Introduction to HPC Workshop

Center for eResearch
(eresearch@nesi.org.nz)

Outline

About Us

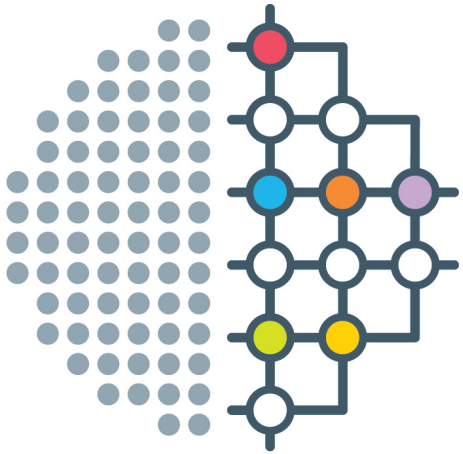
CeR: Center for eResearch

- Part of the University of Auckland
- User support and system maintenance

NeSI : New Zealand eScience Infrastructure

- **NeSI** provides
  - high performance computing
  - a national data storage and sharing service
  - expert support, including engineering
  - single-sign on across the NZ research sector

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

- We 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.

About Us

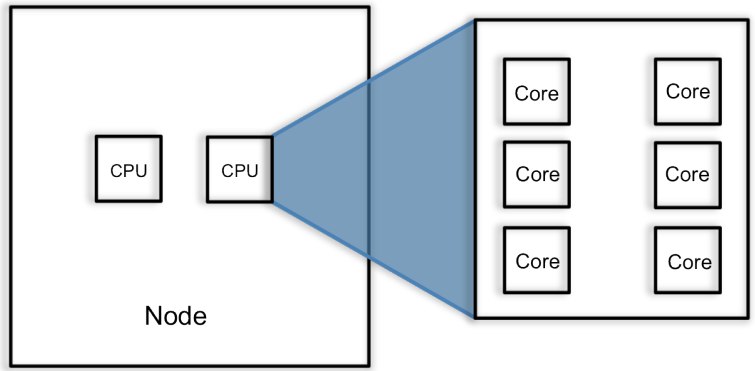
Support

- Email `eresearch@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

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

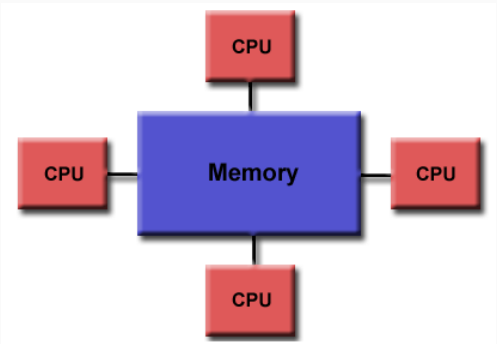
Parallel Programming

- 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

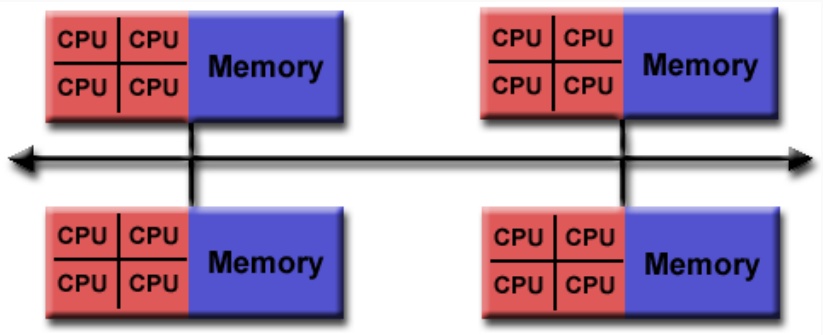
- Symmetric multiprocessing (SMP) : two or more identical processors are connected to a single shared main memory.
- This shared memory may be simultaneously accessed by single program using multiple threads.
- There are different frameworks for utilizing SMP capabilities.



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 (Message Passing Interface).



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

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 3.5 TB of memory and 80 TFLOPS (distributed).
- Shared storage of 400 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

What to expect

Suitable Work

- 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.

