new option additions (any any other improvements for that matter).

## 5.2 Profiles and the Config File

To avoid having to enter all keyword arguments every time, profiles can be used. These profiles can store any of the above keywords and drastically simplify submission. For example:

```
job = submit(my_function, profile='large')
```

Instead of:

```
job = submit(my_funtion, nodes=2, cores=16, mem='64GB', partition='bigjobs',
            features=['highmem'], export='PYTHONPATH')
```

These profiles are saved in a config file at `~/python-cluster` and can be edited in that file directly, or using the below functions. To edit them in the file directly, you must make sure that the section is labelled 'prof\_<name>' where <name> is whatever you want it to be called. e.g.:

```
[prof_default]
nodes = 1
cores = 16
time = 24:00:00
mem = 32000
```

*Note:* a default profile must always exist, it will be added back if it does not exist.

The easiest way to manage profiles is with the `cluster_profile` script in `bin`. It defines several easy methods to manage both profiles and global options, see the scripts section above for information.

Alternatively, the functions `cluster.config_file.set_profile()` and `cluster.config_file.get_profile()` can be used:

```
cluster.config_file.set_profile('small', {'nodes': 1, 'cores': 1,
                                          'mem': '2GB'})
cluster.config_file.get_profile('small')
```

To see all profiles run:

```
config_file.get_profile()
```

Other options are defined in the config file, including the maximum number of jobs in the queue, the time to sleep between submissions, and other options. To see these run:

```
cluster.config_file.get_option()
```

You can set options with:

```
cluster.config_file.set_option()
```

The defaults can be directly edited in `config_file.py`, they are clearly documented.

## 5.3 Job Files

All jobs write out a job file before submission, even though this is not necessary (or useful) with multiprocessing. In local mode, this is a `.cluster` file, in slurm is a `.cluster.sbatch` and a `.cluster.script` file, in torque it is a `.cluster.qsub` file. 'cluster' is set by the suffix keyword, and can be overridden.

To change the directory these files are written to, use the 'filedir' keyword argument to `Job` or `submit`.

**NOTE:** This directory *must* be accessible to the compute nodes!!!

All jobs are assigned a name that is used to generate the output files, including `STDOUT` and `STDERR` files. The default name for the out files is `STDOUT: name.cluster.out` and `STDERR: name.cluster.err`. These can be overwritten with keyword arguments.

All `Job` objects have a `clean()` method that will delete any left over files. In addition there is a `clean_job_files` script that will delete all files made by this package in any given directory. Be very careful with the script though, it can clobber a lot of work all at once if it is used wrong.

## 5.4 Dependency Tracking

Dependency tracking is supported in all modes. Local mode uses a unique queueing system that works similarly to torque and slurm and which is defined in `jobqueue.py`.

To use dependency tracking in any mode pass a list of job ids to `submit` or `submit_file` with the *dependencies* keyword argument.

## 5.5 Logging

I use a custom logging script called `logme` to log errors. To get verbose output, set `logme.MIN_LEVEL` to `'debug'`. To reduce output, set `logme.MIN_LEVEL` to `'warn'`.

## CODE OVERVIEW

There are two important classes for interaction with the batch system: Job and Queue. The essential flow of a job submission is:

```
job = Job(command/function, arguments, name)
job.write()  # Writes the job submission files
job.submit() # Submits the job
job.wait()   # Waits for the job to complete
job.stdout   # Prints the output from the job
job.clean()  # Delete all of the files written
```

You can also wait for many jobs with the Queue class:

```
q = Queue(user='self')
q.wait([job1, job2])
```

The jobs in this case can be either a Job class or a job number.



## ISSUES AND CONTRIBUTING

If you have any trouble with this software add an issue in <https://github.com/MikeDacre/python-cluster/issues>

If you want to help improve it, please fork the repo and send me pull requests when you are done.





## ROADMAP

Right now this software is in `_beta_`, to get to version 1.0 it needs to be tested by users and demonstrated to be stable. In addition, I would like to implement the following features prior to the release of v1.0:

- Auto update Job scripts when attributes are changed until files are already written.
- DONE: Profile managing script in bin
- Update of all bin scripts to work with new options
- Persistent job tracking in an sqlite database stored in \$HOME
- Mac OS X functionality
- Autoadjusting of job options based on queue features (i.e. implement a 'max' option and try to guess the max cores available for a request on any machine)
- Allow users to define their own keyword arguments in their configuration

If you have any other feature suggestions please email them to me at [mike.dacre@gmail.com](mailto:mike.dacre@gmail.com) or open an issue.



