UNIVERSITY OF CAMBRIDGE

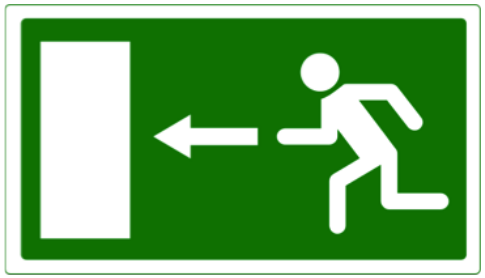
An Introduction to High Performance Computing

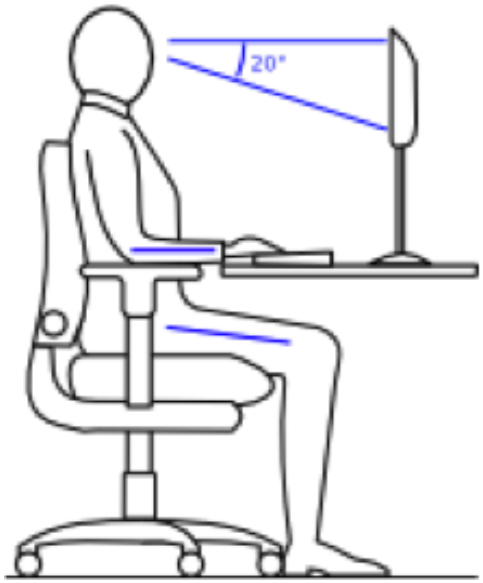
Stuart Rankin

sjr20@cam.ac.uk

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

Health and Safety





Welcome

- Please sign in on the attendance sheet.
- Keep your belongings with you.
- Please ask questions and let us know if you need assistance.

UIS: Research Computing Services

Your trainers for today will be:

- Paul Sumption
  Research Computing User Services
- Eleftherios Avramidis
  Research Software Engineering

You may be . . .

- Programmers (or not).
- UNIX power users (or not).
- Researchers wishing to run large, parallel code.
- Researchers wishing to run many, non-parallel cases.
- Researchers interested in big data, machine learning, AI.
- Researchers requiring slightly more than an ordinary workstation.
- Many different disciplines and requirements.

Plan of the Course

Part 1: Basics

Part 2: Research Computing Services HPC

Part 3: Using HPC

10:00	WELCOME
11:00-11:15	Break
12:30-13:30	LUNCH
15:30-15:45	Break
16:30	CLOSE

Prerequisites

- Basic Unix/Linux command line experience:
  Unix: Introduction to the Command Line Interface (self-paced)
  `https://www.training.cam.ac.uk/ucs/Course/ucs-unixintro1`
- Shell scripting experience is desirable:
  Unix: Simple Shell Scripting for Scientists
  `https://www.training.cam.ac.uk/ucs/Course/ucs-scriptsci`

Training accounts

- For our practical exercises we will use CSD3 accounts. You should all have applied for a CSD3 account.
- We have reserved two nodes for todays training.
- The training-cpu accounting group is only valid for today.
- Course material can be downloaded from: `https://www.hpc.cam.ac.uk/training-courses`

Security

- Cambridge IT is under constant attack by would-be intruders.
- Choose strong passwords and keep it (or private key passphrase) safe.
- Your UIS password is used for multiple systems so keep it secure!
- Keep the software on your laptops/tablets/PCs up to date — this includes home computers.
- Check out and install free anti-malware software available for work and home:
  https://help.uis.cam.ac.uk/service/security/stay-safe-online/malware
- Don't share accounts (this is against the rules, and anyone can get their own).

Part I: **Basics**

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.

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.

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):