Less suited

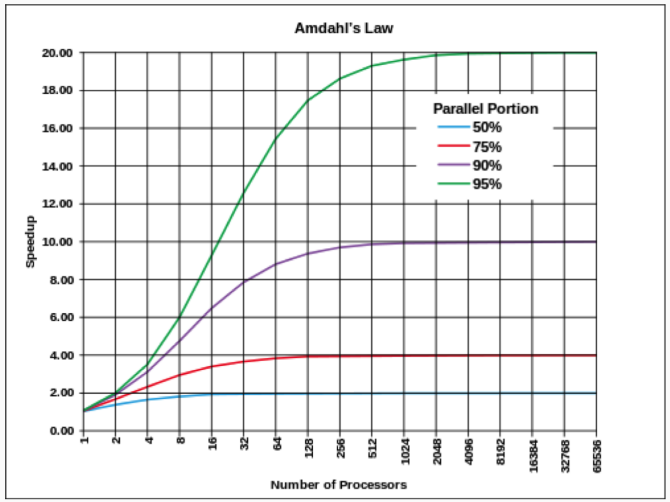
- Windows only software $\mapsto$ Aspirational Research Virtual Machine Farm.
- Interactive software, e.g. GUI, only available for development.

What to expect

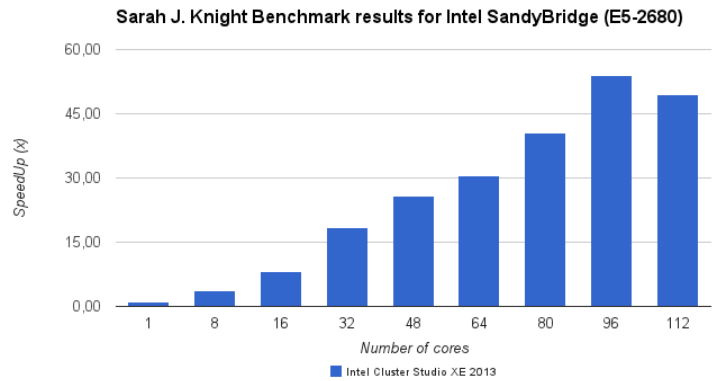
Suitable Work

- 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



Real Case: more cores ≠ more speed

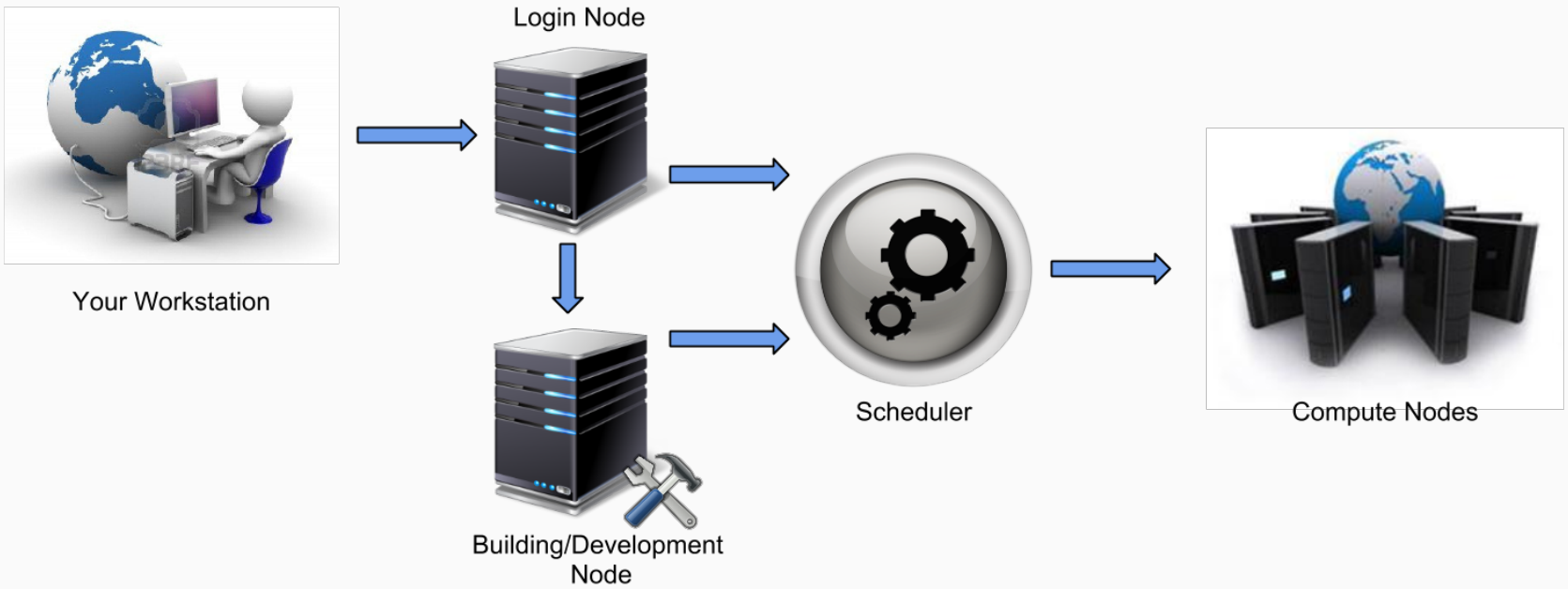


Parallel execution time

- Single core computation time: computation only.
- Parallel computation time: computation + communication + waiting.
- E.g.
  - writing results (to one file) is often a bottleneck.
  - Small problem on many cores: communication cost will dominate.
  - Unbalanced load: one core will mainly wait on the other.
- Conclusion: Test which number of cores is best suited for your problem.

