Center for Mathematical Modeling
University of Chile

CMM
Center for
Mathematical
Modeling

HPC 101

Scientific Computing on HPC systems

By

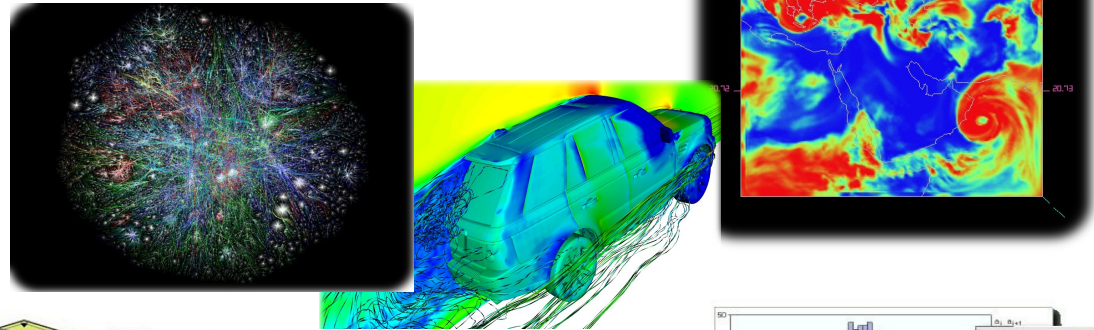**Juan Carlos Maureira B.**
<*jcm@dim.uchile.cl*>

Second La Serena School for Data Science: Applied Tools for Astronomy.
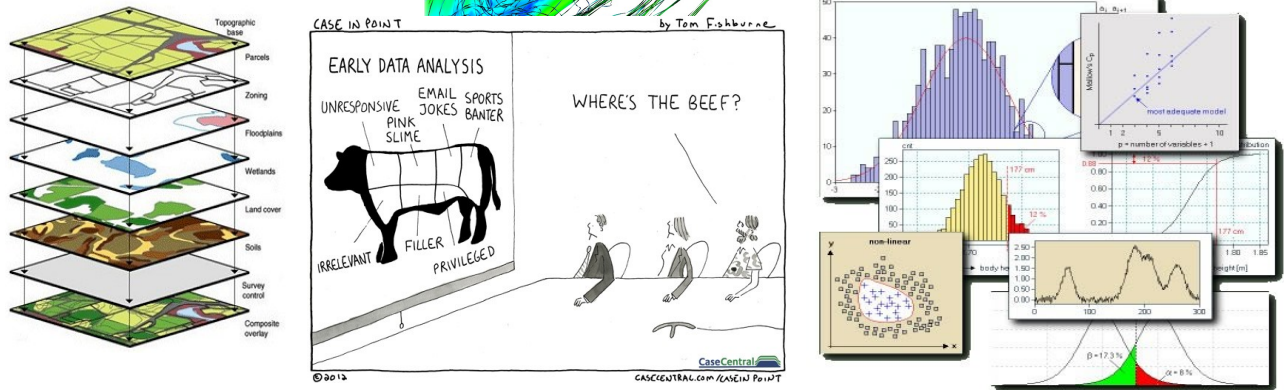La Serena – Chile – 17/08/2014

Overview

- Concepts & Definitions.

- Working with a HPC system.

- Best Practices.

- Hands-on: My first sextraction

- Closing words: The take aways.
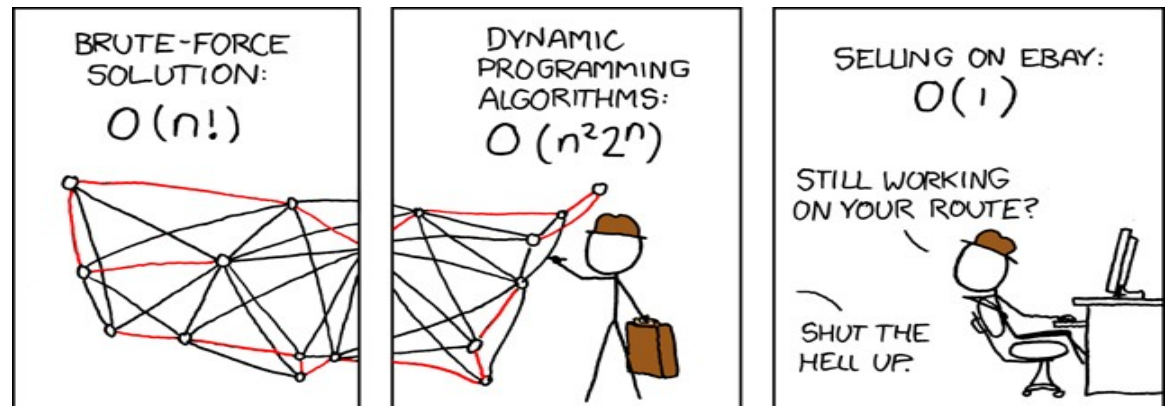
Scientific Computing

- Simulations

- Data Analysis

- Computational Optimization

Concepts & Definitions

HPC system Architecture

- Areas
  - Computing, Storage, Support, Networking
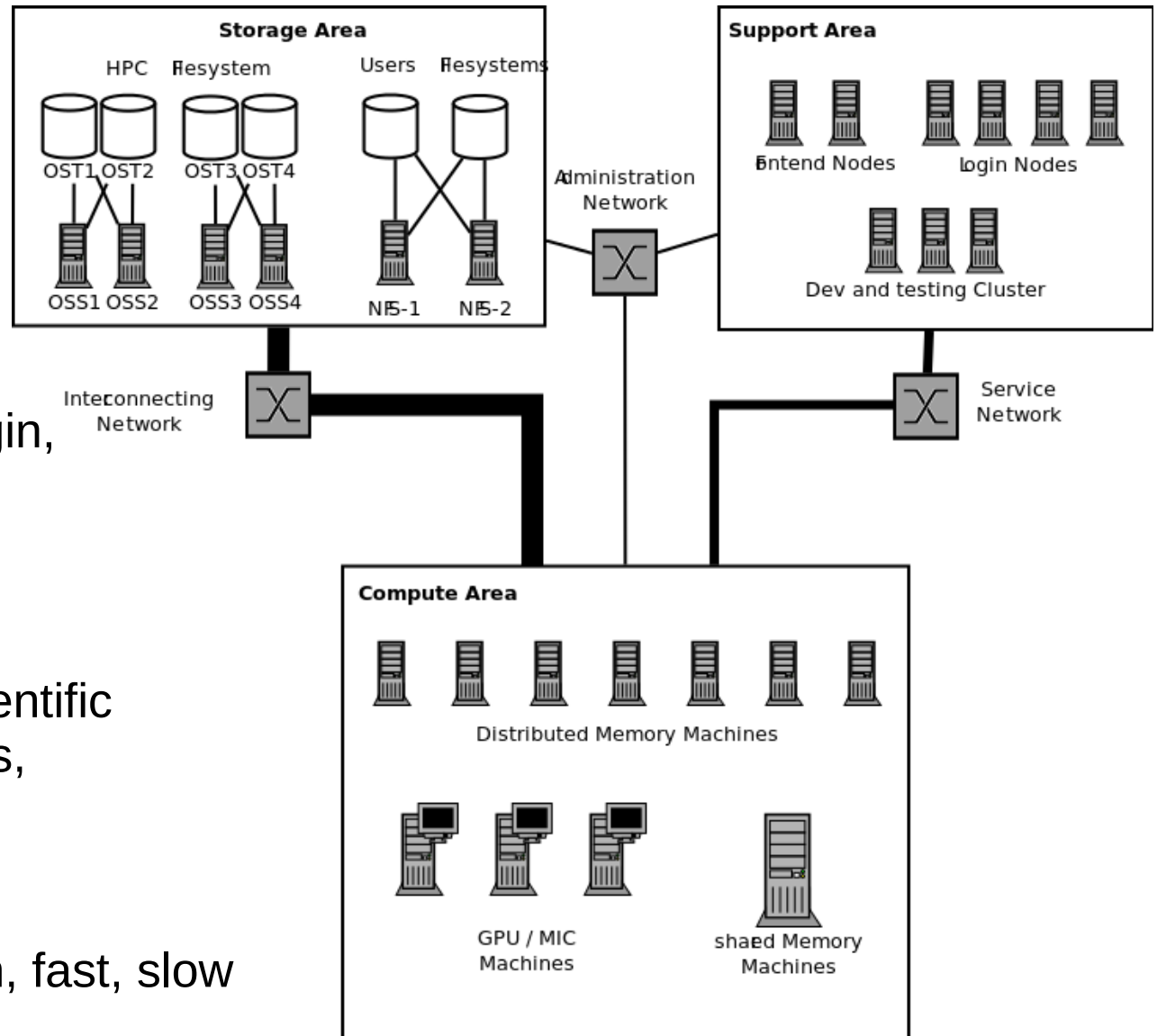- Servers roles
  - Compute, frontend, login, storage, backup, devel monitoring, etc.
- Software
  - Operating System, scientific software, analysis tools, libraries, etc.
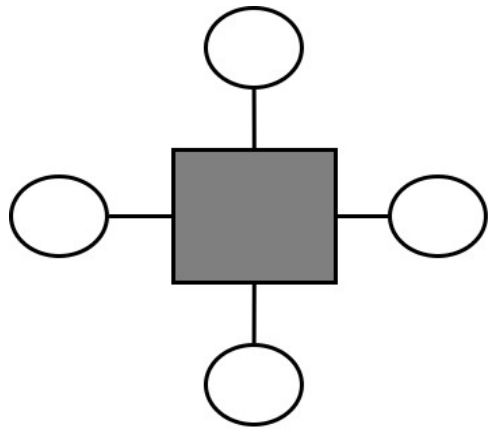- Storage
  - Local, working, scratch, fast, slow