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

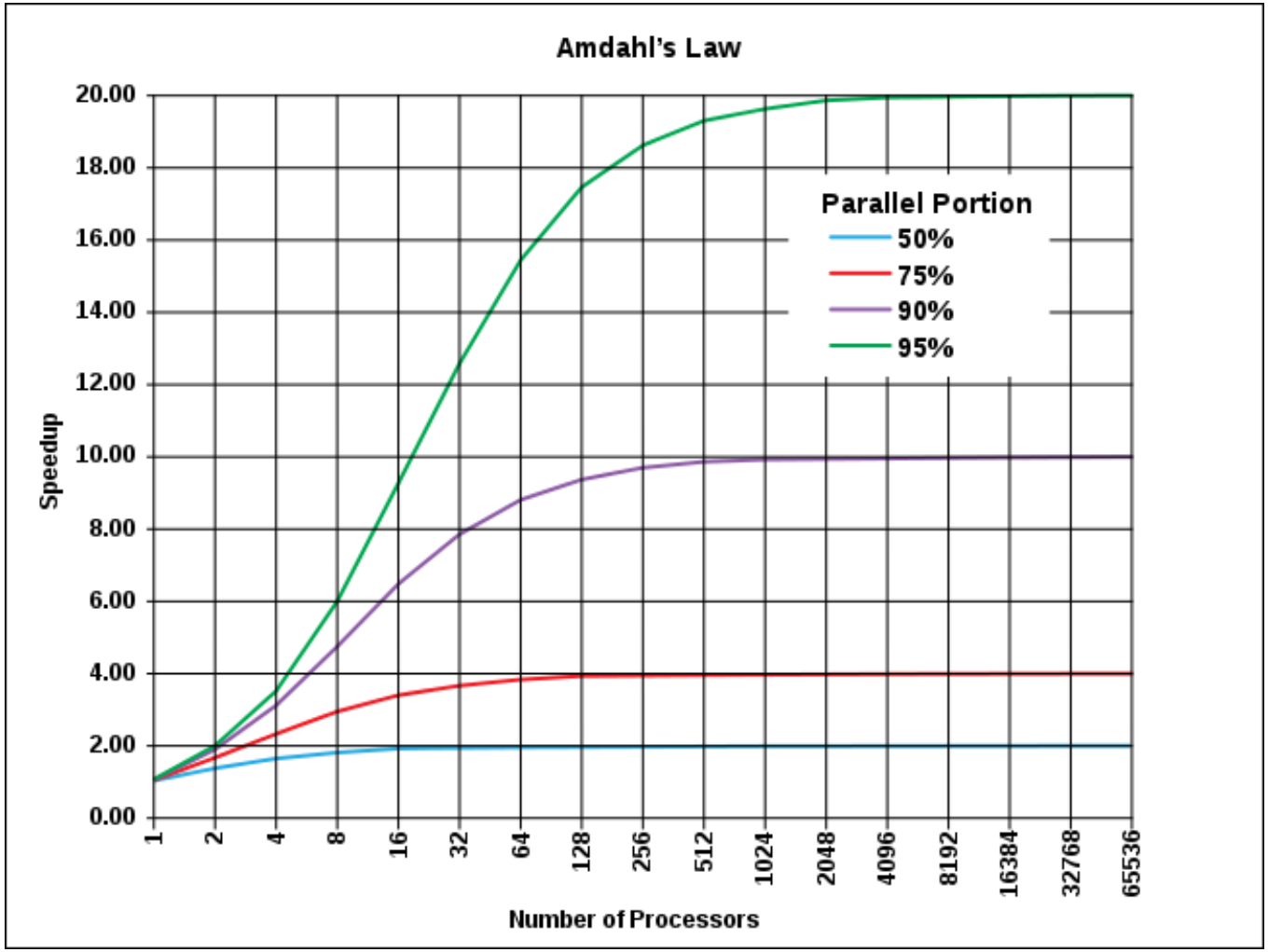
where

$S(N)$ 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.

Basics: Amdahl's Law



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

The Bottom Line

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

Basics: Data Intensive Problems

- Distribute the data for a single problem across multiple CPUs to reduce the overall execution time.
- The *same* work may be done on each data segment.
- Rapid movement of data to and from disk is more important than inter-CPU communication.
- Big Data problems of great current interest -
- Hadoop/MapReduce
- Life Sciences (genomics) and elsewhere.

Basics: High Throughput

- Distribute independent, multiple problems across multiple CPUs to reduce the overall execution time.
- Workload is trivially (or *embarrassingly*) parallel:
  - Workload breaks up naturally into *independent* pieces.
  - Each piece is performed by a separate process/thread on a separate CPU (concurrently).
  - Little or no inter-CPU communication.
- Emphasis is on throughput over a period, rather than on performance on a single problem.
- Compute intensive capable $\Rightarrow$ high throughput capable (not conversely).

If you are using lots of R or python, you are probably high throughput, and possibly data intensive or compute intensive.