## SCRIPTS

This package contains a few little helper scripts to make your life easier. These are not required in order to use the cluster library.

## 9.1 clean\_job\_files

```
usage: clean_job_files [-h] [-d DIR] [-s SUFFIX] [-q {torque,slurm,local}]
                        [-n] [-v VERBOSE]
```

Clean **all** intermediate files created by the cluster module **from this** dir.

=====

```
AUTHOR: Michael D Dacre, mike.dacre@gmail.com
ORGANIZATION: Stanford University
LICENSE: MIT License, property of Stanford, use as you wish
CREATED: 2016-34-15 15:06
Last modified: 2016-06-16 10:42
```

```
DESCRIPTION: Uses the cluster.job.clean_dir() function
```

```
CAUTION: The clean() function will delete **EVERY** file with
          extensions matching those these::
          .<suffix>.err
          .<suffix>.out
          .<suffix>.sbatch & .cluster.script for slurm mode
          .<suffix>.qsub for torque mode
          .<suffix> for local mode
          _func.<suffix>.py
          _func.<suffix>.py.pickle.in
          _func.<suffix>.py.pickle.out
```

=====

optional arguments:

```
-h, --help            show this help message and exit
-d DIR, --dir DIR     Directory to clean
-s SUFFIX, --suffix SUFFIX
                        Directory to clean
-q {torque,slurm,local}, --qtype {torque,slurm,local}
                        Limit deletions to this qtype
-n, --no-confirm       Do not confirm before deleting (for scripts)
```

```
-v VERBOSE, --verbose VERBOSE
                        Show debug information
```

- [search](#)

## API DOCUMENTATION

The following documentation is primarily built from the docstrings of the actual source code and can be considered an API reference.

### 10.1 Queueing

The most import thing is the *Queue()* class which does most of the queue mangement. In addition, *get\_cluster\_environment()* attempts to autodetect the cluster type (torque, slurm, normal) and sets the global cluster type for the whole file. Finally, the *wait()* function accepts a list of jobs and will block until those jobs are complete.

The Queue class is actually a wrapper for a few simple queue parsers, these call *qstat -x* or *squeue* and *sacct* to get job information, and return a simple tuple of that data with the following members:

<code>job_id, name, userid, partition, state, node-list, node-count, cpu-per-node, exit-code</code>
---

The Queue class then converts this information into a *Queue.QueueJob* object and adds it to the internal *jobs* dictionary within the Queue class. This list is now the basis for all of the other functionality encoded by the Queue class. It can be accessed directly, or sliced by accessing the *completed*, *queued*, and *running* attributes of the Queue class, these are used to simply divided up the jobs dictionary to make finding information easy.

**class** `cluster.Queue` (*user=None, qtype=None, partition=None*)

Handle torque, slurm, or multiprocessing objects.

All methods are transparent and work the same regardless of queue type.

`Queue.queue` is a list of jobs in the queue. For torque and slurm, this is all jobs in the queue for the specified user. In local mode, it is all jobs added to the pool, Queue must be notified of these by adding the job object to the queue directly with `add()`.

**exception** `QueueError`

Simple Exception wrapper.

**class** `Queue.QueueJob`

Only used for torque/slurm jobs in the queue.

`Queue.can_submit` (*max\_queue\_len=None*)

Return True if R/Q jobs are less than `max_queue_len`.

If `max_queue_len` is None, default from config is used.

`Queue.update` ()

Refresh the list of jobs from the server, limit queries.

`Queue.wait` (*jobs*)

Block until all jobs in `jobs` are complete.

Update time is dependant upon the `queue_update` parameter in your `~/python-cluster` file.

In addition, `wait()` will not return until between 1 and 3 seconds after a job has completed, irrespective of `queue_update` time. This allows time for any copy operations to complete after the job exits.

**Jobs** A job or list of jobs to check. Can be one of: Job or `multiprocessing.pool.ApplyResult` objects, job ID (int/str), or a object or a list/tuple of multiple Jobs or job IDs.

**Returns** True on success False or None on failure.

`Queue.wait_to_submit (max_queue_len=None)`

Wait until R/Q jobs are less than `max_queue_len`.

If `max_queue_len` is None, default from config is used.

`cluster.queue.get_cluster_environment ()`

Detect the local cluster environment and set MODE globally.

Uses which to search for sbatch first, then qsub. If neither is found, MODE is set to local.

