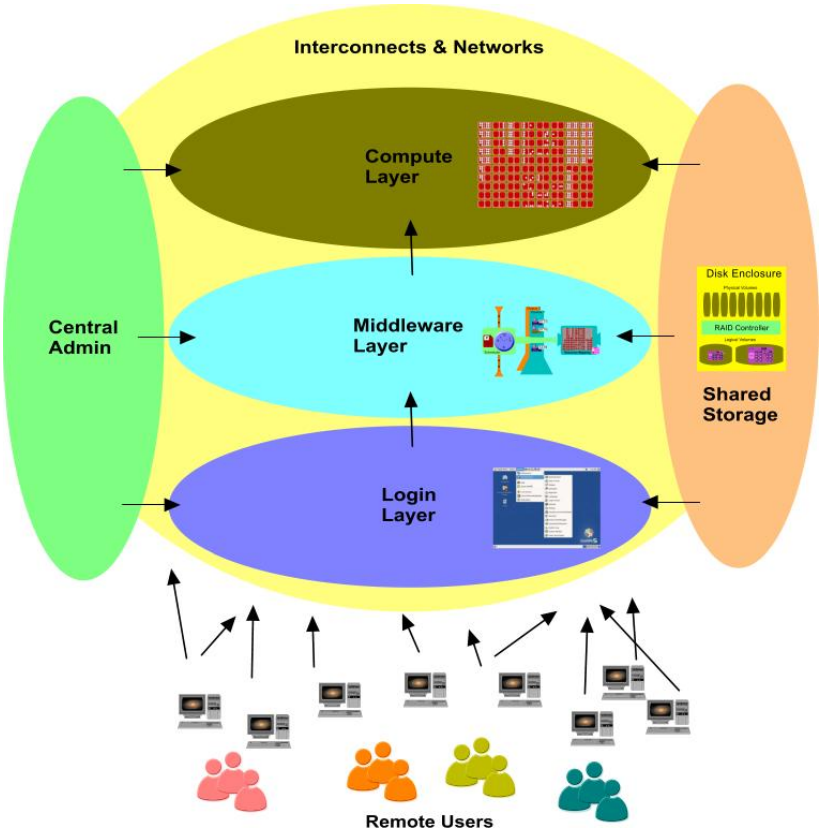
HPC Software and Management



Overview

- Common phrases and building blocks
- Memory models (reviewed)
- Managing software / Modules
- Schedulers and resource managers
- Being a good HPC citizen

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Common Phrases

- Login Server – The machine you connect to from your desktop (laptop).
- Computer server/node – A machine in the compute pool (3700 cores). Node = PC
- Job – A task to be completed by the compute pool. Will comprise of a program and some meta data (size,time etc)
- Queue – The place where jobs wait before they start.
- Lustre storage – Large project data area
- NFS storage - $HOME, the area you log into.
- Batch / Interactive jobs – job type sent to queues.

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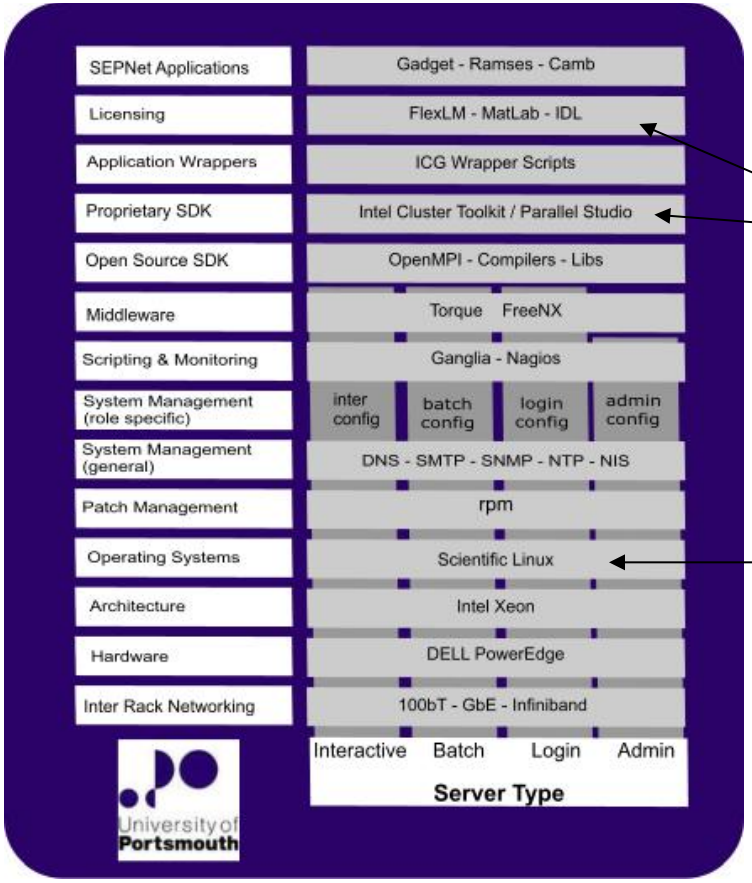
The STACK - Open Source HPC Stack

Two main Enterprise Linux players:-

RedHat & SUSE

Stability is all important. No need for latest and greatest (Fedora 16)



Licensed

RedHat Clone

(CERN)

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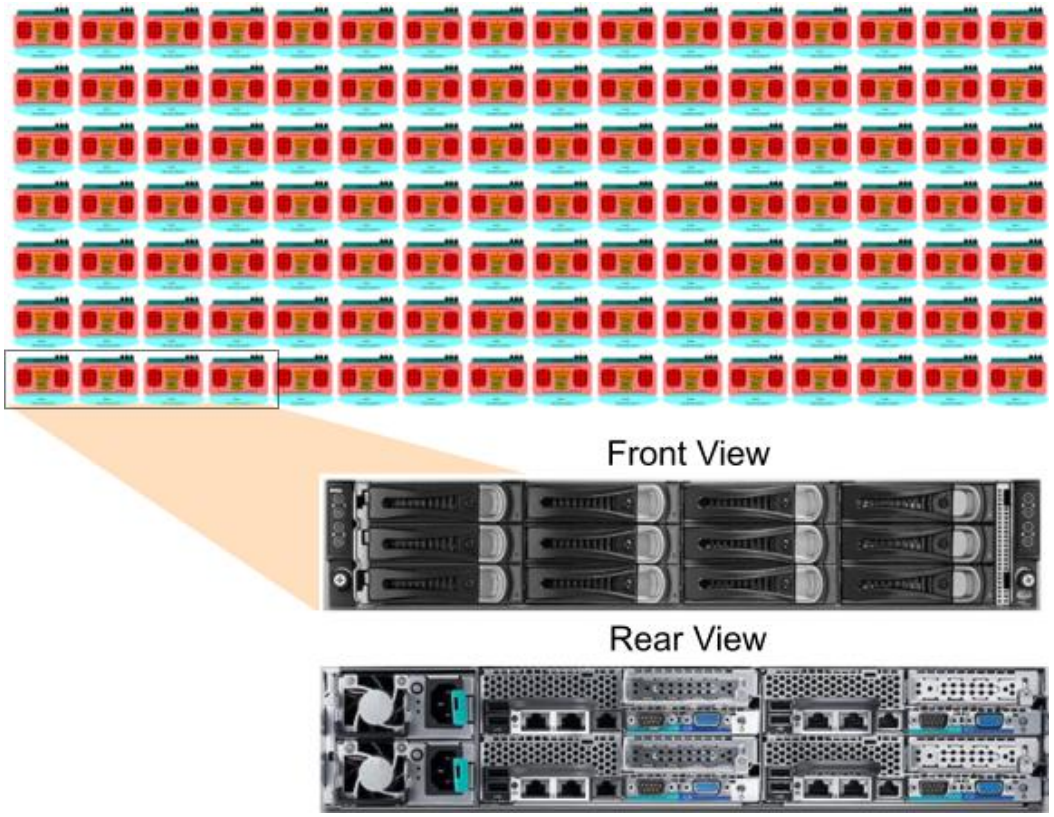
Memory Models

