Introduction to HPC Workshop

NeSI Computational Science Team
(support@nesi.org.nz)

Outline

About Us

NeSI : New Zealand eScience Infrastructure

- **NeSI** provides access to New Zealand's HPC facilities and support.
- **NeSI** includes HPC facilities at the **University of Auckland**, **NIWA** and the **University of Canterbury**.
- NZ researchers involved in funded peer reviewed research
  - access to most appropriate site
  - access to expert support services
  - highest priority in the job queue
- Collaborator institutions at each site have default access

About Us

NeSI

New Zealand eScience Infrastructure

THE UNIVERSITY OF AUCKLAND NEW ZEALAND
Te Whare Wānanga o Tāmaki Makaurau

UC UNIVERSITY OF CANTERBURY

NIWA Taihoro Nukurangi

ministry of science + innovation

Manaaki Whenua Landcare Research

UNIVERSITY of OTAGO Te Whare Wānanga o Otāgo NEW ZEALAND

About Us

Computational Science Team

- NeSI's team support researchers to get the most out of our platforms and services.
- The CS Team has a lot of experience in HPC that spans many science domains.
- Collaboratively enhance the performance of research software codes.
  - Troubleshoot memory and other or I/O bottlenecks.
  - Connect researchers and scientific software experts.
  - The team is available to support researchers across any research institution in New Zealand.
- More information at

  `https://www.nesi.org.nz/computational-science-team`.

About Us

Support

- Email `support@nesi.org.nz`
- Creates a support 'ticket' where we can track the history of your request
- You can also arrange to meet us to discuss any issues

Our Facilities

NeSI Facilities

- NeSI provides several kind of HPC architectures and solutions to cater for various needs.
  - Bluegene/P
  - Power6 and Power7
  - Intel Westmere
  - Intel SandyBridge
  - Kepler and Fermi GPU servers
  - Intel Xeon Phi Co-Processor
- Supported applications can run on across several NeSI architectures.
- We can install and study the scalability in all the NeSI resources and find the most suitable environment for your case.
- See NeSI website for facility specs and application details.

Our Facilities

BlueFern Supercomputing Center

- Funded by the **BlueFern, University of Canterbury** with co-investment from the NZ Government through **NeSI**.
- Currently have 8612 CPU cores across 2061 hosts.
- About 9.6 TB of memory and 71.4 TFLOPS (distributed).
- Shared storage of 172 TB with a 3D Torus interconnect and IB network.
- Linux SLES 11SP2 and AIX

Our Facilities

NeSI BlueFern Supercomputing Center

Architecture	**BlueGene/P**	**Power7**
Model	PowerPC 450	P755
Clock Speed	0.8 GHz	3.3 GHz
Cache	8MB	32MB
Cores/socket	4	8
Cores/node	4	32
Mem/node	4GB	128GB
GFLOPS/node	13.6	422.4
# nodes	2048	13

Our Facilities

NIWA Supercomputing Center

- Funded by the **NIWA** with co-investment from the NZ Government through **NeSI**.
- Currently have 3488 CPU cores across 109 hosts.
- About 8.7 TB of memory and 65.57 TFLOPS (distributed).
- Shared storage of 200 TB with a 40 Gbit/s Infiniband network.
- AIX

Our Facilities

NIWA Supercomputing Center (FitzRoy & Barometer)

Architecture	**Power6**	**Power6**
Model	P575	P575
Clock Speed	4.7 GHz	4.7GHz
Cache	32MB	32MB
Cores/socket	16	16
Cores/node	32	32
Mem/node	64,128GB	64GB
GFLOPS/node	601.6	601.6
# nodes	94	15

Our Facilities

NeSI CeR Supercomputing Center

- funded by the **University of Auckland**, **Landcare Research** and the **University of Otago** with co-investment from the NZ Government through **NeSI**.
- Currently have around 5,000 Intel CPU cores across about 300 hosts.
- About 35 TB of memory and 80 TFLOPS (distributed).
- Shared storage of 200 TB with a 40 Gbit/s Infiniband network.
- Linux RHEL 6.3

Our Facilities

NeSI Pan Cluster

Architecture	Westmere	SandyBridge	LargeMem
Model	X5660	E5-2680	E7-4870
Clock Speed	2.8 GHz	2.7 GHz	2.4GHz
Cache	12MB	20MB	30MB
Intel QPI speed	6.4GT/s	8 GT/s	6.4GT/
Cores/socket	6	8	10
Cores/node	12	16	40
Mem/node	96GB	128GB	512GB
GFLOPS/node	134.4	345.6	384.0
# nodes	76	194	4