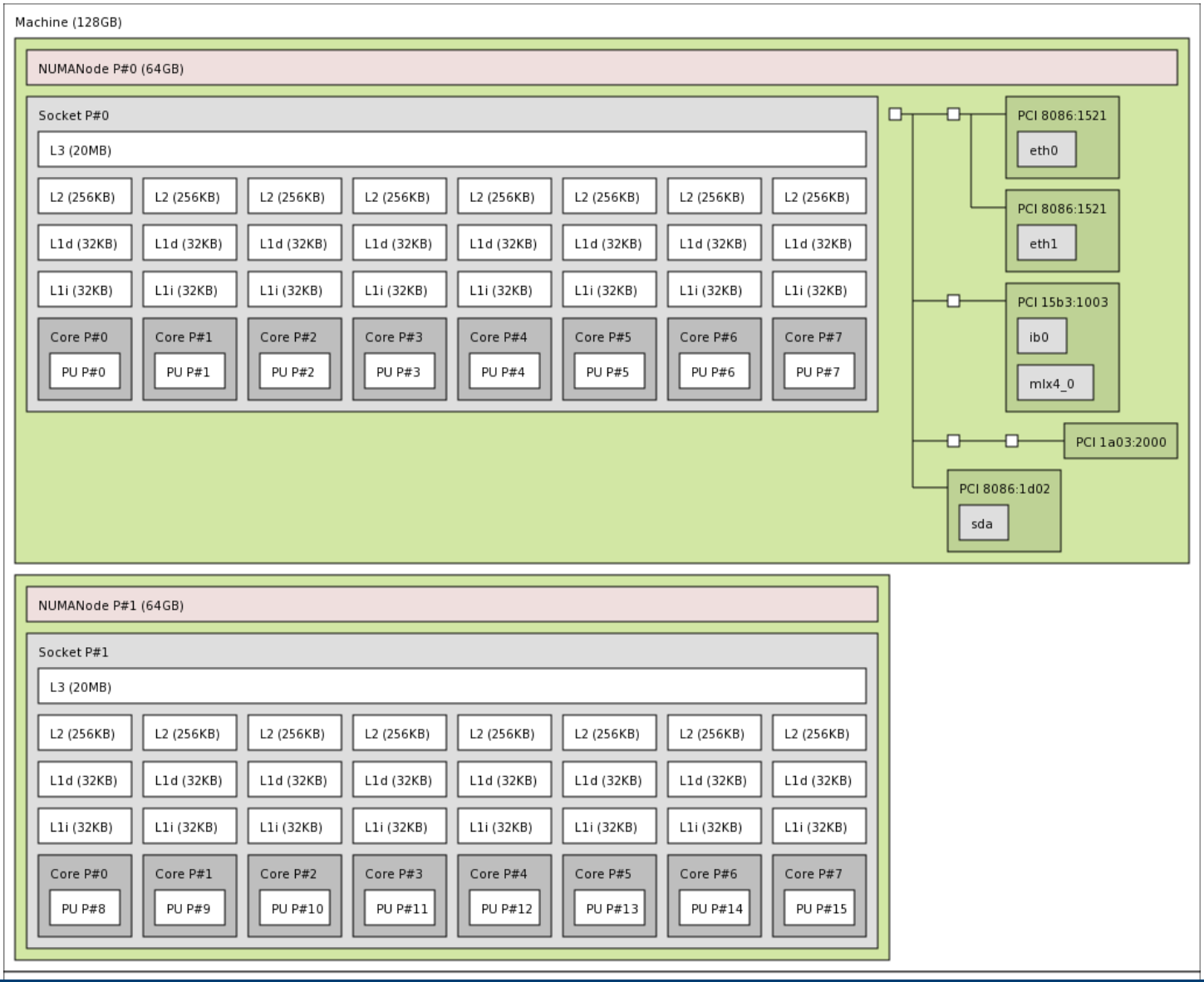
Basics: Putting it All Together

- Each of these types of problem requires combining many CPUs and memory modules.
- Nowadays, there can be many CPUs and memory modules inside a single commodity PC or server.
- HPC involves combining many times more than this.

Basics: Inside a Modern Computer

- Today's commodity servers already aggregate both CPUs and memory to make a single system image in a single box.
- Even small computers now have multiple cores (fully functional CPUs) per socket.
- Larger computers have multiple sockets (each with their own local memory).

Basics: Inside a Modern Computer



Basics: How to Build a Supercomputer

- A supercomputer aggregates contemporary CPUs and memory to obtain increased computing power.
- Usually today these are clusters.

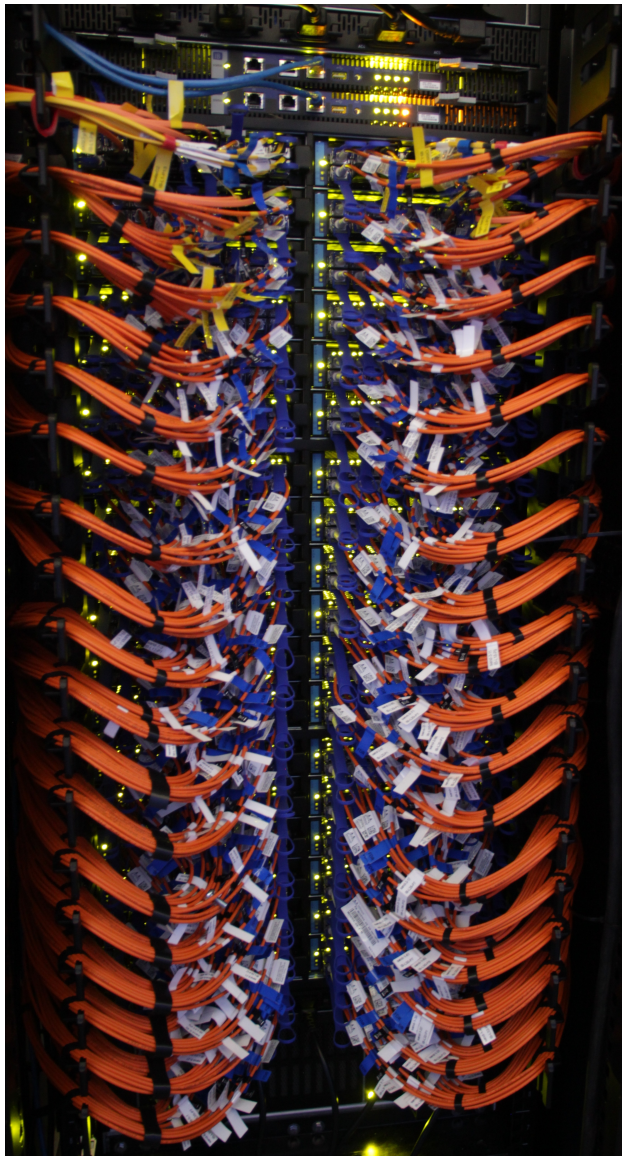
1. Take some (multicore) processors plus some memory to make a node.
   - Could be an off-the-shelf server, or something more special.