Distributed Memory Model



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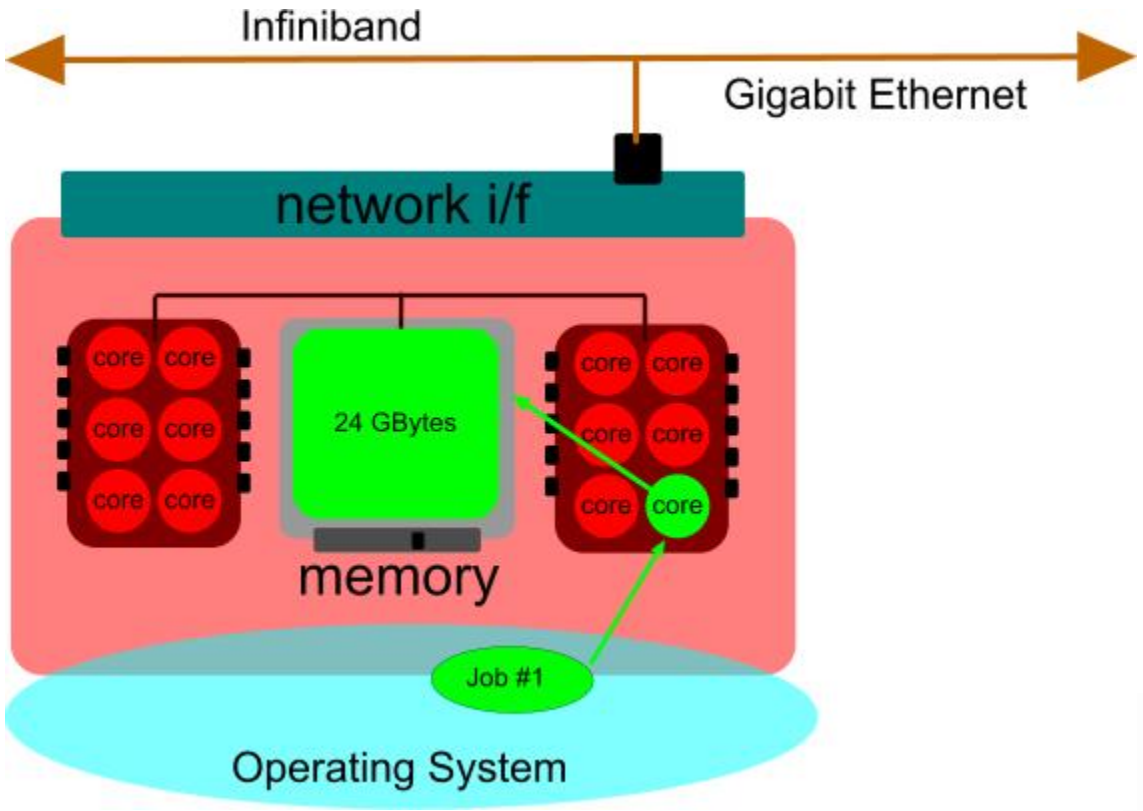
Largest (sensible) job is 24/64Gbytes in this distributed memory model

Paging

Swapping

OOM killer



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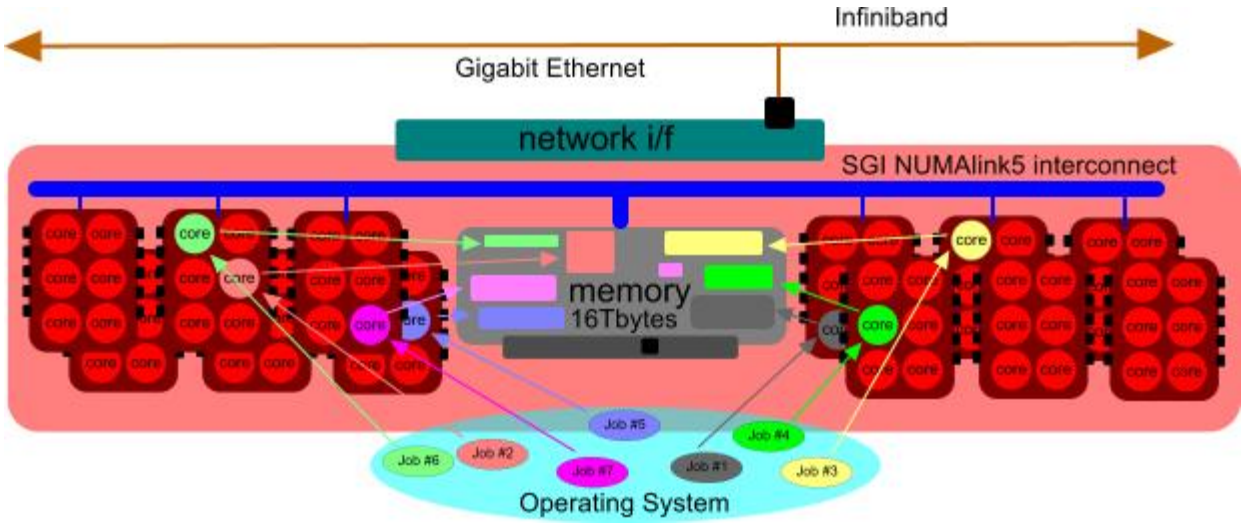
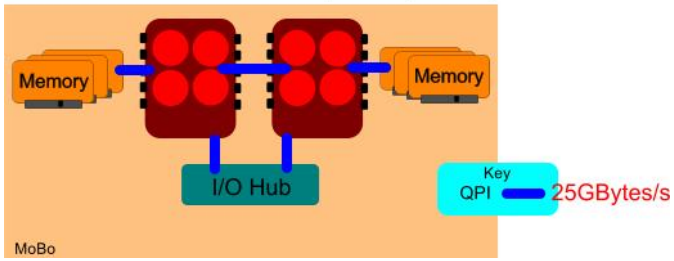
Shared Memory Model



Intel Quick Path Interconnect (Formally - FSB)



15GB/s peak

(3.2Gbytes)

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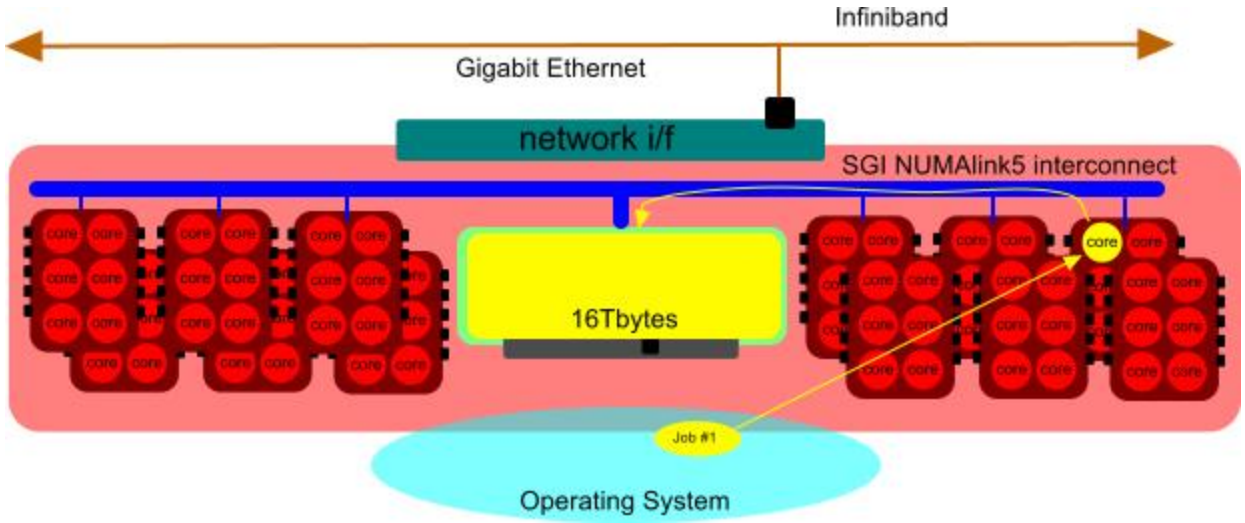
Shared Memory Models Can Support very large processes



Cosmos
Universe

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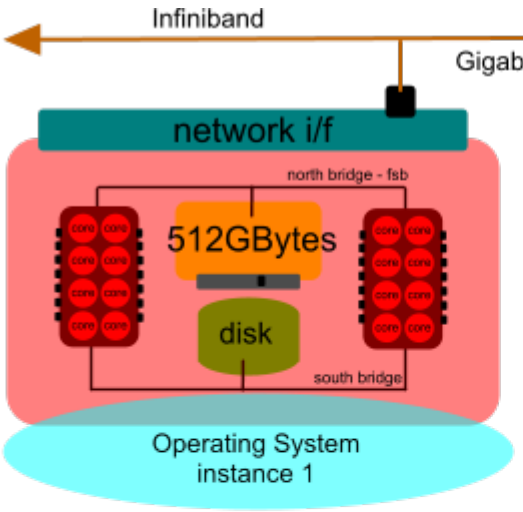
Fat Node



Fat Node
16 Cores
512 GBytes
32 GBytes / Core

Can install 2TBytes
In stand node.

