

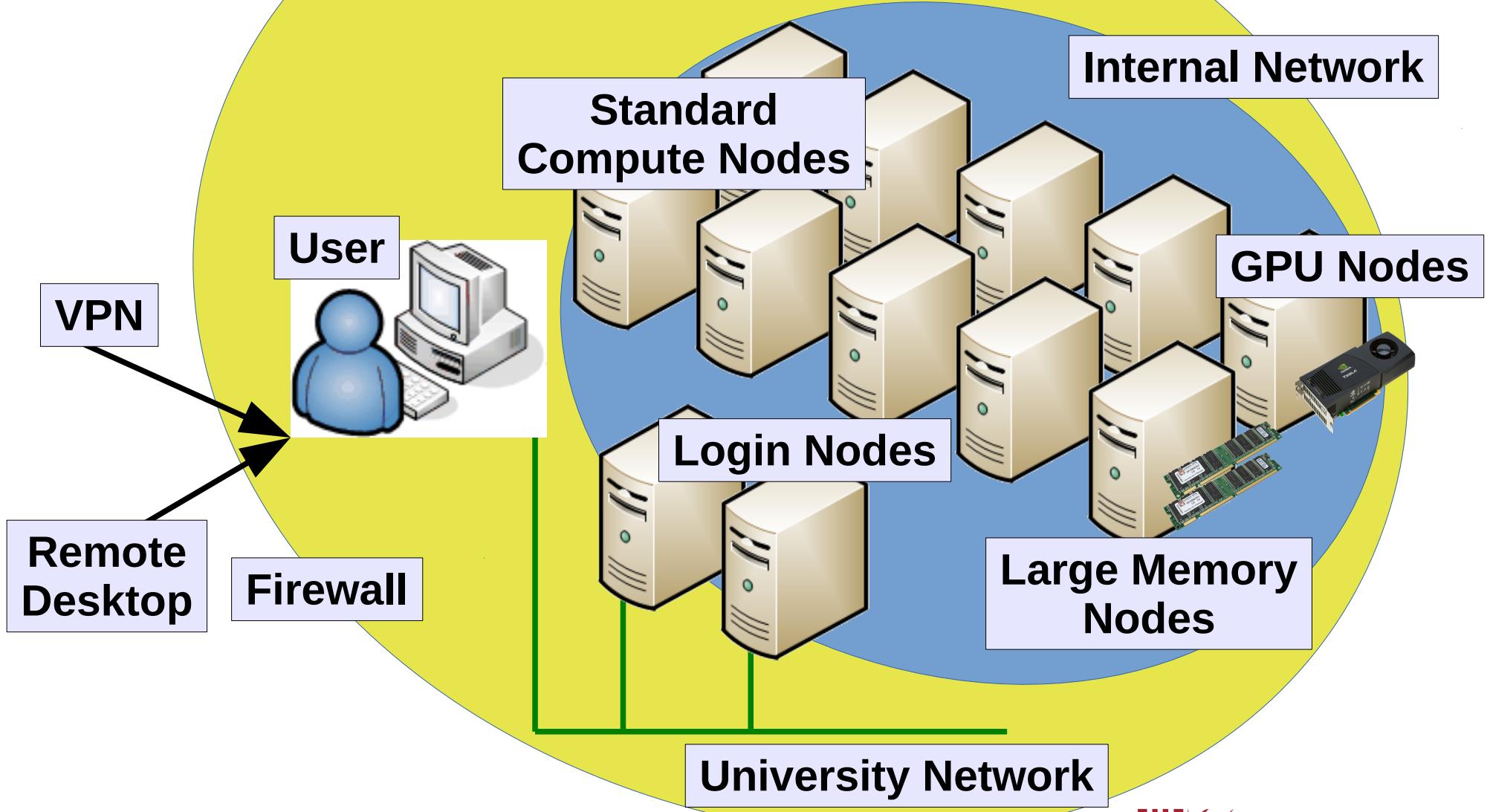
# Introduction to BlueCrystal



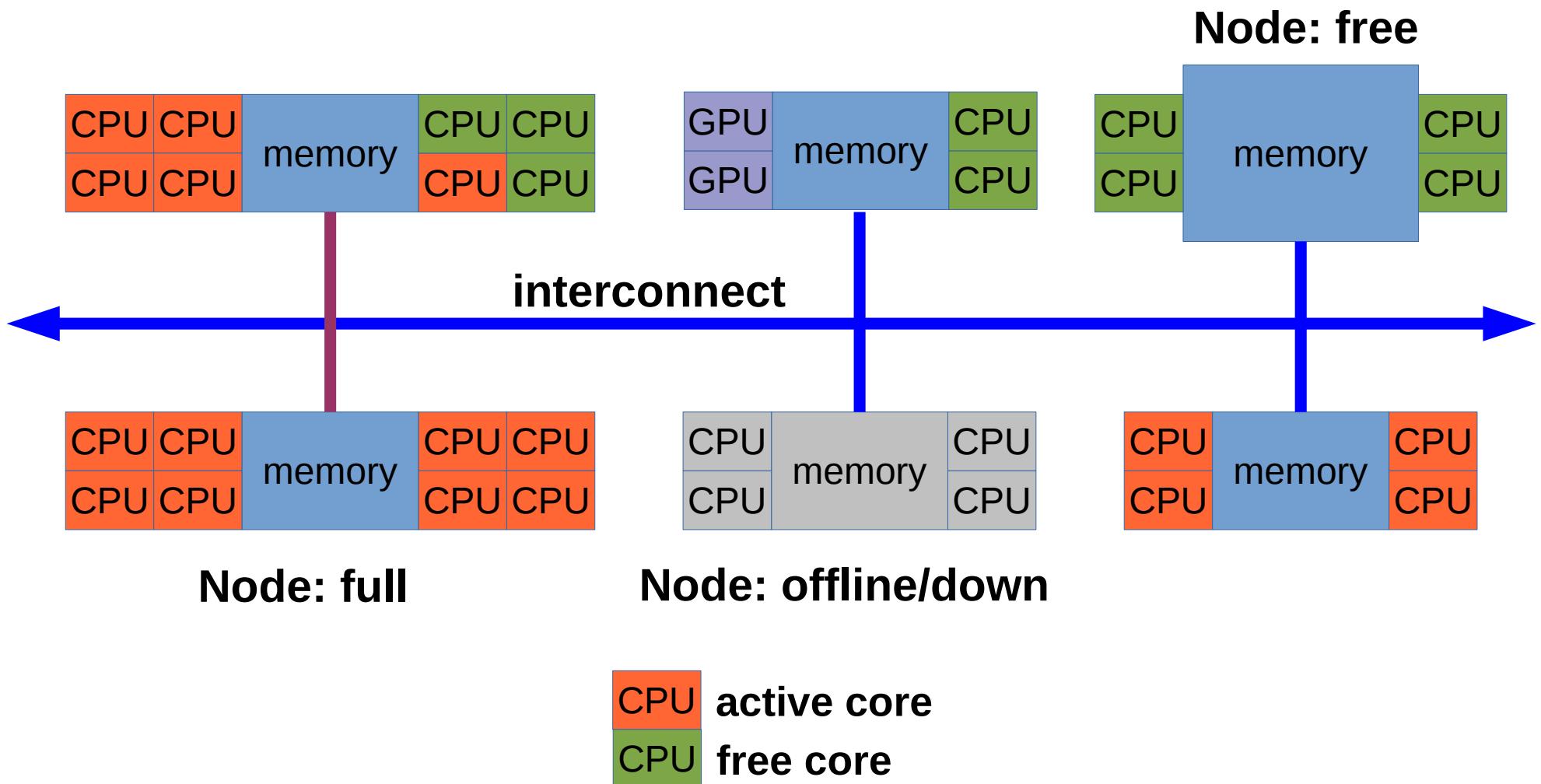
# Overview

- Schematic of a Cluster
- BlueCrystal, please show yourself.
- Logging in.
- The queuing system.
- A job submission script.
- Submitting, tracking and deleting a job.
- Environment Modules.

# BlueCrystal: A 'Commodity Cluster' Supercomputer

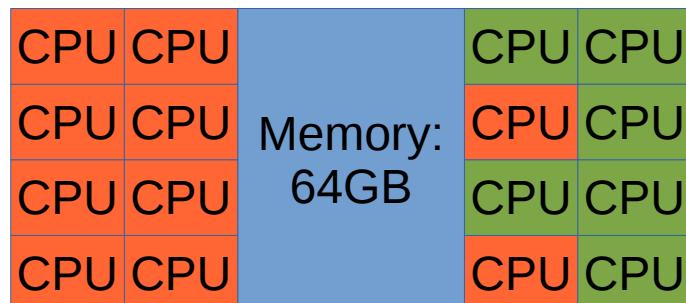


# A Cluster of Heterogeneous Nodes



# BlueCrystal Phase 3

## Standard node



- 8 cores/socket
- 16 cores/node
- Intel SandyBridge (E5-2670, 2.60GHz)