Basics: How to Build a Supercomputer

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

   Gbit Ethernet: 100 MB/sec
   Omni-Path: 10 GB/sec

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



Basics: How to Build a Supercomputer

3. Allocate CPUs & memory to workload
   - Clusters consist of distinct nodes (i.e. separate Linux computers), networked together and controlled centrally by a scheduler.
     * Each process/thread can see only its local node's CPUs and memory (without help from e.g. MPI).
     * Each process/thread must fit within a single node's memory.
   - More expensive machines logically bind nodes into a single system.
     * Logically one big node.
     * A single process can see the entire system.
     * E.g. SGI UV.

Basics: Running Applications on a Cluster

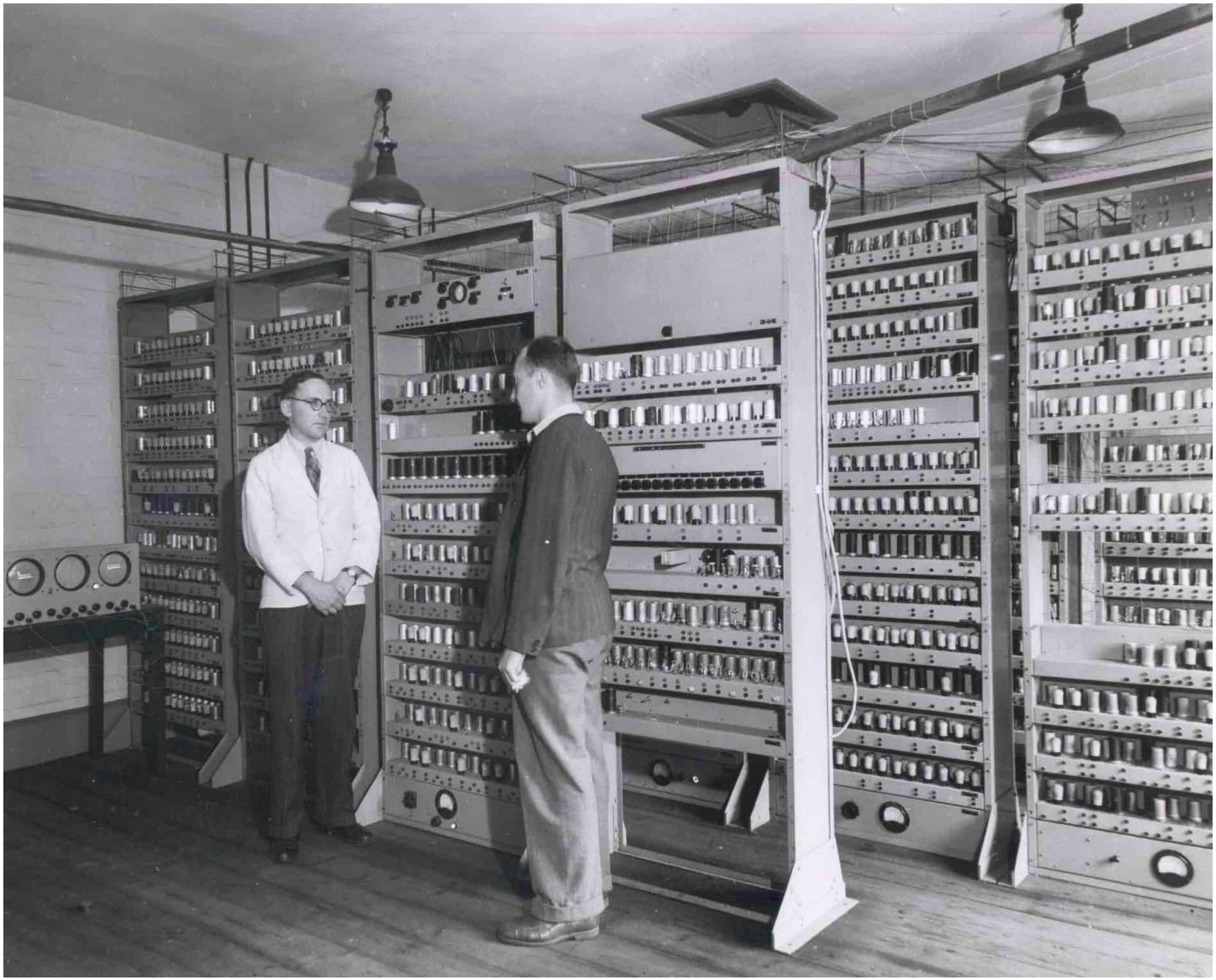
- Non-parallel (serial) code
  - For a single node as for a workstation.
  - Typically run as many copies per node as CPUs, assuming node memory is sufficient.
  - Or simply use the memory accompanying the remaining CPUs.
  - Can replicate this across multiple nodes.
- Parallel code
  - Thread parallelism works only within a node.
    E.g. pthreads, OpenMP.
  - MPI parallelism works both intra- and inter-node.
  - Some hybrid codes use both forms of parallel programming.