General overview

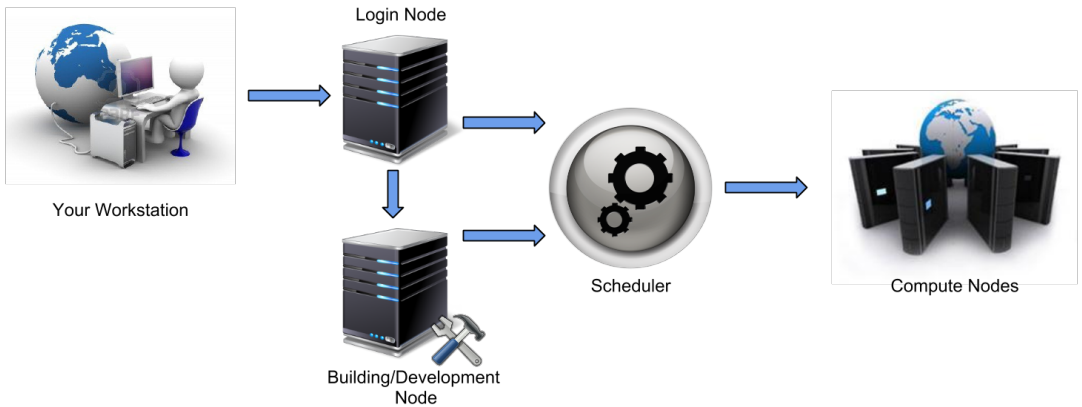
Using the cluster



Using the Cluster

Overview

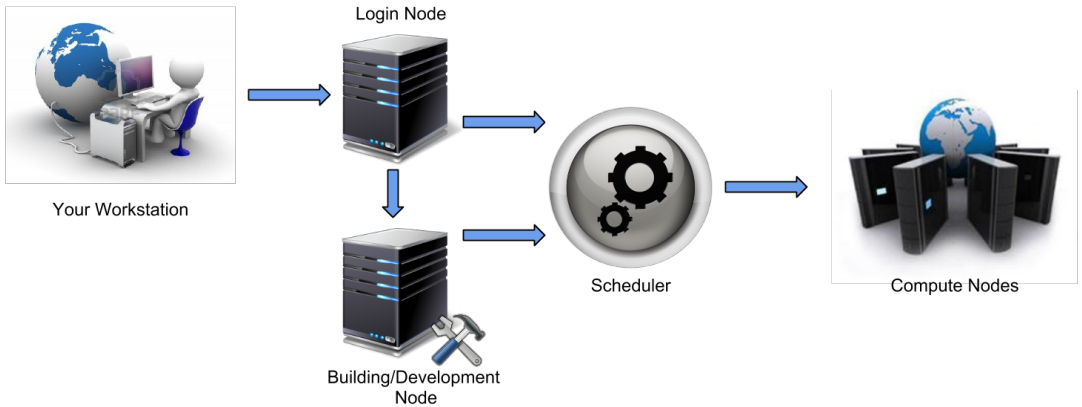
- The cluster is a shared resource and work must be scheduled.
- Jobs are queued and are executed on the compute nodes.
- The login node is not for running jobs, it is only for file management and job submission.



Using the Cluster

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

Connection via SSH

Each terminal client has its 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 `jbon007@login.nesi.org.nz`

Using the Cluster

Each NeSI Supercomputing Center has one or more Login Nodes

- CeR
  - `login.uoa.nesi.org.nz` which is the RHEL linux login node.
- 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.