**Returns** MODE variable ('torque', 'slurm', or 'local')

`cluster.queue.wait (jobs)`

Wait for jobs to finish.

**Jobs** A single job or list of jobs to wait for. With torque or slurm, these should be job IDs, with local mode, these are multiprocessing job objects (returned by `submit()`)

`cluster.queue.check_queue (qtype=None)`

Raise exception if MODE is incorrect.

`cluster.queue.queue_parser (qtype=None, user=None, partition=None)`

Call either torque or slurm qtype parsers depending on qtype.

**Qtype** Either 'torque' or 'slurm', defaults to current MODE

**User** optional user name to pass to queue to filter queue with

**Yields** job\_id, name, userid, partition, state, nodelist, numnodes, ntpernode, exit\_code

`cluster.queue.torque_queue_parser (user=None, partition=None)`

Iterator for torque queues.

Use the `qstat -x` command to get an XML queue for compatibility.

**User** optional user name to pass to qstat to filter queue with

**Partiton** optional partition to filter the queue with

**Yields** job\_id, name, userid, partition, state, nodelist, numnodes, ntpernode, exit\_code

numcpus is currently always 1 as most torque queues treat every core as a node.

`cluster.queue.slurm_queue_parser (user=None, partition=None)`

Iterator for slurm queues.

Use the `squeue -O` command to get standard data across implementation, supplement this data with the results of `sacct`. `sacct` returns data only for the current user but retains a much longer job history. Only jobs not returned by `squeue` are added with `sacct`, and they are added to the end of the returned queue, i.e. *out of order with respect to the actual queue*.

**User** optional user name to filter queue with

**Partition** optional partition to filter queue with

**Yields** job\_id, name, userid, partition, state, nodelist, numnodes, ntpernode, exit\_code

## 10.2 Job Management

Job management is handled by the *Job()* class, full instructions on using this class are above, in particular review the ‘Keyword Arguments’ section above.

The methods of this class are exposed by a few functions that aim to make job submission easier. The foremost of these is *submit()* which can take as little as a single command and execute it. *make\_job()* and *make\_job\_file()* work similarly but just return a Job object, or write the file and then return the Job object respectively. *clean()* takes a list of Job objects and runs their internal *clean()* methods, deleting all written files.

There are two additional functions that are completely independent of the Job object: *submit\_file()* and *clean\_dir()*. *submit\_file()* uses similar methods to the Job class to submit a job to the cluster, but it does not involve the job class at all, instead just submitting an already created job file. It can do dependency tracking in the same way as a job file, but that is all. *clean\_dir()* uses the file naming convention established in the Job class (and defined separately here) to delete all files in a directory that look like they could be made by this module. It has an autoconfirm feature that can be activated to avoid accidental clobbering.

**class** `cluster.Job` (*command, args=None, name=None, path=None, qtype=None, profile=None, \*\*kws*)

Information about a single job on the cluster.

Holds information about submit time, number of cores, the job script, and more.

*submit()* will submit the job if it is ready *wait()* will block until the job is done *get()* will block until the job is done and then unpickle a stored output (if defined) and return the contents *clean()* will delete any files created by this object

Printing the class will display detailed job information.

Both *wait()* and *get()* will update the queue every two seconds and add queue information to the job as they go.

If the job disappears from the queue with no information, it will be listed as ‘completed’.

All jobs have a *.submission* attribute, which is a Script object containing the submission script for the job and the file name, plus a ‘written’ bool that checks if the file exists.

In addition, SLURM jobs have a *.exec\_script* attribute, which is a Script object containing the shell command to run. This difference is due to the fact that some SLURM systems execute multiple lines of the submission file at the same time.

Finally, if the job command is a function, this object will also contain a *.function* attribute, which contains the script to run the function.

**clean** (*delete\_outputs=False*)

Delete all scripts created by this module, if they were written.

If *delete\_outputs* is True, also delete the stdout and stderr files, but get their contents first.

**get** ()

Block until job completed and return *exit\_code*, *stdout*, *stderr*.

**get\_exitcode** (*update=True*)

Try to get the exitcode.

**get\_stderr** (*update=True*)

Read stdout file if exists and set *self.stdout*, return it.

**get\_stdout** (*update=True*)

Read stdout file if exists and set *self.stdout*, return it.

**submit** (*max\_queue\_len=None*)

Submit this job.

**Max\_queue\_len** if specified (or in defaults), then this method will block until the queue is open enough to allow submission.

To disable `max_queue_len`, set it to 0. None will allow override by the default settings in the config file, and any positive integer will be interpreted to be the maximum queue length.