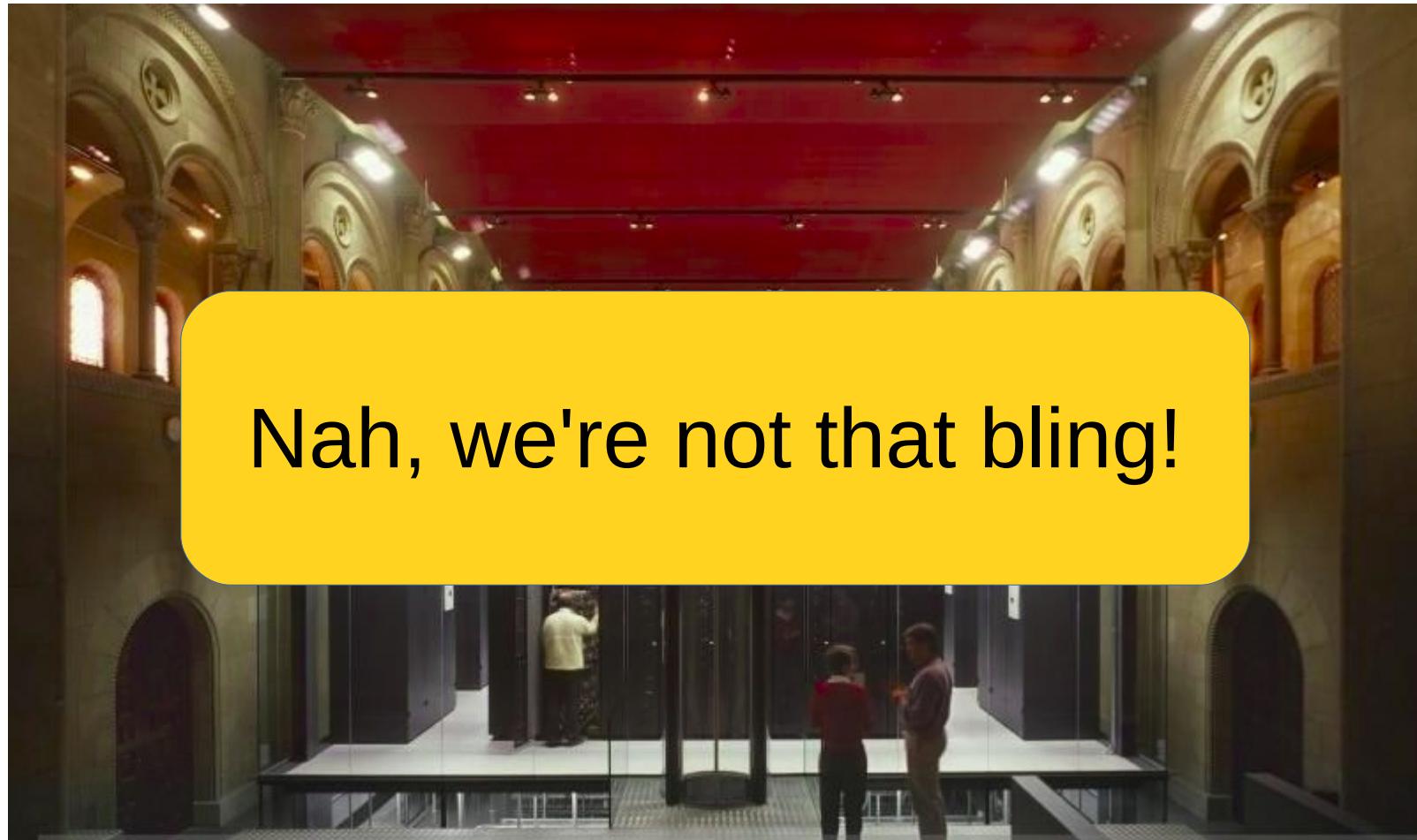
- Interconnect: QDR InfiniBand

Around 350 nodes, 5,500 cores, ~200TFlops  
(but cost £2M compared to US\$273M for world #1..)