Our Facilities

NeSI Pan Cluster - Co-Processors

Architecture	Nvidia Fermi	Nvidia Kepler	Intel Phi
Main CPU	X5660/E5-2680	E5-2680	E5-2680
Model	M2090	K20X	5110P
Clock Speed	1.3GHz	0.732GHz	1.053GHz
Cores/Dev.	512	2688	60 (240)
Dev./node	2	2	2
Mem/Dev.	6GB	6GB	8GB
TFLOPS/Dev	1.33	1.17	1.01
# nodes	16	5	2

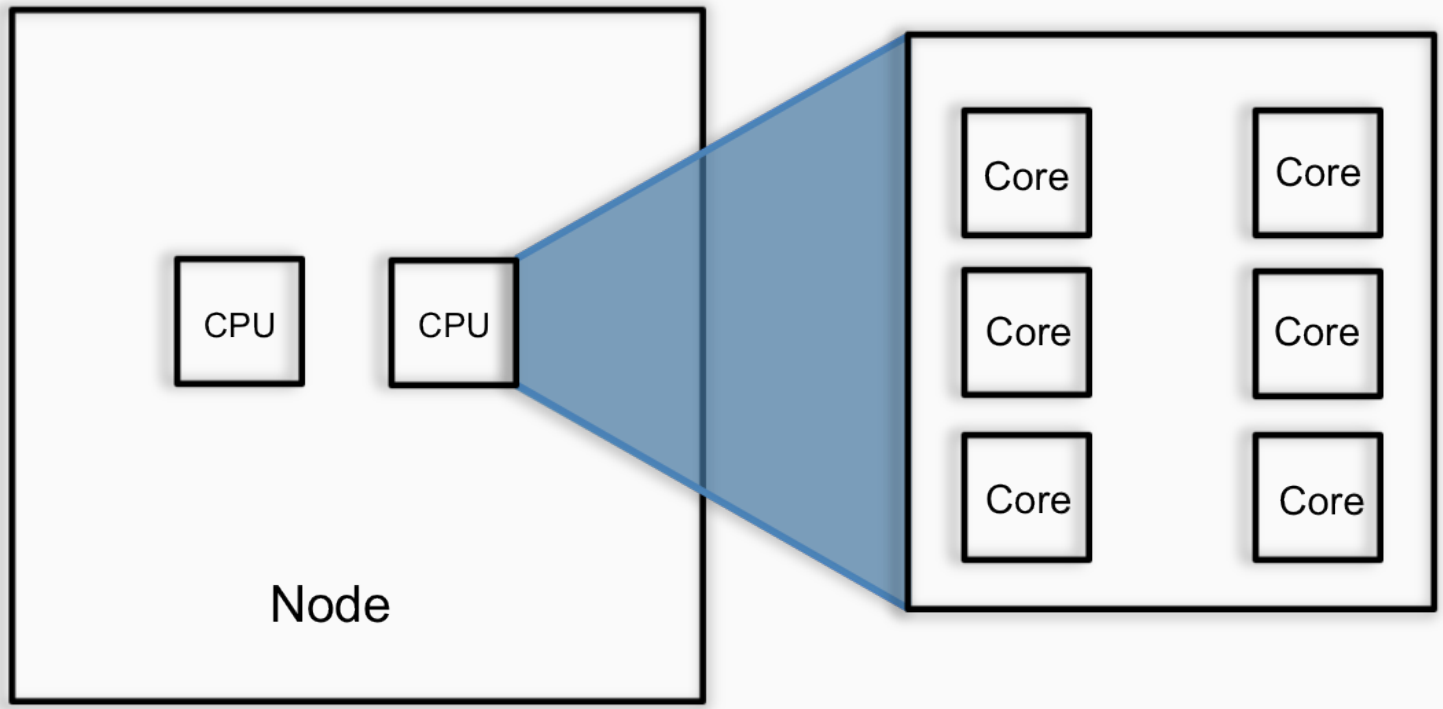
Key Concepts

What is a cluster

- A cluster is a network of computers, sometimes called nodes or hosts.
- Each computer has several processors.
- Each processor has several cores.
- A core does the computing.
- If your application uses more than one core, it can run faster on our cluster.