Basics: Summary

- Why have a supercomputer?
  - Single problems requiring great time or big data; many problems.
- Most current supercomputers are clusters of separate nodes.
- Each node has multiple CPUs and (non-uniform, shared) memory.
- Parallel code may use pthreads/OpenMP/MPI within a node, or MPI across multiple nodes.
- Serial code uses a single CPU and the memory of one node, but may be copied across many nodes.

Part II: **Research Computing Services HPC**

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!
- Used in meteorology, genetics, theoretical chemistry, numerical analysis, radioastronomy.
- *"On a few occasions it worked for more than 24 hours."*

Central HPC in Cambridge

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.
User base:	Includes external STFC & EPSRC plus industrial users.
Plus:	Dedicated group nodes and research projects.

History of Performance

http://www.top500.org

1997 76.8 Gflop/s

2002 1.4 Tflop/s

2006 18.27 Tflop/s

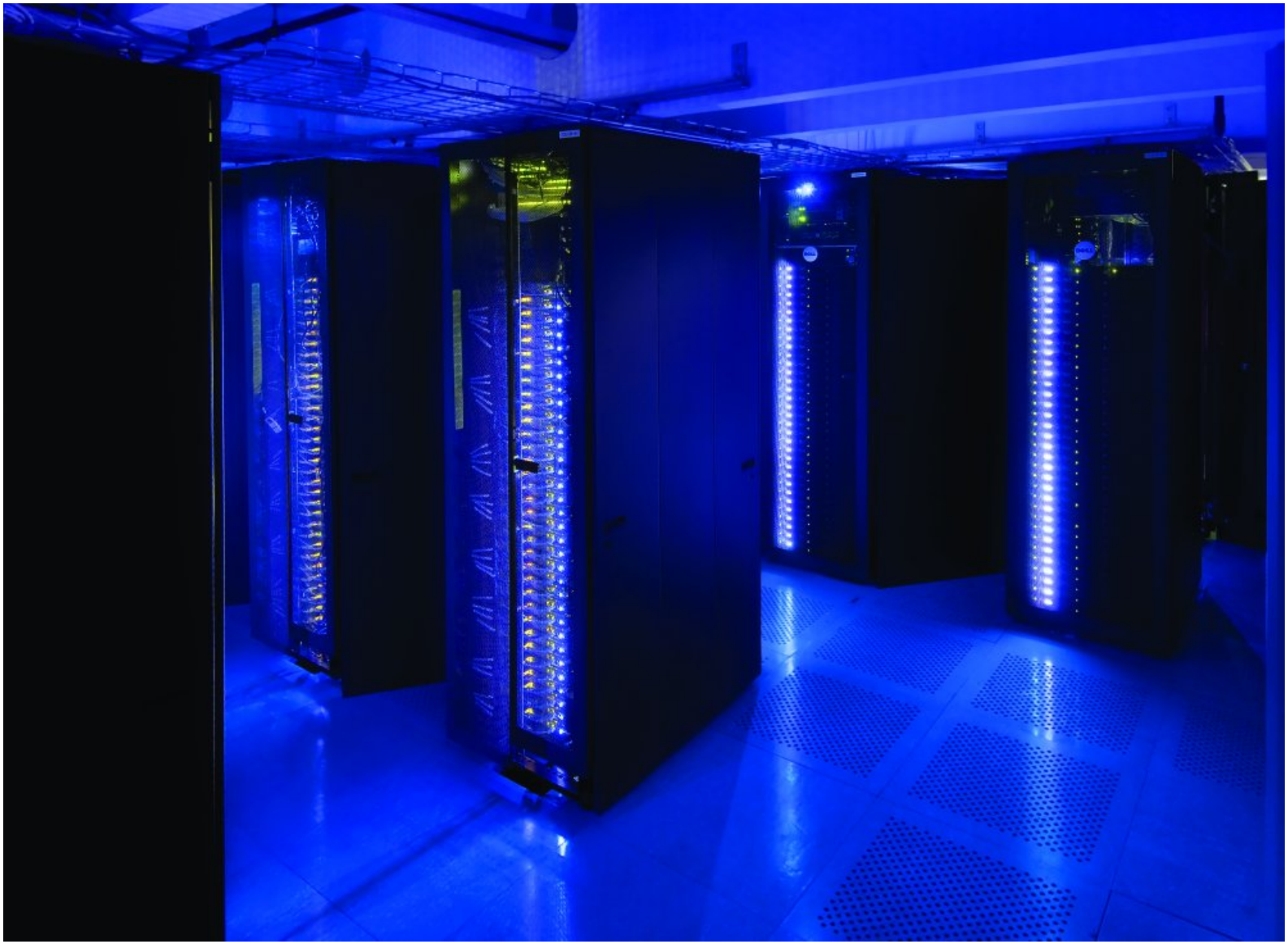
2010 30 Tflop/s

2012 183.38 Tflop/s

2013 183.38 CPU + 239.90 GPU Tflop/s

2018 2.271 CPU + 1.193 GPU Pflop/s

Darwin1 (2006–2012)