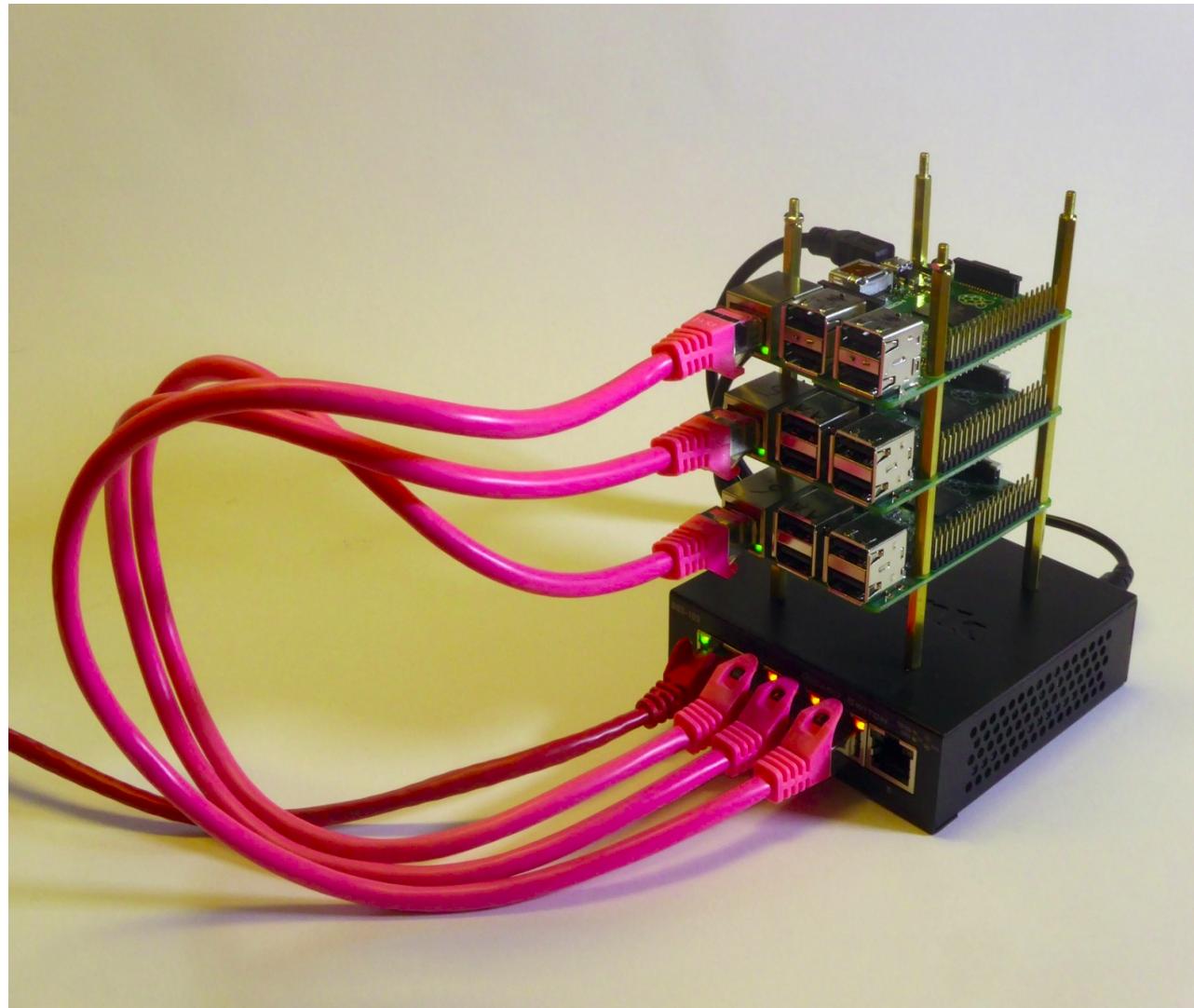
# BlueCrystal



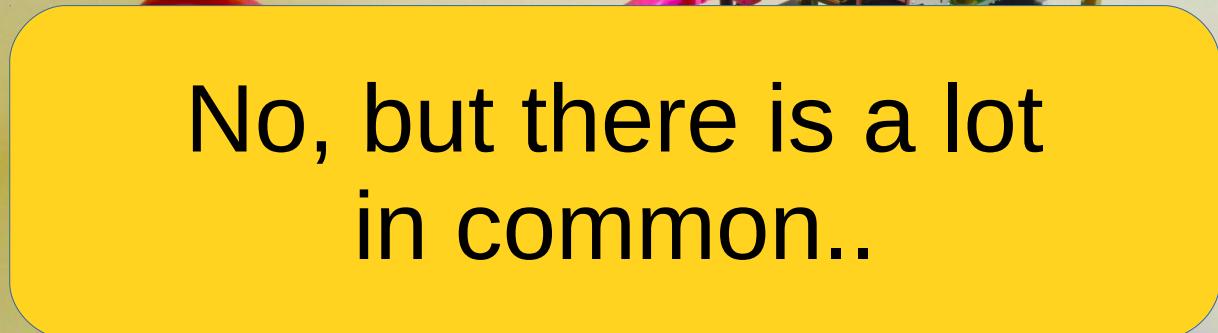
# BlueCrystal



# BlueCrystal



# BlueCrystal



No, but there is a lot  
in common..



