Using CSC computing facilities

An introduction

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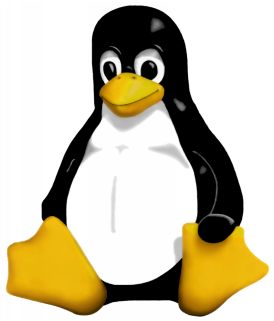
Centre for Scientific Computing

- Research center with seven member departments (including physics).
- Hosts research computing facilities.

- A centrally managed desktop computing environment.
- A distributed computing infrastructure (the CoW).
- A 2500 core high performance computer (`minerva`).
- A 3500 core high performance computer (`tinis`).

You should think of these facilities as research equipment, just like experimental kit. You must not use them without ***explicit*** permission from your supervisor. Using them inappropriately can *very easily* disrupt other (important) research within the university!

The CSC Managed Desktop



GNU / Linux based

- Provides various compilers
  - Fortran, C/C++, Java, Python etc
- General purpose packages
  - Maple, Mathematica, Matlab, Comsol, IDL
- Specific software
  - Abinit, NAMD + many more
- Centrally stored files / settings
  - Log in from anywhere to access your data

Using a CSC workstation

- You may be given access to a CSC-managed PC.

- You must ***not***
  - –turn it off or attempt to install your own operating system
  - –leave the screen unlocked when unattended
  - –unplug it from the network
  - –run long computations without permission

- You ***must***
  - –logout when leaving
  - –obey the usage policy

Remote access via X2Go

Access from ITS workrooms or your own PC is available using free NX client software (`http://wiki.x2go.org`).

Remote desktop hosted by `godzilla.csc.warwick.ac.uk`

- This is a *shared resource*, there may be dozens of people logged in at any time.
- To be used for editing files, compiling code, plotting simple graphs or submitting computational jobs to the CoW *only*.
- You must ***NOT*** run significant computations of any kind on godzilla. This includes calculations within Matlab / Mathematica.
- Very strict ‘three strikes’ policy on this.

The CSC CoW

- Cluster of Workstations, system for assigning calculations to desktops.
- Suitable for high compute, low memory, low I/O calculations.
  - –Any other jobs will disrupt the person working at that PC.
  - –Some dedicated (`taskfarm`) nodes for higher memory jobs.
  - –Some research groups have their own dedicated nodes.

```
#!/bin/bash
#PBS -l nodes=1:ppn=1,pvmem=100mb,walltime=08:00:00
#PBS –V

cd $PBS_O_WORKDIR   # Change into working directory

./myprog.exe        # Run my program
```

Submit job script to CoW, it will run on the next available workstation.

Final Points

- Read and obey the usage policy!
  - –Don't do anything illegal.
  - –Don't do anything stupid.
- Do not run calculations on any PCs without explicit permission
  - –Don't assume currently idle machines are fair game!
  - –All substantial calculations will need to run via the COW.
- If in doubt – ask!
  - –First point of call is always your supervisor.
  - –Some research groups have a nominated CSC mentor.