UNIVERSITY OF CAMBRIDGE

An Introduction to High Performance Computing

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Research Computing Services (http://www.hpc.cam.ac.uk/ http://www.csd3.cam.ac.uk/)
University Information Services (http://www.uis.cam.ac.uk/)

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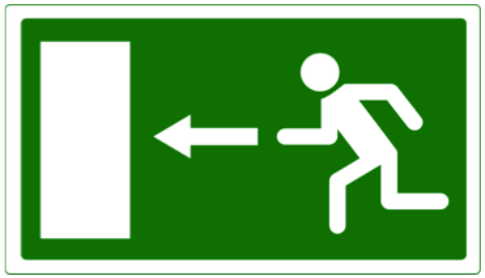
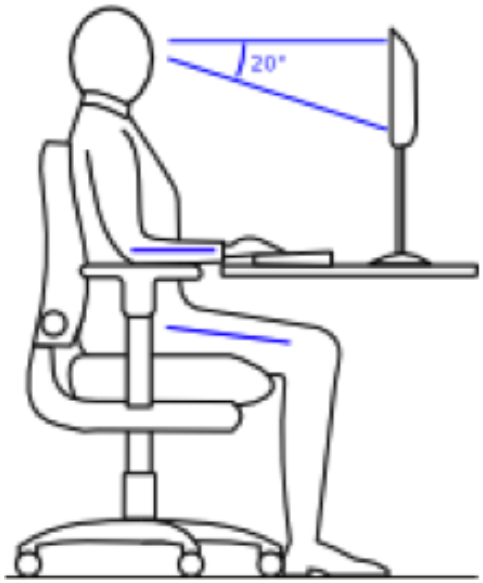
Health and Safety





Welcome

- Please sign in on the attendance sheet.
- Please fill in the online feedback at the end of the course:
  `http://feedback.training.cam.ac.uk/ucs/form.php`
- Keep your belongings with you.
- The printer will not work.
- Please ask questions and let us know if you need assistance.

Plan of the Course

Part 1: Basics

Part 2: High Performance Computing Service

Part 3: Using a HPC Facility

09:30	WELCOME
11:00-11:30	Practical and break
12:00-12:30	Practical
12:30-13:30	LUNCH
14:00-14:30	Practical
14:45-15:15	Practical
15:30-CLOSE	Further discussion

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Part I: **Basics**

Basics: Outline

Why Buy a Big Computer?

Inside a Modern Computer

How to Build a Supercomputer

Programming a Multiprocessor Machine

Basics: Why Buy a Big Computer?

What types of big problem might require a "Big Computer"?

Compute Intensive: A single problem requiring a large amount of computation.

Memory Intensive: A single problem requiring a large amount of memory.

Data Intensive: A single problem operating on a large amount of data.

High Throughput: Many unrelated problems to be executed in bulk.

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Basics: Compute Intensive Problems

- Distribute the work for a single problem across multiple CPUs to reduce the execution time as far as possible.
- Program workload must be *parallelised*:

  Parallel programs split into copies (processes or threads).

  Each process/thread performs a part of the work on its own CPU, concurrently with the others.

  A well-parallelised program will fully exercise as many CPUs as there are processes/threads.
- The CPUs typically need to exchange information rapidly, requiring specialized communication hardware.
- Many use cases from Physics, Chemistry, Engineering, Astronomy, Biology...
- The traditional domain of HPC and the Supercomputer.

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Basics: Scaling & Amdahl's Law

- Using more CPUs is not necessarily faster.
- Typically parallel codes have a scaling limit.
- Partly due to the system overhead of managing more copies, but also to more basic constraints;
- Amdahl's Law (idealized):

$$S(N) = \frac{1}{(1 - p + \frac{p}{N})}$$

where

$S(N)$ is the fraction by which the program has sped up relative to $N = 1$

p is the fraction of the program which can be parallelized

N is the number of CPUs.

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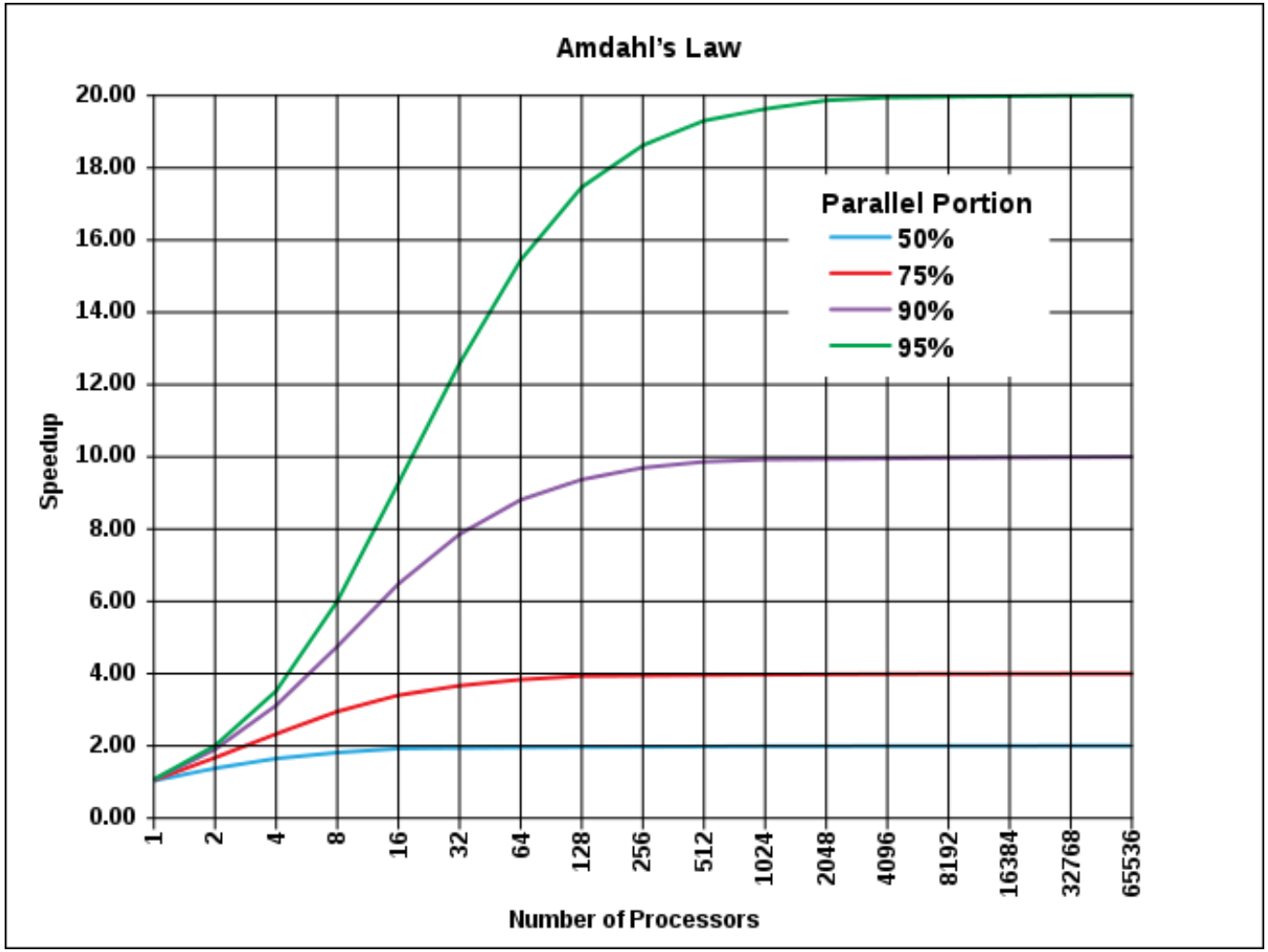

http://en.wikipedia.org/wiki/File:AmdahlsLaw.svg

The Bottom Line

- Parallelisation requires effort:
  - There are libraries to help (e.g. OpenMP, MPI).
  - First optimise performance on one CPU, then make p as large as possible.
- The scaling limit: eventually using more CPUs becomes detrimental instead of helpful.

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- Rapid movement of data to and from disk is more important than inter-CPU communication.
- Big Data problems of great current interest -
- Hadoop/MapReduce
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Basics: Memory Intensive Problems

- Require aggregation of large memory rather than multiple CPUs.

  NB Memory (fast, volatile) vs disk (slow, non-volatile).
- Technically more challenging to build machines (interconnecting memory and CPUs).
- Coding/porting easier (memory appears seamless, allowing a single system image).
- Optimisation harder (nonuniform memory produces latency).
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- Nowadays, similar techniques are applicable to commodity servers.

