HPC Cluster intro

Today plan

The presentation is based on the officials HPC-Ghent tutorials

http://users.ugent.be/~kehoste/hpcugent-intro-20171110.pdf

and general manual is under following link (subtitute „linux” with „windows” or „mac” to get tutorial fo your OS)

http://hpcugent.github.io/vsc_user_docs/pdf/intro-HPC-linux-gent.pdf

I will specifically use the information from these chapters from the manual manual:

- 1/ Introduction to HPC

  3/ Connecting to the HPC
- 4/ Running batch jobs
- 6/ Running jobs with input/output data

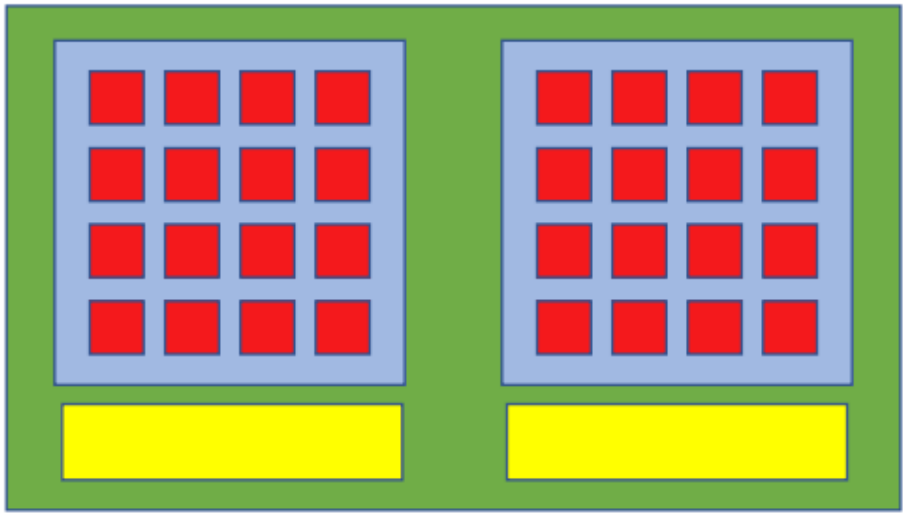
What is High Performance Computing?

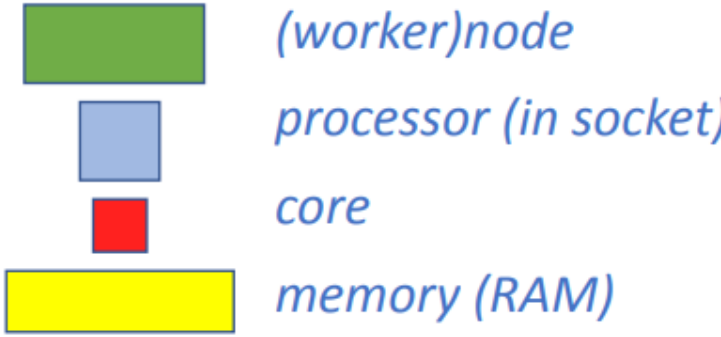
- A computer clusterconsists of a set of loosely or tightly connected computers that work together so that in many respects they can be viewed as a single system.
- harness power of multiple interconnected cores/nodes/processing units

Cores vs processors vs sockets vs nodes

- Modern servers, also referred to as (worker) nodes in the context of hpc,
- include one or more sockets, each housing a multi-core processor (next to memory, disk(s), network cards, …).
- A modern (micro)processor consists of multiple cpus or cores that areu sed to execute computations.

example: node with two 16-core processors





Parallel vs sequential programs

- In parallel software, many calculations are carried out simultaneously. They are based on the principle that large problems can often be divided into smaller ones, which are then solved concurrently ("in parallel").
- Sequential (a.k.a. serial) software does not do calculations in parallel, i.e. it only uses one single core of a single worker node. (Sequential) software does not become faster by just throwing cores at it…
- You can run multiple instances at the same time on a cluster. e.g., you can easily run a Python script 20 times at once to quickly analyse 20 datasets