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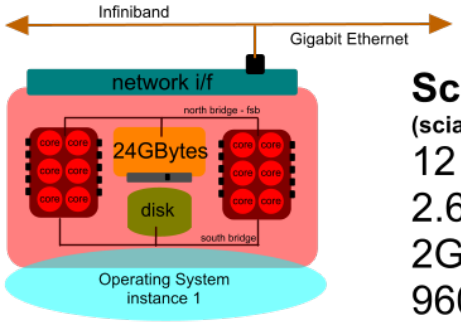
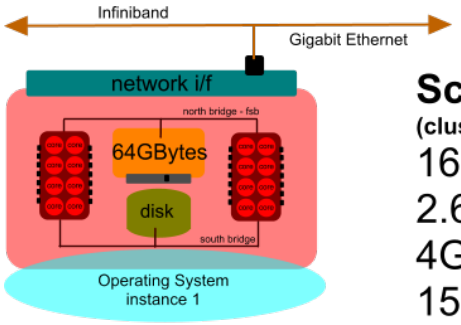
You need to know your HPC Building Block

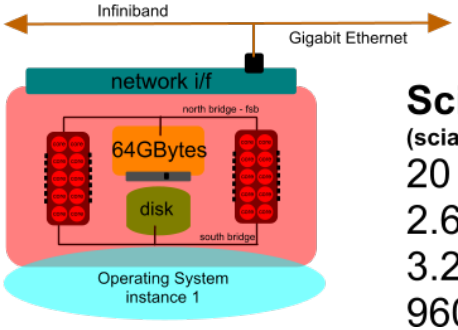
You need to know :-
Architecture – Intel/AMD
No. Cores
How much memory
Clock rate



Sciama 1 Node
(sciama1.q)
12 cores
2.6G Westmere
2GByte / Core
960 Cores



Sciama 2 Node
(cluster.q)
16 cores
2.6G Ivy Bridge
4GByte / Core
1536 Cores



Sciama 3 Node
(sciama3.q)
20 cores
2.6G Haswell
3.2GByte / Core
960 Cores

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Managing software / Modules

Running Programs on an HPC - 3 Scenarios

- Run an application already loaded in the environment.
  - Use selection tool (“module avail”) to check what is installed and select.
- Get a new application installed so you can run it.
  - Unless very specific its best to get administrators to install centrally.
  - Others may want – saves space, often quicker.
- Compile your own application from source code.
  - You will need to select the compiler(s) and libraries using the “module” command described. Request dependencies to be installed but not always possible.

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Many “modules” (probably) available

```
(Training)[burtong@login6(sciama) ~]$module avail

------------------------------------------------------------------------------------------------------ /opt/apps/modulefiles/core -------------------------------------------------------------------------------------------------------
bundles/2016.0/parallel     bundles/2016.0/serial       bundles/tools              services/torque/2.5.13      system/intel64(default)     system/sciama-2
bundles/2016.0/parallel_oss bundles/2016.0/serial_oss   services/maui/3.3.1        system/ia32                 system/sciama-1             system/sciama-3

---------------------------------------------------------------------------------------------------- /opt/apps/modulefiles/compilers ----------------------------------------------------------------------------------------------------
gnu_comp/4.3.5    gnu_comp/4.4.7    gnu_comp/4.9.4    intel_comp/2011.0 intel_comp/2013.2 intel_comp/2016.2 intel_comp/2018.2
gnu_comp/4.4.5    gnu_comp/4.8.4    gnu_comp/5.4.0    intel_comp/2013.1 intel_comp/2016.1 intel_comp/2017.2

---------------------------------------------------------------------------------------------------- /opt/apps/modulefiles/libraries ----------------------------------------------------------------------------------------------------
arpack-ng/3.5.0              cfitsio/3.37                glibc/2.17                  healpix/3.20                lapack/3.7.0                openmpi/1.8.2               Qhull/2015.2
atlas/3.10.2                 cfitsio/3.39                glibc/2.21                  healpix/3.31                libconfig/1.4.9             openmpi/1.8.4               qrupdate/1.1.2
atlas/3.10.3                 cfitsio/3.41                glibc/2.23                  intel_mpi/2017.2            libconfig/1.5               openmpi/2.0.1               root/6.10.8
bdwgc/7.2                    copter/0.8.7                glpk/4.61                   intel_mpi/4.1.0(default)    libpng/1.5.28               openmpi/2.0.2               ssh2/1.4.3
blas/3.7.0                   cuba/3.0                    graphicsmagic/1.3.19        intel_mpi/4.1.3             libz/1.2.11                 oracle-jdk/1.8.0_131        SuiteSparse/4.2.1
blitz/0.10                   cuba/4.2                    graphicsmagic/1.3.25        intel_mpi/5.1.2             llvm/4.0.1                  oracle-jre/1.8.0_131        SuiteSparse/4.3.1
blitz/0.9                    curl/7.54.0                 gsl/1.16                    intel_mpi/5.1.3             llvm/5.0.0                  pcre/8.35                   SuiteSparse/4.4.1
boost/1.53.0                 ffi/3.1                     gsl/2.3                     lalsuite/lal/6.18.0         log4cplus/1.1.1             pcre/8.40                   SuiteSparse/4.4.4
boost/1.59.0                 fftw/2.1.5                  hdf4/4.2.12                 lalsuite/lalburst/1.4.4     metaio/8.4.0                pcre2/10.23                 SuiteSparse/4.5.5
boost/1.62.0                 fftw/3.3.6                  hdf5/1.10.0-patch1          lalsuite/lalframe/1.4.3     mpich/3.2                   petsc/3.0.0                 swig/3.0.12
boost/1.63.0                 fftw_mpi/2.1.5              hdf5/1.10.1                 lalsuite/lalinspiral/1.7.7  netcdf/4.3.2                petsc/3.4.5                 unistring/0.9.3
boost_mpi/1.57.0             fftw_mpi/3.3.6              hdf5/1.6.10                 lalsuite/lalmetaio/1.3.1    openmpi/1.10.2              petsc/3.5.3(default)        wcs/4.16
boost_mpi/1.63.0             fgsl/0.9.4                  hdf5/1.8.17                 lalsuite/lalpulsar/1.16.0   openmpi/1.10.6              petsc/3.6.3                 wcs/4.23
bzip2/1.0.6                  fltk/1.3.4                  hdf5_mpi/1.10.0-patch1      lalsuite/lalsimulation/1.7.3 openmpi/1.4.3              plplot/5.10                 wcs/4.24
cblas/3.7.0                  frame/8.30                  hdf5_mpi/1.6.10             lalsuite/lalstochastic/1.1.20 openmpi/1.6.4             pqxx/4.0.1                  wxwidgets/3.0.1
cfitsio/2.5.10               glew/1.13                   hdf-java/3.2.1              lalsuite/lalxml/1.2.4       openmpi/1.8.1               qdbm/1.8.77                 xml2/2.9.7

-------------------------------------------------------------------------------------------------- /opt/apps/modulefiles/applications --------------------------------------------------------------------------------------------------
abaqus/6.10-2                bison/3.0/gcc-4.4.7         emacs/24.5                  gromacs/5.1.2               matlab/R2017a               Qt/5.3.1                    tex/2015
abaqus/6.12-1                blast/2.3.0                 enzo/2.1.1                  gtkplus/2.12.121            meqtrees/aug14              R/3.2.2                     tips/1.0
abaqus/6.14                  bowtie/1.1.2                enzo/2.4                    guile/1.8.8                 mercurial/aug14             R/3.4.1                     tkdiff/4.2
abaqus/6.9-2                 bowtie2/2.2.7               enzo/2.5                    gv/3.5.8                    minuit2/5.34.14             radmc-3d/0.27               tmux/1.6
anaconda/1.0                 bwa/0.7.12                  enzo/2.5-mc                 heasoft/6.16                montepython/2.2.2           rclone/1.38                 tmv/0.70
anaconda/2.2.0               casa/4.2.1                  enzo/2.5-mc-intel           help2man/1.47.5             mpss/3.0                    rna-seq/1.0                 topcat/4.2
anaconda/2.4.0               casa-core-rest/1.7.0/gcc-4.4.7 ez/0.3.1                 htslib/1.3                  multinest/3.6               rockstar/0.99.9-RC3+        tophat/2.1
anaconda/2.4.1               cgal/4.8                    ffmpeg/3.1                  idl/8.0                     music/oct15                 rrdtool/1.6.0               vcftools/0.1.13
anaconda3/2.1.0              class/2.6.1                 fluidstructures/17.1        idl/8.3                     nlopt/2.4.2                 samtools/1.3                visit/2.10.2
anaconda3/2.5.0              cloudy/13.04                freetypes/2.6.2             idl/8.5                     octave/4.2.1                scamp/2.0.4                 vmd/1.9.2
anaconda3/2.5.0-2            cmake/2.8.3/gcc-4.4.7       fv/5.3                      igv/2.3.68                  OpenCV/2.4.10               sextractor/2.19.5           vtk/6.1.0
anaconda-atlas/2.2.0         cmake/3.0.0/gcc-4.4.7       gadgetviewer/1.0.4          ImageMagick/6.9.2-8         parallel/1.0                SNANA/v10_36e               vtk/6.1.0-a
anaconda-intel/2.2.0         cmake/3.10.0                gadgetviewer/1.0.7          iraf/2.16.1                 paraview/5.0.1              SNANA/v10_40b               vtk/6.1.0-mod
ant/1.10.1                   cmake/3.10.1                galsim/1.3                  java/1.8.0_131              parosol/jun16               splotch/4.4                 wcstools/3.9.0
appspack/5.0.1-C3            cmake/3.6.2                 gdl/0.9.4                   java-ide/apr15              perl/5.26                   splotch/6.0                 weka/3.6.11
autoconf/2.69                cpython/2.7.13              ghostscript/9.14            knime/3.2.1                 pgplot/5.2                  splotch/6.0a                xv/3.10a
autogen/5.13                 cpython/3.6.1               git/2.9.4                   libtool/2.4.6               pgplot/5.2-gcc              starccm/10.06.010           xvfb/2.4
autogen/5.18.1               crime/1.3                   gnuplot/4.4.3               lofar/oct13                 pgplot/5.2-sept15           starccm/10.06.010-r8        xz/5.2.3
automake/1.13.1              cufflinks/2.2.1             gnuplot/4.6.6               lofar/oct13-pybdsm          pigz/2.3.3                  starccm/9.06.011            yasm/1.3.0
automake/1.15                doxygen/1.8.13              go/1.4                      m4/1.4.17                   plc/2.0                     swarp/2.38.0
axesim/apr15                 dtfe/1.1.1                  go/1.9.1                    make/4.2                    pybdsm/1.8.2                syn++/0.98
bcftools/1.3                 ecl/jul17                   grace/5.1.25                mathematica/10.4.0          Qt/4.5.3                    tcllib/1.17
binutils/2.28                elements/3.8                gromacs/3.3                 mathematica/11.0.0          Qt/4.8.4                    tcllib/1.18
```