Distributed and Shared Memory Systems

Shaed Memory
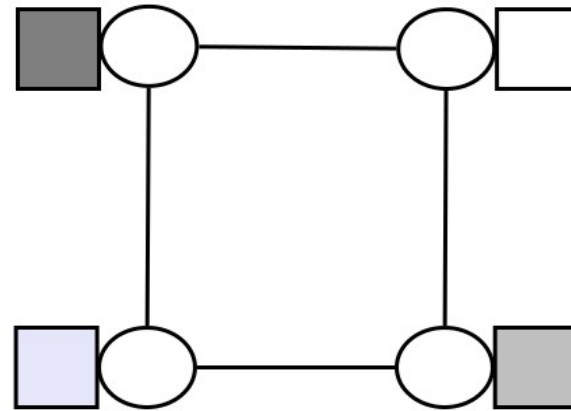
Distributed Memory
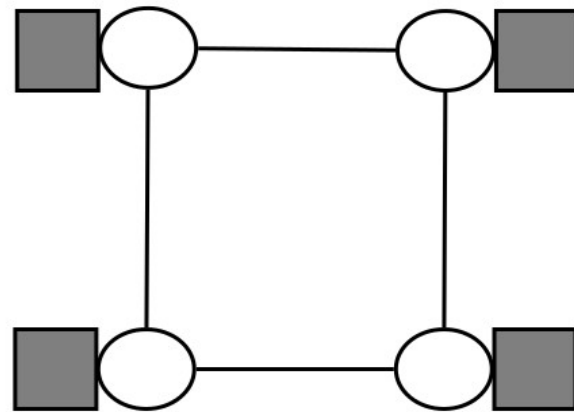
Distributed Shaed Memory

Interconnects

- Ethernet
  - latency ~ 0.05 ms
  - Throughput ~ 10 Gbps

- Infiniband
  - latency ~5 usec
  - Throughput ~ 40/56 Gbps

- QPI / NUMA
  - Latency ~ 100 nsec
  - Throughput ~ 100 - 200 Gbps
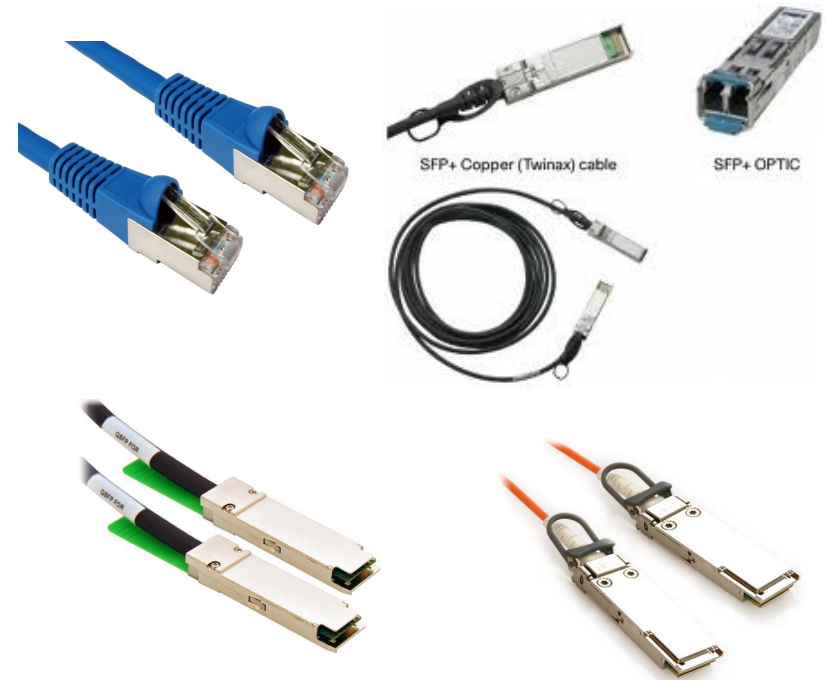
File-systems Types
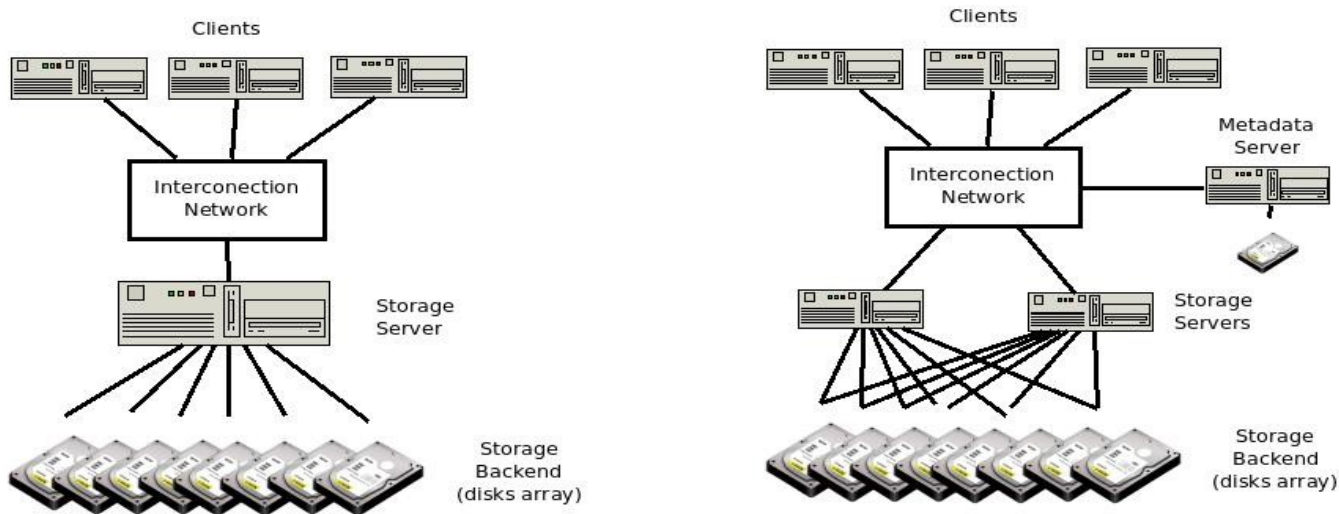
Serial
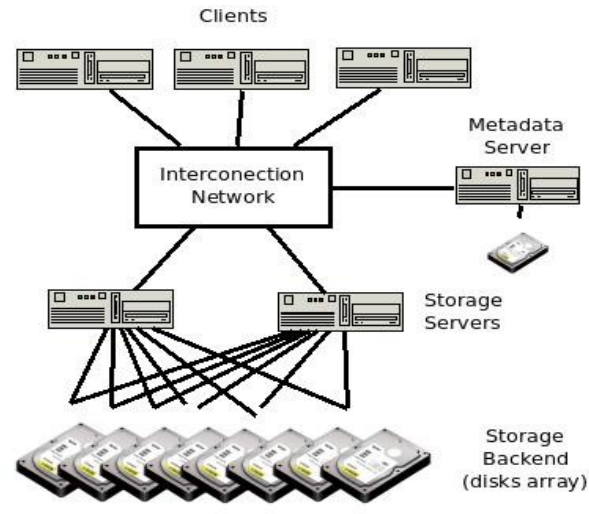
Distributed
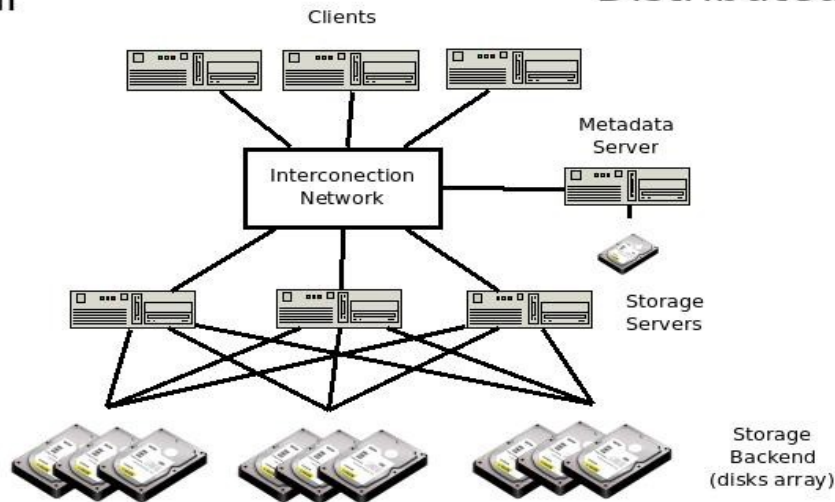
Parallel