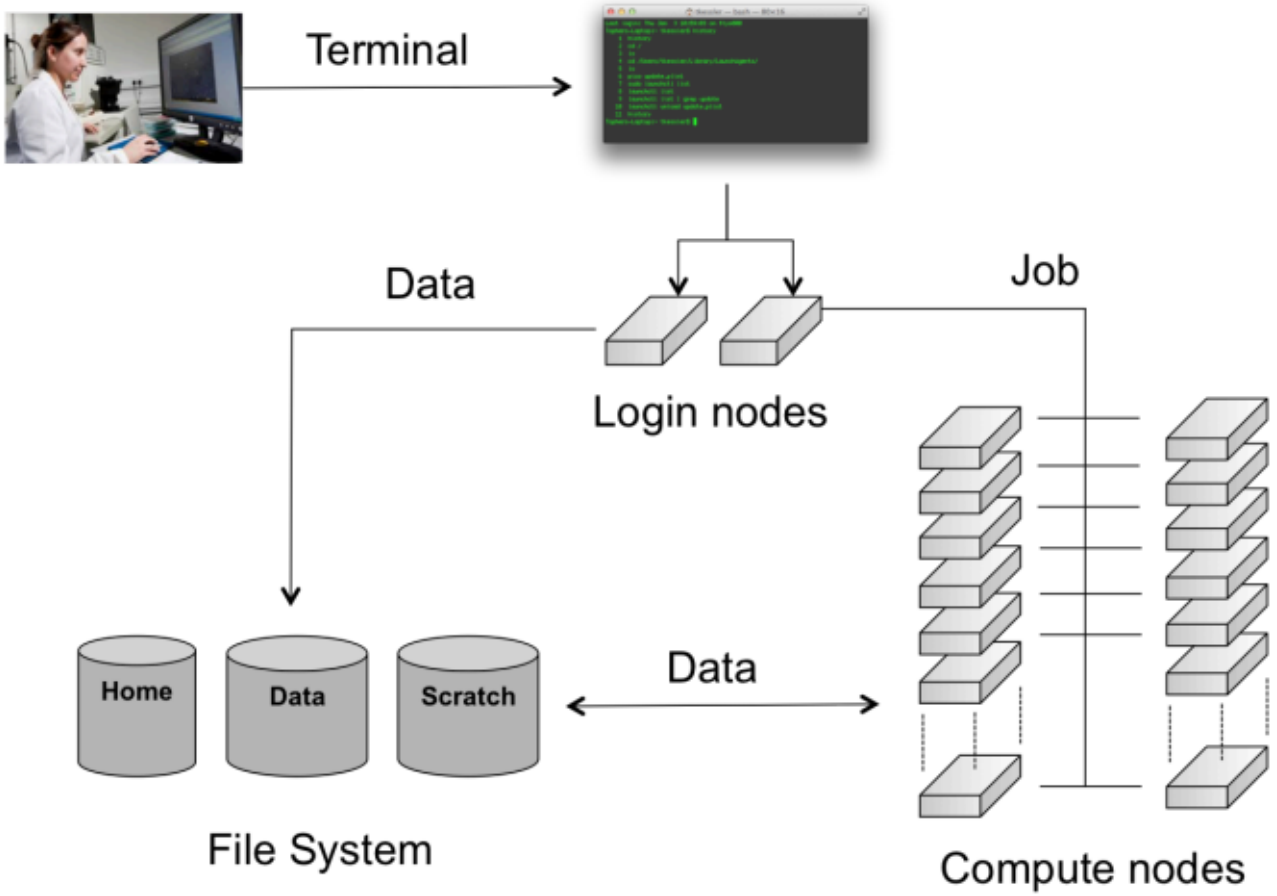
How to login

Use public/private ssh key pairs for user authentication

How to login

- But before login you need to create an account!
- Follow chapter 2 from the manual to create pair of the public/private keys (http://hpcugent.github.io/vsc_user_docs/pdf/intro-HPC-linux-gent.pdf)
- Visit https://account.vscentrum.be/ to register your account
- After filling short form you will be asked to upload you public key through the browser
- Within one day, you should receive a welcome e-mail with your VSC account details.

Running batch jobs



Workflow on HPC infrastructure

1. Connect to login nodes
2. Transfer your files
3. (Compile your code and test it)
4. Create a job script
5. Submit your job
6. Be patient
   - Your job gets into the queue
   - Your job gets executed
   - Your job finishes
7. Move your results

HPC worklfow

- Users interact with the infrastructure via the login nodes
- No direct access to the worker nodes
- Except when a job is running on it!
- Default time (short job) is 1 hour, it cannot be more than 72hours!