# BlueCrystal



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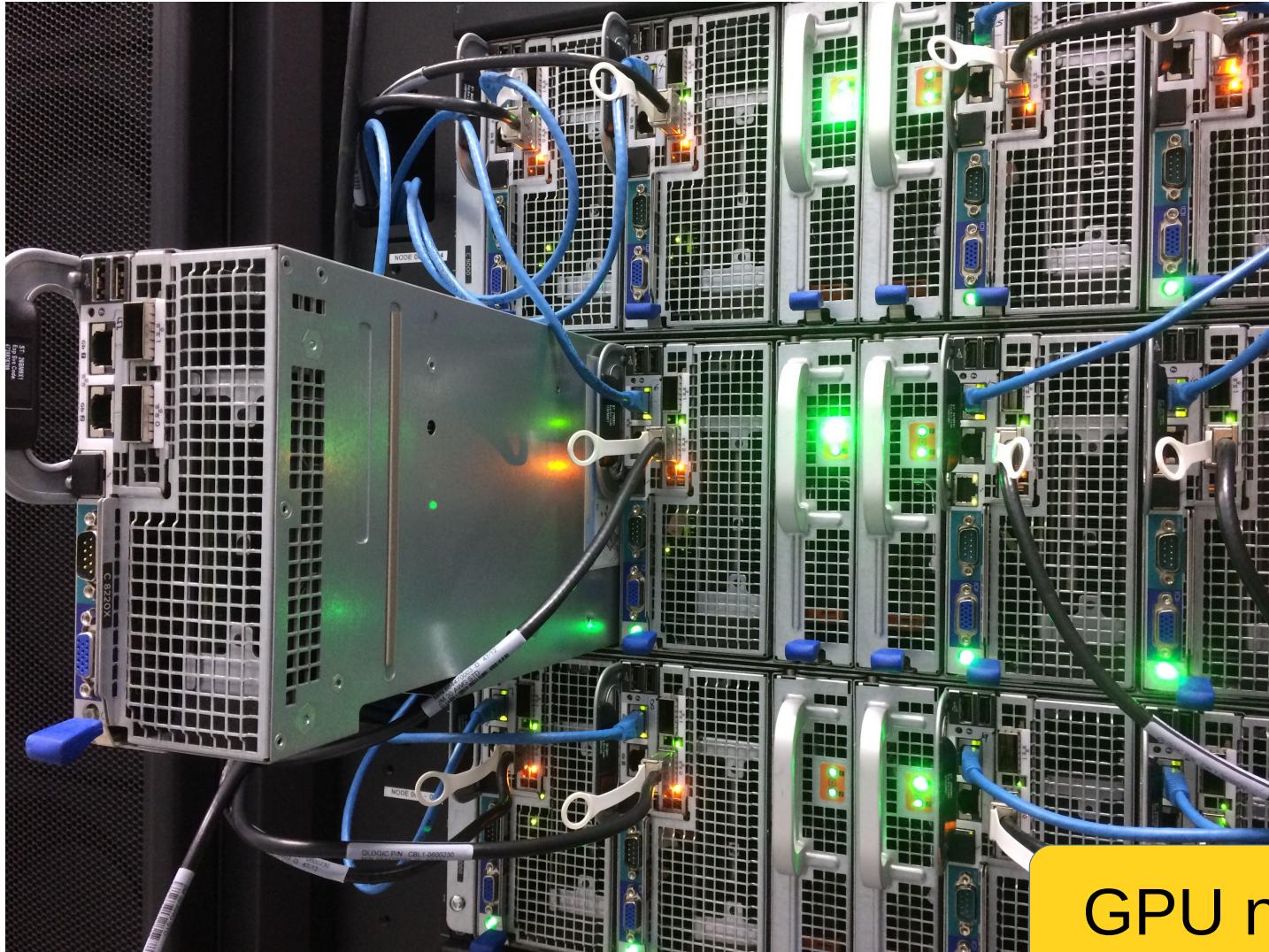
# BlueCrystal