- Serial
  - NFS, ZFS

- Distributed
  - pNFS
  - GFS
  - Gluster

- Parallel
  - Lustre
  - GPFS

Storage Layouts

- **Working ($Home)**
  - Safe and Slow storage.
  - Cheep
  - Bad for I/O

- **Scratch**
  - Unsafe and Fast storage
  - Expensive
  - Volatile and great for I/O
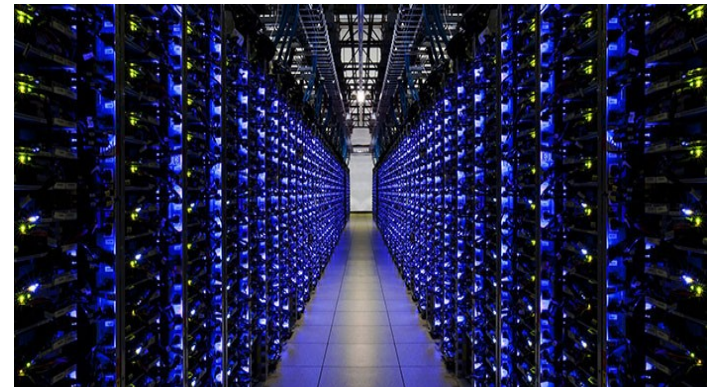
- **Archiving**
  - disaster-proof storage
  - Incredible slow (random) access
  - Backup Policies

Software Layout

Your are here!	**Job Scripts**
Queue	**Resource Scheduler**
Tools chains	**Applications & libraries**
Resources	**Operating System**
	Cores · **Memory** · **Storage** · **Network**
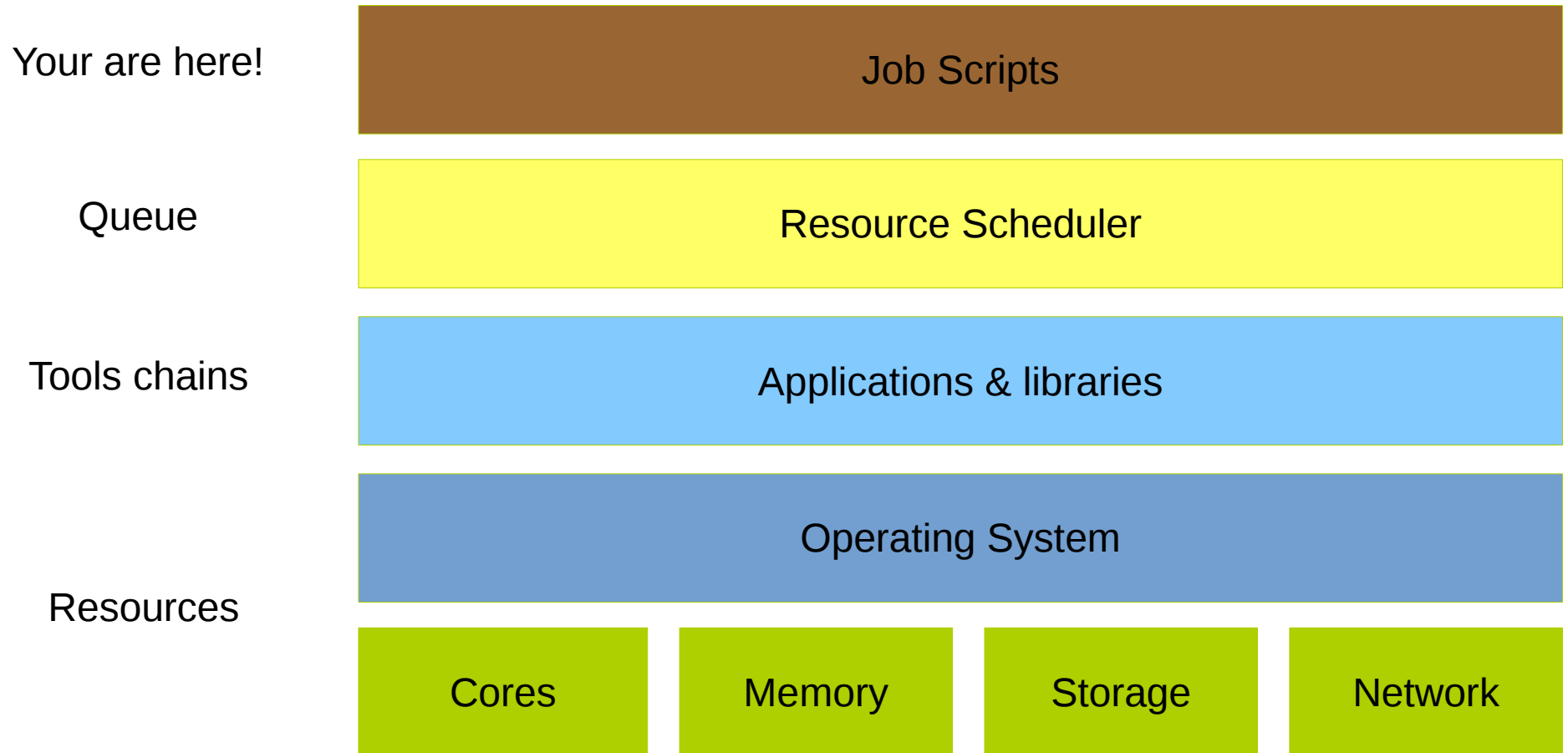
Tool Chains

- Set of self-standing libraries and applications to perform a class of jobs. (e.g. astro, bioinfo, optimization, etc).

- System wide (one for all).

  – Compiled and Installed by admins.

- User Space (each one has its own).

  – Compiled and installed by the user in their homes.

Resource Schedulers

- **Scheduler**: allocate resources to perform a job.

- **Job**: set of instructions and resources to perform a task.

- **Task**: involves preparing the environment

  and input data needed to run an application.