Using the Cluster

Remote File System Access

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

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

Using the Cluster

Data

- Upload input data to the login node for use on the cluster.
- Download results from the login node to your local drive.
- The home directory has a rather small quota, project directories can be larger.
- For long term storage and back-up, ask your IT department.
- Things do go wrong, make sure to have a back-up.
- Files on the login node are shared across the build and compute nodes

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/CER/`
- 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

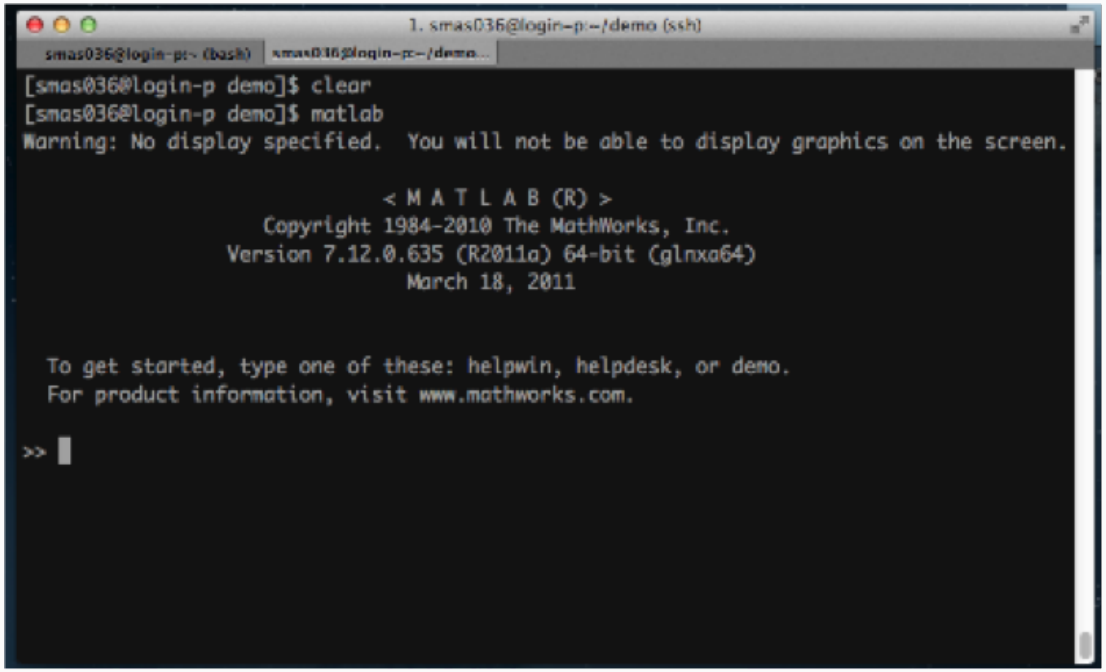
Submitting a Job

Basic Job Properties

- **Name** So you can identify the output later.
- **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, Project 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

Outputs



Jobs have no interactive interface, but command line output and can write to files. Graphical tools are, however, available on the login and build/development nodes.

Submitting a Job

Outputs

- Information output while the job runs 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 (see job Name)
- 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

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

Quick introduction Slurm

- You need to access the login node and work from a terminal.
- Requires basic knowledge of the 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 with SLURM: example job file

Job Description Example : Serial

```
#!/bin/bash
#SBATCH -J Serial_JOB
#SBATCH -A uoa99999          # Project Account
#SBATCH --time=01:00:00      # Walltime
#SBATCH --mem-per-cpu=4096   # memory/core (in MB)

srun cat ~/inputfile.txt
```

Also see `https://wiki.auckland.ac.nz/display/CER/Slurm+User+Guide`

Submitting a job with Slurm: example MPI job file

SLURM job Description Example : MPI

```
#!/bin/bash
#SBATCH -J MPI_JOB
#SBATCH -A uoa99999          # Project Account
#SBATCH --time=01:00:00      # Walltime
#SBATCH --ntasks=2           # number of tasks
#SBATCH --mem-per-cpu=4096 # memory/core (in MB)

module load myModule
srun mpi_binary
```

Also see `https://wiki.auckland.ac.nz/display/CER/Slurm+User+Guide`

Submitting a Job with Slurm: Send the job to the queue

Slurm

- To submit a job:

```
sbatch myJob.sl
```

- To monitor your jobs:

```
squeue -u <myUserId>
```

- To cancel:

```
scancel <jobId>
```

Notes for Windows Users

- Be careful of Windows end of line (EOL) characters, sometimes Linux will not handle them correctly.
- MobaXterm has a build in text file editor.
- 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.

Software

- We have many specialized 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:
  - Linux version of the software.
  - Command line mode without user interaction.
  - Interaction possible for small tests on the build nodes.
  - We don't provide licenses.
  - You can install software in your home directory if it is really esoteric.

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 wall-time, it will help the scheduler to efficiently schedule the jobs.
- Be aware that you are sharing resources with other researchers.
- 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 behavior 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