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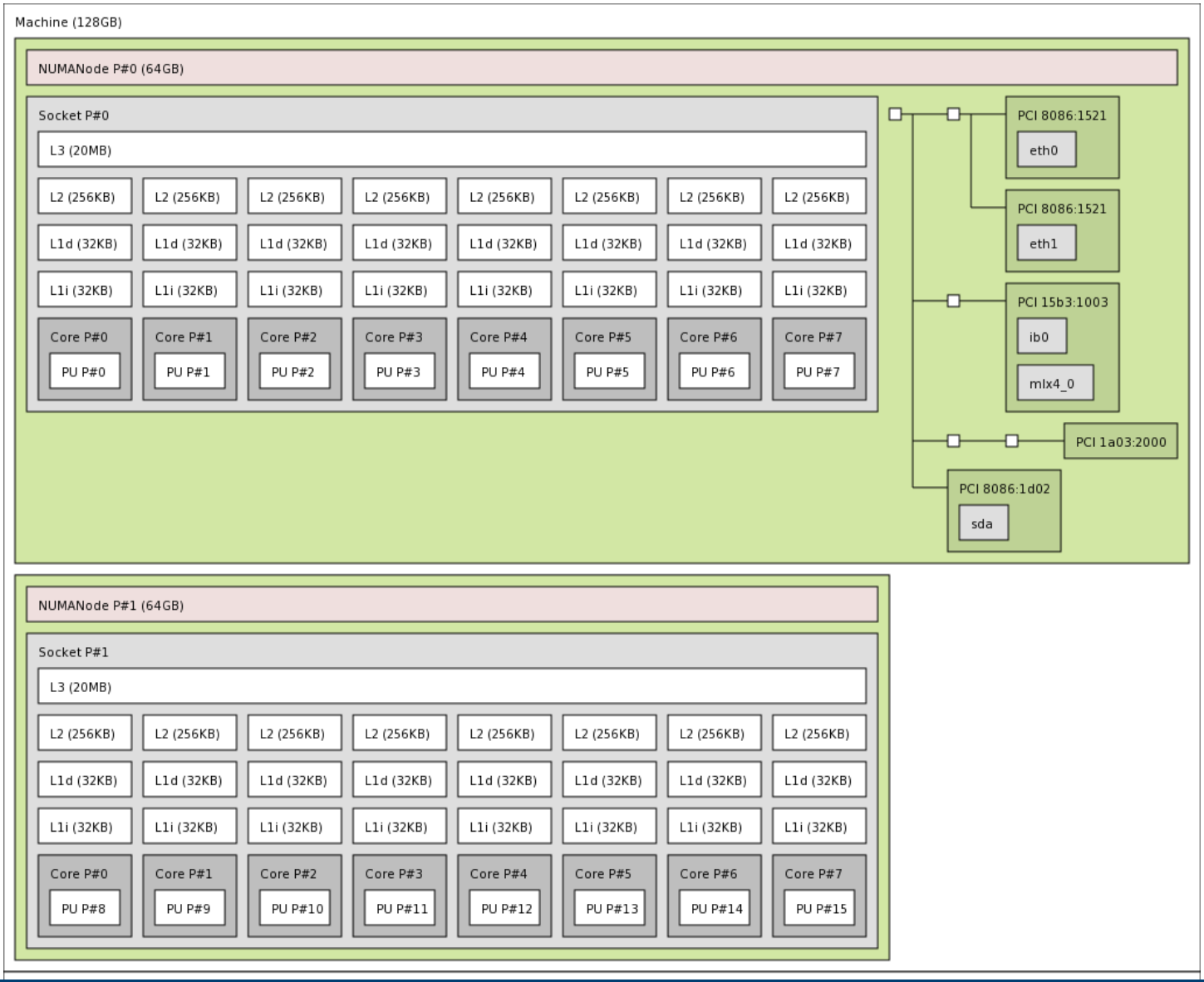

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  with Non-Uniform Memory Architecture (NUMA)
  but users still see a single computer (single system image).

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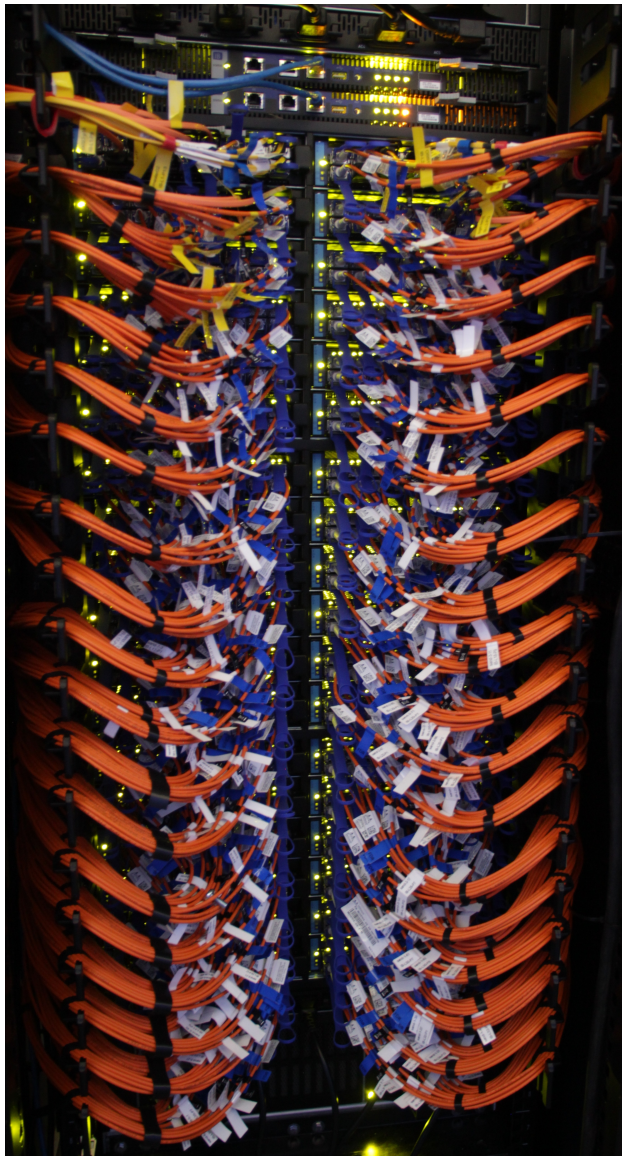
2. Connect the nodes with one or more networks. E.g.

   Gbit Ethernet: 100 MB/sec
   FDR Infiniband: 5 GB/sec

   Faster network is for inter-CPU communication across nodes.
   Slower network is for management and provisioning.
   Storage may use either.



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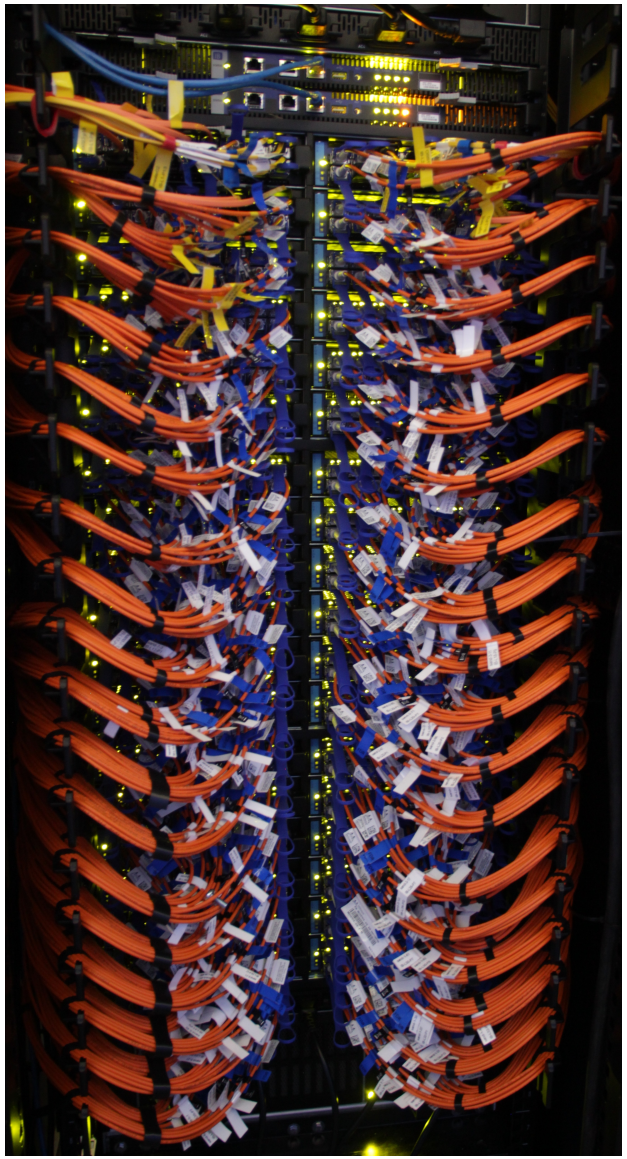

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3. Logically bind the nodes
   - Clusters consist of distinct nodes (i.e. separate Linux computers) on common private network(s) and controlled centrally.
     * Private networks allow CPUs in different nodes to communicate.
     * Clusters are distributed memory machines:
       Each process/thread sees only its local node's CPUs and memory (without help).
     * Each process/thread must fit within a single node's memory.
   - More expensive machines logically bind nodes into a single system i.e. CPUs and memory.
     * E.g. SGI UV (COSMOS system in DAMTP).
     * Private networks allow CPUs to see CPUs and memory in other nodes.
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- Non-parallel code uses the memory of one node, but may be copied across many.

Basics: Summary

- Why have a supercomputer?
  - Big single problems, many problems, Big Data.
- Most current supercomputers are clusters of separate nodes.
- Each node has multiple CPUs and non-uniform shared memory.
- Parallel code uses shared memory (pthreads/OpenMP) within a node, distributed memory (MPI) spanning multiple nodes.
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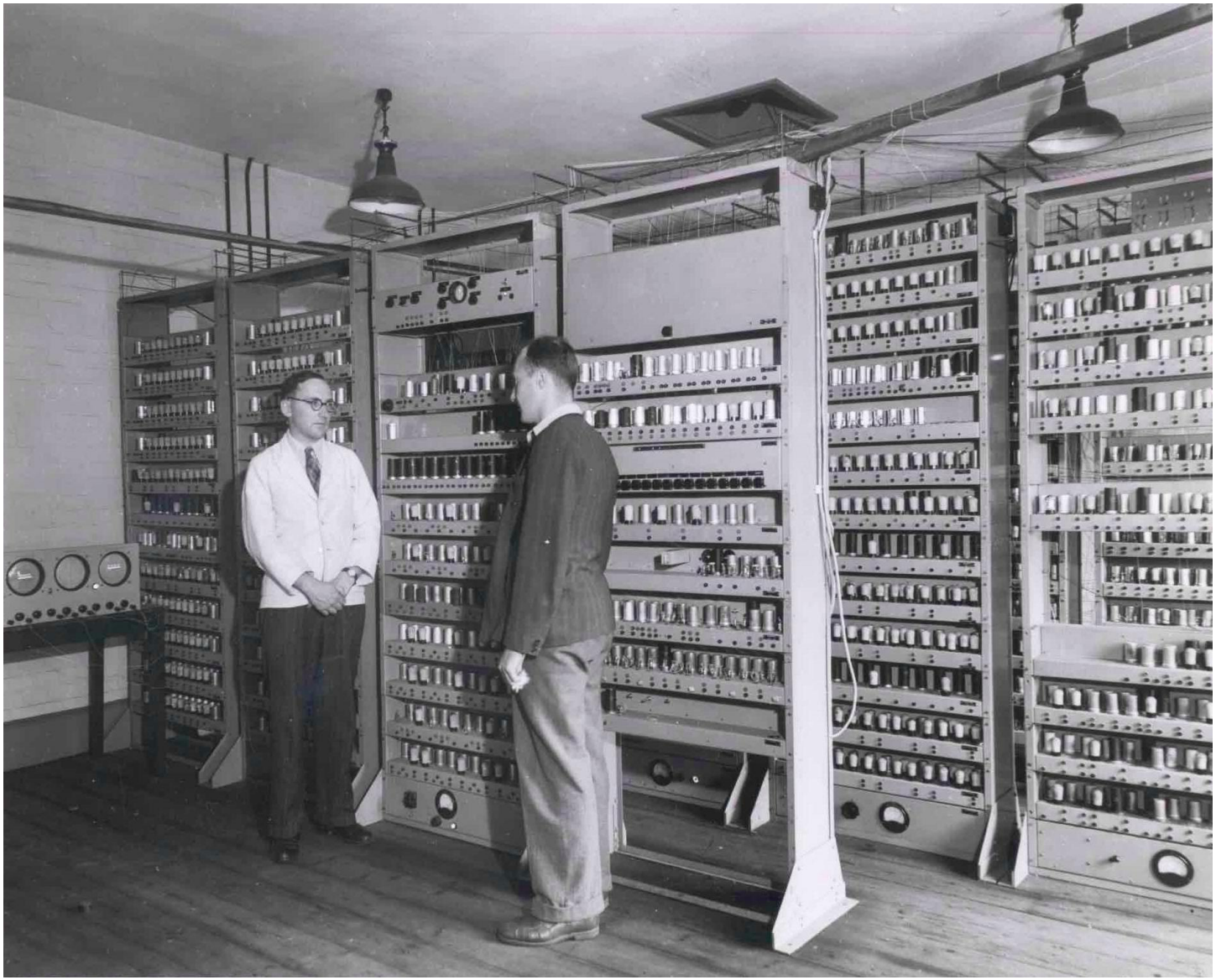
Part II: **The High Performance Computing**