> **Resource specifications**
> **+**
> **Instructions to perform a task**

Jobs: Parallel v/s Distributed
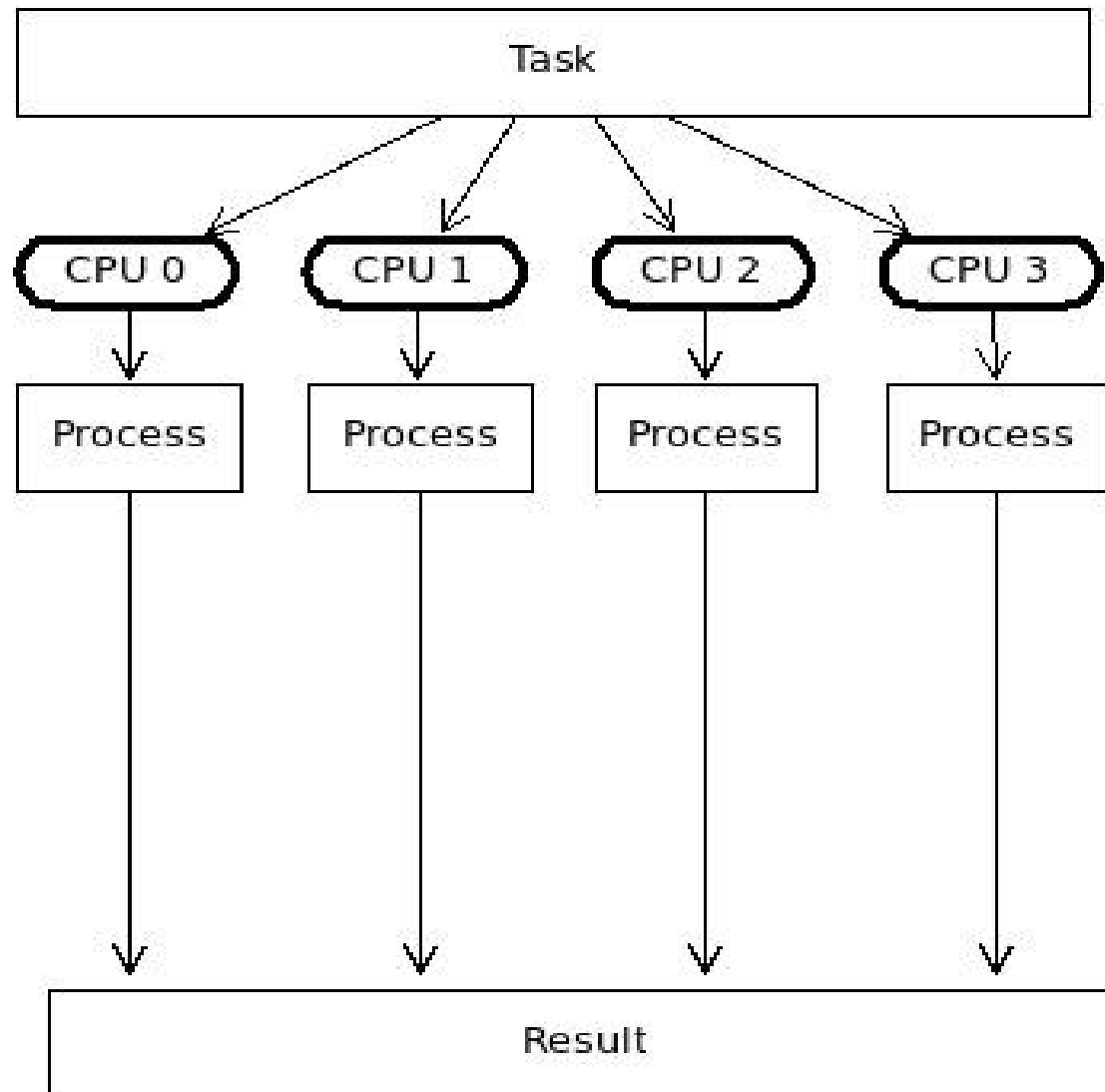
Jobs: Parallel v/s Distributed
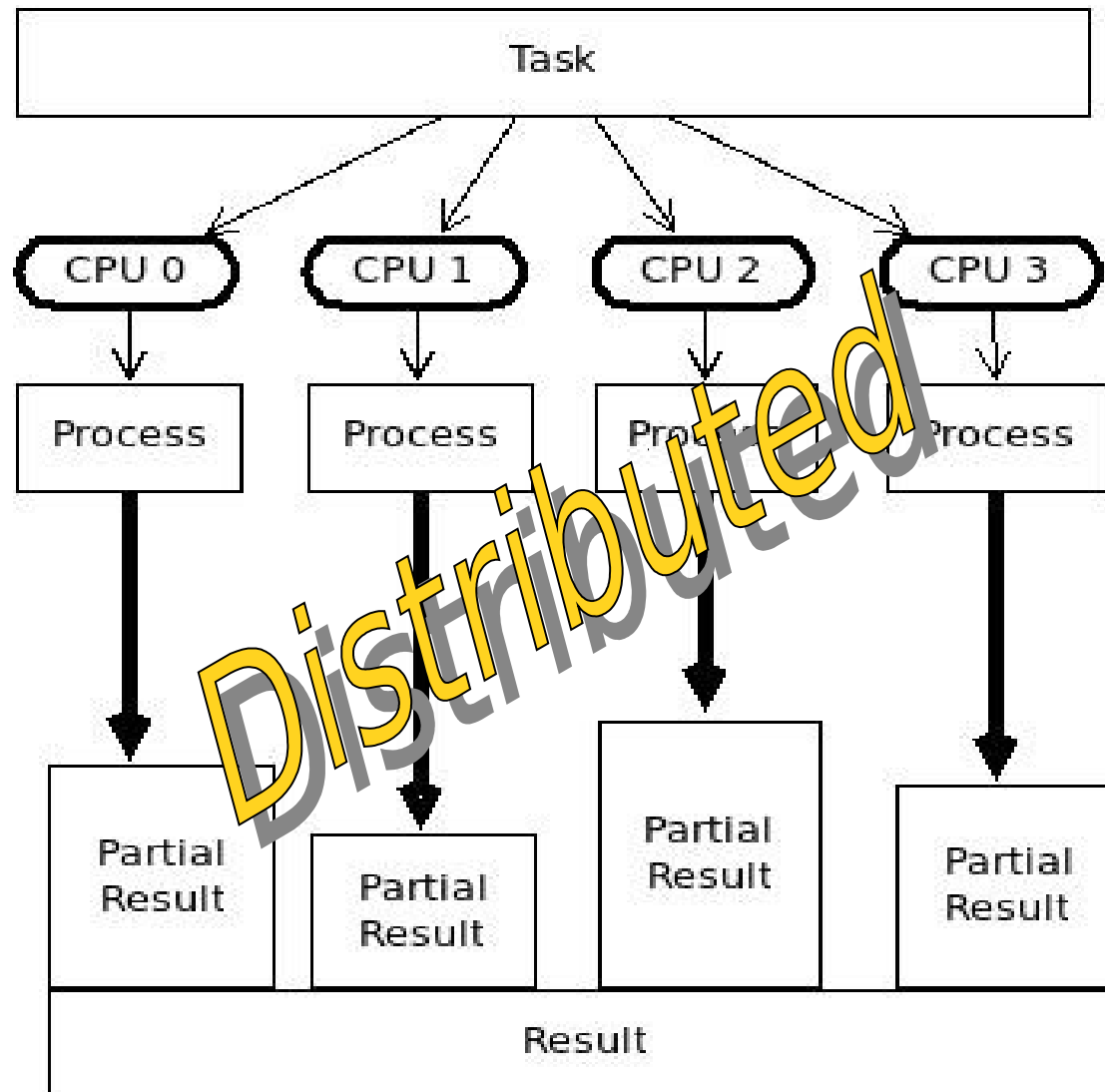
Jobs: Parallel v/s Distributed
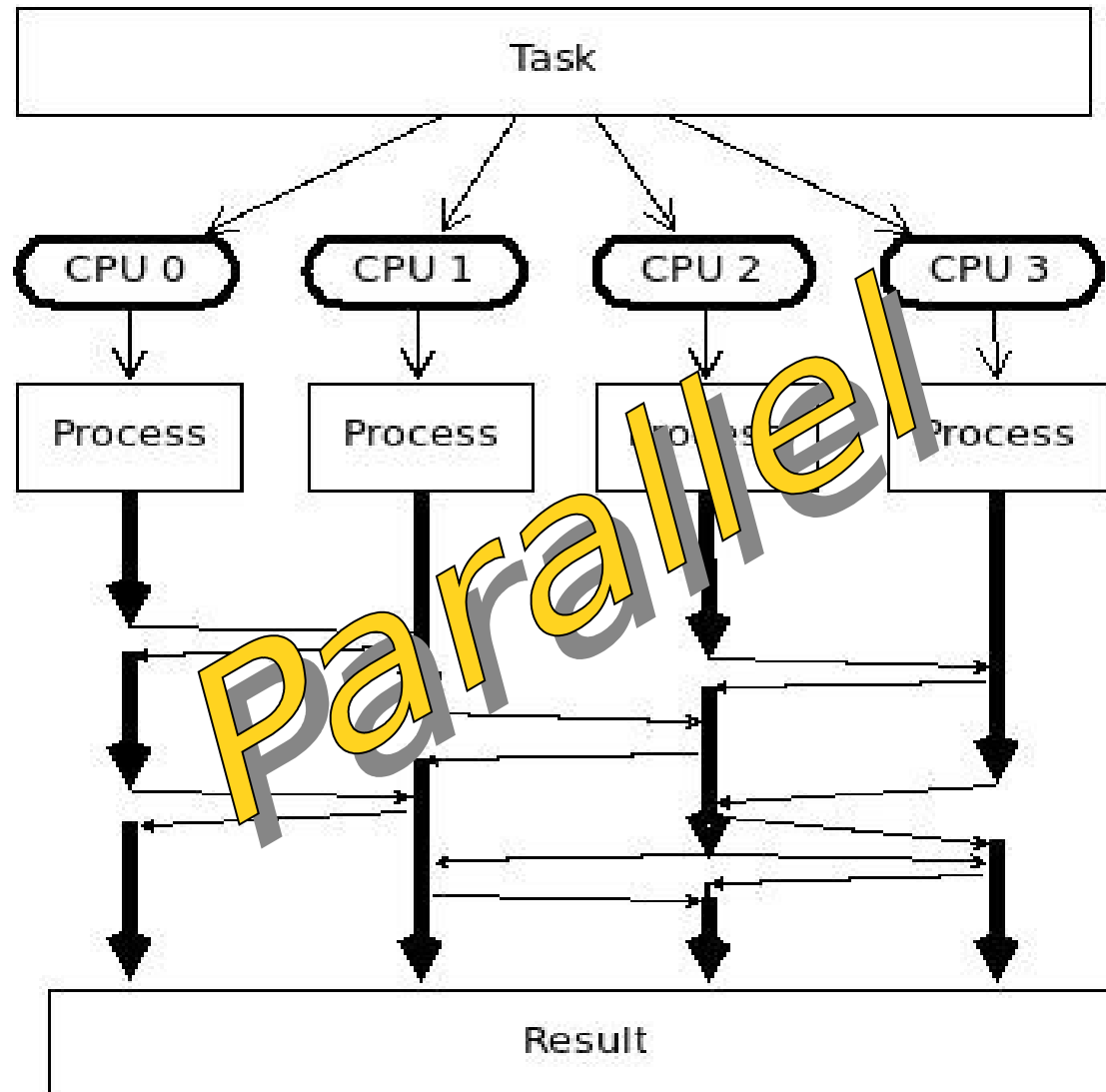
Working with a HPC System