**Returns** self

**update()**

Update status from the queue.

**update\_queue\_info()**

Set `queue_info` from the queue even if done.

**wait()**

Block until job completes.

**write(overwrite=True)**

Write all scripts.

`cluster.submit(command, args=None, name=None, path=None, qtype=None, profile=None, **kwargs)`

Submit a script to the cluster.

**Command** The command or function to execute.

**Args** Optional arguments to add to command, particularly useful for functions.

**Name** The name of the job.

**Path** Where to create the script, if None, current dir used.

**Qtype** 'torque', 'slurm', or 'normal'

**Profile** The name of a profile saved in the `config_file`

**Kwargs** Keyword arguments to control job options

There are many keyword arguments available for cluster job submission. These vary somewhat by queue type. For info run:

```
cluster.options.option_help()
```

**Returns** Job object

`cluster.job.submit_file(script_file, dependencies=None, threads=None, qtype=None)`

Submit a job file to the cluster.

If `qtype` or `queue.MODE` is torque, `qsub` is used; if it is slurm, `sbatch` is used; if it is local, the file is executed with `subprocess`.

This function is independent of the Job object and just submits a file.

**Dependencies** A job number or list of job numbers. In slurm: `-dependency=afterok:` is used For torque: `-W depend=afterok:` is used

**Threads** Total number of threads to use at a time, defaults to all. ONLY USED IN LOCAL MODE

**Returns** job number for torque or slurm multiprocessing job object for local mode

`cluster.job.make_job(command, args=None, name=None, path=None, qtype=None, profile=None, **kwargs)`

Make a job file compatible with the chosen cluster.

If mode is local, this is just a simple shell script.



**Command** The command or function to execute.

**Args** Optional arguments to add to command, particularly useful for functions.

**Name** The name of the job.

**Path** Where to create the script, if None, current dir used.

**Qtype** 'torque', 'slurm', or 'normal'

**Profile** The name of a profile saved in the config\_file

There are many keyword arguments available for cluster job submission. These vary somewhat by queue type. For info run:

```
cluster.options.option_help()
```

**Returns** A Job object

`cluster.job.make_job_file(command, args=None, name=None, path=None, qtype=None, profile=None, **kwargs)`

Make a job file compatible with the chosen cluster.

If mode is local, this is just a simple shell script.

**Command** The command or function to execute.

**Args** Optional arguments to add to command, particularly useful for functions.

**Name** The name of the job.

**Path** Where to create the script, if None, current dir used.

**Qtype** 'torque', 'slurm', or 'normal'

**Profile** The name of a profile saved in the config\_file

**Kwargs** Keyword arguments to control job options

There are many keyword arguments available for cluster job submission. These vary somewhat by queue type. For info run:

```
cluster.options.option_help()
```

**Returns** Path to job script

`cluster.job.clean(jobs)`

Delete all files in jobs list or single Job object.

`cluster.job.clean_dir(directory='.', suffix='cluster', qtype=None, confirm=False)`

Delete all files made by this module in directory.

**CAUTION: The clean() function will delete EVERY file with**

**extensions matching those these::** .<suffix>.err .<suffix>.out .<suffix>.sbatch & .<suffix>.script for  
slurm mode .<suffix>.qsub for torque mode .<suffix> for local mode \_func.<suffix>.py  
\_func.<suffix>.py.pickle.in \_func.<suffix>.py.pickle.out

**Directory** The directory to run in, defaults to the current directory.

**Qtype** Only run on files of this qtype

**Confirm** Ask the user before deleting the files

**Returns** A set of deleted files

## 10.3 Options

All keyword arguments are defined in dictionaries in the *options.py* file, alongside function to manage those dictionaries. Of particular importance is *option\_help()*, which can display all of the keyword arguments as a string or a table. *check\_arguments()* checks a dictionary to make sure that the arguments are allowed (i.e. defined), it is called on all keyword arguments in the package.

The way that option handling works in general, is that all hardcoded keyword arguments must contain a dictionary entry for ‘torque’ and ‘slurm’, as well as a type declaration. If the type is `NoneType`, then the option is assumed to be a boolean option. If it has a type though, *check\_argument()* attempts to cast the type and specific idiosyncracies are handled in this step, e.g. memory is converted into an integer of MB. Once the arguments are sanitized *format()* is called on the string held in either the ‘torque’ or the ‘slurm’ values, and the formatted string is then used as an option. If the type is a list/tuple, the ‘sjoin’ and ‘tjoin’ dictionary keys must exist, and are used to handle joining.