Early History: EDSAC (1949–1958)



Early History: EDSAC (1949–1958)

- **E**lectronic **D**elay **S**torage **A**utomatic **C**alculator
- The second general use, electronic digital (Turing complete) stored program computer
- 3,000 valves
- 650 instructions per second
- 2KB memory in mercury ultrasonic delay lines
- One program at a time!
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HPCS: A Brief History

Created: 1996 (as the HPCF).

Mission: Delivery and support of a large HPC resource for use by the University of Cambridge research community.

Self-funding: Paying and non-paying service levels.

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2010 30 Tflop/s

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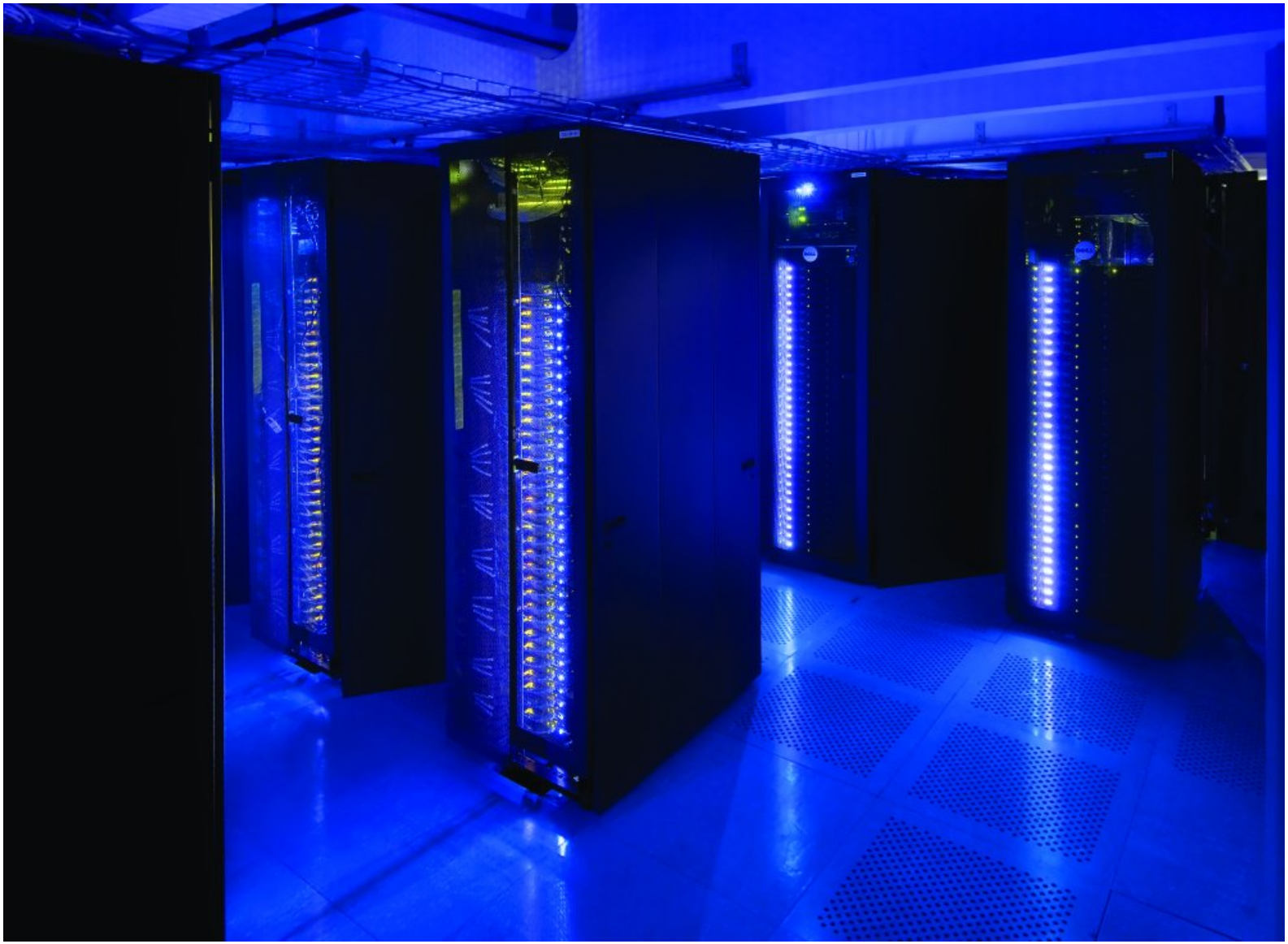

Darwin3 (2012)(b) & Wilkes (2013)(f)

Darwin: an Infiniband CPU Cluster

- Each compute node:
  - 2x8 cores, Intel Sandy Bridge 2.6 GHz.
  - 64 GB RAM (63900 MB usable).
  - 56 Gb/sec (4X FDR) Infiniband.
- 600 compute nodes (300 belong to Cambridge).
- 8 login nodes (login.hpc.cam.ac.uk).

Darwin: an Infiniband CPU Cluster

- Each compute node:
  - 16 cores
  - 63900 MB
  - 5 GB/sec Infiniband (for MPI and storage)
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- 1 Petaflop upgrade availability October 2017

Wilkes: a Dual-Rail Infiniband GPU Cluster

- Each compute node:
  - $2 \times$ NVIDIA Tesla K20c GPU.
  - 2x6 cores, Intel Ivy Bridge 2.6 GHz.
  - 64 GB RAM (63900 MB usable).
  - 2×56 Gb/sec (4X FDR) Infiniband.
- 128 compute nodes.
- 8 login nodes (login.hpc.cam.ac.uk).
- Environment shared with Darwin (same filesystems, user environment, scheduler).
- 1 Petaflop upgrade (Wilkes2) early access June 2017

Wilkes: a Dual-Rail Infiniband GPU Cluster

- Each compute node:
  - 2 GPUs
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- Multi-petabytes split across multiple filesystems with tape.
- Lustre cluster filesystem:
  - Multiple RAID6 back-end disk volumes.
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  - Single metadata server.
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Service Level 1 Paying, intended for large projects with long-term, consistent requirement.

Service Level 2 Paying, intended for medium-sized projects with irregular requirement.

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Very low priority, very restricted, very limited. Best efforts continuation.

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The West Cambridge Data Centre

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- The PI should be someone senior enough to have funding.
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Part III: **Using HPC**

Using HPC: Security

- Boring but very, very important . . .
- Cambridge IT is under constant attack by would-be intruders.
- Your data and research career is threatened by intruders.
- Big systems are big, juicy targets.
- Anything in the University of Cambridge is a big, juicy target.
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- WinSCP
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- TurboVNC (remote desktop, 3D optional)
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Connecting: Login

- From Linux/MacOSX/UNIX (or Cygwin):
  ssh -Y **abc123**@login.hpc.cam.ac.uk
- From graphical clients:
  Host: login.hpc.cam.ac.uk
  Username: **abc123** (your UCAM account name)
- login.hpc will map to a random login node
  i.e. one of login-sand1, login-sand2, . . . , login-sand8
  NB Not darwin.hpc (the head node).
- Non-registered addresses will fail with "Connection refused".
- Similarly for other systems (e.g. cardio-login.hpc, login-mrc-bsu.hpc, . . .).

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- Similarly for other systems (e.g. cardio-login.hpc, login-mrc-bsu.hpc,. . .).

Connecting: Login

- From Linux/MacOSX/UNIX (or Cygwin):
  ssh -Y **abc123**@login.hpc.cam.ac.uk
- From graphical clients:
  Host: login.hpc.cam.ac.uk
  Username: **abc123** (your UCAM account name)
- login.hpc will map to a random login node
  i.e. one of login-sand1, login-sand2, . . . , login-sand8
  NB Not darwin.hpc (the head node).
- Non-registered addresses will fail with "Connection refused".
- Similarly for other systems (e.g. cardio-login.hpc, login-mrc-bsu.hpc,. . .).