Job Scripting

Input data and results	Data
Instructions to perform a task	Applications Algorithms Binary · Python · Perl · R · etc
Command Interpreter	(Bash / tch / csh) · Scheduler Resources
Job	Scripts
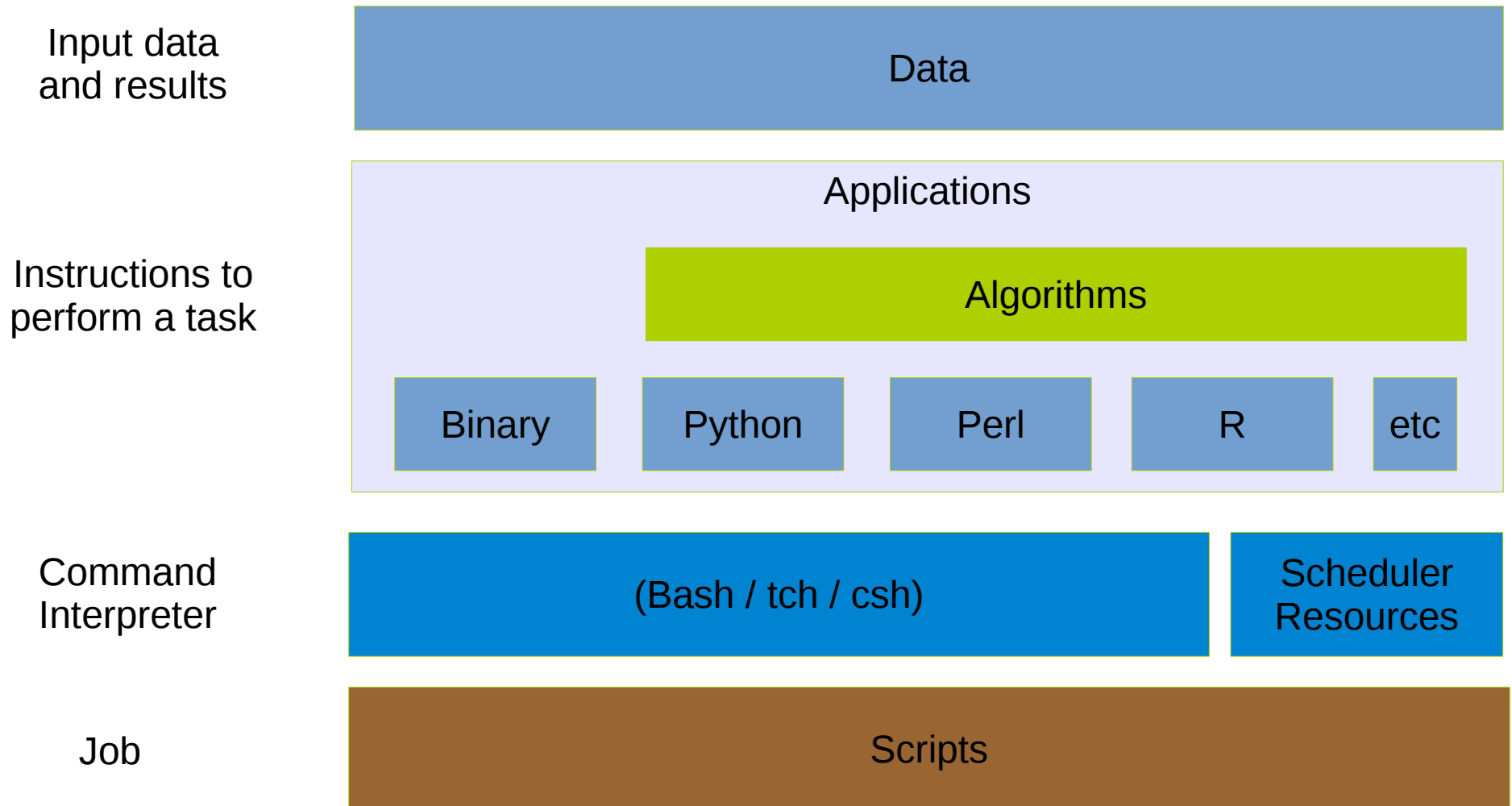
Job Scheduler Directives

```
#!/bin/bash
# Resource specification
#$ -l h_rt=1:00:00
#$ -cwd
#$ -j y
#$ -V
#$ -notify
# User Notification
#$ -m abes
#$ -M myemail@domain.com
# Job name
#$ -N jobname
# Command interpreter
#$ -S /bin/bash
# Parallel environment: openmpi,openmp,etc
#$ -pe openmpi 128
# Job Array
#$ -te 1:1000
# Queue to use
#$ -q all.q
```

- **Grid Engine**

- PBS

- Condor

Job Scheduler Directives

```bash
#!/bin/bash
# number of nodes and processes per node
#PBS -l select=4:mpiprocs=8
# resources
#PBS -l mem=213mb
#PBS -l walltime=2:00:00
#PBS -l cput=1:00:00
# name of job
#PBS -N jobname
# User notificacion
#PBS -m bea
#PBS -M myemail@domain.com
# Use submission environment
#PBS -V
# Queue to use
#PBS -q default
```

- Grid Engine

- **PBS**

- Condor

Job Scheduler Directives

```
## executable file
Executable = my_program.exe
## Specify Condor execution environment.
Universe = vanilla
## execution machines
Requirements = ((OpSys == "LINUX")
## Define input files and arguments
Input = stdin.txt.$(Process)
Arguments = in.$(Process)  out.$(Process)
## Define output/error/log files
Output = logs/stdout.$(Process).txt
Error = logs/stderr.$(Process).txt
Log = logs/log.$(Process).txt
## files need to be transferred and when.
Transfer_input_files = files/in1.$(Process)
Transfer_output_files = out.$(Process)
Transfer_executable = true
Should_transfer_files = YES
When_to_transfer_output = ON_EXIT
## Add 100 copies of the job to the queue
Queue 100
```

- Grid Engine

- PBS

- **Condor**

Environment Modules

- Configure the environment to run a particular application (or a set of applications)
  - Environmental variables:
    - PATH
    - LD_LIBRARY_PATH
    - LD_RUN_PATH}
  - Library versions and locations
    - BOOST_HOME, ATLAS_HOME, etc
  - Compilation & execution flags
    - CFLAGS, LDFLAGS, CXXFLAGS, etc.

Environment Modules

- Example: module available

```
[astrouser@levque ~]$ module available

------------------------ /usr/share/Modules/modulefiles ----------------------
dot            module-cvs  module-info modules      null        use.own

----------------------------- /etc/modulefiles -------------------------------
R/3.1.0                 intel/12.1.5         openmpi_gcc44/1.4.3
adf/2012.01             intelmpi/4.0.2       openmpi_intel/1.4.3
astro/1.1               intelmpi/4.0.3       openmpi_intel/1.6.5
cplex/12.1.0            lsst/9.2             openmpi_pgi/1.4.3
cplex/12.2.0            namd/2.7             opl/6.3
cplex/9.1.0             namd/2.8             pgi/10.9
espresso/5.1            namd/2.9             python/2.6.6
gaussian/09B1           namd_intel/2.8       siesta/3.2
gnuplot/4.6.5           octave/3.8.1         stata/11.0
gromacs/4.6.5           openmpi/1.4.2
gromacs_single/4.5.3 openmpi/1.4.3

[astrouser@levque ~]$
```

Environment Modules

- module show {module name/version}

```
[astrouser@levque ~]$ module show lsst

---------------------------------------------------------------
/etc/modulefiles/lsst/9.2:

module-whatis      Sets up the LSST Astro toolchain (Self-standing edition)
                   in you enviornment
prepend-path       PATH /home/apps/lsst/bin
prepend-path       PATH /home/apps/lsst/sbin
prepend-path       LD_LIBRARY_PATH /home/apps/lsst/lib
prepend-path       LD_LIBRARY_PATH /home/apps/lsst/lib64
prepend-path       MANPATH /home/apps/lsst/share/man
---------------------------------------------------------------

[astrouser@levque ~]$
```

Environment Modules

- module load {module name/version}

- module list

```
[student01@syntagma ~]$ module load lsst

[student01@syntagma ~]$ module list
Currently Loaded Modulefiles:
  1) lsst/9.2

[astrouser@development ~]$ echo $LD_LIBRARY_PATH
/home/apps/lsst/lib64:/home/apps/lsst/lib:/opt/intel/Compiler/11.1/072/lib/intel64:
/opt/intel/Compiler/11.1/072/ipp/em64t/sharedlib:/opt/intel/Compiler/11.1/072/mkl/lib
/em64t:/opt/intel/Compiler/11.1/072/lib/intel64:/opt/intel/Compiler/11.1/072/ipp/em64t
/sharedlib:/opt/intel/Compiler/11.1/072/mkl/lib/em64t

[astrouser@development ~]$ echo $PATH
/home/apps/lsst/sbin:/home/apps/lsst/bin:/opt/gridengine/bin/lx24-amd64:/usr/lib64
/qt-3.3/bin:/usr/kerberos/bin:/opt/intel/Compiler/11.1/072/bin/intel64:/opt/intel
/Compiler/11.1/072/bin/intel64:/usr/local/bin:/bin:/usr/bin:/home/uchile/cmm
/astrolab/astrouser/bin
```