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Application, Libraries and Compilers

- Use the “module” command (>man module)
- “> module avail” to see available modules.
- “>module add <mod path>”
- “>module delete <mod path>”
- “>module list”
- “>module initadd <mod path>”
- $HOME/.modules

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Ex. Selecting a different version of Python

1.) Current Python version

```
(Training)[burtong@login6(sciama) ~]$
(Training)[burtong@login6(sciama) ~]$python -V
Python 2.6.6
(Training)[burtong@login6(sciama) ~]$module avail anaconda

------------------------------------------------------------------------ /opt/apps/modulefiles/applications -
anaconda/1.0         anaconda/2.4.0       anaconda3/2.1.0      anaconda3/2.5.0-2    anaconda-intel/2.2.0
anaconda/2.2.0       anaconda/2.4.1       anaconda3/2.5.0      anaconda-atlas/2.2.0
(Training)[burtong@login6(sciama) ~]$
(Training)[burtong@login6(sciama) ~]$module add anaconda3/2.5.0
(Training)[burtong@login6(sciama) ~]$
(Training)[burtong@login6(sciama) ~]$python -V
Python 3.5.2 :: Anaconda custom (64-bit)
(Training)[burtong@login6(sciama) ~]$
(Training)[burtong@login6(sciama) ~]$module list
Currently Loaded Modulefiles:
  1) anaconda3/2.5.0
(Training)[burtong@login6(sciama) ~]$
```

2.) Check available versions

3.) Select required version

4.) New version

5.) Modules loaded

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Environmental Variables

- Env's customise your environment.
- Run the command "env" .
- $PATH is important – search path for commands.
- "echo $PATH"
- "export PATH="/usr/bin:/usr/local/bin/:/bin"

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“module show”

```
[burtong@login8(sciama) ~]$ module show libs/wcs/4.16/gcc-4.4.7
-------------------------------------------------------------------
/opt/apps/modules//libs/wcs/4.16/gcc-4.4.7:

module-whatis   loads the necessary `wcs-4.16' library paths
setenv          WCSINCLUDE /opt/apps/libs/wcs/4.16/gcc-4.4.7/include
setenv          WCSLIB /opt/apps/libs/wcs/4.16/gcc-4.4.7/lib
setenv          WCSBIN /opt/apps/libs/wcs/4.16/gcc-4.4.7/bin
prepend-path    PATH /opt/apps/libs/wcs/4.16/gcc-4.4.7/bin
prepend-path    LD_LIBRARY_PATH /opt/apps/libs/wcs/4.16/gcc-4.4.7/lib/
prepend-path    MANPATH /opt/apps/libs/wcs/4.16/gcc-4.4.7/share/man/
prepend-path    C_INCLUDE_PATH /opt/apps/libs/wcs/4.16/gcc-4.4.7/include/
prepend-path    CPLUS_INCLUDE_PATH /opt/apps/libs/wcs/4.16/gcc-4.4.7/include/
prepend-path    --delim  CPPFLAGS  -I/opt/apps/libs/wcs/4.16/gcc-4.4.7/include
prepend-path    --delim  CFLAGS  -I/opt/apps/libs/wcs/4.16/gcc-4.4.7/include
prepend-path    --delim  LDFLAGS  -L/opt/apps/libs/wcs/4.16/gcc-4.4.7/lib/
-------------------------------------------------------------------
```

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Prepending $PATH

[burtong@login8(sciama) ~]$ echo $PATH
/usr/lib64/qt-3.3/bin:/usr/local/sbin:/usr/local/bin:/usr/sbin:
/usr/bin:/sbin:/bin:/bin:/usr/bin:/usr/X11R6/bin:/users/
burtong/bin:/users/burtong/bin

[burtong@login8(sciama) ~]$ module add libs/wcs/4.16/gcc-4.4.7

[burtong@login8(sciama) ~]$ echo $PATH
/opt/apps/libs/wcs/4.16/gcc-4.4.7/bin:/usr/lib64/qt-3.3/bin:
/usr/local/sbin:/usr/local/bin:/usr/sbin:/usr/bin:/sbin:/bin:/bin:
/usr/bin:/usr/X11R6/bin:/users/burtong/bin:/users/burtong/bin

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Compilers, libraries and bundles

1.) Select the system (hardware specific)

```
services/torque/2.5.13      system/intel64(default)     system/sciama-2
system/ia32                 system/sciama-1            system/sciama-3
```

```
------------------------------------------------------------------------------ /opt/apps/modulefiles/compilers ------------------
gnu_comp/4.3.5    gnu_comp/4.4.7    gnu_comp/4.9.4    intel_comp/2011.0 intel_comp/2013.2 intel_comp/2016.2 intel_comp/2018.2
gnu_comp/4.4.5    gnu_comp/4.8.4    gnu_comp/5.4.0    intel_comp/2013.1 intel_comp/2016.1 intel_comp/2017.2
```

2.) Select Compiler

```
intel_comp/2016.2 \
intel_mpi/5.1.3 \
fftw_mpi/3.3.6 \
hdf5_mpi/1.10.0-patch1 \
gsl/2.3 \
boost_mpi/1.63.0 \
```

3.) Select the libraries

4.) Alternatively select Bundle

```
------------------------------------------------------------------------------
bundles/2016.0/parallel     bundles/2016.0/serial       bundles/tools
bundles/2016.0/parallel_oss bundles/2016.0/serial_oss   services/maui/3.3.1
```

5.) Compatible libaries selected

```
[jschewts@login7(sciama) ~]$ module add system/intel64
[jschewts@login7(sciama) ~]$ module add bundles/2016.0/parallel_oss
[jschewts@login7(sciama) ~]$ module list
Currently Loaded Modulefiles:
  1) services/torque/2.5.13       3) system/intel64             5) openmpi/2.0.2              7) hdf5_mpi/1.10.0-patch1      9) boost_mpi/1.63.0
  2) services/maui/3.3.1          4) gnu_comp/5.4.0             6) fftw_mpi/3.3.6             8) gsl/2.3                    10) bundles/2016.0/parallel_oss
[jschewts@login7(sciama) ~]$
```