Connecting: First time login

- The first connection to a particular hostname produces the following:

```
The authenticity of host 'login-sand2.hpc.cam.ac.uk (131.111.1.214)'
can't be established.
RSA key fingerprint is
0b:ef:59:90:fb:13:4a:c9:56:82:7b:cd:4b:2b:e1:3b.
Are you sure you want to continue connecting (yes/no)? yes
Warning: Permanently added 'login-sand2.hpc.cam.ac.uk' (RSA) to the
list of known hosts.
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- One should always check the fingerprint before typing "yes".
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SHA256:sSkVfzpwjwiFvxLcdPoDpN8IsN3kt0ZSywhDhPKZPAg

MD5:34:9b:f2:d2:c6:b3:5c:63:99:b7:27:da:5b:c8:16:fe
SHA256:HsiY1Oe0M8tS6JwR76PeQQA/VB7r8675BzG5OYQ4h34

MD5:64:7c:7c:ff:05:9d:0e:dc:06:fe:f1:c2:10:37:7a:85
SHA256:wq9ljBfPa7lXXpQq+rk5JTBXLJO/kXjOc5A7rp4ENzA
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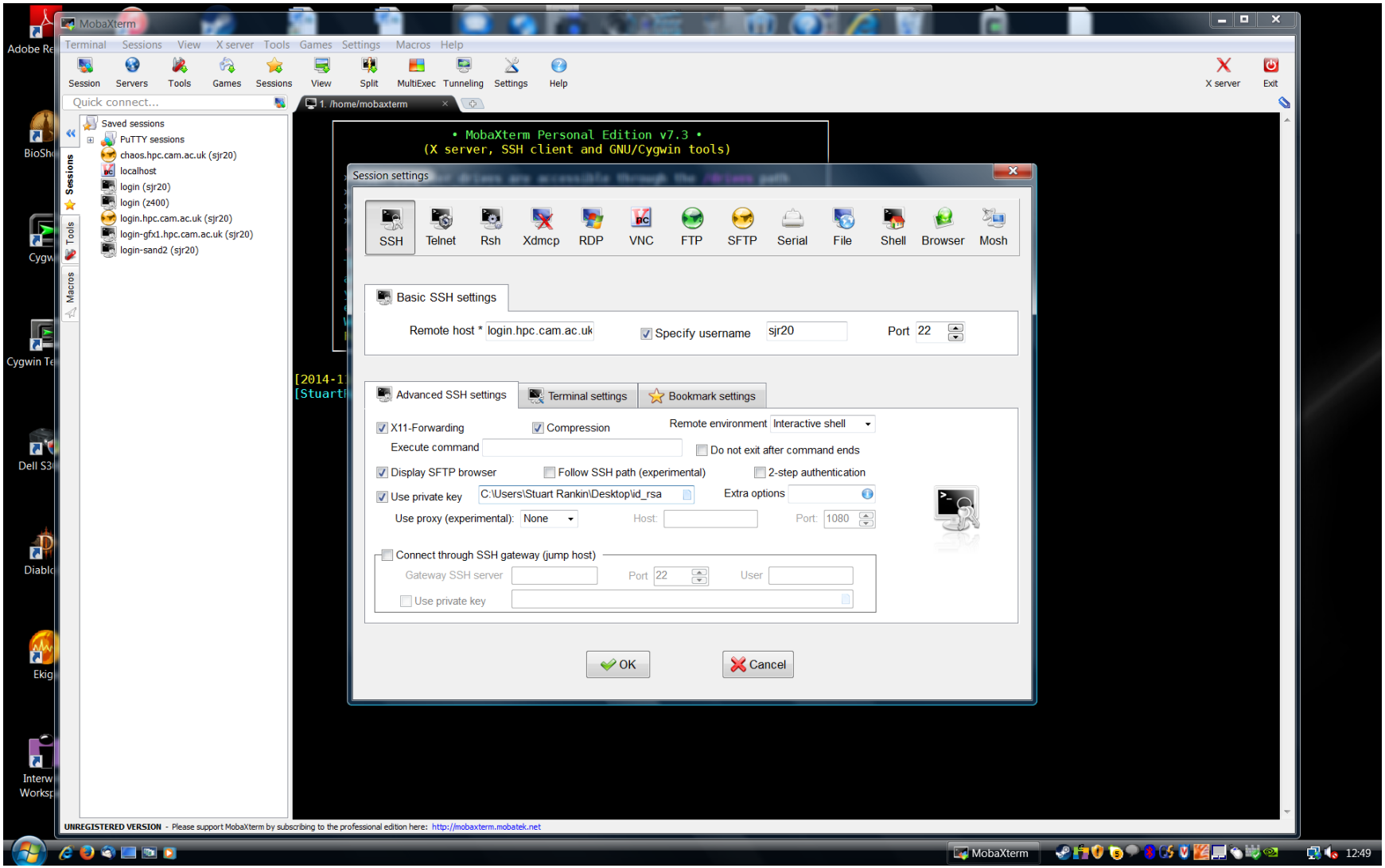
MD5:34:9b:f2:d2:c6:b3:5c:63:99:b7:27:da:5b:c8:16:fe
SHA256:HsiY1Oe0M8tS6JwR76PeQQA/VB7r8675BzG5OYQ4h34

MD5:64:7c:7c:ff:05:9d:0e:dc:06:fe:f1:c2:10:37:7a:85
SHA256:wq9ljBfPa7lXXpQq+rk5JTBXLJO/kXjOc5A7rp4ENzA
```

- Exercise 1 - Log into your HPCS training account.

MobaXterm SSH (Windows)



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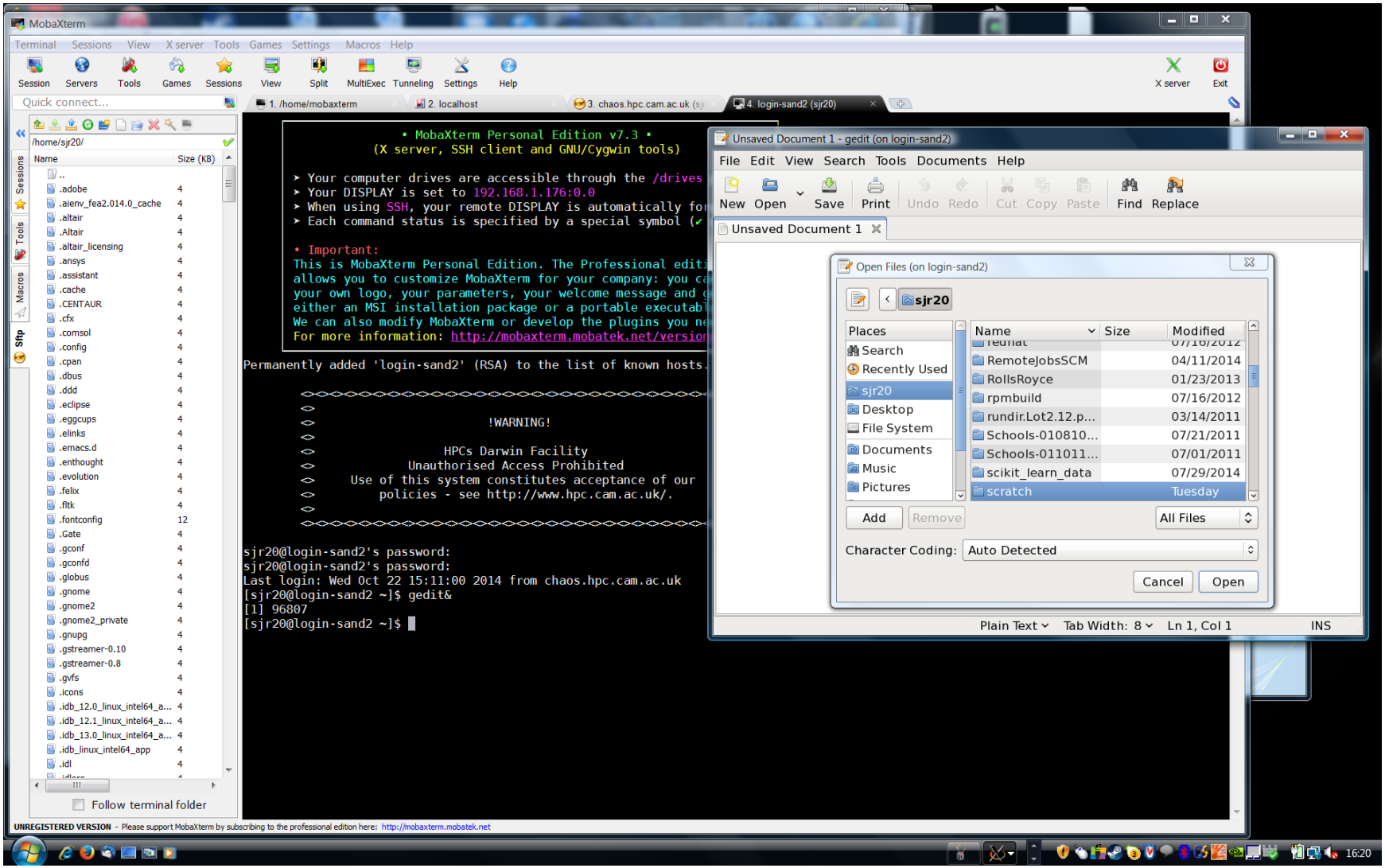

Connecting: File Transfer

- From Linux/MacOSX/UNIX (or Cygwin):

  rsync -av **old_directory/** abc123@login.hpc.cam.ac.uk:scratch/new_directory

  copies contents of old_directory to ~/scratch/new_directory.

  rsync -av **old_directory** abc123@login.hpc.cam.ac.uk:scratch/new_directory

  copies old_directory (and contents) to ~/scratch/new_directory/old_directory.

  * Rerun to update or resume after interruption.
  * All transfers are checksummed.
  * For transfers in the opposite direction, place the remote machine as the first argument.

- With graphical clients, connect as before and drag and drop.
- Exercise 2 - File transfer.

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- Exercise 2 - File transfer.

Connecting: Remote Desktop

- First time starting a remote desktop:

```
[sjr20@login-sand2 ~]$ vncserver

You will require a password to access your desktops.

Password:
Verify:
Would you like to enter a view-only password (y/n)? n

New 'X' desktop is login-sand2:8

Starting applications specified in /home/sjr20/.vnc/xstartup.turbovnc
Log file is /home/sjr20/.vnc/login-sand2:8.log
```

- For 3D graphics sessions, use login-gfx1 or login-gfx2.

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```

- For 3D graphics sessions, use login-gfx1 or login-gfx2.

Connecting: Remote Desktop

- Remote desktop already running:

```
[sjr20@login-sand2 ~]$ vncserver -list

TurboVNC server sessions:

X DISPLAY #     PROCESS ID
:8              12745
```

- Kill it:

```
[sjr20@login-sand2 ~]$ vncserver -kill :8
Killing Xvnc process ID 12745
```

- Typically you only need one remote desktop.
- Keeps running until killed, or the node reboots.

