HPC Workshop

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Information on the Web

This presentation

https://github.com/Astrophysics-UCL/HPCInfo/

Splinter on the UCL Astrophysics Wiki

https://wiki.ucl.ac.uk/display/PhysAstAstPhysGrp/Splinter+User+Guide

UCL Research Computing Platforms

https://wiki.rc.ucl.ac.uk/wiki/Main_Page

DiRAC

http://www.dirac.ac.uk/

Mailing list

`https://www.mailinglists.ucl.ac.uk/mailman/listinfo/splinter-users`

- please subscirbe
- post any issues regarding splinter

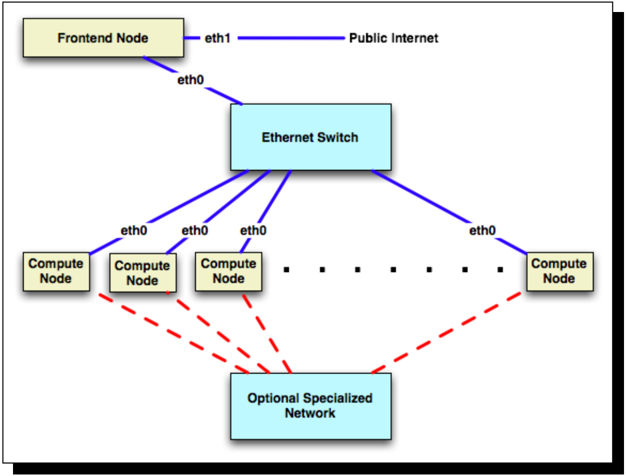
What will you learn?

- Running your programs in HPC machines
- Best practices

Splinter specs

- As of October 22, 2015, *Splinter* has 528, 4TB memory
- 8 nodes, dual 6-core 2.8GHz, 48GB memory
- 20 nodes, dual 8-core 2.0GHz, 128GB memory
- SMP node, 40 2.4GHz cores, 1TB memory
- login node, dual 10-core, 2.4GHz 98GB memory
- head-node, dual 8-core, 2.4GHz, 164GB memory

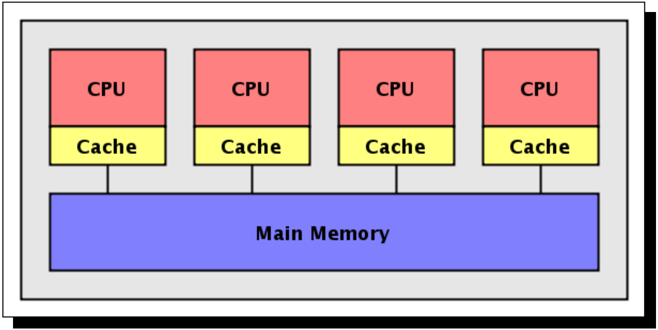
SPLINTER distributed



[1]

[1] http://www.rocksclusters.org/

SPLINTER shared



[2]

[2] http://www.cs.rit.edu/

Workspaces I

/home/user_name

- this is your home directory
- login scripts can be put here
- 1GB quota
- private

/share/splinter/user_name

- create the directory if not already there
- can be used as a workspace
- no quota
- public unless made private

Workspaces II

`/share/data1`

- for storing large data
- you can create a directory for your, .e.g, `/share/data1/SKA`

`/share/apps`

- for installing software
- module-files

Login script

- everytime you login this file will be executed
- this file is in your $HOME
- it is called .login
- you can load modules, envvars, etc.

example

```
# load my aliases
source ~/alisas.csh

# load python
module load dev_tools/nov2014/python-anaconda
```

Modules

- easy and flexible way use software
- available to everyone in splinter

commands

```
# print the available modules
module avail
# load a module
module load module_name
# list the loaded modules
module list
# unload a module
module unload module_name
# unload all modules
module purge
# help
module --help
```

Submitting jobs

- computing jobs should be submitted to the scheudler
- you will have to write a job script
- interactive job

commands

```
# submit a job
qsub job_script
# sumit an interative job
qsub -I
# check the status of a job
checkjob job_id
# list the status of all jobs
qstat
# show the queue
showq
# delete a job
qdel job_id
```

Queues

- `compute`
- `cores16`
- `cores12`
- `smp`

Structure of a job script

```
#!/bin/tcsh
#PBS -q cores12
#PBS -N a_name_for_your_job
#PBS -l nodes=1:ppn=6
#PBS -l mem=32gb
#PBS -l walltime=120:00:00

# set some environment variables
setenv OMP_NUM_THREADS 6

# source paths if needed
source /home/sbalan/libpaths.csh

# run my program
/home/sbalan/hello.exe
```

Jobscripts: things to remember

- Submit the job to the right queue
- Request the correct number of `nodes` and `ppn`
- Specify the memory required
- Always specify the walltime
- If your program is not parallel, please use `nodes=1,ppn=1`
- Use `-q compute` for single processor jobs
- Use `qsub -I` for interative job
- If using most of the resources, please send an email to the mailing list.

More PBS commands

```
# spcify output
#PBS -o path/to/file.out

# specify error output
#PBS -e path/to/file.err

# mail alert at (b)eginning, (e)nd and (a)bortion of
    execution
#PBS -m bea

# send mail to the following address
#PBS -M your_email_id@ucl.ac.uk
```

Using *Gaglia*

`http://splinter.star.ucl.ac.uk/ganglia/`

- is tool for analysing splinter
- can only be loaded from splinter (using firefox)
- will give you load/memory information
- can look into nodes

Collaborative projects

- collaboration between two splinter users
- can share common data in `/share/data1/my_collaboration`
- give read/write permission to other users using `chmod`

Best practices

- Choose the machines that are suited for your problem
- Read the User Guide
- Do not run your programs in the login node
- Install common software locally if and only if absolutely necessary
- Request optimum resouces
- Minimise data transfer between nodes,
- Backup! Backup! Backup!

Exercises

`https://github.com/Astrophysics-UCL/HPCInfo/blob/master/training/workshops_2015/hpc_workshop/exercies/exercises.md`