Creating (Sun Grid Engine) Jobs

Command interpreter	
↓	
Scheduler Information	
↓	
Load the proper environment	
↓	
Define input files	
↓	
Application execution	
↓	
Done	
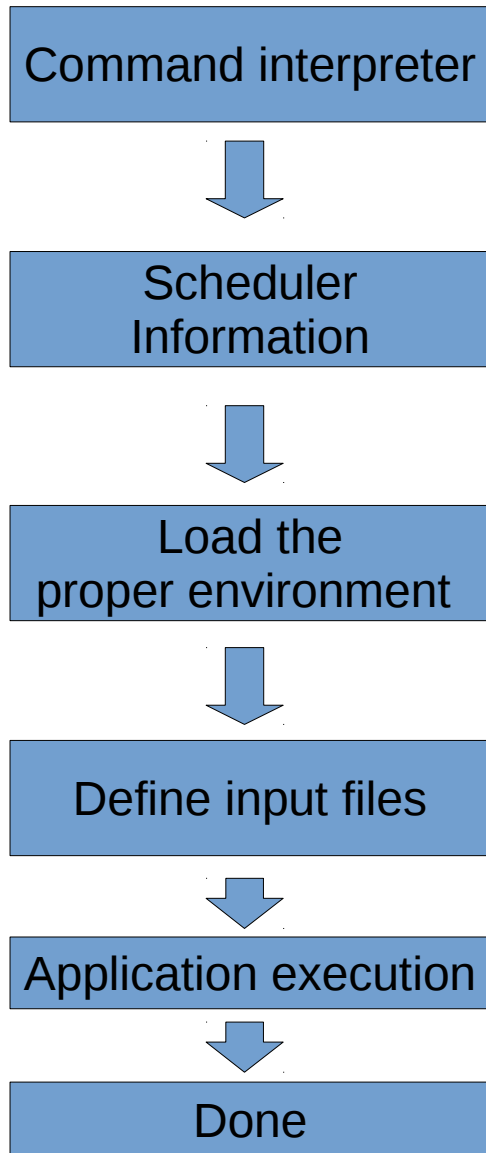
```bash
#!/bin/bash
#$ -cwd
#$ -j y
#$ -V
#$ -notify
#$ -m abes
#$ -M myemail@domain.com
#$ -N my-first-job
#$ -S /bin/bash
#$ -q all.q

module load lsst

echo "Running at `hostname -s`"
echo "Starting at `date '+%c'`"

INPUT_FITS=$1
WEIGHT_FITS=$2

sex $INPUT_FITS -CATALOG_NAME catalogue.cat \
    -WEIGHT_IMAGE $WEIGHT_FITS


echo "done"
```

Interacting with the SGE

- qsub `job_script.sge`
  - Submit *`job_script`* to the queue
- qstat
  - Show only the status of **your jobs** in the queue
- qstat -f
  - Show the status of **jobs** by queue
- qstat -u "`user`"
  - Show the jobs owned by `user`
- qstat -j `Job-ID`
  - Show the status for the job `Job-ID`
- qhost
  - Show the status of each node
- qhost -j
  - Show the status of each node and the jobs running on each one of them
- qdel `Job-ID`
  - Cancel (running) and delete a job from the queue

Submitting & Monitoring Jobs

```
[astrouser@levque ~]$ qsub my_first_job.sge
Your job XXXX ("my-first-job") has been submitted


[astrouser@levque ~]$ qstat
job-ID  prior    name       user     state submit/start at    queue          slots ja-task-ID
-----------------------------------------------------------------------------------------------
XXXX 0.00000 my-first-s astrouser  qw    08/09/2013 23:00:06                  1

[astrouser@levque ~]$ qstat
job-ID  prior    name       user     state submit/start at    queue          slots ja-task-ID
-----------------------------------------------------------------------------------------------
XXXX 0.00000 my-first-s astrouser  r    08/09/2013 23:00:30 all.q@levque001  1
```

- `watch` is your friend

  - `watch -n 1 "qstat"` : show qstat at 1 second interval

- Ganglia is your best friend

Monitoring Jobs

- **Ganglia** is an open source monitoring system developed in the NPACI (UCLA) and used initially by the UCSD to monitor their Rocks clusters.

http://syntagma.cmm.uchile.cl/ganglia

http://levque.dim.uchile.cl/ganglia

- Queue is monitored at "host overview" in the frontend.

- Compute nodes "host overview" gives you the state of your processes (require an extra plug-in)

- Useful metrics such as memory and network consumption are shown in an aggregated way as well as in a host basis way.

Best Practices

Rule 1 : Characterize your job

Because you are not alone in the world,
when submitting your job, please mind:

- The **memory** consumption.
  - Per core
  - Per process
- How **intensive** is on **Input/Output** operations.
  - Is my process able to run in a NFS storage layout?
  - Is my process able to run in a parallel filesystem
  - Do my process need a locking scheme to work?
- Scalability in terms of **cores**.
  - No always the highest, the better

Rule 2 : Monitor your Job

Because your jobs are running together with other people's job, please mind:

- Check continuously the status of the compute nodes where your jobs are running

- Check the load of the filesystem if your job is I/O intensive
  - Ganglia is your friend

- Be sure about how much storage your job is consuming.
  - You don't want to be remembered as the guy who crash everyone else jobs due to "out of space" in the filesystem.

Rule 3 : Do not leave data unattended

Because the storage is expensive and other users have the same right to use it, please mind:

- Remove temporal data and job output files.
  - .o and .e files
  - By applying the Rule 1, you should know if your job produces temporal files that can be deleted at the end of the job.
- When finishing with your results, keep them in other storage than your HPC account.
- Do not leave data in the scratch filesystem – It is volatile, which means it can be wiped out without further notice.
- Get used to backup your work (scripts, jobs, results).

Rule 4: Share your knowledge

Because not all the users have your skills to work with a HPC System, please mind:

- Write documentation by commenting your jobs scripts between lines.

- Write `readme` files specifying how many "*shaolin chambers*" did you have to go through to get your job done.

- Publish your scripts (if you are allowed to)

Hands-On

"My first sextraction"

Accessing the HPC System

SSH Connection

Ssh keys generation
Or Password change
(only first time)

Login OK

```
# ssh astrouser@development.cmm.uchile.cl

astrouser@development.cmm.uchile.cl's password:
Last login: Sat Aug 16 19:08:44 2014 from pc-163-125-
44-190.cm.vtr.net

Bienvenido a Levque

...

[astrouser@development ~]$ ssh-keygen -t rsa

[astrouser@development ~]$ passwd

...

...

[astrouser@development ~]$
```
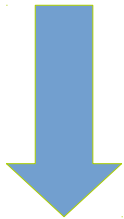
Accessing the HPC System

Checking

Home directory listing

Ready to go!

```
[astrouser@development ~]$ ls -la
total 692
drwx------ 26 astrouser astro     4096 ago 16 19:08 .
drwxr-xr-x 17 root         root     4096 ago 14 20:07 ..
lrwxrwxrwx  1 astrouser astro       16 jun 27 12:30 astro ->
/home/apps/astro
drwxr-xr-x  4 astrouser astro     4096 jul  2 18:15 .astropy
-rw-------  1 astrouser astro    12936 ago 15 15:14 .bash_history
-rw-r--r--  1 astrouser astro       33 jun 25 16:06 .bash_logout
-rw-------  1 astrouser astro       42 ago 14 17:14 .lesshst
lrwxrwxrwx  1 astrouser astro       16 ago 13 10:54 lsst ->
/home/apps/lsst/
drwxr-xr-x  3 astrouser astro     4096 ago 14 19:04 .matplotlib
drwxr-xr-x  2 astrouser astro     4096 ago 14 19:54 .mc
drwxr-xr-x  5 astrouser astro     4096 jul 12 10:08 .mozilla
-rw-r--r--  1 astrouser astro     4322 jul  7 16:26 .recently-used.xbel
drwx------  2 astrouser astro     4096 ago 13 19:09 .ssh
drwxr-xr-x  3 astrouser astro     4096 jun 27 12:46 .subversion
-rw-r--r--  1 astrouser astro      658 jun 25 16:06 .zshrc
[astrouser@development ~]$
```

Getting Cluster State

Checking Hosts
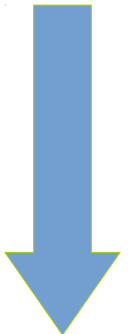
```
[astrouser@development ~]$ qhost
HOSTNAME                ARCH         NCPU  LOAD  MEMTOT  MEMUSE  SWAPTO  SWAPUS
-------------------------------------------------------------------------------
global                  -              -     -       -       -       -       -
levque001               lx24-amd64     8  0.02   23.5G    1.2G    2.0G   64.4M
levque002               lx24-amd64     8  5.00   23.5G    1.9G    2.0G   50.0M
...
levque065               lx24-amd64     8  7.00   23.5G    7.8G    2.0G   88.0K
levque066               lx24-amd64     8  0.00   23.5G  593.3M    2.0G    6.6M
matlab1                 lx24-amd64    16  0.10   23.5G  493.4M    2.0G     0.0
```
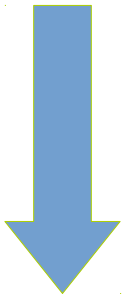
Checking Jobs

```
[astrouser@development ~]$ qstat
job-ID  prior    name      user      state submit/start at      queue                       slots
ja-task-ID
-----------------------------------------------------------------------------------------------------
1239018 0.99951 CR_Blind14 astrouser    r     08/12/2014 11:50:27 all.q@levque062             4 30
1239021 0.00000 doastro_Bl astrouser   hqw    08/06/2014 23:06:30                             4 1
1239022 0.00000 doastro_Bl astrouser   hqw    08/06/2014 23:06:30                             4 1
1239023 0.00000 doastro_Bl astrouser   hqw    08/06/2014 23:06:30                             4 1

[astrouser@development ~]$
```

Ready to go!