Darwin3 (2012–2018)(b) & Wilkes (2013–2018)(f)

Peta4 (2017) Cumulus (2018)

Skylake

- Each compute node:
  - 2x16 cores, Intel Skylake 2.6 GHz32 CPUs
  - 192 GB or 384 GB RAM6 GB or 12 GB per CPU
  - 100 Gb/sec Omni-Path10 GB/sec (for MPI and storage)
- 1152 compute nodes.
- 8 login nodes (login-cpu.hpc.cam.ac.uk).

Coprocessors — GPUs etc

- CPUs are general purpose
- Some types of parallel workload fit vector processing well:
  - Single Instruction, Multiple Data (SIMD)
  - *Think pixels on a screen*
  - GPUs specialise in this type of work
  - Also competitor many-core architectures such as the Intel Phi

Pascal

- Each compute node:
  - 4 × NVIDIA P100 GPU4 GPUs
  - 1x12 cores, Intel Broadwell 2.2 GHz12 CPUs
  - 96 GB RAM96 GB RAM
  - 100 Gb/sec (4X EDR) Infiniband.10 GB/sec (for MPI and storage)
- 90 compute nodes.
- 8 login nodes (login-gpu.hpc.cam.ac.uk).

KNL (Intel Phi)

- Each compute node:
  - 64 cores, Intel Phi 7210256 CPUs
  - 96 GB RAM96 GB RAM
  - 100 Gb/sec Omni-Path10 GB/sec (for MPI and storage)
- 342 compute nodes
- Shared login nodes with Skylake

Cluster Storage

- Lustre cluster filesystem:
  - Very scalable, high bandwidth.
  - Multiple RAID6 back-end disk volumes.
  - Multiple object storage servers.
  - Single metadata server.
  - Tape-backed HSM on newest filesystems.
  - 12 GB/sec overall read or write.
  - Prefers big read/writes over small.

Obtaining an Account and Support

- https://www.hpc.cam.ac.uk/applications-access-research-computing-services
- Email support@hpc.cam.ac.uk

Part III: **Using HPC**

Using HPC: Connecting to the RCS Clusters

- SSH secure protocol only.
  Supports login, file transfer, remote desktop. . .
- SSH access is allowed from anywhere.
  Fail2Ban will ban repeatedly failing clients for 20 minutes.
- Policies for other clusters may differ.

Connecting: Windows Clients

- putty, pscp, psftp
  http://www.chiark.greenend.org.uk/ sgtatham/putty/download.html
- WinSCP
  http://winscp.net/eng/download.php
- TurboVNC (remote desktop, 3D optional)
  http://sourceforge.net/projects/turbovnc/files/
- Cygwin (provides an application environment similar to Linux)
  http://cygwin.com/install.html
  Includes X server for displaying graphical applications running remotely.
- MobaXterm
  http://mobaxterm.mobatek.net/

Connecting: Linux/MacOSX/UNIX Clients

- ssh, scp, sftp, rsync
  Installed (or installable).
- TurboVNC (remote desktop, 3D optional)
  http://sourceforge.net/projects/turbovnc/files/
- On MacOSX, install XQuartz to display remote graphical applications.
  http://xquartz.macosforge.org/landing/

Connecting: Login

- From Linux/MacOSX/UNIX (or Cygwin):
  ssh -Y **abc123**@login-cpu.hpc.cam.ac.uk
- From graphical clients:
  Host: login-cpu.hpc.cam.ac.uk
  Username: **abc123** (your UCAM account name)
- login-cpu.hpc will map to a random login node
  i.e. one of login-e-9, login-e-10, . . . , login-e-16

Connecting: First time login

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

```
The authenticity of host 'login-cpu (128.232.224.50)' can't be established.

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

Are you sure you want to continue connecting (yes/no)? yes
Warning: Permanently added 'login-cpu,128.232.224.50' (ECDSA) to the list of known hosts.
```

- One should always check the fingerprint before typing "yes".
- Graphical SSH clients *should* ask a similar question.
- Designed to detect fraudulent servers.

Connecting: First time login

- Exercise 1 - Log into your RCS account.
- Exercise 2 - Simple command line operations.

Connecting: File Transfer

- With graphical clients, connect as before and drag and drop.
- From Linux/MacOSX/UNIX (or Cygwin):

  rsync -av **old_directory/**

  abc12@login-cpu.hpc.cam.ac.uk:rds/hpc-work/new_directory

  copies contents of old_directory to ~/rds/hpc-work/new_directory.

  rsync -av **old_directory**

  abc12@login-cpu.hpc.cam.ac.uk:rds/hpc-work/new_directory

  copies old_directory (and contents) to ~/rds/hpc-work/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.
- Exercise 3 - File transfer.