The following two functions are used to manage this formatting step.

*option\_to\_string()* will take an option/value pair and return an appropriate string that can be used in the current queue mode. If the option is not implemented in the current mode, a debug message is printed to the console and an empty string is returned.

*options\_to\_string()* is a wrapper around *option\_to\_string()* and can handle a whole dictionary of arguments, it explicitly handle arguments that cannot be managed using a simple string format.

`cluster.options.option_help (qtype=None, mode='string')`

Print a sting to stdout displaying information on all options.

**Qtype** If provided only return info on that queue type.

**Mode** string: Return a formatted string print: Print the string to stdout table: Return a table of lists

`cluster.options.check_arguments (kwargs)`

Make sure all keywords are allowed.

Raises `OptionsError` on error, returns sanitized dictionary on success.

**Note:** Checks in **SYNONYMS** if argument is not recognized, raises **OptionsError** if it is not found there either.

`cluster.options.options_to_string (option_dict, qtype=None)`

Return a multi-line string for slurm or torque job submission.

**Option\_dict** Dict in format {option: value} where value can be None. If value is None, default used.

**Qtype** ‘torque’, ‘slurm’, or ‘local’: override queue.MODE

`cluster.options.option_to_string (option, value=None, qtype=None)`

Return a string with an appropriate flag for slurm or torque.

**Option** An allowed option defined in `options.all_options`

**Value** A value for that option if required (if None, default used)

**Qtype** ‘torque’, ‘slurm’, or ‘local’: override queue.MODE

## 10.4 Config File

Profiles are combinations of keyword arguments that can be called in any of the submission functions. They are handled in the `config_file.py` file which just adds an abstraction layer on top of the builtin python ConfigParser script.

The config file also contains other options that can be managed with the `get_option()` and `set_option()` functions. Profiles are wrapped in a `Profile()` class to make attribute access easy, but they are fundamentally just dictionaries of keyword arguments. They can be created with `cluster.config_file.Profile({kewyws})` and then written to a file with that class' `write()` method. The easiest way to interact with profiles is with the `get_profile()` and `set_profile()` functions. These make it very easy to go from a dictionary of keywords to a profile.

Profiles can then be called with the `profile=` keyword in any submission function or Job class.

**class** `cluster.config_file.Profile(name, kwds)`  
A job submission profile. Just a thin wrapper around a dict.

**write()**  
Write self to config file.

`cluster.config_file.get_option(section=None, key=None, default=None)`  
Get a single key or section.

**Section** The config section to use (e.g. queue, prof)

**Key** The config key to get (e.g. 'max\_jobs')

**Default** If the key does not exist, create it with this default value.

**Returns** None if key does not exist.

`cluster.config_file.set_option(section, key, value)`  
Write a config key to the config file.

`cluster.config_file.set_profile(name, args)`  
Write profile to config file.

**Name** The name of the profile to add/edit.

**Args** Keyword arguments to add to the profile.

`cluster.config_file.get_profile(profile=None)`  
Return a profile if it exists, if None, return all profiles.

Will return None if profile is supplied but does not exist.

**Profile** The name of a profile to search for.

`cluster.config_file.delete(section, key=None)`  
Delete a config item.

If key is not provided deletes whole section.

`cluster.config_file.get_config()`  
Load defaults from file.

## 10.5 Local Queue Implementation

The local queue implementation is based on the multiprocessing library and is not intended to be used directly, it should always be used via the Job class because it is somewhat temperamental. The essential idea behind it is that we can have one JobQueue class that is bound to the parent process, it exclusively manages a single child thread

that runs the `job_runner()` function. The two process communicate using a `multiprocessing.Queue` object, and pass `cluster.jobqueue.Job` objects back and forth between them.

The Job objects (different from the Job objects in `job.py`) contain information about the task to run, including the number of cores required. The job runner manages a pool of `multiprocessing.Pool` tasks directly, and keeps the total running cores below the total allowed (default is the system max, can be set with the `threads` keyword). It backfills smaller jobs and holds on to larger jobs until there is enough space free.

This is close to what torque and slurm do, but vastly more crude. It serves as a stopgap to allow parallel software written for compute clusters to run on a single machine in a similar fashion, without the need for a pipeline alteration. The reason I have reimplemented a process pool is that I need dependency tracking and I need to allow some processes to run on multiple cores (e.g. 6 of the available 24 on the machine).