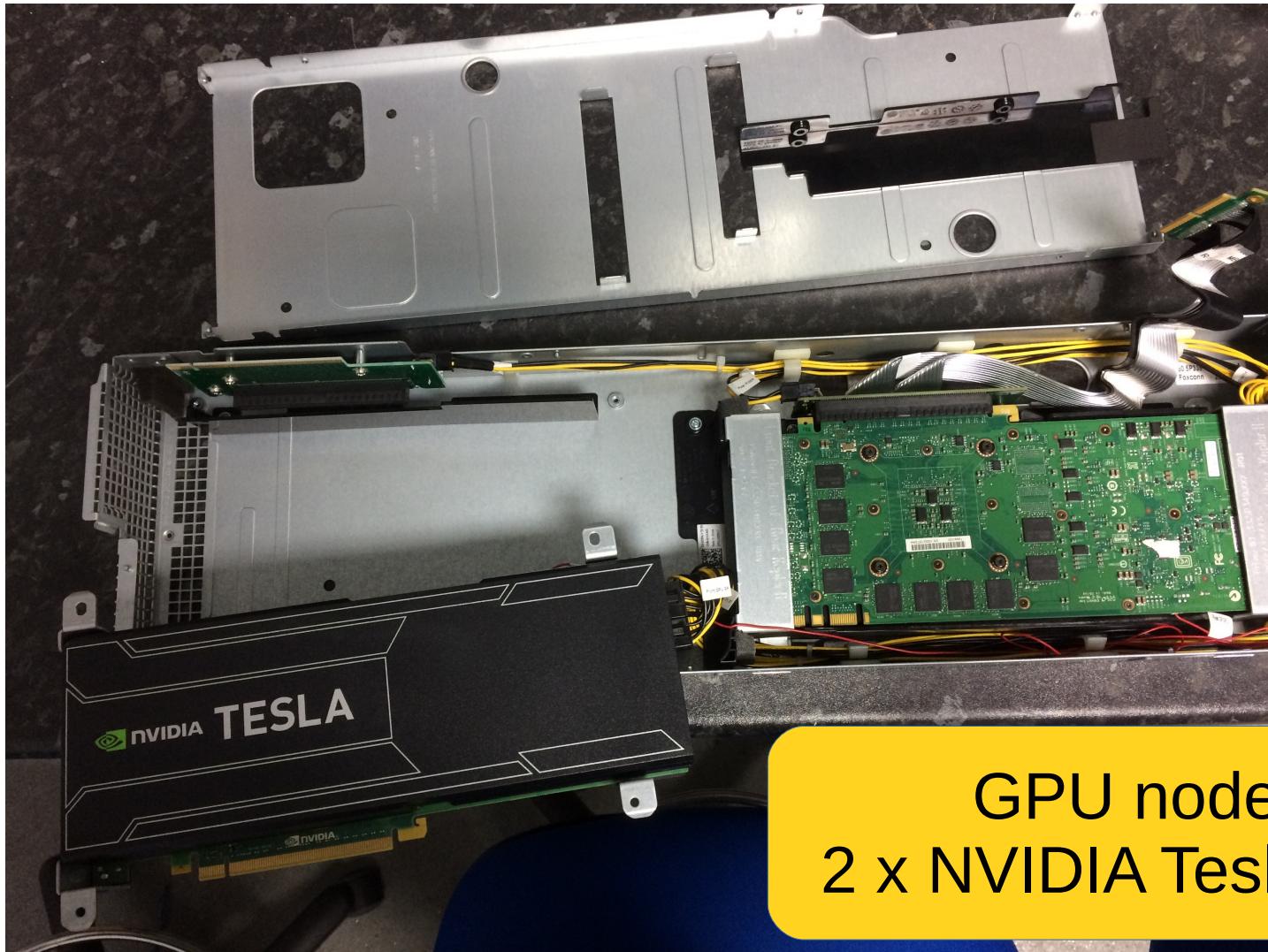
# BlueCrystal: Phase 3



# BlueCrystal: Phase 3



# BlueCrystal: Phase 3



# When you log in

```
[ggdagw@newblue2 ~]$ █
```

# When you log in

```
[ggdagw@newblue2 ~]$ █
```

£2M well spent!

# It's Linux!

```
top - 12:32:34 up 55 days, 16:47, 34 users, load average: 1.60, 2.02, 2.30
Tasks: 803 total, 5 running, 783 sleeping, 13 stopped, 2 zombie
Cpu(s): 9.1%us, 3.6%sy, 0.0%ni, 86.0%id, 0.0%wa, 0.0%hi, 1.3%si, 0.0%st
Mem: 132252088k total, 131862452k used, 389636k free, 3656k buffers
Swap: 11999228k total, 638640k used, 11360588k free, 129722640k cached
```

PID	USER	PR	NI	VIRT	RES	SHR	S	%CPU	%MEM	TIME+	COMMAND
27018	epdab	20	0	270m	168m	772	R	100.0	0.1	64:48.91	grep
7480	am14886	20	0	66396	3640	756	R	51.0	0.0	57:02.83	ssh
5249	root	20	0	0	0	0	S	13.9	0.0	1239:41	qib_cq0
7479	am14886	20	0	60252	488	308	S	12.9	0.0	17:00.95	scp
2324	root	20	0	28392	4936	2236	R	4.6	0.0	0:01.60	ipmi-sensors
20686	yh1714	20	0	60260	896	460	S	3.3	0.0	1:17.91	sftp-server
6208	nslcd	20	0	393m	1164	664	S	3.0	0.0	75:45.10	nslcd
6889	root	20	0	0	0	0	S	2.3	0.0	229:34.83	kpanfs_thpool
6890	root	20	0	0	0	0	S	2.3	0.0	229:42.34	kpanfs_thpool
6891	root	20	0	0	0	0	S	2.3	0.0	229:39.05	kpanfs_thpool
6892	root	20	0	0	0	0	S	2.3	0.0	229:39.55	kpanfs_thpool
6893	root	20	0	0	0	0	S	2.3	0.0	229:42.72	kpanfs_thpool
6894	root	20	0	0	0	0	S	2.3	0.0	229:42.72	kpanfs_thpool
6895	root	20	0	0	0	0	S	2.3	0.0	229:42.72	kpanfs_thpool
6896	root	20	0	0	0	0	S	2.3	0.0	229:42.72	kpanfs_thpool
6898	root	20	0	0	0	0	S	2.3	0.0	229:42.72	kpanfs_thpool
6901	root	20	0	0	0	0	S	2.3	0.0	229:42.72	kpanfs_thpool

'top' should show a modest load on the login nodes

# It's Linux!

- For those familiar:
  - Same tools as those you are used to on your laptop, desktop, workstation or remote server..
- For those unfamiliar:
  - You'll need to get familiar with:
    - The command line and shell
    - Starting up a text editor (emacs, gedit etc.)
    - redirecting I/O streams etc.