Key Concepts

HPC node overview



Key Concepts

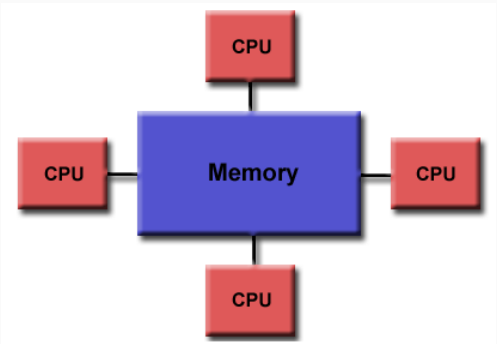
Parallel Programming

- There are several ways to make a program use more cores and hence run faster.
- Many scientific software applications will be able to use multiple cores in some way. But this is often done explicitly by the user, not automagically.
- We can help you improve the performance of your code or make better use of your application.

Key Concepts

Shared Memory

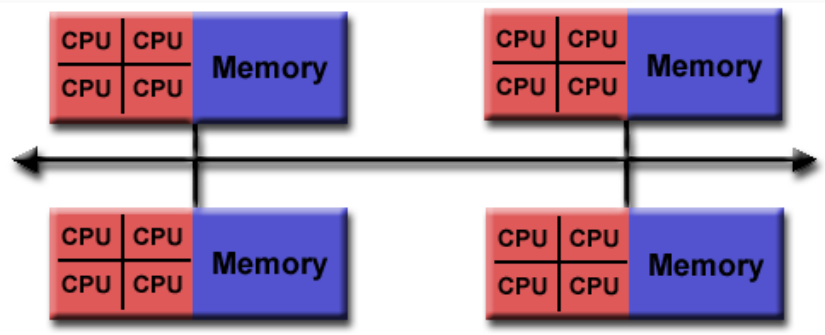
- Symmetric multiprocessing (SMP) : two or more identical processors are connected to a single shared main memory.
- This shared memory may be simultaneously accessed by single program using multiple threads.
- There are different frameworks for utilizing SMP capabilities.



Key Concepts

Distributed Memory

- Multiple-processor computer system in which each process has its own private memory.
- Computational tasks can only operate on local data.
- If remote data is required, the computational task must communicate with one or more remote processors.
- The most popular parallel programming paradigm is MPI.



Key Concepts

Useful Quick References

- VI Quick Reference
- BASH Quick Reference
- Linux Quick Reference
- OpenMP Fortran Syntax
- OpenMP C/C++ Syntax
- MPI Quick Reference

Using the Cluster

Overview

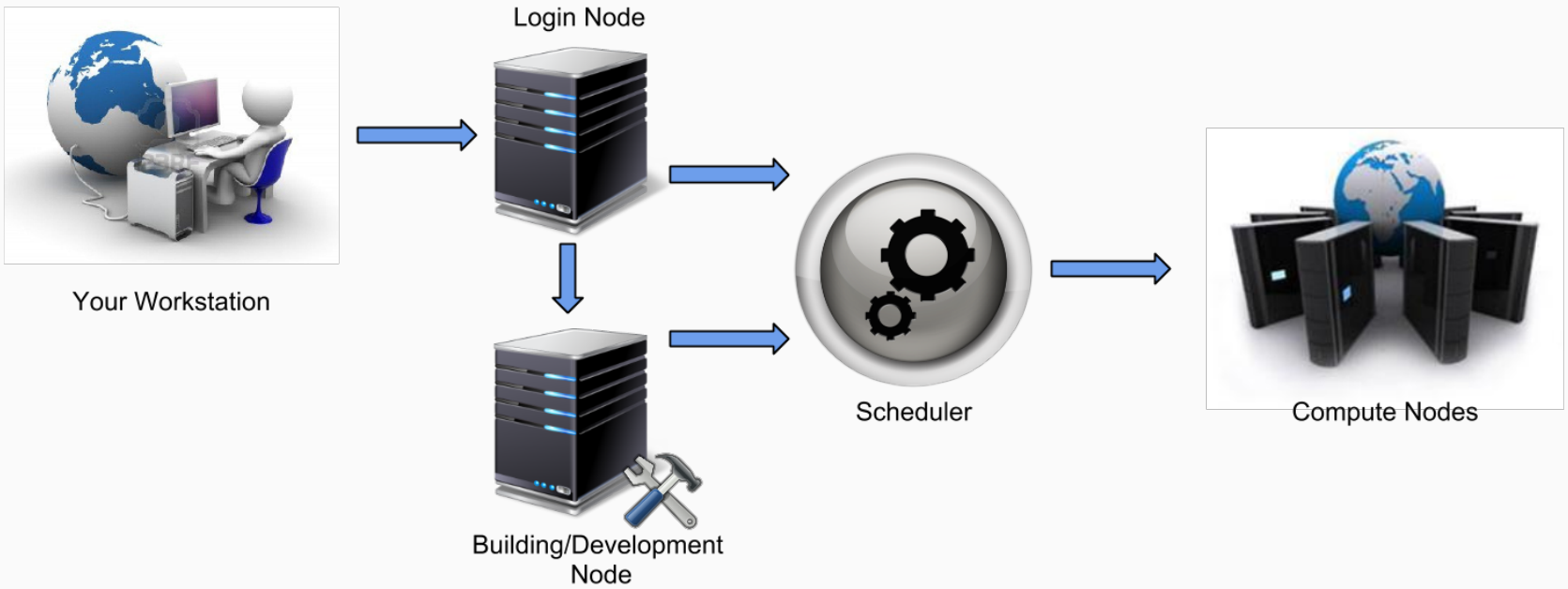
- The cluster is a shared resource and work must be scheduled.
- Jobs are queued by LoadLeveler (LL) and are executed on the compute nodes.
- The login node is not for running jobs, it is only for file management and job submission.