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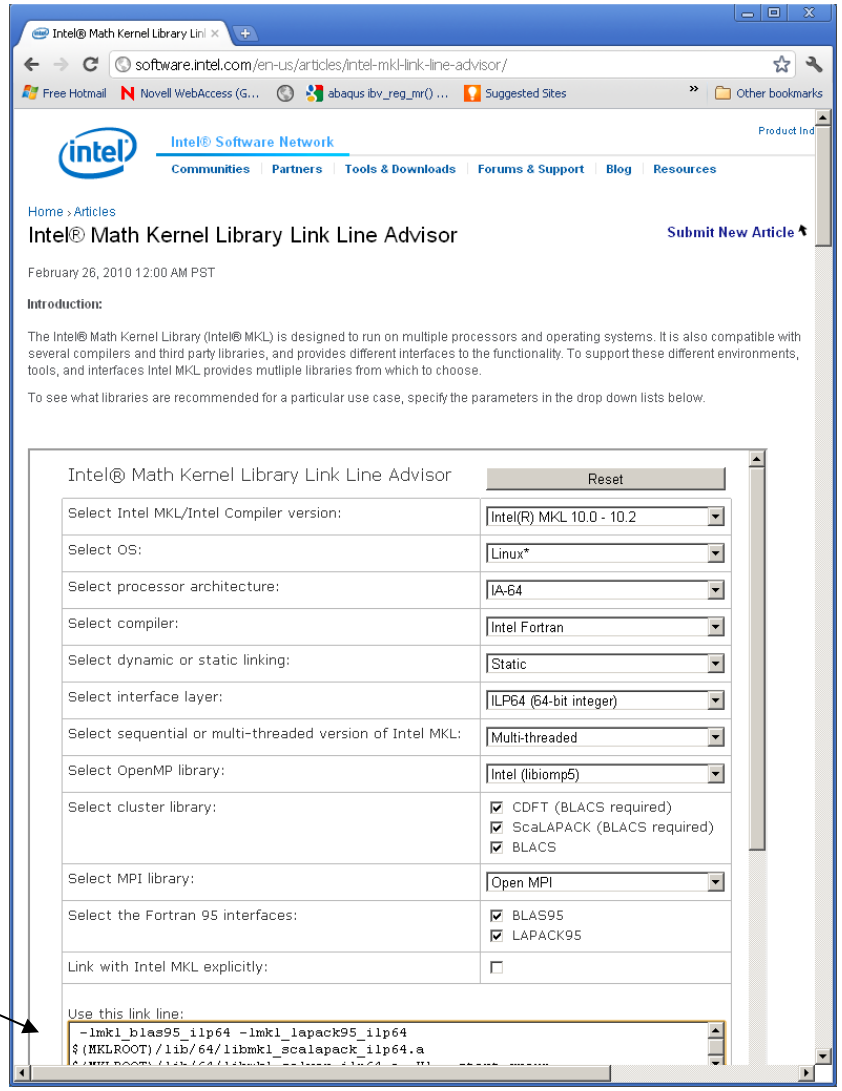
Compile Options



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Schedulers and Resource managers

Creating a job

- Once an application has been selected or compiled it can be run.
- This is done by setting up a “job”.
- A jobs has two components:-
  - The program
  - The “meta data”
- A job script is needed (bash script)
- We need to submit the job

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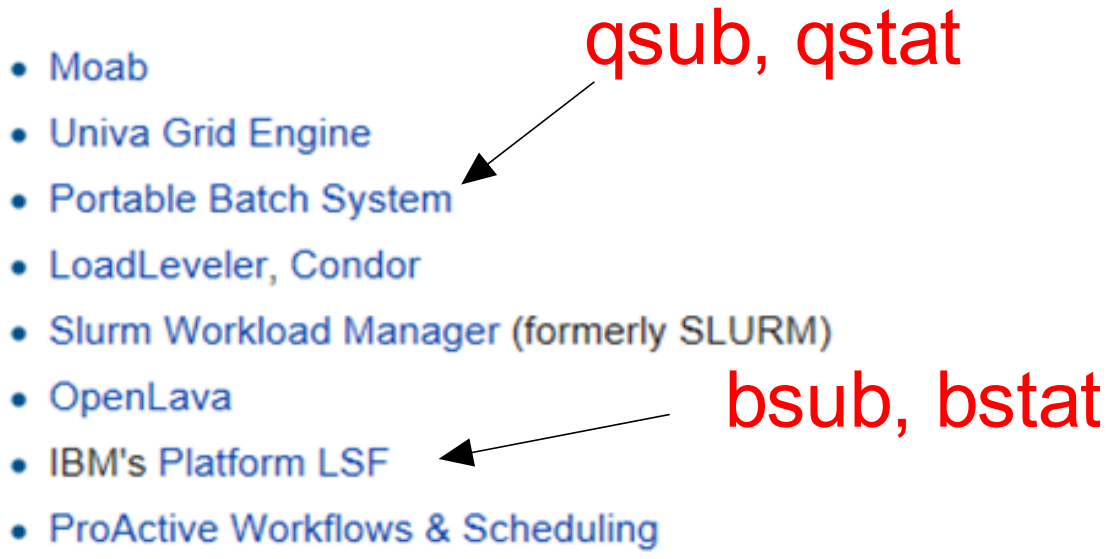
Schedulers and Resource Managers (The Queueing System)

- We use Torque and Maui based on PBS (Portable Batch System)
- Mainly because its free (open source).
- We only use basic functionality.



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Job Script Example

```
#!/bin/bash
#PBS -l nodes=10:ppn=12
#PBS -l walltime=6:00:00
#PBS -N gadget
#PBS -o out_gadget_blind8001.o$PBS_JOBID
#PBS -e err_gadget_blind8001.e$PBS_JOBID
#PBS -m abe
#PBS -M gary.burton@port.ac.uk
#PBS -V
#PBS -q cluster.q
```

Queuing System Directives

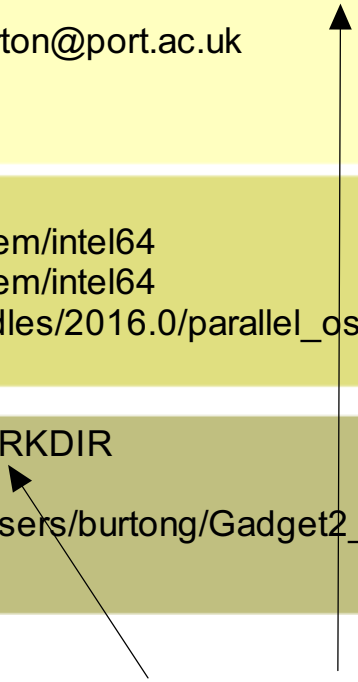
```
module purge
module load system/intel64
module load system/intel64
module add  bundles/2016.0/parallel_oss
```

Module selection

```
cd $PBS_O_WORKDIR

mpirun -np 780 /users/burtong/Gadget2_grid2400  /users/burtong/Gadget_Oriana_Bli
nd_ir8001.param
```

Program to Run



Internal Variables

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Running Jobs

- You should never run any large processes on a login server. Login servers are shared by others so any intense processing will slow down the responsiveness others experience.
- All major applications / compilations should be done on a compute node
- There are two ways to do this both using the “qsub” command to submit a job to a queue :-
  - Create an interactive shell on a compute node:-

    qsub –IX # I=Interactive X=allow X server windows

    This will give you a command prompt in the current shell.
  - Run a batch job on a compute node(s) :-

    qsub <job-script>

    This will start / queue a job according to the directives specified in the job script.

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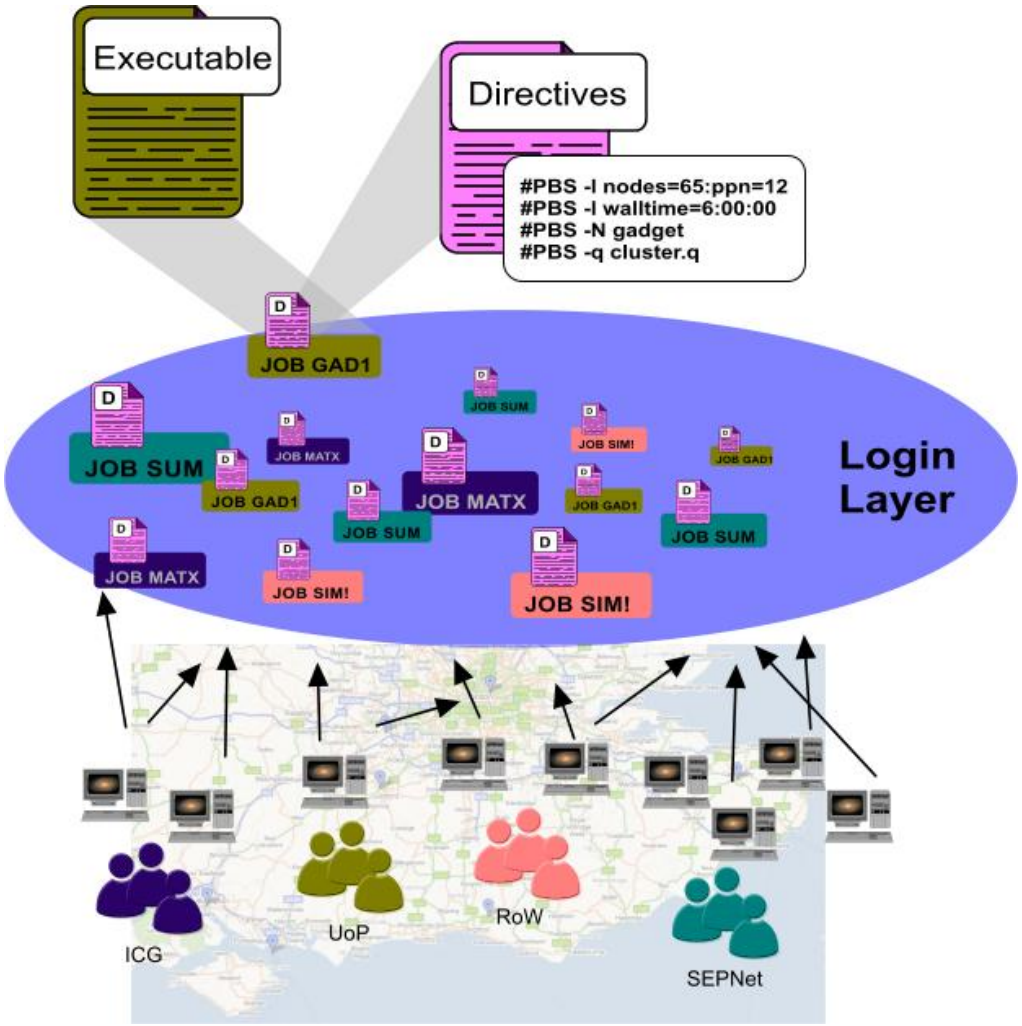
Executable and Jobscript setup in Login Layer