Connecting: Remote Desktop

- To connect to the desktop from Linux:

```
[sjr20@themis ~]$ vncviewer -via sjr20@login-sand2.hpc.cam.ac.uk localhost:8
Connected to RFB server, using protocol version 3.8
Enabling TightVNC protocol extensions
Performing standard VNC authentication
Password:
```

- Press F8 to bring up the control panel.
- Exercise 3 - Remote desktop

Connecting: Remote Desktop

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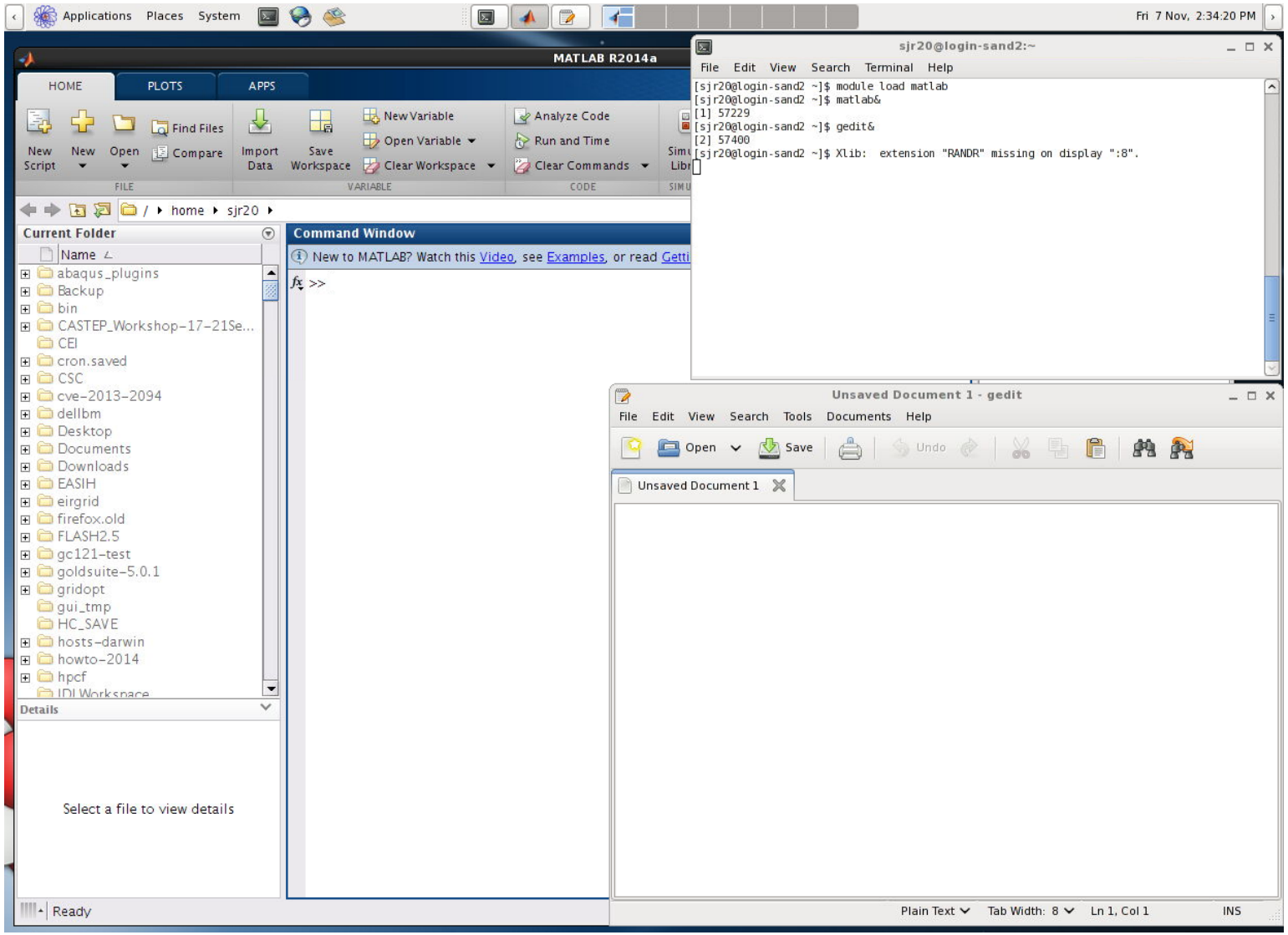
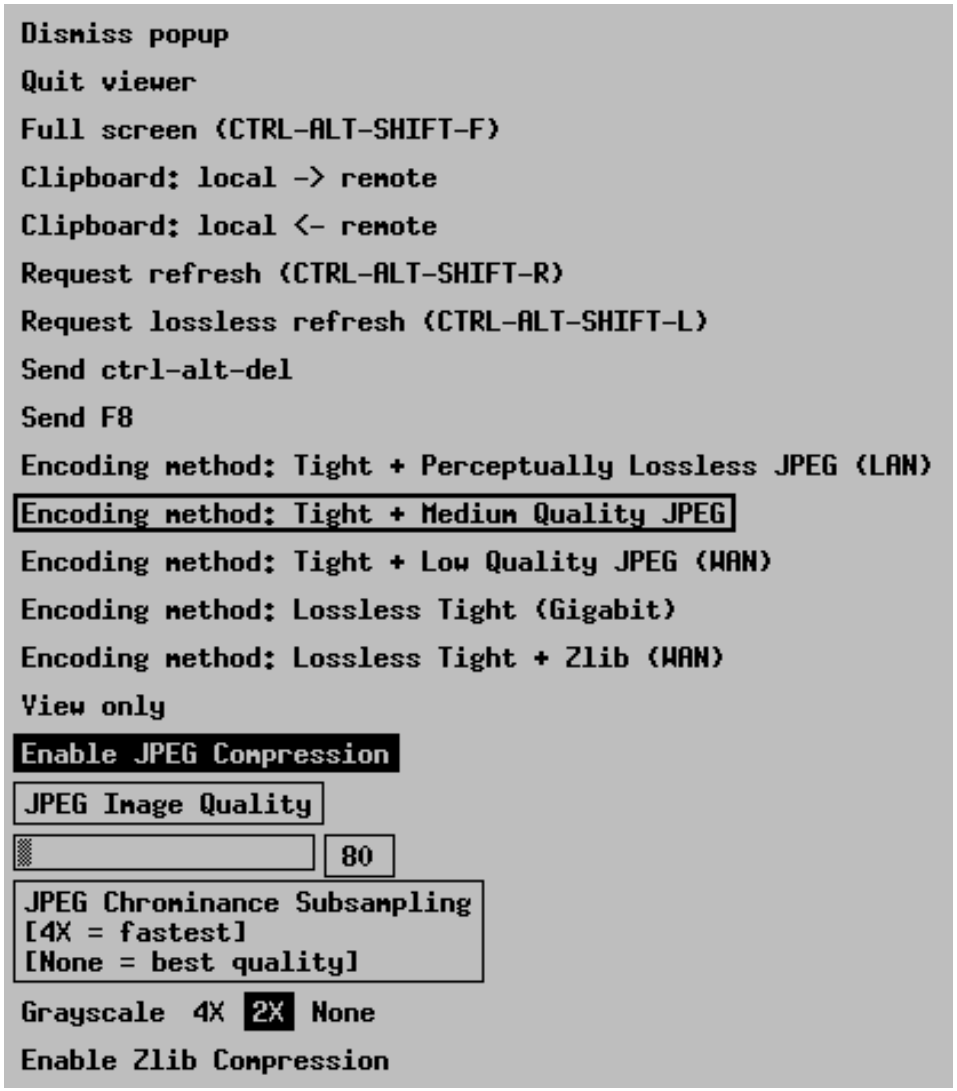
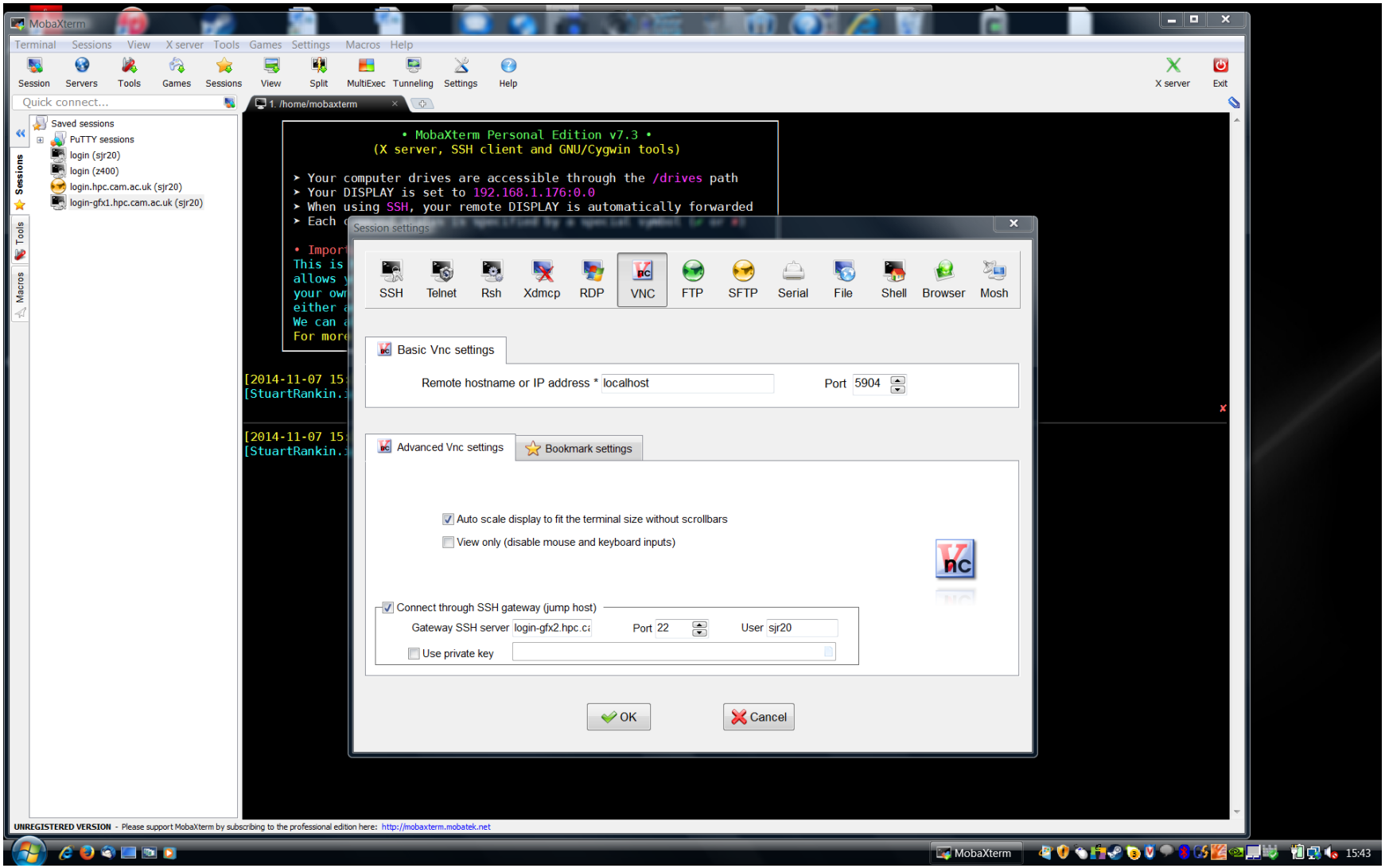
HPCS TurboVNC Session



