FIMM Atlas Cluster

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Start

official guideline

1. Get rights for accessing services:

- General account: Go to https://userportal.giu.fi/
- Access to special service, like `sisu_impute.q`: Contact Olle Hansson (olle.hansson@helsinki.fi)
- Access to different data folders: Contact Jarmo Harju

2. Connect to Atlas:

- Server: `atlas.fimm.fi`
- Command line: `ssh <username>@atlas.fimm.fi`
- Windows: Using ssh clients, like `Putty`.

3. Transfer files

- local to remote: `scp /path/to/local_file username@atlas.fimm.fi:/path/to/remote_file`
- remote to local: `scp username@atlas.fimm.fi:/path/to/remote_file /path/to/local_file`
- Windows: Using SCP servers, like `WinSCP`

Environment

Nodes

1. Login node

- Do:
  - File operations (copy, edit, create, move, etc).
  - Submit jobs to cluster nodes.
  - Monitor the status of jobs on cluster nodes.
  - Login interactive node: `qlogin -q interactive.q`
- Don't:
  - Run intensive tasks.

2. Interactive node

- Do:
  - Run interactive tasks, like running R codes in R console.
- Don't:
  - Submit jobs to cluster nodes.
  - Run time-consuming tasks, because you have to connect with server during the processing.

3. Cluster node

- Do:
  - Run user submitted jobs.
  - Automatic *queue* system for allocating jobs.

Queues

- express.q: mem < 2G, timeout limmit 90 min;
- all.q: mem < 2G;
- medmem.q: mem 2-5G;
- highmem.q: mem 5-10G;
- hugemem.q: mem 10-20G.

Job management commands

1. Submit queue (Run in `login node`)

1. `qsub <option> <command>`

Options:

- Basic setting:
  - `-A <username>`: add the job to your own queue;
  - `-N <job_name>`: informative name for later job status lookup;
  - `-q <queue_type>`: select the type of queue;
- Job specific setting:
  - `-l h_vmem=<n>G`: specify hard limit on memory;
  - `-l h_rt=hh:mm:ss`: specify hard limit on runtime;
  - `-b <y/n>`: `y`, run binary code;`n`, run non-binary codes (like shell script);
  - `-shell n`: do not create a new bash shell but run the command immediately;
  - `-c n`: no checkpoint performed;
  - `-V`: export all active environment variables to the job;
  - `-w e`: validate the submission. If error stop immediately;
- Output setting:
  - `-e /path/to/error_log_file/`: set the file for error log;
  - `-o /path/to/basic_log_file/`: set the file for output log.

2. `grun.py`: a queue submit wrapper

Options:

- `-h` or `--help`: show help message;
- Basic setting
  - `-c <command>` or `--command <command>`: set the commands that will run on cluster nodes. Wrap your command with `"`;
  - `-n <name>` or `--name <name>`: set the name of the jobs;
  - `-q <queue_type>` or `--queue <queue_type>`: select the type of queues;
  - `-l` or `--list`:
  - `-N <nodes>` or `--nodes <nodes>`: specify nodes;
- Notation setting:
  - `-M`:
    - `<your.email@provider.fi>`: set the email for receive the notations;
    - `n`: don't send any mails.
  - `-m <mail>` or `--mail <mail>`:
    - `a`: send mail if jobs aborts/fails;
    - `b`: send mail when jobs begin;
    - `e`: send mail when jobs end;
    - `n`: don's send any mails.
- Other setting:
  - `-L <logdir>` or `--log-dir <logdir>`

- `-s <sync>` or `--sync <sync>`
- `-S <slots>` or `--slots <slots>`
- `-R [<resources> [<resources> ...]]` or `--resources [<resources> [<resourses> ...]]`
- `--hold-jid [<hold_jid> [<hold_jid> ...]]`

You can add default set for sending mails in file `/homes/<username>/.grun.ini`

2. Monitor the jobs and node

1. Query job status with `qstat`

Options:

- `-u <username>`: check all your current running jobs
- `-j <job_id>`: check a specific job.
- `-g c`: check queues usage

2. Delete submitted jobs with `qdel`

Options:

- `-j <job_id>`: kill job by its ID;
- `<job_name>`: kill job by its name;

3. Monitor global environment with `qhost`

Option:

- : Without option it will show the nodes information of the cluster
- `-j`: It will show all nodes and **all** jobs currently running on the cluster