Compiling and Testing Software

- In each NeSI facility you will find building/development nodes.
- We have the most up to date development tools ready to use.
- You can build and test your software and then submit a job.

Using the Cluster

Using the cluster



What to Expect

Suitable Work

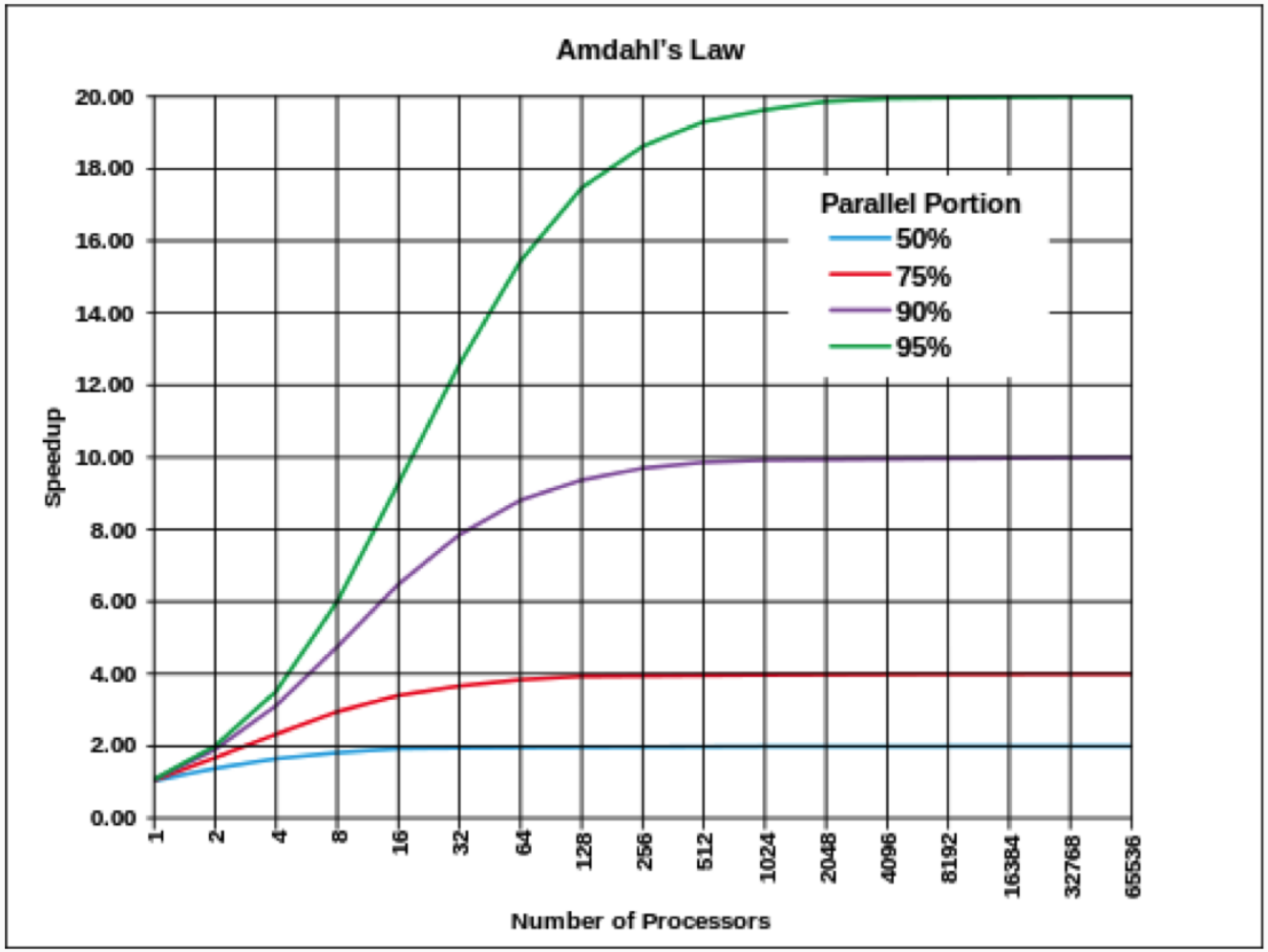
- Not all work is suitable for our HPC facilities (e.g. interactive work)
  - Suitable work includes
  - Problems that can be solved with parallel processing
  - Problems that consume large amounts of memory
  - Problems that render your desktop useless for long periods of time