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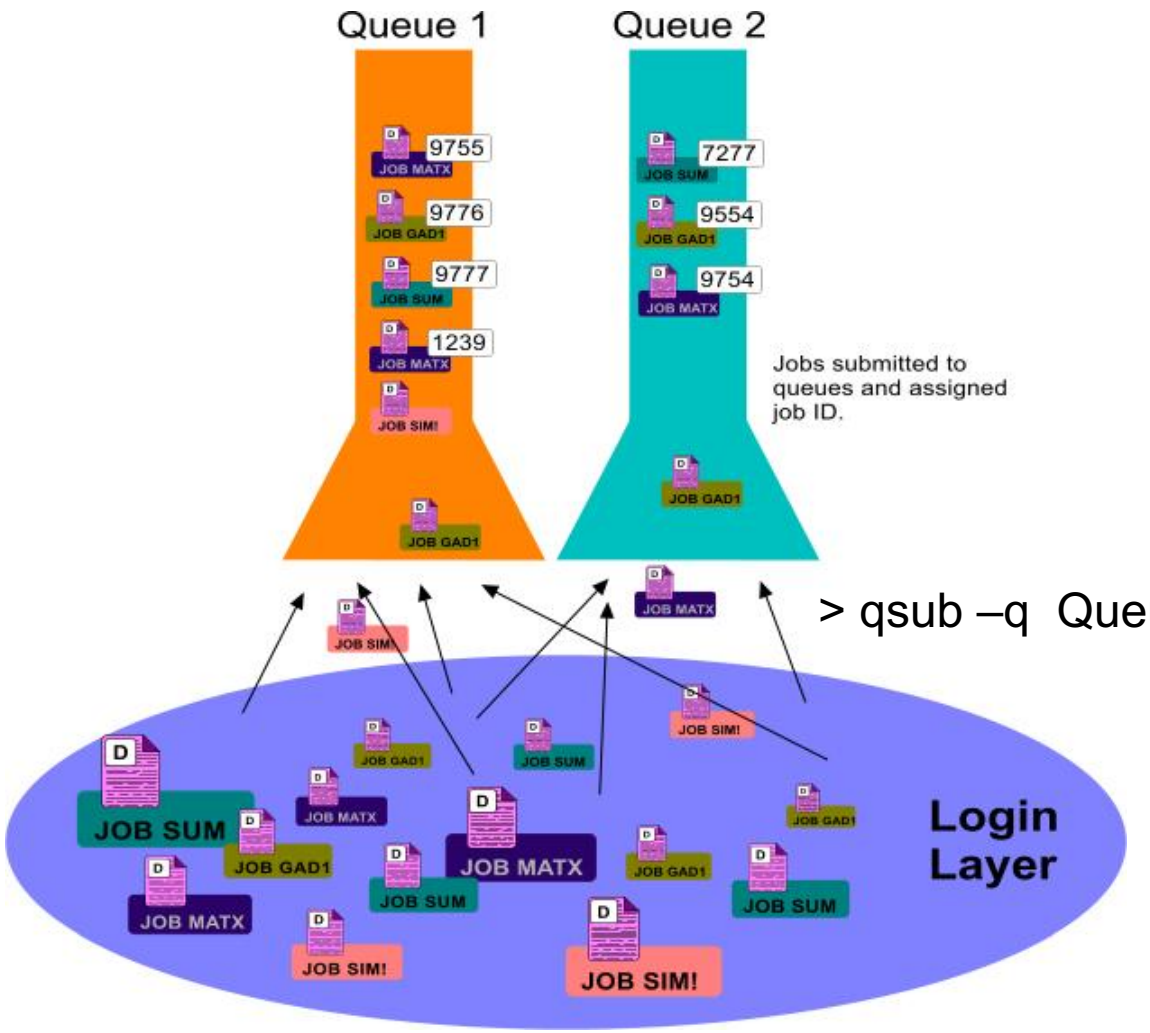
Jobs submitted to the queues



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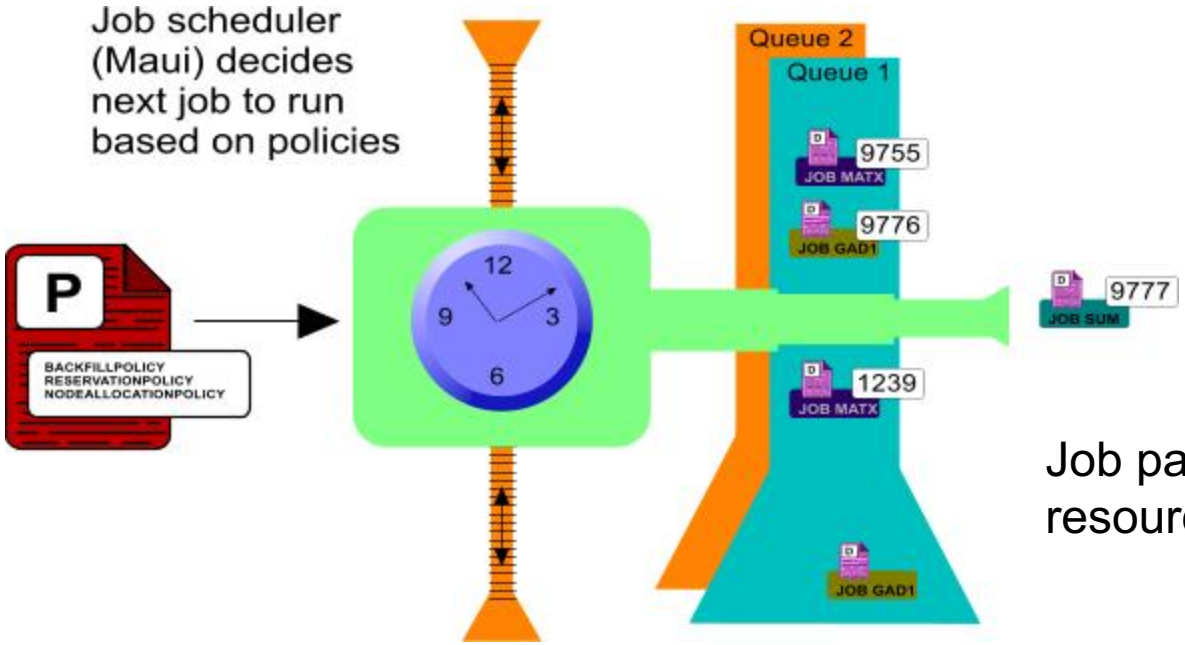
Scheduler prioritises and deems a job ready to run.