Connecting: Remote Desktop

- First time use of TurboVNC (recommended):

```
[sjr20@login-e-1 ~]$ 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 'login-e-1:99 (sjr20)' desktop is login-e-1:99

Starting applications specified in /home/sjr20/.vnc/xstartup
Log file is /home/sjr20/.vnc/login-e-1:99.log
```

- NB Choose a different password for VNC to protect your desktop from other users.
- Note the unique host and display number (login-e-1 and :99 here).

Connecting: Remote Desktop

- Remote desktop already running:

```
[sjr20@login-e-1 ~]$ vncserver -list

TigerVNC server sessions:

X DISPLAY #     PROCESS ID
:99             130655
```

- Kill it:

```
[sjr20@login-e-1 ~]$ vncserver -kill :99
Killing Xvnc process ID 130655
```

- 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:

  ```
  vncviewer -via abc12@login-e-1.hpc.cam.ac.uk localhost:99
  ```

- The display number :99 will be different in general and unique to each desktop.
- You will be asked firstly for your cluster login password, and secondly for your VNC password.
- Press F8 to bring up the control panel.

Using HPC: User Environment

- Scientific Linux 7.x (Red Hat Enterprise Linux 7.x rebuild)
  - bash shell
  - Gnome or XFCE4 desktop (if you want)
  - GCC, Intel, PGI compilers and other development software.
- But you don't need to know that.
- NOT Ubuntu or Debian!
- CentOS 7 is OK.

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.
- /rds/user/abc123/hpc-work a.k.a. /home/abc123/rds/hpc-work
  - Visible equally from all nodes.
  - Larger and faster (1TB initial quota).
  - Intended for job inputs and outputs.
  - Not backed up.
  - Research Data Storage
  - https://www.hpc.cam.ac.uk/research-data-storage-services

Filesystems: Quotas

- quota

```
[abc123@login-e-1 ~]$ quota
Filesystem  GiBytes    quota   limit   grace    files    quota    limit   grace User/group
/home          10.6     40.0    40.0       0    ----- No ZFS File Quotas  ----- U:abc123
/rds-d2         1.0   1024.0  1126.4       -        8  1048576  1048576       - G:abc123
```

- 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.

Filesystems: Quotas

- quota

```
[abc123@login-e-1 ~]$ quota
Filesystem  GiBytes    quota   limit   grace    files    quota    limit   grace User/group
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- 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.

Filesystems: Permissions

- Be careful and if unsure, please ask support.
  - 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.

User Environment: Software

- Free software accompanying Red Hat Enterprise Linux is (or can be) provided.
- Other software (free and non-free) is available via modules.
- Some proprietary software may not be generally accessible.
- New software may be possible to provide on request.
- Self-installed software should be properly licensed.
- *sudo will not work.* (You should be worried if it did.)
- Docker-compatible containers can now be downloaded and used via singularity.

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                                 9) intel/impi/2017.4/intel
  2) slurm                              10) intel/libs/idb/2017.4
  3) turbovnc/2.0.1                     11) intel/libs/tbb/2017.4
  4) vgl/2.5.1/64                       12) intel/libs/ipp/2017.4
  5) singularity/current                13) intel/libs/daal/2017.4
  6) rhel7/global                       14) intel/bundles/complib/2017.4
  7) intel/compilers/2017.4             15) rhel7/default-peta4
  8) intel/mkl/2017.4
```

- Available:

```
module av
```

User Environment: Environment Modules

- Whatis:

```
module whatis openmpi-1.10.7-gcc-5.4.0-jdc7f4f
openmpi-1.10.7-gcc-5.4.0-jdc7f4f: The Open MPI Project is an open source...
```

- Load:

```
module load openmpi-1.10.7-gcc-5.4.0-jdc7f4f
```

- Unload:

```
module unload openmpi-1.10.7-gcc-5.4.0-jdc7f4f
```

User Environment: Environment Modules

- Matlab

```
module load matlab/r2017b
```

- 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.
- MATLAB Parallel Server is also available.

User Environment: Environment Modules

- Purge:

```
module purge
```

- Defaults loaded on login (vary by cluster):

```
module show rhel7/default-peta4
-------------------------------------------------------------------
/usr/local/Cluster-Config/modulefiles/rhel7/default-peta4:

module-whatis    default user environment for Peta4 nodes with Intel MPI
setenv           OMP_NUM_THREADS 1
module           add dot slurm turbovnc vgl singularity
module           add rhel7/global
module           add intel/bundles/complib/2017.4
-------------------------------------------------------------------
module load rhel7/default-peta4
```

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

Exercise 5: 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 node
  — not itself 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.

Using HPC: Job Submission

- Jobs may use part or all of one or more nodes
  — the owner can specify `--exclusive` to force exclusive node access (automatic on KNL).
- 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-e-1]$ sbatch slurm_submission_script
Submitted batch job 790299
```

Job Submission: Show Queue

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

```
[abc123@login-e-1]$ squeue -u abc123
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
            790299   skylake     Test3  abc123 PD       0:00      2 (PriorityResourcesAssocGrpCPUMinsL
            790290   skylake     Test2  abc123  R   27:56:10      2 cpu-e-[1,10]
```

Job Submission: Monitor Job

- Examine a particular job:

```
[abc123@login-e-1]$ scontrol show job=790290
```

Job Submission: Accounting Commands

- How many core hours available do I have?