What to expect

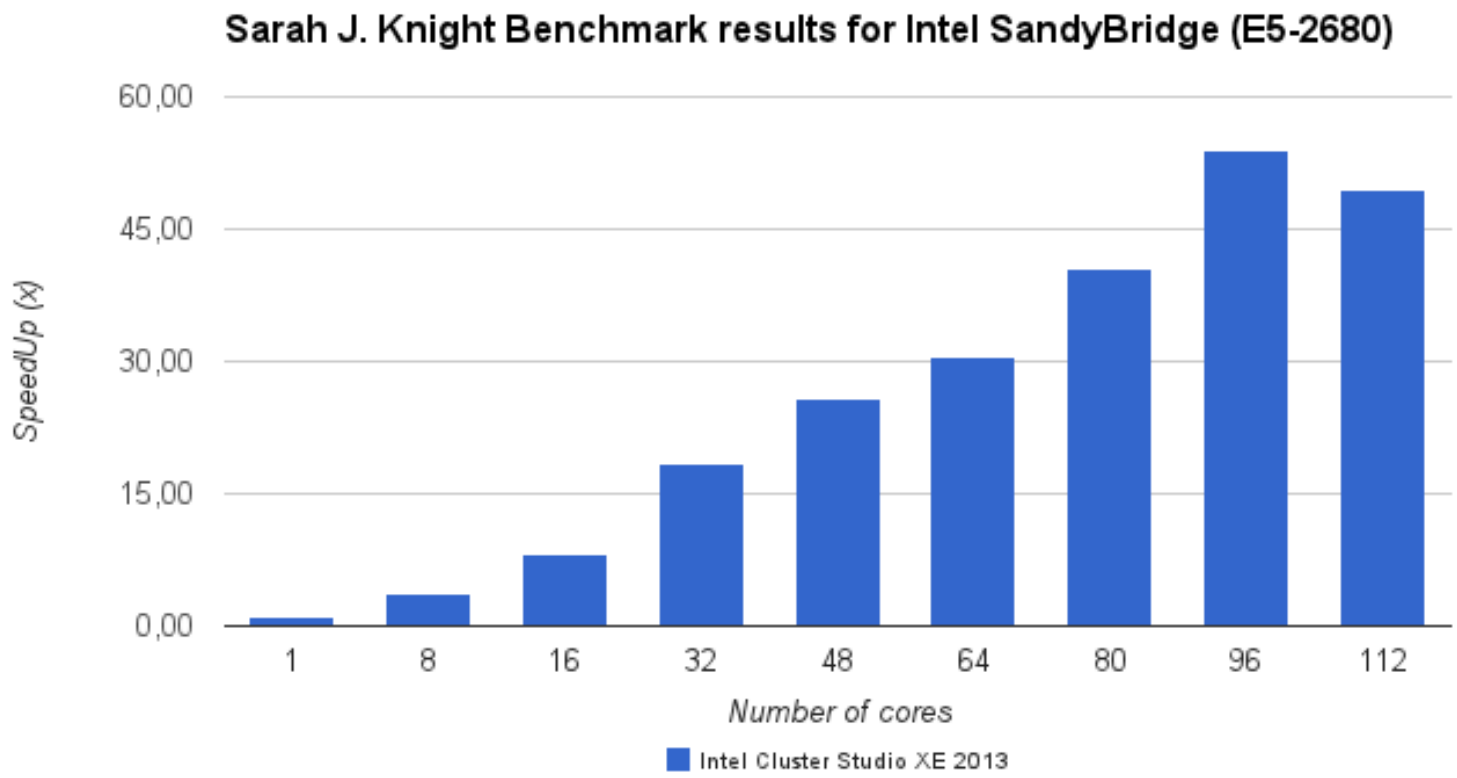
Suitable Work

- Some problems are 'embarrassingly parallel' i.e. it is trivial to divide the problem and solve independently.
  e.g. run simulation with 1000 different initial conditions
- Approximately linear speedup
- Other problems have dependencies, they cannot be separated
  e.g. simulate the weather
- Speed up depends what % of the program runtime can be parallelised