Getting Cluster State

Via web

Ready to go!

http://levque.cmm.uchile.cl/ganglia
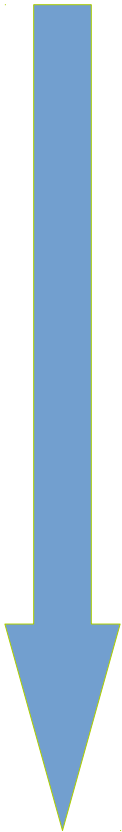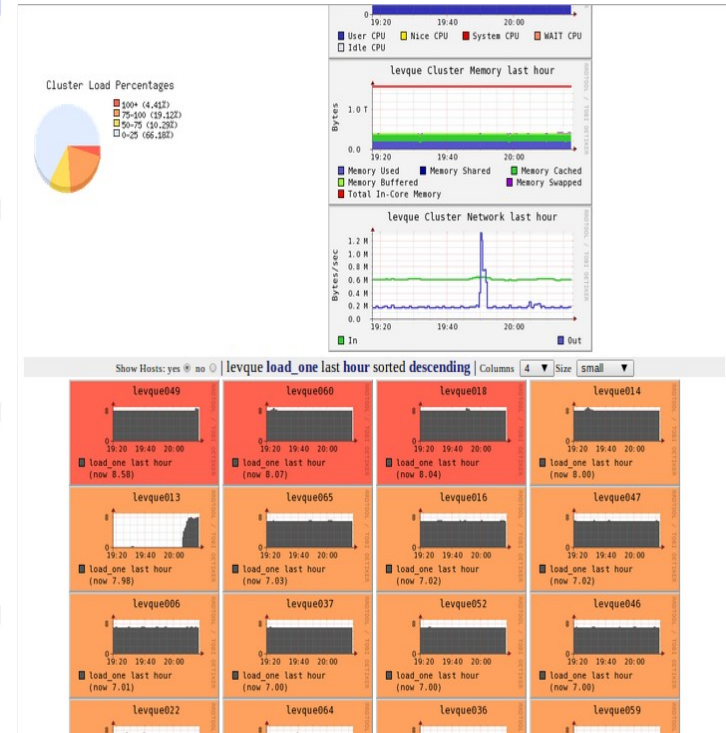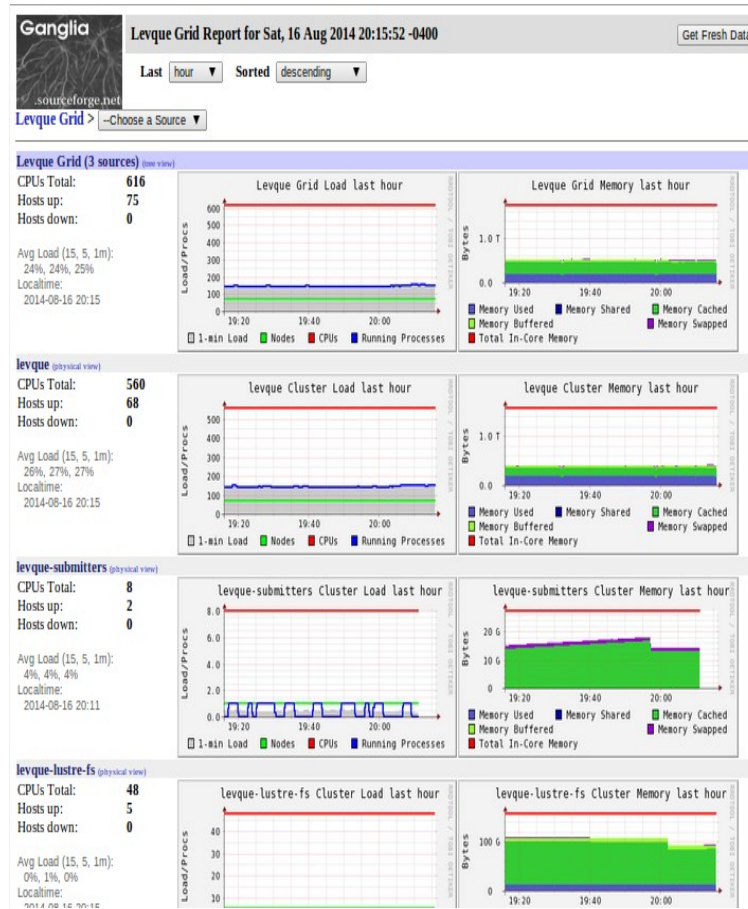
Preparing My Data

Cloning base files

```
[astrouser@levque demos]$ git clone  http://git.cmm.uchile.cl/demo-sextractor.git
git clone  http://git.cmm.uchile.cl/demo-sextractor.git
```

⬇

Create working directory

```
[astrouser@levque demos]$ mkdir -p workdir
```

⬇

Copy input files

```
[astrouser@levque demos]$ cp demo-sextractor/Blind_03_N1_01* workdir
```

⬇

Copy sextractor default files & job script

```
[astrouser@levque demos]$ cp demo-sextractor/default.* workdir/

[astrouser@levque demos]$ cp demo-sextractor/*.sge workdir/
```

⬇

Getting into the cwd

```
[astrouser@levque demos]$ cd workdir
```

⬇

Ready to go!

```
[astrouser@levque demos/workdir]$
```

Preparing My Job

Edit the job script

Ready to go!
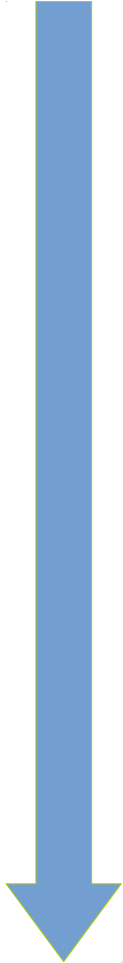
```
[astrouser@levque demos/workdir]$ cat my-first-sextraction.sge
#!/bin/bash
# My First Sextraction (by using sextractor)
# usage: my-first-sextraction.sge {input_fits} {weight_fits}
#
# By Francisco Forster and Juan-Carlos Maureira
# CMM. University of Chile
############################################################
#$ -cwd
#$ -j y
#$ -notify
#$ -m abes
#$ -M your-email@mail.com
#$ -N my-first-sextraction
#$ -S /bin/bash

# load the proper enviroment module
module load astro

# check for arguments
if [ $# != 2 ]; then
   echo "usage: $0 {input_fits} {weight_fits}"
   Exit 1
Fi

# get the input arguments (see usage)
INPUT_FITS=$1
WEIGHT_FITS=$2

if [ ! -f "$INPUT_FITS" ] || [ ! -f "$WEIGHT_FITS" ]; then
   echo "input files not found."
   Exit 1
Fi

# perform the source extraction and generate the file cataloge.cat
sex $INPUT_FITS -CATALOG_NAME cataloge.cat -WEIGHT_IMAGE $WEIGHT_FITS

echo "done"
[astrouser@levque demos/workdir]$
```

Characterizing My Job

Open two terminals

1: execute the getProcessMemoryStatus

2: execute the script by hand

```
[astrouser@levque demos/workdir]$ ./getProcessMemoryStatus sex
Sample VmPeak: VmSize: VmLck: VmHWM: VmRSS: VmData: VmStk: VmExe: VmLib:
VmPTE: VmSwap:
1 81220 81216 0 12116 12116 22080 92 1368 37268 124 0
2 81220 81216 0 12120 12112 22080 92 1368 37268 124 0
3 81220 81212 0 12124 12120 22076 92 1368 37268 124 0
4 81220 81212 0 12124 12116 22076 92 1368 37268 124 0
5 96908 96908 0 23128 23128 37772 92 1368 37268 132 0
6 105392 105392 0 37296 37296 46256 92 1368 37268 136 0
7 106408 105612 0 38016 37432 46476 92 1368 37268 136 0
8 106408 105612 0 38016 37456 46476 92 1368 37268 136 0
9 106408 105612 0 38016 37460 46476 92 1368 37268 136 0
10 106408 105612 0 38016 37548 46476 92 1368 37268 136 0
11 106408 105944 0 38016 37788 46808 92 1368 37268 136 0
12 114240 105468 0 45796 37512 46332 92 1368 37268 136 0
13 114240 105624 0 45796 37556 46488 92 1368 37268 136 0
14 114240 105624 0 45796 37564 46488 92 1368 37268 136 0
15 114240 78328 0 45796 11304 19192 92 1368 37268 116 0
^C
[astrouser@levque demos/workdir]$
```

```
[astrouser@levque demos/workdir]$ ./my-first-
sextraction.sge \
        Blind_03_N1_01.fits.fz_proj.fits \
        Blind_03_N1_01_wtmap.fits.fz_proj.fits
Running at development.cmm.uchile.cl
Starting time : Sat 10 Aug 2013 12:41:00 AM CLT
.
----- SExtractor 2.18.9 started on 2013-08-10 at
00:41:00 with 1 thread

Setting catalog parameters.
Reading detection filter.
Initializing catalog.
Looking for Blind_03_N1_01.fits.fz_proj.fits.
----- Measuring from: Blind_03_N1_01.fits.fz_p

...

[astrouser@levque demos/wordir]$
```