# It's a *Shared* System

```
[ggdagw@newblue2 ~]$ who | head -20
aexbz    pts/1      2017-09-21 09:50 (it025412.users.bris.ac.uk)
epdab    pts/2      2017-09-21 10:31 (it051705.users.bris.ac.uk)
mt14481   pts/3      2017-09-11 13:26 (it025331.users.bris.ac.uk)
ts12436   pts/4      2017-09-21 10:26 (it065525.users.bris.ac.uk)
am14886   pts/9      2017-09-21 09:12 (vpn-user-248-148.nomadic.bris.ac.uk)
rs15164   pts/10     2017-09-21 11:28 (vpn-user-249-121.nomadic.bris.ac.uk)
lm15898   pts/12     2017-09-09 16:05 (it033733.users.bris.ac.uk)
sm15511   pts/13     2017-09-19 10:46 (it062184.users.bris.ac.uk)
ah12410   pts/15     2017-09-18 12:14 (it000473.users.bris.ac.uk)
at15963   pts/17     2017-09-06 13:59 (it062400.users.bris.ac.uk)
ce16990   pts/22     2017-09-20 14:04 (it064058.wks.bris.ac.uk)
chmahk    pts/23     2017-09-21 09:31 (it060015.users.bris.ac.uk)
sz14869   pts/24     2017-09-13 09:26 (it021619.users.bris.ac.uk)
eejrp     pts/26     2017-09-19 10:15 (it025844.wks.bris.ac.uk)
lk12325   pts/25     2017-09-20 09:14 (it062728.users.bris.ac.uk)
mu13199   pts/27     2017-09-21 11:03 (vpn-user-248-018.nomadic.bris.ac.uk)
kh1627    pts/28     2017-09-21 09:55 (it061938.users.bris.ac.uk)
me12288   pts/29     2017-09-19 12:06 (it062613.users.bris.ac.uk)
ieudata   pts/30     2017-09-21 12:11 (it017385.users.bris.ac.uk)
rs17282   pts/31     2017-09-18 15:52 (it050010.users.bris.ac.uk)
[ggdagw@newblue2 ~]$ who | wc
      34      170     2296
[ggdagw@newblue2 ~]$ █
```

# It has a Queuing System

Queue	Memory	CPU	Time	Walltime	Node	Run	Que	Lm	State
gaia	--	--		720:00:0	--	1	0	--	E R
gpu	--	--		360:00:0	--	5	0	--	E R
ghlc	--	--		480:00:0	--	0	0	--	E R
long	--	--		360:00:0	--	313	0	--	E R
paleo	--	--		360:00:0	--	0	0	--	E R
galaxy-std	--	--		240:00:0	--	0	0	--	E R
cfdgroup	--	--		480:00:0	--	4	0	--	E R
medium	--	--		240:00:0	--	134	0	--	E R
testq	--	--		01:00:00	--	1	1	--	E R
veryshort	--	--		12:00:00	--	6	0	--	E R
visualisation	--	--		576:00:0	--	0	0	--	E R
himem	--	--		360:00:0	--	8	0	--	E R
vsmp	--	--		360:00:0	--	0	0	--	E R
system	--	--		240:00:0	--	0	0	--	E R
galaxy-high	--	--		240:00:0	--	1	0	--	E R
short	--	--		120:00:0	--	466	58	--	E R
default	--	--		--	--	0	0	--	E R
bridge	--	--		360:00:0	--	1	0	--	E R
teaching	--	--		24:00:00	--	0	0	--	E R
accis	--	--		360:00:0	--	8	2	--	E R
glaciol	--	--		360:00:0	--	0	0	--	E R
amd-gpu	--	--		360:00:0	--	0	0	--	E R
						948	61		

# It has a Queuing System

```
6113426          jr15286  Running   1 13:23:51:02  Wed Sep 20 12:25:26
6113429          jr15286  Running   1 13:23:51:34  Wed Sep 20 12:25:58
6113428          jr15286  Running   1 13:23:51:34  Wed Sep 20 12:25:58
6113430          jr15286  Running   1 13:23:52:06  Wed Sep 20 12:26:30
6113431          jr15286  Running   1 13:23:52:06  Wed Sep 20 12:26:30
6113432          jr15286  Running   1 13:23:52:38  Wed Sep 20 12:27:02
6113986          lc0415   Running   1 14:04:01:46  Wed Sep 20 16:36:10
6085406          pc14830  Running   1 16:08:35:11  Thu Sep  7 21:09:35

946 active jobs      4379 of 5760 processors in use by local jobs (76.02%)
                      279 of 361 nodes active      (77.29%)

eligible jobs-----
JOBID           USERNAME    STATE PROCS    WCLIMIT    QUEUETIME
6118912          xs7126     Idle   16  5:00:00:00  Thu Sep 21 12:08:41
6118921          col2181    Idle   16  1:16:00:00  Thu Sep 21 12:21:35

2 eligible jobs

blocked jobs-----
JOBID           USERNAME    STATE PROCS    WCLIMIT    QUEUETIME
6118621          epdjc      Idle   4   5:00:00:00  Thu Sep 21 11:16:34
6118622          epdjc      Idle   4   5:00:00:00  Thu Sep 21 11:16:35
6118623          epdjc      Idle   4   5:00:00:00  Thu Sep 21 11:16:35
6118624          epdjc      Idle   4   5:00:00:00  Thu Sep 21 11:16:36
6118625          epdjc      Idle   4   5:00:00:00  Thu Sep 21 11:16:36
6118626          epdjc      Idle   4   5:00:00:00  Thu Sep 21 11:16:37
6118627          epdjc      Idle   4   5:00:00:00  Thu Sep 21 11:16:37
:■
```