Amdahl's Law


Amdahl's Law
Speedup
20.00
18.00
16.00
14.00
12.00
10.00
8.00
6.00
4.00
2.00
0.00
Parallel Portion
50%
75%
90%
95%
1
2
4
8
16
32
64
128
256
512
1024
2048
4096
8192
16384
32768
65536
Number of Processors

Real Case: more cores ≠ more speed



Using the Cluster

Data

- You need to upload data to the login node for use on the cluster
- Home directory has limited quota space, but more can be requested.
- Not an archive or long term storage
- Backup important data elsewhere and download results after your job is finished
- Files on the login node are shared across to the build and compute nodes

Using the Cluster

Suggested Terminal Clients

Each terminal client has it's own way of using the Secure Shell (SSH) protocol

- Windows: mobaxterm
- MacOSX: Terminal(Included in the OS), iTerm2
- Linux: Konsole, GnomeTerminal, yakuake

On Unix based systems you need to do something like:
ssh myuserid@LOGINNODE

Using the Cluster

Each NeSI Supercomputing Center has one or more Login Nodes

- **Bluefern**
  - kerr.canterbury.ac.nz which is the AIX unix login node.
  - beatrice.canterbury.ac.nz which is the SUSE linux login node.
  - foster.canterbury.ac.nz which is the BlueGene/P login node
  - popper.canterbury.ac.nz which is the Visualization Cluster login node.
- **NIWA**
  - fitzroy.nesi.org.nz which is the AIX unix login node.
- **CeR**
  - login.uoa.nesi.org.nz which is the RHEL Linux login node.

Using the Cluster

Remote File System Access

In order to access the file system (/home) remotely from your machine, we recommend:

- **Konqueror** (KDE) : type fish://user@host:port
- **Nautilus** (Gnome) : type sftp://user@host:port
- **mobaxterm** (Windows) : mobaxterm
- **SSHFS** (MacOSX) : `http://code.google.com/p/macfuse/`
- **SSHFS** (Linux) : `http://fuse.sourceforge.net/sshfs.html`
- **SSHFS** (Windows) : `http://code.google.com/p/win-sshfs/`

Submitting a Job

Documentation

- Center specific documentation:
  - Bluefern : `http://wiki.canterbury.ac.nz/display/BlueFern`
  - NIWA : `http://teamwork.niwa.co.nz/display/HPCF/NIWA+HPCF+User+Documentation`
  - CeR : `http://wiki.auckland.ac.nz/display/CERES/`
- Examples for submitting jobs are on our Wiki page
- See the "Getting Started section"
- Take a look to the Quick Reference Guide. `http://goo.gl/ytbRWy`
- You will also find links to available software on the cluster

Submitting a Job

Basic Job Properties

- **Name** So you can identify it later
- **Job Type** How many processes and how many threads?
- **Walltime** How long the job can run for. The job will be cancelled if the walltime is exceeded.
- **Memory** How much memory to use? Job will die if memory is exceeded
- **CPU cores** How many to use? Your program may try to use more than you request e.g MATLAB
- **Account or Group information** Especially important for access to licensed software and funded research allocations
- **Emails** Notification of job starting, also scheduler errors.