Submitting My Job

```
[astrouser@levque demos/workdir]$ qsub my-first-sextraction.sge \
        Blind_03_N1_01.fits.fz_proj.fits \
        Blind_03_N1_01_wtmap.fits.fz_proj.fits

Your job 9762 ("my-first-sextraction") has been submitted


[astrouser@levque demos/workdir]$ qstat



job-ID  prior    name        user          state submit/start at        queue                        slots ja-task-ID
-----------------------------------------------------------------------------------------------------------------------
  9762 0.00000 my-first-s astrouser    qw    08/09/2013 23:00:06                                      1


[astrouser@levque demos/workdir]$ qstat

job-ID  prior    name        user          state submit/start at        queue                        slots ja-task-ID
-----------------------------------------------------------------------------------------------------------------------
  9762 0.00000 my-first-s astrouser     r    08/09/2013 23:00:16 all.q@levque001                      1



[astrouser@levque demos/workdir]$
```

Submit the job

Check submission status

You got an Email!

Monitoring My Job

```
[astrouser@levque demos/workdir]$  watch –n 1 'qstat'

Every 1.0s: qstat                                                    Fri Aug  9 23:12:52 2013

job-ID  prior    name        user          state submit/start at      queue                        slots ja-task-ID
-----------------------------------------------------------------------------------------------------------------
   9762 0.00000 my-first-s astrouser    qw     08/09/2013 23:00:06                                     1
```

```
[astrouser@levque demos/workdir]$ watch –n 1 "qstat –u '*'"

Every 1.0s: qstat –u "*"                                             Fri Aug  9 23:13:12 2013

job-ID  prior    name        user          state submit/start at      queue                        slots ja-task-ID
-----------------------------------------------------------------------------------------------------------------
   9051 0.50500 QLOGIN      dtravisany    r      07/09/2013 16:14:16 all.q@levque003                   1
   9683 0.50500 QLOGIN      adigenova     r      07/28/2013 18:21:19 all.q@levque034                   1
   9703 0.60500 V6O18H12_s wcanon        r      08/02/2013 13:44:15 all.q@levque023                   8
   9704 0.60500 V6O18H12_s wcanon        r      08/02/2013 13:51:45 all.q@levque056                   8
   9741 0.50500 QLOGIN      mcortes       r      08/08/2013 15:18:02 all.q@levque043                   1
   9759 0.60500 BIphenFeCs wcanon        r      08/09/2013 19:52:31 all.q@levque065                   8
   9761 0.60500 BIphenFeC2 wcanon        r      08/09/2013 20:28:16 all.q@levque042                   8
   9762 0.00000 my-first-s astrouser    r      08/09/2013 23:00:16 astro.q@levque001                  1
   9760 0.60500 BIphenFeC2 wcanon        qw     08/09/2013 20:10:11                                    8


[astrouser@levque demos/workdir]$
```

Getting My Job Status

```
[astrouser@levque demos/workdir]$ qstat -j 9762
==============================================================
job_number:              9762
submission_time:         Fri Aug  9 23:05:29 2013
owner:                   astrouser
Uid:                     18010
group:                   demo
Gid:                     11056
sge_o_home:              /home/uchile/cmm/astrolab/astrouser
sge_o_log_name:          astrouser
sge_o_shell:             /bin/bash
sge_o_workdir:           /home/uchile/cmm/astrolab/astrouser/demos/workdir
sge_o_host:              login-1-0
account:                 sge
cwd:                     /home/uchile/cmm/astrolab/astrouser/demos/workdir
merge:                   y
mail_options:            abes
mail_list:               jcm@dim.uchile.cl
notify:                  TRUE
job_name:                my-first-sextraction
Jobshare:                0
shell_list:              NONE:/bin/bash
error reason    1:       08/09/2014 01:07:49 [15086:29399]: error: can't open output file "/home/apps/astro/logs/XXXXXX.o
env_list:
job_args:                Blind_03_N1_01.fits.fz_proj.fits,Blind_03_N1_01_wtmap.fits.fz_proj.fits
scheduling info:         queue instance "all.q@levque001" dropped because it is temporarily not available
                         queue instance "all.q@levque002" dropped because it is temporarily not available
                         queue instance "all.q@levque003" dropped because it is disabled
                         queue instance "all.q@levque004" dropped because it is disabled
                         queue instance "all.q@levque065" dropped because it is disabled
                         queue instance "all.q@levque066" dropped because it is full
                         queue instance "all.q@matlab1" dropped because it is full
                         job dropped because of job dependencies

[astrouser@levque demos/workdir]$
```

Job information

Why the job is not
In that compute node
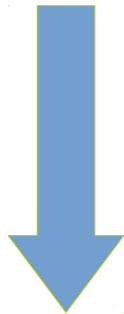
Getting My Results

Looking for result files

Checking results contents

YES!!!

```
[astrouser@levque demos/workdir]$ ls -la
total 119732]
drwxr-xr-x 3 astrouser astro      4096 ago 16 19:13 .
drwxr-xr-x 3 astrouser astro      4096 ago 16 19:10 ..
-rw-r--r-- 1 astrouser astro 61228800 ago 16 19:10 Blind_03_N1_01.fits.fz_proj.fits
-rw-r--r-- 1 astrouser astro     40958 ago 16 19:10 Blind_03_N1_01.fits.fz_proj.fits-
catalogue.dat
-rw-r--r-- 1 astrouser astro 61228800 ago 16 19:10 Blind_03_N1_01_wtmap.fits.fz_proj.fits
-rw-r--r-- 1 astrouser astro     42702 ago 16 19:11 catalogue.cat
-rw-r--r-- 1 astrouser astro       804 ago 16 19:10 default.conv
-rw-r--r-- 1 astrouser astro        82 ago 16 19:10 default.param
-rw-r--r-- 1 astrouser astro     11520 ago 16 19:10 default.psf
-rw-r--r-- 1 astrouser astro      3620 ago 16 19:10 default.sex
-rwxr-xr-x 1 astrouser astro       865 ago 16 19:10 getProcessMemoryStatus
drwxr-xr-x 8 astrouser astro      4096 ago 16 19:13 .git
-rwxr-xr-x 1 astrouser astro      1042 ago 16 19:10 my-first-sextraction.sge
-rw-r--r-- 1 astrouser astro       711 ago 16 19:10 README.seaf
-rw-r--r-- 1 astrouser astro      3620 ago 16 19:10 my-first-sextraction.o9762

[astrouser@levque demos/workdir]$ head -n 5 my-first-sextraction.o9762
Running at levque001
Starting time : Fri 09 Aug 2013 11:00:16 PM CLT
.
----- SExtractor 2.18.9 started on 2013-08-09 at 23:24:46 with 1 thread

[astrouser@levque demos/workdir]$ tail -n 5 my-first-sextraction.o9762
     433 1477.1 2924.3   3.4   3.2       115090 _____
     434 1914.5 3765.5   2.3   2.1       646.094 _____
     435  806.2 2865.6   2.9   2.6       2201.14 _____
     436 1699.9 2835.1   2.3   2.0       522.624 _____
     Objects: detected 443     / sextracted 436

Closing files.
.
Ending time : Fri 09 Aug 2013 11:24:47 PM CLT
done

[astrouser@levque demos/workdir]$
```
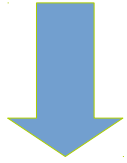
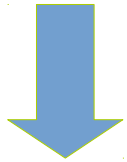# Hands-on: My first job in HPC@CMM
Saving and Cleaning up

Return to your $HOME	`[astrouser@levque demos/workdir]$` `cd`
Save results files	`[astrouser@levque demos]$` `cp workdir/cataloge.cat demo-sextractor`
Clean the working directory	`[astrouser@levque demos]$` `rm -rf workdir`
logout	`[astrouser@levque demos]$` `logout`

The Take Aways

- Definitions needed to understand a HPC system.

- Overview about architecture and components of a HPC system.

- Software, Applications, tools-chains

- Best practices when working with a HPC system.

- Follow an example of how to work with generic HPC system.