Linux TurboVNC Control Panel



Connecting: Remote Desktop (MobaXterm)



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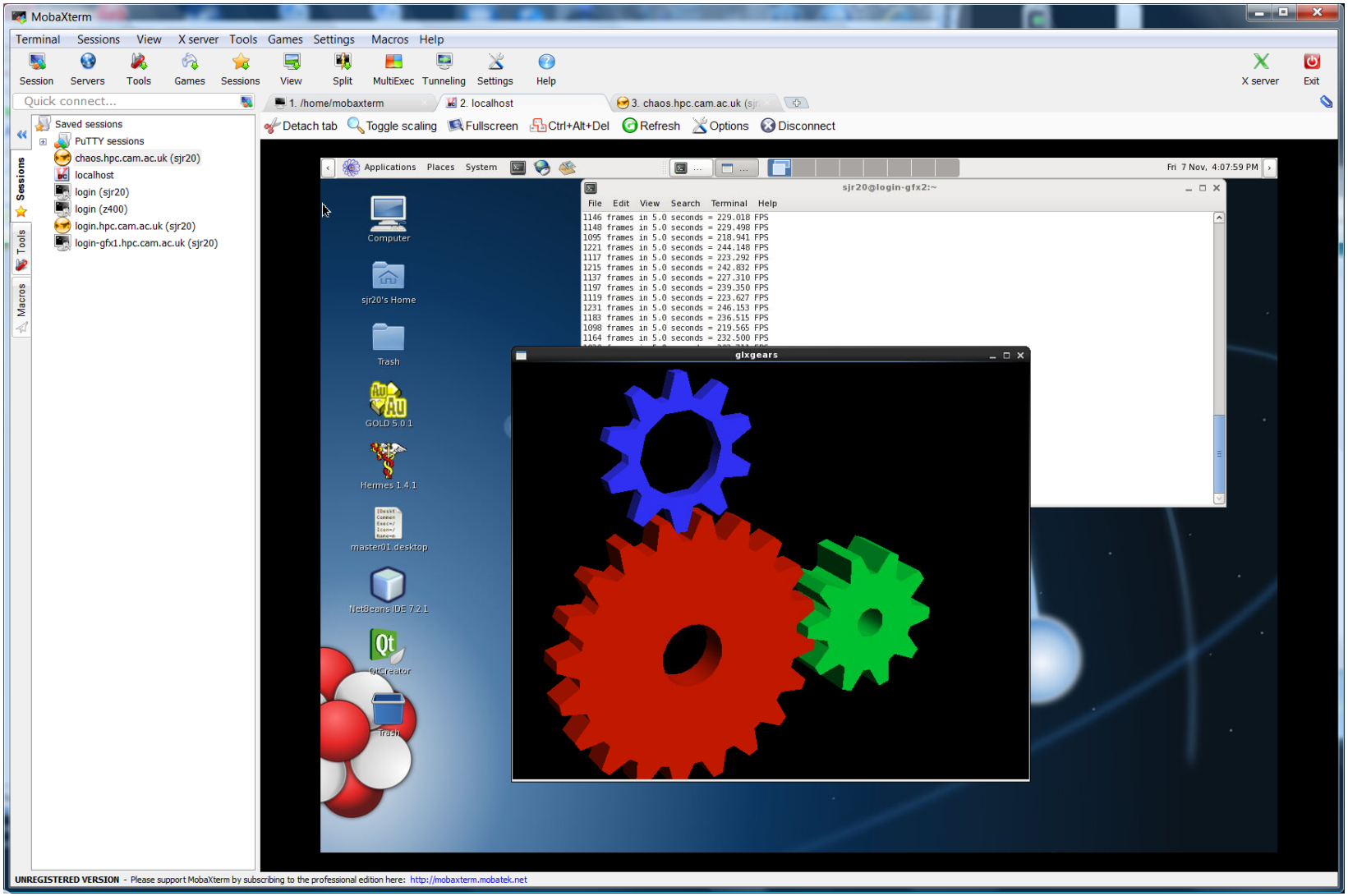
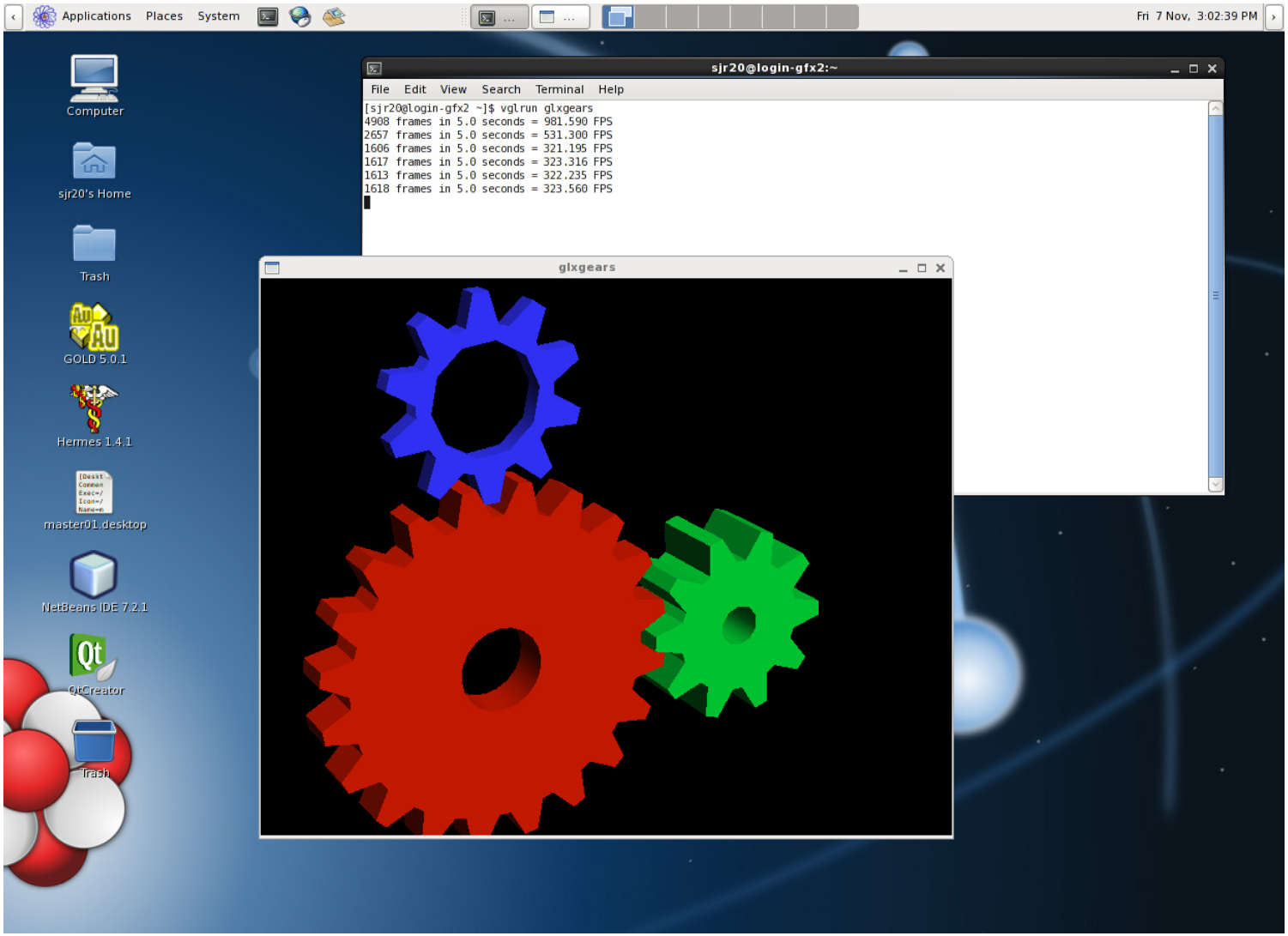


3D Remote Visualization



3D Remote Visualization

- Choose login-gfx2.
- Launch any application requiring 3D (OpenGL) with vglrun.
- May need to adjust the compression level for your network connection.

Using HPC: User Environment

- Scientific Linux 6.8 (Red Hat Enterprise Linux 6.8 rebuild)
  - bash
  - GNOME2 or XFCE4 desktop (if you want)
- Lustre 2.4.1 (patched), Mellanox OFED 3.3, CUDA 8.0
- But you don't need to know that.
- Upgrade to Scientific Linux/Red Hat Enterprise Linux 7 underway (Wilkes already upgraded).

Using HPC: User Environment

Red Hat Enterprise Linux 6

CUDA 8

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User Environment: Filesystems

- /home/abc123
  - 40GB quota.
  - Visible equally from all nodes.
  - Single storage server.
  - Hourly, daily, weekly snapshots copied to tape.
  - Not intended for job outputs or large/many input files.
- /scratch/abc123
  - Visible equally from all nodes.
  - Larger and faster (1TB initial quota).
  - Intended for job inputs and outputs.
  - Not backed up.
  - Changes coming post-upgrade.
  - http://www.uis.cam.ac.uk/initiatives/storage-strategy/storage-services

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Filesystems: Quotas

- quota

```
==========================================================================================
Usage on /scratch (lfs quota -u abc123 /scratch):
==========================================================================================
Disk quotas for user abc123 (uid 456):
      Filesystem  kbytes   quota   limit   grace   files   quota   limit   grace
 /scratch/abc123 9298708  1073741824 1181116006   -   165588       0       0       -
...
```

- Aim to stay below the soft limit (*quota*).
- Once over the soft limit, you have 7 days grace to return below.
- When the grace period expires, or you reach the hard limit (*limit*), no more data can be written.
- It is important to rectify an out of quota condition ASAP.

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Filesystems: Backups

- Disk snapshots and tape (as of May 2017).
- They are not an undelete - take care when deleting.
- Successful restoration depends on:
  - The file having existed long enough to have been backed up at all.
  - The last good version existing in a current backup.
  - Request restoration as soon as possible with *location* and *exact time of loss*.