Submitting a Job

Two main tools for submitting a job

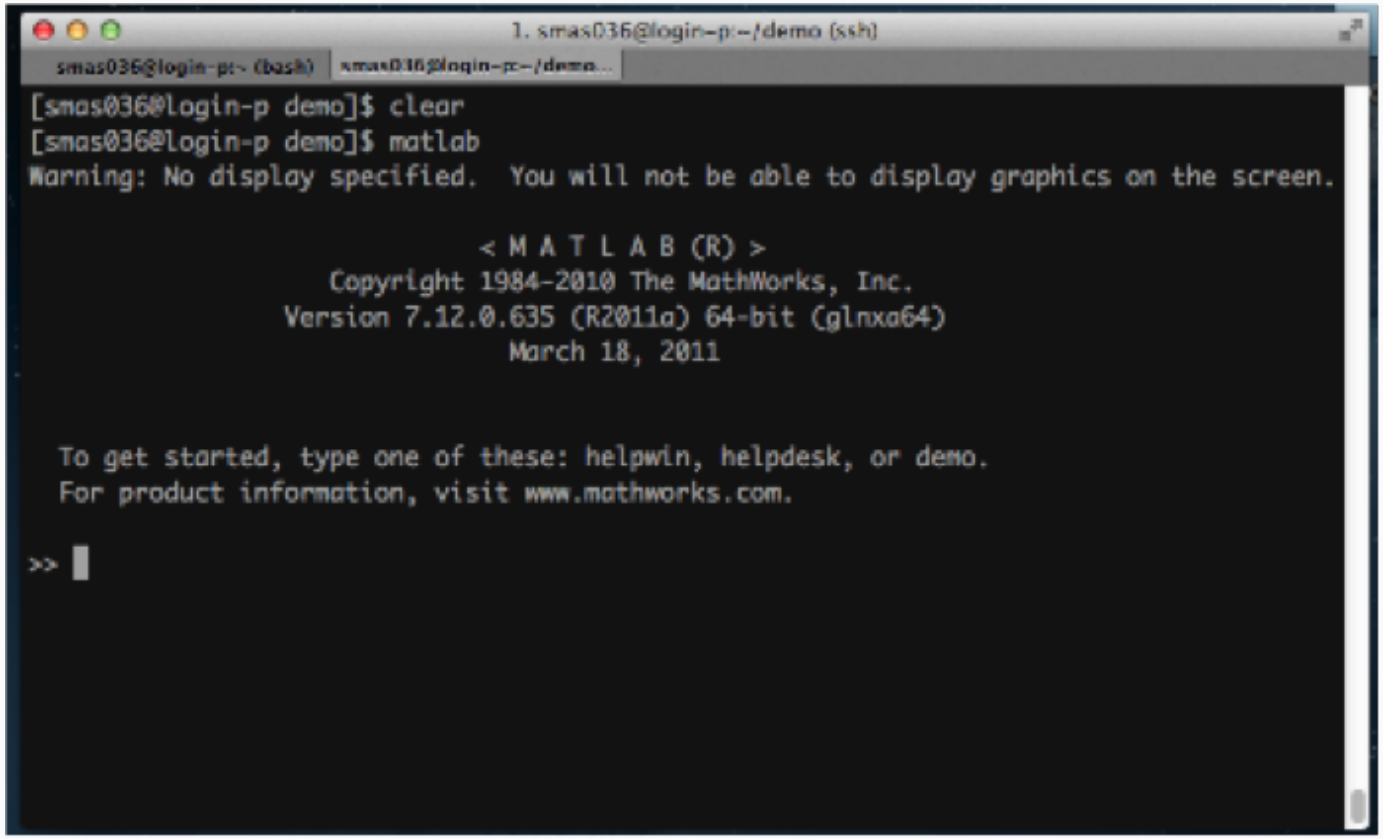
- LoadLeveler – for people comfortable with the Linux command line
- Grisu Template Client – for a graphical interface

Which one to use? In general

- LL for complex workflows or large numbers of jobs
- Grisu for simple workflows or few jobs

Submitting a Job

Outputs



Jobs have no interactive interface, only command line output, but graphical tools are available on the login and build/development

Submitting a Job

Outputs

- Since there is no interactive terminal to display output, output it is written to a text file
- Standard output goes to stdout, standard error goes to stderr
- These should have unique names for a given job directory
- If your application writes to other files e.g. output data, that stays the same
- When your job fails, first look at stdout and stderr for clues

Submitting a Job

Quick Intro to Grisu

- Cross platform Java client: Windows, Mac, Linux
- Grisu interfaces with LoadLeveler to submit and monitor jobs
- Basic workflow:
- Login
- Set requirements
- Attach files
- Submit job
- Wait . . . check status
- Download results

Submitting a Job

Quick Intro to LoadLeveler

- You need to access the login node and work from a terminal
- Requires working knowledge of Linux command line:
  - How to navigate file system and edit files
  - Shell scripting is very useful for automation
  - Tutorials available online at Software Carpentry – computing basics aimed at researchers

Submitting a Job

Setup a Job Description

Can use macros in job attributes

```
e.g. #@ output = $(job_name).$(jobid).out
```

MPI jobs

```
#@ job_type = MPICH | parallel
#@ total_tasks = 16
#@ blocking = 4 | unlimited
```

Submitting a Job

Setup a Job Description

GPUs

```
#@ resources = ... GPUDev(1)
```

Specific architectures

```
#@ requirements = (Feature==‘‘sandybridge’’)
#@ requirements = (Feature==‘‘Kepler’’)
```