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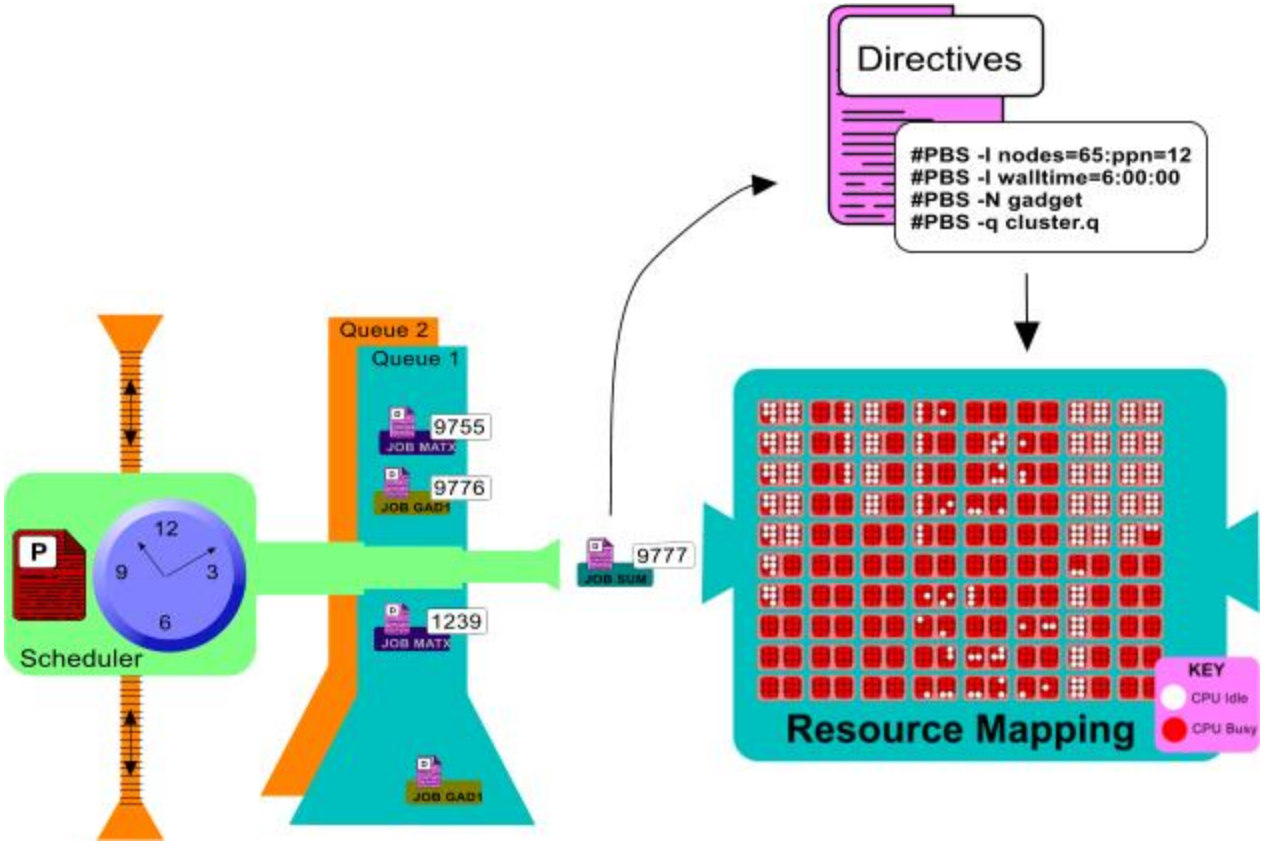
Resource manager (Torque) checks for available resources.



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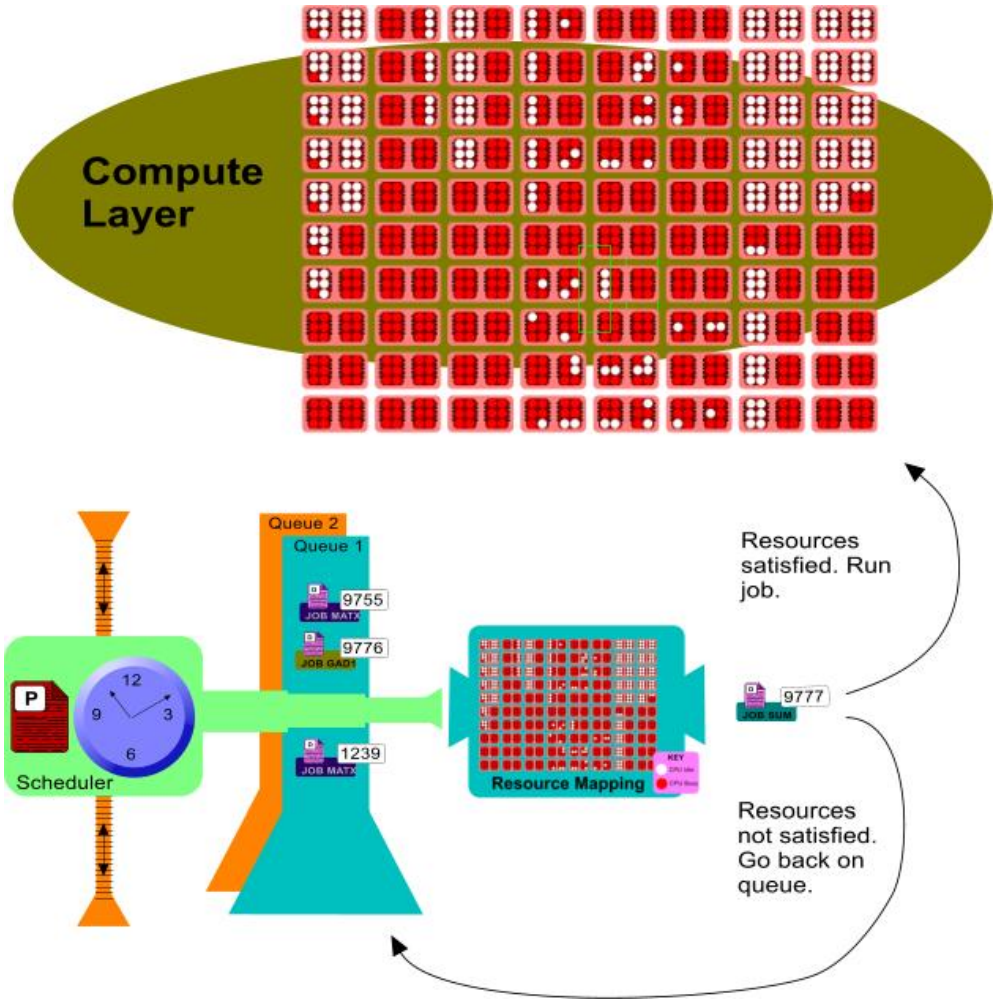
Job either runs in the compute pool or returns to queue



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Common Queue Commands

- Qsub, Qstat, Qdel

-tn1ru

```
[burtong@login8(sciama) ~]$ qstat                                cksim

headnode1.prv.sciama.cluster:
                                                                  Req'd    Req'd       Elap
Job ID                  Username    Queue    Jobname         SessID  NDS   TSK   Memory  Time    S  Time
----------------------- ----------- -------- --------------- ------ ----- ------ ------ --------- - ---------
2839001.headnode1.prv.  cksim       cluster. job2_1           67977     1    16    --  400:00:00 R 366:25:56
node105/15+node105/14+
2862199.headnode1.prv.  cksim       cluster. job3_1            2734     1    16    --  400:00:00 R 279:32:25
node158/15+node158/14+
2868380.headnode1.prv.  cksim       cluster. job3             75690     1    16    --  400:00:00 R 208:20:13
node193/15+node193/14+
2868381.headnode1.prv.  cksim       cluster. job4             40446     1    16    --  400:00:00 R 208:20:13
node159/15+node159/14+
```

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Being a Good HPC Citizen

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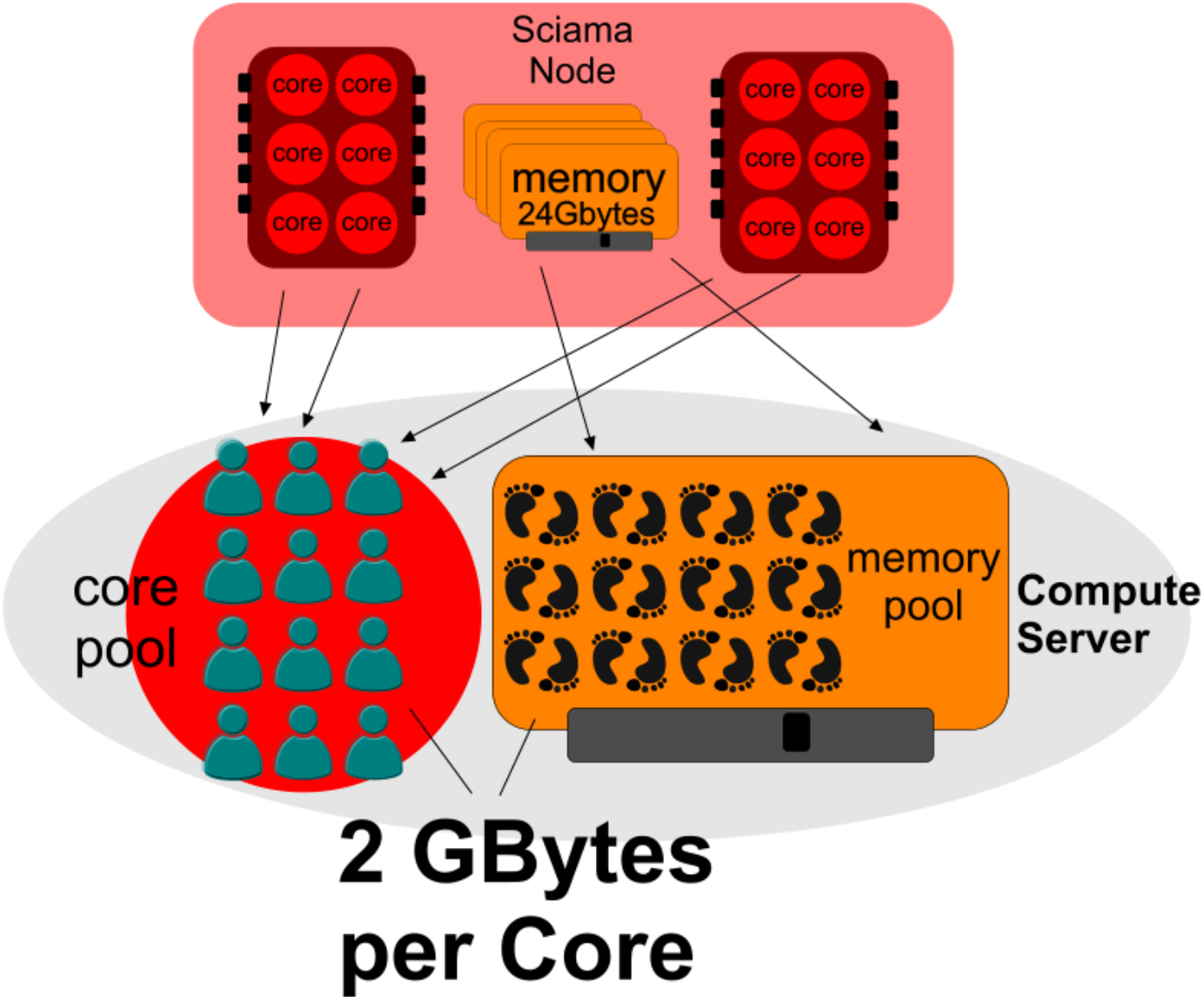