```
mybalance

User           Usage |        Account     Usage | Account Limit Available (hours)
---------- --------- + ------------- --------- + ------------- ---------
sjr20              3 |    SUPPORT-CPU     2,929 |    22,425,600 22,422,671
sjr20              0 |    SUPPORT-GPU         0 |        87,600    87,600
```

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

```
gbalance -p SUPPORT-CPU

User           Usage |        Account     Usage | Account Limit Available (hours)
---------- --------- + ------------- --------- + ------------- ---------

pfb29          2,925 |    SUPPORT-CPU     2,929 |    22,425,600 22,422,671
sjr20 *            3 |    SUPPORT-CPU     2,929 |    22,425,600 22,422,671
...
(Use -u for user.)
```

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

```
gstatement -p SUPPORT-CPU  -u xyz10 -s "2018-04-01-00:00:00" -e "2018-04-30-00:00:00"
       JobID      User    Account    JobName  Partition                 End ExitCode      State  CompHrs
------------ --------- ---------- ---------- ---------- ------------------- -------- ---------- --------
263              xyz10 support-c+ _interact+    skylake 2018-04-18T19:44:40      0:0    TIMEOUT      1.0
264              xyz10 support-c+ _interact+    skylake 2018-04-18T19:48:07      0:0 CANCELLED+      0.1
275              xyz10 support-c+ _interact+    skylake             Unknown      0:0    RUNNING      0.3
...
```

Job Submission: Cancel Job

- Cancel a particular job:

```
[abc123@login-e-1]$ scancel 790290
```

Job Submission: Scripts

- SLURM
  In /usr/local/Cluster-Docs/SLURM, see examples: slurm_submit.peta4-skylake, slurm_submit.wilkes2.

```
#!/bin/bash
#! Name of the job:
#SBATCH -J myjob
#! 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*32)
#SBATCH --ntasks=116
#! How much wallclock time will be required?
#SBATCH --time=02:00:00
#! Select partition:
#SBATCH -p skylake
...
```

- #SBATCH lines are *structured comments*
  — correspond to sbatch command line options.
- The above job will be given 1 cpu16 cpus on 1 node for 2 hours (by default there is 1 task per node, and 1 cpu per task).

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=5990
# 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=1
# Default is 1 cpu (core) per task
#SBATCH --mem=5990
# 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=32 # Whole node

#SBATCH --mem=5990
# 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=32  # For OpenMP across 32 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  # Half node

#SBATCH --mem=5990
# 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=32 # Whole node

#SBATCH --mem=5990
# 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 (using all memory)
$application $options
...
```

Job Submission: MPI Jobs

- Parallel job across multiple nodes.

```
#!/bin/bash
...
#SBATCH --nodes=4
#SBATCH --ntasks=128      # i.e. 32x4 MPI tasks in total.
#SBATCH --cpus-per-task=2
...
mpirun -np 128 $application $options
...
```

- SLURM-aware MPI launches remote tasks via SLURM (doesn't need a list of nodes).

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 -ppn 16 -np 64 $application $options
...
```

- SLURM-aware MPI launches remote tasks via SLURM (doesn't need a list of nodes).

Job Submission: Hybrid Jobs

- Parallel jobs using both MPI and OpenMP.

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

- This job uses 128 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=2
...
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 6–8 - Submitting Jobs.

Job Submission: Interactive

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

```
sintr -A TRAINING-CPU -N1 -n8 -t 1:0:0
```

- Within the window (screen session):
  - Launches a shell on the first node (when the job starts).
  - Graphical applications should display correctly (if they did from the login node).
  - 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.

Job Submission: Array Jobs

- *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-e-1]$ sbatch --array=1-7:21,3,5,7 -A TRAINING-CPU submit_script
Submitted batch job 791609

[abc123@login-e-1]$ squeue -u abc123
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
         791609_1 skylake      hpl    abc123  R       0:06      1 cpu-a-6
         791609_3 skylake      hpl    abc123  R       0:06      1 cpu-a-16
         791609_5 skylake      hpl    abc123  R       0:06      1 cpu-a-7
         791609_7 skylake      hpl    abc123  R       0:06      1 cpu-a-7
```

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).
- Exercise 9 - Array Jobs.

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.
  - Demands that the higher priority jobs not be delayed.
  - Relies on reasonably accurate wall time requests for this to work.
  - Jobs of default length will not backfill readily.

Wait Times

- 36 hour job walltimes are permitted.
- This sets the timescale at busy times (*without* backfilling).
- Use backfilling when possible.
- Short (1 hour or less) jobs have higher throughput.

Checkpointing

- Insurance against failures during long jobs.
- Restart from checkpoints to work around finite job length.
- Application native methods are best. Failing that, one can try DMTCP:

  http://dmtcp.sourceforge.net/index.html

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.