Linux intro

- „ls” list the files
- „Pwd” show your current directory
- cd ‘path’ change directory to ‘path’
- cd without parameters move you to your home folder
- use cp to copy files
- use mv to change name or move files

Basic commands

- to login: ssh vsc40000@login.hpc.ugent.be (where vsc40000 have to be your login)
- To list specific module(in example matlab): module av 2>&1 | grep -i -e "matlab"
- module load MATLAB
- module unload MATLAB
- to list all active modules: module list

Running batch jobs

- In order to have access to the compute nodes of a cluster, you have to use the job system.
- The system software that handles your batch jobs consists of two pieces: the queue- and resource manager TORQUE and the scheduler Moab.
- Together, TORQUE and Moab provide a suite of commands for submitting jobs, altering some of the properties of waiting jobs (such as reorderingor deleting them), monitoring their progress and killing ones that are having problems or are no longer needed.

Running batch jobs

- cp -r /apps/gent/tutorials/Intro-HPC/examples ~/examples
- cd ~/examples/Running-batch-jobs
- ./fibo.pl (running program as a script on a login node)
- qsub fibo.pbs (running as a job on a computing node)
- more fibo.pbs.o123456 (look into printed output of a script)
- more fibo.pbs.e123456 (look into errors during execution)

Monitoring and managing your job

- Get status: qstat <jobid> or simply qstat
- qdel <jobid>

  The state S can be any of the following:
- Q The job is queued and is waiting to start.
- R The job is currently running.
- E The job is currently exiting after having run.
- C The job is completed after having run.
- H The job has a user or system hold on

  How long is the queque?
- qstat -q

- Generate your own e-mail notifications (add the following to your script)

  #PBS -m abe

  #PBS -M <your e-mail address>

Example of parameters (resources)

- qsub -l some parameters (walltime=2:30:00)
- nodes=1:ppn=1,mem=2gb)

it could also specified as #PBS-directive

```
#!/bin/bash -l
#PBS -l nodes=1:ppn=1
 #PBS -l mem=2gb
cd $PBS_O_WORKDIR
./fibo.pl
```

Interactive sessions

- Working interactively
- hostname -f
- qsub -I (will wait for assigment of the node)
- hostname -f
- exit

Job scheduling

- No guarantees on when job will start, so plan ahead!

Job priority is determined by:

- historical usage
  - aim is to balance usage over users
  - infrequent/frequent users => higher/lower priority
- requested resources (# nodes/cores, walltime, memory, …)
  - large resource request => lower priority
- time waiting in queue
  - queued jobs get higher priority over time
- user limits
  - avoid that a single user fillsup an entire cluster

Running jobs with input/output data

- cd ~/examples/Running-jobs-with-input-output-data
- qsub file1a.pbs

Pre-defined user directories (substitute to echo $VAR to print your location)

- $VSC_HOME /user/gent/xxx/<vsc-account> (Your home directory)
- $VSC_DATA /data/gent/xxx/<vsc-account>
- $VSC_SCRATCH_NODE
- $VSC_SCRATCH

The quota of disk space and number of files for each HPC user is:

Volume	Max. disk space	Max. # Files
HOME	3 GB	20000
DATA	25 GB	100000
SCRATCH	25 GB	100000

Miscellaneous

- Request software installations via hpc@ugent.be
- Installing itself software is also possible
- Use filezilla (https://filezilla-project.org/) to copy files
- Matlab toolboxes → copy them!
- We could set up a virtual organisation so w can share data with others in our group, and get more storage quota, http://hpc.ugent.be/userwiki/index.php/User:VSCVos
- We could get around the 72h walltime limit for jobs http://hpc.ugent.be/userwiki/index.php/User:Checkpointing
- submitting chains of jobs is also possible

Documentation & training

Documentation is available at:

- https://www.vscentrum.be/en/user-portal
- (http://hpc.ugent.be/userwiki, being phased out)
- HPC tutorial: http://hpcugent.github.io/vsc_user_docs/pdf/intro-HPC-linux-gent.pdf
- Basic Linux: http://hpc.ugent.be/userwiki/index.php/Tips:Introduction_to_Linux