2 GBytes per Core

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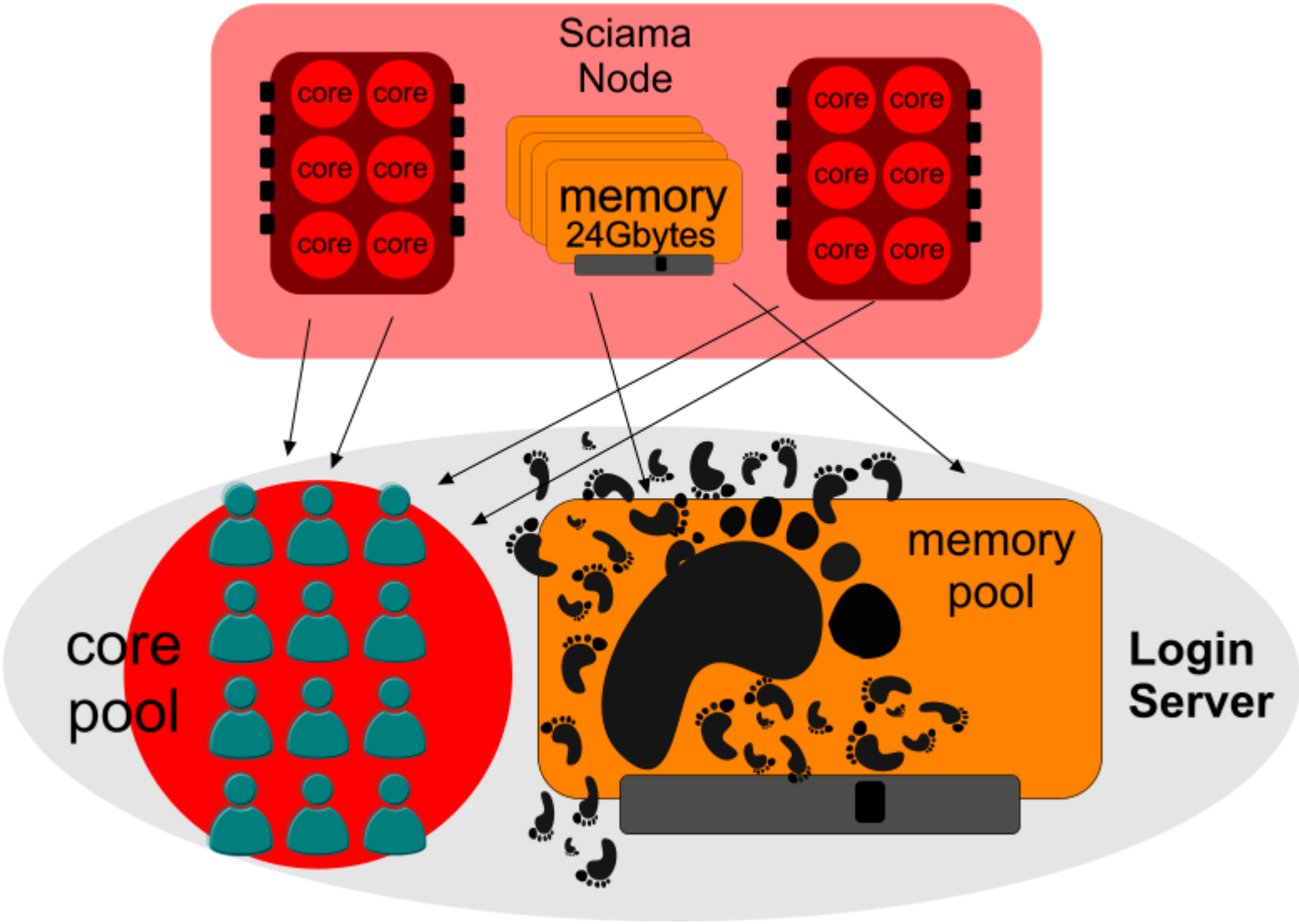

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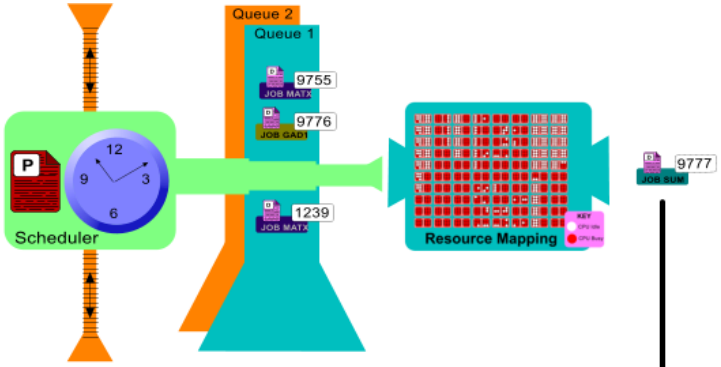
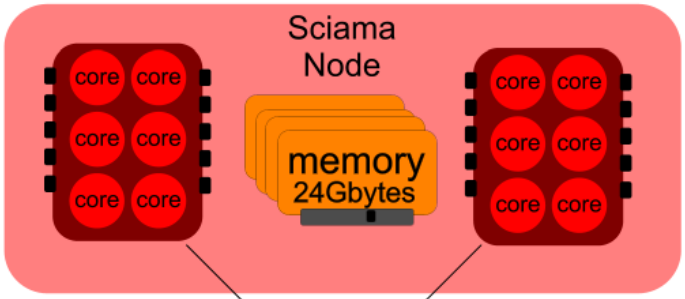
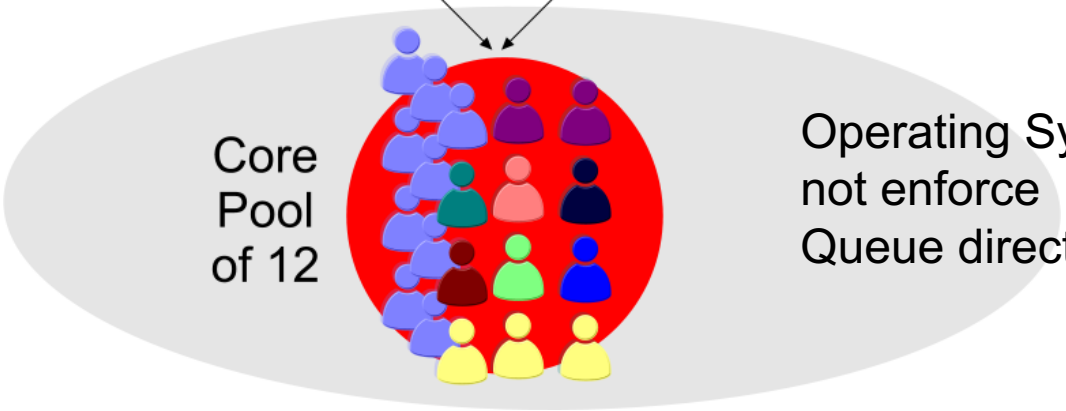


Beware Multi-threaded Programs





Operating System does not enforce Queue directives.

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Sciama has few enforced limits

- Don’t run big jobs on the login nodes.
- Stick to the memory / core limits (over allocate).
- Restrict Openmp cores (omp_num_cores)
- If unsure allocated the whole node to check the resources used (-l nodes=1:ppn=16)
- If you require more than 100GBytes storage then request a “Lustre” (project) area.
- Don’t install packages without checking.
- If you sense something is wrong then tell us.

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