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  - Scratch files are not backed up.

Filesystems: Automounter

- Directories under /scratch are automounted.
- They only appear under /scratch when explicitly referenced.
- Thus when browsing /scratch may appear too empty
  — use *ls* or *cd* to reference /scratch/abc123 explicitly.

Filesystems: Permissions

- Be careful and if unsure, please ask support@hpc.cam.ac.uk.
  - Can lead to accidental destruction of your data or account compromise.
- Avoid changing the permissions on your home directory.
  - Files under /home are particularly security sensitive.
  - Easy to break passwordless communication between nodes.

Using HPC: Software

- Free software accompanying Red Hat Enterprise is (or can be) provided.
- Other software (free and non-free) is available via modules.
- Some proprietary software may not be generally accessible.
- See http://www.hpc.cam.ac.uk/using-clusters/software.
- New software may be possible to provide on request.
- Self-installed software must be properly licensed.
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User Environment: Environment Modules

- Modules load or unload additional software packages.
- Some are required and automatically loaded on login.
- Others are optional extras, or possible replacements for other modules.
- Beware unloading default modules in ~/.bashrc.
- Beware overwriting environment variables such as PATH and LD_LIBRARY_PATH in ~/.bashrc. If necessary append or prepend.

User Environment: Environment Modules

- Currently loaded:

```
module list
Currently Loaded Modulefiles:
  1) dot                       6) intel/impi/4.1.3.045   11) default-impi
  2) scheduler                 7) global
  3) java/jdk1.7.0_60          8) intel/cce/12.1.10.319
  4) turbovnc/1.1              9) intel/fce/12.1.10.319
  5) vgl/2.3.1/64             10) intel/mkl/10.3.10.319
```

- Available:

```
module av
```

User Environment: Environment Modules

- Show:

```
module show castep/impi/7.0.3
-------------------------------------------------------------------
/usr/local/Cluster-Config/modulefiles/castep/impi/7.0.3:

module-whatis    adds CASTEP 7.0.3 (Intel MPI) to your environment

Note that this software is restricted to registered users.

prepend-path     PATH /usr/local/Cluster-Apps/castep/impi/7.0.3/bin:/usr/local/...
-------------------------------------------------------------------
```

- Load:

```
module load castep/impi/7.0.3
```

- Unload:

```
module unload castep/impi/7.0.3
```

User Environment: Environment Modules

- Matlab

```
module load matlab/r2015b
```

- Invoking matlab in batch mode:
  matlab -nodisplay -nojvm -nosplash command
  where the file command.m contains your matlab code.
- The University site license contains the Parallel Computing Toolbox.

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User Environment: Environment Modules

- Purge:

```
module purge
```

- Defaults:

```
module show default-impi
module unload default-impi
module load default-impi-LATEST
```

- Run time environment must match compile time environment.

User Environment: Compilers

Intel: icc, icpc, ifort (recommended)

```
icc -O3 -xHOST -ip code.c -o prog
mpicc -O3 -xHOST -ip mpi_code.c -o mpi_prog
```

GCC: gcc, g++, gfortran

```
gcc -O3 -mtune=native code.c -o prog
mpicc -cc=gcc -O3 -mtune=native mpi_code.c -o mpi_prog
```

PGI: pgcc, pgCC, pgf90

```
pgcc -O3 -tp=sandybridge code.c -o prog
mpicc -cc=pgcc -O3 -tp=sandybridge mpi_code.c -o mpi_prog
```

Exercise 4: Modules and Compilers

User Environment: Compilers

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```

Exercise 4: Modules and Compilers

Using HPC: Job Submission

Using HPC: Job Submission

- Compute resources are managed by a scheduler:
  SLURM/PBS/SGE/LSF/...
- Jobs are submitted to the scheduler
  — analogous to submitting jobs to a print queue
  — a file (*submission script*) is copied and queued for processing.

Using HPC: Job Submission

- Jobs are submitted from the login nodes
  — not themselves managed by the scheduler.
- Jobs may be either non-interactive (batch) or interactive.
- Batch jobs run a shell script on the first of a list of allocated nodes.
- Interactive jobs provide a command line on the first of a list of allocated nodes.

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Using HPC: Job Submission

- The HPCS has used SLURM since February 2014.
- Jobs may use part or all of one or more nodes
  — the owner can specify `--exclusive` to force exclusive node access (automatic on Wilkes but may change post-upgrade).
- Template submission scripts are available under /usr/local/Cluster-Docs/SLURM.

Job Submission: Using SLURM

- Prepare a shell script and submit it to SLURM:

```
[abc123@login]$ sbatch slurm_submission_script
Submitted batch job 790299
```

Job Submission: Show Queue

- Submitted job scripts are copied and stored in a queue:

```
[abc123@login]$ squeue -u abc123
             JOBID PARTITION     NAME     USER  ST       TIME  NODES NODELIST(REASON)
            790299 sandybrid     Test3  abc123 PD       0:00      8 (Priority)
            790290 sandybrid     Test2  abc123  R   27:56:10      8 sand-6-[38-40],sand-7-[27-31]
```

Job Submission: Show Queue

- Submitted job scripts are copied and stored in a queue:

```
[abc123@login]$ squeue -u abc123
             JOBID PARTITION     NAME     USER  ST       TIME  NODES NODELIST(REASON)
            790299 sandybrid     Test3  abc123 PD       0:00      8 (Resources)
            790290 sandybrid     Test2  abc123  R   27:56:10      8 sand-6-[38-40],sand-7-[27-31]
```

Job Submission: Show Queue

- Submitted job scripts are copied and stored in a queue:

```
[abc123@login]$ squeue -u abc123
             JOBID PARTITION     NAME     USER  ST       TIME  NODES NODELIST(REASON)
            790299 sandybrid     Test3  abc123 PD       0:00      8 (AssocGrpCPUMinsLimit)
            790290 sandybrid     Test2  abc123  R   27:56:10      8 sand-6-[38-40],sand-7-[27-31]
```

Job Submission: Monitor Job

- Examine a particular job:

```
[abc123@login]$ scontrol show job=790299
```

Job Submission: Cancel Job

- Cancel a particular job:

```
[abc123@login]$ scancel 790299
```

Job Submission: Scripts

- SLURM

  See slurm_submit.darwin, slurm_submit.wilkes.

```
#!/bin/bash
#! Name of the job:
#SBATCH -J darwinjob
#! Which project should be charged:
#SBATCH -A CHANGEME
#! How many whole nodes should be allocated?
#SBATCH --nodes=1
#! How many tasks will there be in total? (<= nodes*16)
#SBATCH --ntasks=1
#! How much wallclock time will be required?
#SBATCH --time=02:00:00
#! Select partition:
#SBATCH -p sandybridge
...
```

- #SBATCH lines are *structured comments*

  — correspond to sbatch command line options.

- The above job will be given 1 cpu on 1 node for 2 hours (by default there is 1 task per node, and 1 cpu per task).

Job Submission: Scripts

- SLURM

  See slurm_submit.darwin, slurm_submit.wilkes.

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#! How many whole nodes should be allocated?
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#SBATCH --ntasks=16
#! How much wallclock time will be required?
#SBATCH --time=02:00:00
#! Select partition:
#SBATCH -p sandybridge
...
```

- #SBATCH lines are *structured comments*

  — correspond to sbatch command line options.

- The above job will be given 16 cpus on 1 node for 2 hours (by default there is 1 task per node, and 1 cpu per task).

Job Submission: Accounting Commands [HPCS]

- How many core hours available do I have?

```
mybalance

User            Usage |        Account     Usage | Account Limit Available (CPU hrs)
---------- --------- + ------------- --------- + ------------- ---------
abc123             18 |          STARS       171 |       100,000    99,829
abc123             18 |      STARS-SL2        35 |       101,000   100,965
abc123            925 |         BLACKH    10,634 |       166,667   156,033
```

- How many core hours does some other project or user have?

```
gbalance -p HALOS

User           Usage |   Account     Usage | Account Limit Available (CPU hrs)
---------- --------- + --------- --------- + ------------- ---------

pq345              0 |     HALOS   317,656 |       600,000   282,344
xyz10         11,880 |     HALOS   317,656 |       600,000   282,344

(Use -u for user.)
```

- List all jobs charged to a project/user between certain times:

```
gstatement -p HALOS  -u xyz10 -s "2014-01-01-00:00:00" -e "2014-01-20-00:00:00"
       JobID      User   Account  JobName  Partition                End      NCPUS CPUTimeRAW ExitCode      State
------------ --------- ---------- -------- ---------- ------------------- ---------- ---------- -------- ----------
14505             xyz10     halos       help sandybrid+ 2014-01-07T12:59:40         16         32      0:9  COMPLETED
14506             xyz10     halos       help sandybrid+ 2014-01-07T13:00:11         16         48      2:0     FAILED
...
```

Job Submission: Single Node Jobs

- Serial jobs requiring large memory, or OpenMP codes.

```
#!/bin/bash
...
#SBATCH --nodes=1
#SBATCH --ntasks=1
# Default is 1 task per node
#SBATCH --cpus-per-task=

#SBATCH --mem=3994
# Memory per node in MB - default is pro rata by cpu number
# Increasing --mem or --cpus-per-task implicitly increases the other
...
export OMP_NUM_THREADS=  # For OpenMP across  cores
$application $options
...
```

Job Submission: Single Node Jobs

- Serial jobs requiring large memory, or OpenMP codes.

```
#!/bin/bash
...
#SBATCH --nodes=1
#SBATCH --ntasks=1
# Default is 1 task per node
#SBATCH --cpus-per-task=

#SBATCH --mem=3994
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```
#!/bin/bash
...
#SBATCH --nodes=1
#SBATCH --ntasks=1
# Default is 1 task per node
#SBATCH --cpus-per-task=1
# Default is 1 cpu (core) per task
#SBATCH --mem=3994
# Memory per node in MB - default is pro rata by cpu number
# Increasing --mem or --cpus-per-task implicitly increases the other
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# Default is 1 cpu (core) per task
#SBATCH --mem=3994
# Memory per node in MB - default is pro rata by cpu number
# Increasing --mem or --cpus-per-task implicitly increases the other
...
export OMP_NUM_THREADS=  # For OpenMP across  cores
$application $options
...
```

Job Submission: Single Node Jobs

- Serial jobs requiring large memory, or OpenMP codes.