The `job_runner()` and `Job` objects should never be accessed except by the `JobQueue`. Only one `JobQueue` should run at a time (not enforced), and by default it is bound to `cluster.jobqueue.JQUEUE`. That is the interface used by all other parts of this package.

**class** `cluster.jobqueue.JobQueue` (`cores=None`)

Monitor and submit `multiprocessing.Pool` jobs with dependencies.

**add** (`function`, `args=None`, `kwargs=None`, `dependencies=None`, `cores=1`)

Add function to local job queue.

**Function** A function object. To run a command, use the `run.cmd` function here.

**Args** A tuple of args to submit to the function.

**Kwargs** A dict of keyword arguments to submit to the function.

**Dependencies** A list of job IDs that this job will depend on.

**Cores** The number of threads required by this job.

**Returns** A job ID

**get** (`job`)

Return the output of a single job

**restart** (`force=False`)

Kill the job queue and restart it.

**update** ()

Get fresh job info from the runner.

**wait** (`jobs=None`)

Wait for a list of jobs, all jobs are the default.

**class** `cluster.jobqueue.Job` (`function`, `args=None`, `kwargs=None`, `depends=None`, `cores=1`)

An object to pass arguments to the runner.

`cluster.jobqueue.job_runner` (`jobqueue`, `outputs`, `cores=None`, `jobno=None`)

Run jobs with dependency tracking.

Must be run as a separate `multiprocessing.Process` to function correctly.

**Jobqueue** A `multiprocessing.Queue` object into which Job objects must be added. The function continually searches this Queue for new jobs. Note, function must be a function call, it cannot be anything else. function is the only required argument, the rest are optional. tuples are required.

**Outputs** A `multiprocessing.Queue` object that will take outputs. A dictionary of job objects will be output here with the format:: {job\_no => Job} **NOTE:** function return must be picklable otherwise this will raise an exception when it is put into the Queue object.

**Cores** Number of cores to use in the multiprocessing pool. Defaults to all.

**Jobno** What number to start counting jobs from, default 1.

## 10.6 Logme

This is a package I wrote myself and keep using because I like it. It provides syslog style leveled logging (e.g. 'debug'->'info'->'warn'->'error'->'critical') and it implements colors and timestamped messages.

The minimum print level can be set module wide at runtime by changing `cluster.logme.MIN_LEVEL`.

```
cluster.logme.log(message, level='info', logfile=None, also_write=None, min_level=None,
                  kind=None)
```

Print a string to logfile.

**Message** The message to print.

**Logfile** Optional file to log to, defaults to STDERR. Can provide a logging object

**Level** 'debug'|'info'|'warn'|'error'|'normal' Will only print if level > MIN\_LEVEL

'debug':	'<timestamp> DEBUG -> '
'info':	'<timestamp> INFO -> '
'warn':	'<timestamp> WARNING -> '
'error':	'<timestamp> ERROR -> '
'critical':	'<timestamp> CRITICAL -> '

**Also\_write** 'stdout': print to STDOUT also. 'stderr': print to STDERR also. These only have an effect if the output is not already set to the same device.

**Min\_level** Retained for backwards compatibility, min\_level should be set using the logme.MIN\_LEVEL constant.

**Kind** synonym for level, kept to retain backwards compatibility

## 10.7 Other Functions

Some other wrapper functions are defined in `run.py`, these are just little useful knick-knacks that make function submission and queue management possible.

```
cluster.run.cmd(command, args=None, stdout=None, stderr=None, tries=1)
```

Run command and return status, output, stderr.

**Command** Path to executable.

**Args** Tuple of arguments.

**Stdout** File or open file like object to write STDOUT to.

**Stderr** File or open file like object to write STDERR to.

**Tries** Int: Number of times to try to execute 1+

**Returns** exit\_code, STDOUT, STDERR

```
cluster.run.which(program)
```

Replicate the UNIX which command.

**Taken verbatim from:** [stackoverflow.com/questions/377017/test-if-executable-exists-in-python](http://stackoverflow.com/questions/377017/test-if-executable-exists-in-python)

**Program** Name of executable to test.

**Returns** Path to the program or None on failure.

`cluster.run.open_zipped(infile, mode='r')`

Open a regular, gzipped, or bz2 file.

Returns text mode file handle.

If `infile` is a file handle or text device, it is returned without changes.

`cluster.run.split_file(infile, parts, outpath='', keep_header=True)`

Split a file in parts and return a list of paths.

NOTE: Linux specific (uses `wc`).

**Outpath** The directory to save the split files.

**Keep\_header** Add the header line to the top of every file.

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