Submitting a Job

```
#!/bin/bash
# Optimized for run parallel job of 12 Cores in NeSI (Pandora-westmere)
#################################################################################
#@ job_name = Gaussian
#@ class = default
#@ notification = never
#@ group = nesi
#@ account_no = uoa
#@ wall_clock_limit = 1:00
#@ initialdir = $(home)
#@ output = $(home)/$(job_name).txt
#@ error = $(home)/$(job_name).err
#@ job_type = serial
#@ resources = ConsumableMemory(2048mb) ConsumableVirtualMemory(2048mb)
#@ parallel_threads = 12
#@ environment = COPY_ALL,OMP_NUM_THREADS=12
#@ queue
#################################################################################
module load g09/C.01
cd $SCRATCH_DIR
cp -r $HOME/Gaussian/h2o_opt.dat .
setenv GAUSS_SCRDIR $SCRATCH_DIR
###  Run the Parallel Program
g09 < ./h2o_opt.dat > h2ol_opt.log
###  Transfering the results to the home directory ($HOME)
cp -pr $TMP_DIR $HOME/results/
```

Submitting a Job

```
#!/bin/bash
# Optimized for run parallel job of 512 Cores at NeSI (Pandora-SandyBridge)
#################################################################################
#@ job_name = LAMMPS_TEST
#@ class = default
#@ group = nesi
#@ notification = never
#@ account_no = uoa
#@ wall_clock_limit = 00:30:00
#@ resources = ConsumableMemory(4096mb) ConsumableVirtualMemory(4096mb)
#@ job_type = MPICH
#@ blocking = unlimited
#@ node_usage = not_shared
#@ output = $(job_name).$(jobid).out
#@ error = $(job_name).$(jobid).err
#@ requirements = (Feature=="sandybridge")
#@ initialdir = /share/src/LAMMPS/lammps-12Aug13/bench
#@ total_tasks = 512
#@ queue
#################################################################################
module load lammps/12Aug13-sandybridge
cd $SCRATCH_DIR
cp /share/test/LAMMPS/* .
###  Run the Parallel Program
export OMP_NUM_THREADS=1
MPIRUN lmp_mpi -var x 20 -var y 20 -var z 20 -in in.lj > lj-512.out
###  Transfering the results to the home directory ($HOME)
cp -pr $SCRATCH_DIR $HOME/OUT/lammps/
```

Submitting a Job

Environment Modules

- Modules are a convenient way to provide access to applications on the cluster
- They prepare the environment you need to run the application
- Commands
  - **module avail** - lists available modules
  - **module show module_name** - displays full information about the module with name *module_name*.
  - **module load module_name** - loads the module with name *module_name* and its dependencies.
  - **module unload module_name** - unload the module with name *module_name* and its dependencies.
  - **module list** - list all modules currently loaded.
- Grisu loads a module when you select an application

Submitting a Job

LoadLeveler

- To submit a job
  llsubmit myjob.ll
- To monitor a job
  llq –u “myuserid”
- Shows job id and status – R, I, etc
- To cancel
  llcancel “jobid”

Submitting a Job

Notes for Windows Users

- Be careful of Windows end of line (EOL) characters, sometimes Linux will not handle them correctly
- Notepad++ lets you convert between Windows and Unix style line endings
- Even though you can avoid using the Linux command line, having a basic understanding will help you debug your jobs

Submitting a Job

Software

- We have many specialised software packages.
- Best way to see what we have is by checking the wiki.
- The Wiki also has a software section
- We can install software that you need, but . . .
  - It must run on Linux
  - It must run in batch mode – no user interaction
  - You must have the required licenses
  - You can install software in your home directory if it is really esoteric

Submitting a Job

Best practices and advice

- Share with us a short test and we will study the scalability of your application.
- Try to be accurate with the walltime, it will help to the LL to schedule the jobs better.
- Be aware that you are sharing resources with other researchers.
- If you need to run a test for a long time (>2h) use tLL.
- A wrong memory request or a wrong job description setup can potentially affect others.
- If we find some case like that, we may be forced to cancel the job with this behaviour and inform the owner by email.

Our Expectations

Our Expectations

- We have an acceptable use policy that follows the NeSI IT policies
- We conduct regular reviews of projects to :
  - see how you are going and if you could use some help
  - collect any research outputs from your work on our facility
  - determine how the cluster has helped your research
  - look at the potential for feature stories on your work
- Please contact us if you have any questions
- Please acknowledge us in your publications

Questions & Answers