```
#!/bin/bash
...
#SBATCH --nodes=1
#SBATCH --ntasks=1
# Default is 1 task per node
#SBATCH --cpus-per-task=16 # Whole node

#SBATCH --mem=3994
# Memory per node in MB - default is pro rata by cpu number
# Increasing --mem or --cpus-per-task implicitly increases the other
...
export OMP_NUM_THREADS=16  # For OpenMP across 16 cores
$application $options
...
```

Job Submission: Single Node Jobs

- Serial jobs requiring large memory, or OpenMP codes.

```
#!/bin/bash
...
#SBATCH --nodes=1
#SBATCH --ntasks=1
# Default is 1 task per node
#SBATCH --cpus-per-task=8  # Half node

#SBATCH --mem=3994
# Memory per node in MB - default is pro rata by cpu number
# Increasing --mem or --cpus-per-task implicitly increases the other
...
export OMP_NUM_THREADS=8   # For OpenMP across 8 cores
$application $options
...
```

Job Submission: Single Node Jobs

- Serial jobs requiring large memory, or OpenMP codes.

```
#!/bin/bash
...
#SBATCH --nodes=1
#SBATCH --ntasks=1
# Default is 1 task per node
#SBATCH --cpus-per-task=16 # Whole node

#SBATCH --mem=3994
# Memory per node in MB - default is pro rata by cpu number
# Increasing --mem or --cpus-per-task implicitly increases the other
...
export OMP_NUM_THREADS=8   # For OpenMP across 8 cores (using all memory)
$application $options
...
```

Job Submission: MPI Jobs

- Parallel job across multiple nodes.

```
#!/bin/bash
...
#SBATCH --nodes=4
#SBATCH --ntasks=64      # i.e. 16x4 MPI tasks in total.
#SBATCH --cpus-per-task=2
...
mpirun -np 64 $application $options
...
```

- SLURM-aware MPI launches remote tasks via SLURM.
- The template script uses $SLURM_TASKS_PER_NODE to set PPN.

Job Submission: MPI Jobs

- Parallel job across multiple nodes.

```
#!/bin/bash
...
#SBATCH --nodes=4
#SBATCH --ntasks=32     # i.e.  8x4 MPI tasks in total.
#SBATCH --cpus-per-task=2
...
mpirun -ppn 8 -np 32 $application $options
...
```

- SLURM-aware MPI launches remote tasks via SLURM.
- The template script uses $SLURM_TASKS_PER_NODE to set PPN.

Job Submission: MPI Jobs

- Parallel job across multiple nodes.

```
#!/bin/bash
...
#SBATCH --nodes=4
#SBATCH --ntasks=32     # i.e.  8x4 MPI tasks in total.
#SBATCH --cpus-per-task=2
...
mpirun -ppn 8 -np 32 $application $options
...
```

- SLURM-aware MPI launches remote tasks via SLURM.
- The template script uses $SLURM_TASKS_PER_NODE to set PPN.

Job Submission: Hybrid Jobs

- Parallel jobs using both MPI and OpenMP.

```
#!/bin/bash
...
#SBATCH --nodes=4
#SBATCH --ntasks=32      # i.e.  8x4 MPI tasks in total.
#SBATCH --cpus-per-task=2
...
export OMP_NUM_THREADS=2   # i.e. 2 threads per MPI task.
mpirun -ppn 8 -np 32 $application $options
...
```

- This job uses 64 CPUs (each MPI task splits into 2 OpenMP threads).

Job Submission: Hybrid Jobs

- Parallel jobs using both MPI and OpenMP.

```
#!/bin/bash
...
#SBATCH --nodes=4
#SBATCH --ntasks=32      # i.e.  8x4 MPI tasks in total.
#SBATCH --cpus-per-task=2
...
export OMP_NUM_THREADS=2   # i.e. 2 threads per MPI task.
mpirun -ppn 8 -np 32 $application $options
...
```

- This job uses 64 CPUs (each MPI task splits into 2 OpenMP threads).

Job Submission: High Throughput Jobs

- Multiple serial jobs across multiple nodes.
- Use srun to launch tasks (job steps) within a job.

```
#!/bin/bash
...
#SBATCH --nodes=4
...
cd directory_for_job1
srun --exclusive -N 1 -n 1 $application $options_for_job1 > output 2> err &
cd directory_for_job2
srun --exclusive -N 1 -n 1 $application $options_for_job2 > output 2> err &
...
cd directory_for_job64
srun --exclusive -N 1 -n 1 $application $options_for_job64 > output 2> err &
wait
```

- Exercise 5 & 6 - Submitting Jobs.

Job Submission: High Throughput Jobs

- Multiple serial jobs across multiple nodes.
- Use srun to launch tasks (job steps) within a job.

```
#!/bin/bash
...
#SBATCH --nodes=4
...
cd directory_for_job1
srun --exclusive -N 1 -n 1 $application $options_for_job1 > output 2> err &
cd directory_for_job2
srun --exclusive -N 1 -n 1 $application $options_for_job2 > output 2> err &
...
cd directory_for_job64
srun --exclusive -N 1 -n 1 $application $options_for_job64 > output 2> err &
wait
```

- Exercise 5 & 6 - Submitting Jobs.

Job Submission: High Throughput Jobs

- Multiple serial jobs across multiple nodes.
- Use srun to launch tasks (job steps) within a job.

```
#!/bin/bash
...
#SBATCH --nodes=4
...
cd directory_for_job1
srun --exclusive -N 1 -n 1 $application $options_for_job1 > output 2> err &
cd directory_for_job2
srun --exclusive -N 1 -n 1 $application $options_for_job2 > output 2> err &
...
cd directory_for_job64
srun --exclusive -N 1 -n 1 $application $options_for_job64 > output 2> err &
wait
```

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Job Submission: High Throughput Jobs

- Multiple serial jobs across multiple nodes.
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```
#!/bin/bash
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cd directory_for_job2
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...
cd directory_for_job64
srun --exclusive -N 1 -n 1 $application $options_for_job64 > output 2> err &
wait
```

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Job Submission: High Throughput Jobs

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#!/bin/bash
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...
cd directory_for_job64
srun --exclusive -N 1 -n 1 $application $options_for_job64 > output 2> err &
wait
```

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Job Submission: High Throughput Jobs

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...
cd directory_for_job64
srun --exclusive -N 1 -n 1 $application $options_for_job64 > output 2> err &
wait
```

- Exercise 5 & 6 - Submitting Jobs.

Job Submission: Interactive [HPCS]

- Compute nodes are accessible via SSH while you have a job running on them.
- Alternatively, submit an interactive job:

```
sintr -A MYPROJECT -N2 -n16 -t 2:0:0
```

- Within the window (screen session):
  - Launches a shell on the first node (when the job starts).
  - Graphical applications should display correctly.
  - Create new shells with ctrl-a c, navigate with ctrl-a n and ctrl-a p.
  - ssh or srun can be used to start processes on any nodes in the job.
  - SLURM-aware MPI will do this automatically.

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Job Submission: Array Jobs

- This feature varies between versions.
- *http://slurm.schedmd.com/job_array.html*
- Used for submitting and managing large sets of similar jobs.
- Each job in the array has the same initial options.
- SLURM

```
[abc123@login]$ sbatch --array=1-7 -A STARS-SL2 submission_script
Submitted batch job 791609
```

```
[abc123@login-sand2]$ squeue -u abc123
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
          791609_1 sandybrid      hpl    abc123  R       0:06      1 sand-6-32
          791609_3 sandybrid      hpl    abc123  R       0:06      1 sand-6-37
          791609_5 sandybrid      hpl    abc123  R       0:06      1 sand-6-59
          791609_7 sandybrid      hpl    abc123  R       0:06      1 sand-7-27
```

791609_1, 791609_3, 791609_5, 791609_7

i.e. ${SLURM_ARRAY_JOB_ID}_${SLURM_ARRAY_TASK_ID}

SLURM_ARRAY_JOB_ID = SLURM_JOBID for the first element.

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```
[abc123@login]$ sbatch --array=1-7:2 -A STARS-SL2 submission_script
Submitted batch job 791609
```

```
[abc123@login-sand2]$ squeue -u abc123
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
          791609_1 sandybrid      hpl    abc123  R       0:06      1 sand-6-32
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- SLURM

```
[abc123@login]$ sbatch --array=1,3,5,7 -A STARS-SL2 submission_script
Submitted batch job 791609

[abc123@login-sand2]$ squeue -u abc123
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
          791609_1 sandybrid      hpl    abc123  R       0:06      1 sand-6-32
          791609_3 sandybrid      hpl    abc123  R       0:06      1 sand-6-37
          791609_5 sandybrid      hpl    abc123  R       0:06      1 sand-6-59
          791609_7 sandybrid      hpl    abc123  R       0:06      1 sand-7-27
```

791609_1, 791609_3, 791609_5, 791609_7

i.e. ${SLURM_ARRAY_JOB_ID}_${SLURM_ARRAY_TASK_ID}

SLURM_ARRAY_JOB_ID = SLURM_JOBID for the first element.

Job Submission: Array Jobs (ctd)

- Updates can be applied to specific array elements using ${SLURM_ARRAY_JOB_ID}_${SLURM_ARRAY_TASK_ID}
- Alternatively operate on the entire array via ${SLURM_ARRAY_JOB_ID}.
- Some commands still require the SLURM_JOB_ID (sacct, sreport, sshare, sstat and a few others).

Scheduling

- SLURM scheduling is multifactor:
  - QoS — payer or non-payer?
  - Age — how long has the job waited?
    Don't cancel jobs that seem to wait too long.
  - Fair Share — how much recent usage?
    Payers with little recent usage receive boost.
  - sprio -j jobid
- Backfilling
  - Promote lower priority jobs into gaps left by higher priority jobs.
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- The cluster is currently very busy and we do not preempt.
- 36 or 12 hour job walltimes are permitted.
- This sets the timescale at busy times (*without* backfilling).
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Checkpointing

- Insurance against failures during long jobs.
- Restart from checkpoints to work around finite job length.
- Application native methods are best. Failing that . . .
- Darwin & Wilkes nodes currently provide Berkeley Lab Checkpoint/Restart (BLCR)

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Job Submission: Scheduling Top Dos & Don'ts

- **Do . . .**
  - Give reasonably accurate wall times (allows backfilling).
  - Check your balance occasionally (mybalance).
  - Test on a small scale first.
  - Implement checkpointing if possible (reduces resource wastage).
- **Don't . . .**
  - Request more than you need
    — you will wait longer and use more credits.
  - Cancel jobs unnecessarily
    — priority increases over time.