# What is a Queuing System?

**resource manager**

- monitors nodes
- load balances

**scheduler**

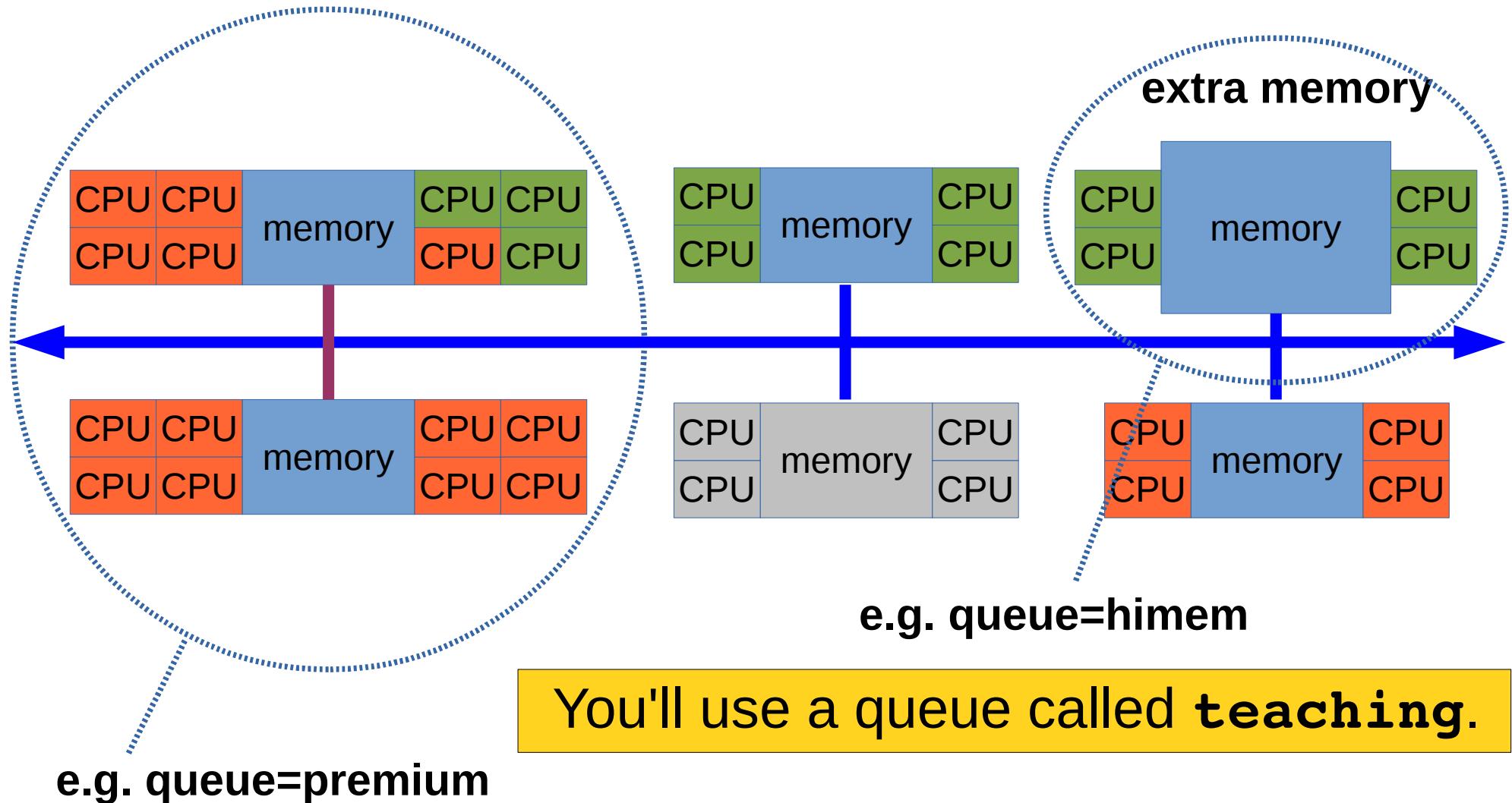
- ordered by priority
- key features:
  - job ID
  - state
  - resource request

Batch system

job	user	state	proc	time
114976	peter	running	4	00:10:00
114977	paul	running	1	01:00:00
114978	mary	idle	16	00:30:00
114979	peter	idle	256	24:00:00

Jobs are run when they are deemed the highest priority  
and some resources become free which match the request

# Typically Multiple Queues



# Submitting a Job

```
#!/bin/bash          A shell script

#PBS -q teaching      queue
#PBS -l nodes=1:ppn=4,walltime=00:05:00  resource request

#! application name
application="./hello_c.exe"      The program to run

cd $PBS_O_WORKDIR      where
export OMP_NUM_THREADS=$numnodes    environment

#! Run the executable
$application $options      Invoke the executable
```

**qsub <options> openmp\_submit**

# Queuing Systems Gotchas

- A shared memory job:

```
qsub -l nodes=2:ppn=4.
```

- Request is for 2 nodes, 4 processes per node.

- What's the problem here?

- Another request to BC3:

```
qsub -l nodes=1:ppn=32.
```

- What is the problem this time?

- **Don't** run 'e.g. watch qstat -u' – you'll prevent jobs from running – yours and others.

# There is a User Guide

The screenshot shows the homepage of the Advanced Computing Research Centre (ACRC) at Bristol University. The page features a dark blue header with the University of Bristol logo and the text "Advanced Computing Research Centre". Below the header is a banner with a blue crystalline background. The main content area has a white background. On the left, there is a sidebar with links to "ACRC home", "About HPC", "Members", "Training and Support", "Storage", "News and Events", and "People". The main content area includes a heading "Welcome to the Advanced Computing Research Centre", a paragraph about the centre's mission, and a photograph of server racks. A text box at the bottom states: "BlueCrystal is the University's High Performance Computing (HPC) machine." To the right, there are two columns: "News and Events" with three bullet points and "Training and Support" with four bullet points. At the bottom of the page, a yellow box contains the URL: <https://www.acrc.bris.ac.uk/pdf/bc-user-guide.pdf>.

# Let's Submit a Job

# 'qdel' To Delete a Job..

- ***If the job is still queued..*** no problems.
- ***If the job is running..*** make sure that the node is cleaned up afterward:
  - 'qstat -n'
  - ssh to the node(s) in question
  - 'killall -u'

# Environment Modules

```
[ggdagw@newblue2 ~]$ module list
Currently Loaded Modulefiles:
 1) shared
 2) dot
 3) torque/4.2.4.1
 4) moab/7.2.9
 5) default-environment
 6) openmpi/intel/64/1.6.5
 7) tools/git-1.8.4.2
 8) intel-cluster-studio/compiler/64/13.1/117
 9) intel-cluster-studio/mkl/64/13.1/117
10) cuda60/toolkit/6.0.37
[ggdagw@newblue2 ~]$ █
```

# .bashrc

```
[ggdagw@newblue2 ~]$ cat .bashrc
# .bashrc

# Source global definitions
if [ -f /etc/bashrc ]; then
    . /etc/bashrc
fi

export EDITOR=emacs

# User specific aliases and functions
module add shared default-environment
# MPI library
module add openmpi/intel/64/1.6.5
# git
module add tools/git-1.8.4.2
# Intel compiler
module add intel-cluster-studio/compiler/64/13.1/117
```

# Environment Modules

apps/charmm	intel-cluster-checker/2.0
apps/comsol-4.3b	intel-cluster-runtime/3.4
apps/comsol-4.3b-zone-e	intel-cluster-studio/compiler/32/13.1/117
apps/comsol-4.4	intel-cluster-studio/compiler/64/13.1/117
apps/comsol-5-zone-e	intel-cluster-studio/impi/32/4.1.0/024
apps/comsol-5.2-zone-e	intel-cluster-studio/impi/64/4.1.0/024
apps/comsol-5.2a-zone-e	intel-cluster-studio/ipp/32/2013.1.117
apps/comsol-5.3-zone-e	intel-cluster-studio/ipp/64/2013.1.117
apps/comsol-51-jg	intel-cluster-studio/itac/impi4/64/8.1.0.024
apps/cp2k-2.6.2-sopt	intel-cluster-studio/itac/mpich/64/8.1.0.024
apps/crystal-14-mpi	intel-cluster-studio/mkl/32/13.1/117
apps/crystal-14-v1.0.4-mpi	intel-cluster-studio/mkl/64/13.1/117
apps/crystal-14-v1.0.4-mpi.original	intel-cluster-studio/openmp/32/13.1/117
apps/cst-studio.2015	intel-cluster-studio/openmp/64/13.1/117
apps/cuda-5.5.22	intel-cluster-studio/src-ck/32/13.1/117
apps/cufflinks-2.2.1	intel-cluster-studio/src-ck/64/13.1/117
apps/depict	intel-cluster-studio/tbb/32/2013.1.117
apps/diffs splice-0.1.2	intel-cluster-studio/tbb/64/2013.1.117
apps/eman2.12	intel-cluster-studio/vtune/vtune-2013
apps/emboss-6.6.0	intel-cluster-studio/vtune/vtune-2015
apps/epacts	intel-mpi/32/4.0.3/008
apps/exabayes-1.2.1	intel-mpi/64/4.0.3/008
apps/fastqc-0.11.2	intel-mpi/64/4.1.0/024
apps/fastqc-0.11.5	intel-tbb-oss/ia32/40_20120613oss
apps/fc gene-1.0.7	intel-tbb-oss/intel64/40_20120613oss
apps/fda-gromacs-4.0.5	iozone/3_398
apps/ferret-v7.2	iperf/2.0.5
apps/freesurfer-5.3.0	languages/R-2.15.1
apps/fsl	languages/R-2.15.1-ATLAS
apps/galaxy	languages/R-3.0.2
apps/galaxy.backup	languages/R-3.0.2-ATLAS
apps/garli-2.01	languages/R-3.1.1-ATLAS
apps/gcta-1.24.3	languages/R-3.2.0-ATLAS
apps/gdal-1.11.1	languages/R-3.2.2-ATLAS
apps/geany-1.23.1	languages/R-3.2.4-ATLAS

# Environment Modules

The screenshot shows a web browser window with the following details:

- Title Bar:** Resources - ACRC, Univ
- Address Bar:** https://www.acrc.bris.ac.uk/acrc/resources.htm
- Left Sidebar (Menu):**
  - ACRC home
  - About HPC
  - Members
  - Training
  - Resources** (selected)
  - Support**
  - Storage
  - News and Events
  - People
- Content Area:**

### Guides for BlueCrystal users

Please also refer to the [Support](#) page for links to BlueCrystal user guides and details of how to request help with a specific problem.

#### Reference guides

<p><b>BlueCrystal quick reference guide</b></p> <p>This quick reference guide for both new and experienced users gives a summary of useful commands when using BlueCrystal.</p> <p>Topics include:</p> <ul style="list-style-type: none"><li>■ Configuring your environment</li><li>■ Using the queueing system</li><li>■ Useful commands</li></ul>	<p><b>Emacs reference card</b></p> <p>Emacs is a text editor that offers more support to programmers, through its various modes, than more generic editors, such as gedit or nano. Emacs uses a large number of key combinations as time-saving short cuts. The guide is a handy quick reference to the most commonly used key combinations.</p> <p>Topics include:</p> <ul style="list-style-type: none"><li>■ Files</li><li>■ Formatting</li><li>■ Regular expressions</li></ul>
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#### ACRC 'How-To' guides

We have developed some short 'How-To' guides. Let us know if there are other topics you would like to see in this series.

<a href="#">Getting Started with Compiler Flags</a>	<a href="#">Using Accelerators - GPUs and Co-processors - on BlueCrystal Phase 3</a>
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<https://www.acrc.bris.ac.uk/acrc/pdf/customising-environment-variables.pdf>

# Summary

- You now know what BlueCrytsal is and what it looks like.
- How to login, query the queue(s), submit, track and delete a job.
- How to control your environment.
- For better or for worse it's a Linux machine, with a command line, editors such as vi, emacs etc.