



DATA SCIENCE &
SCIENTIFIC COMPUTING



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L02: HPC software stack

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Agenda

- A first look at the Software stack for HPC (part 1)
 - Middleware
 - Compilers
 - Libraries
 - Scientific software
 - How to compile scientific software
- HPC Concepts (part 2)
 - Parallel programming paradigms
 - Evolution of paradigms
 - Ahmdal law / Gustafson law
 - Strong/weak scalability

System stack of a general HPC platform

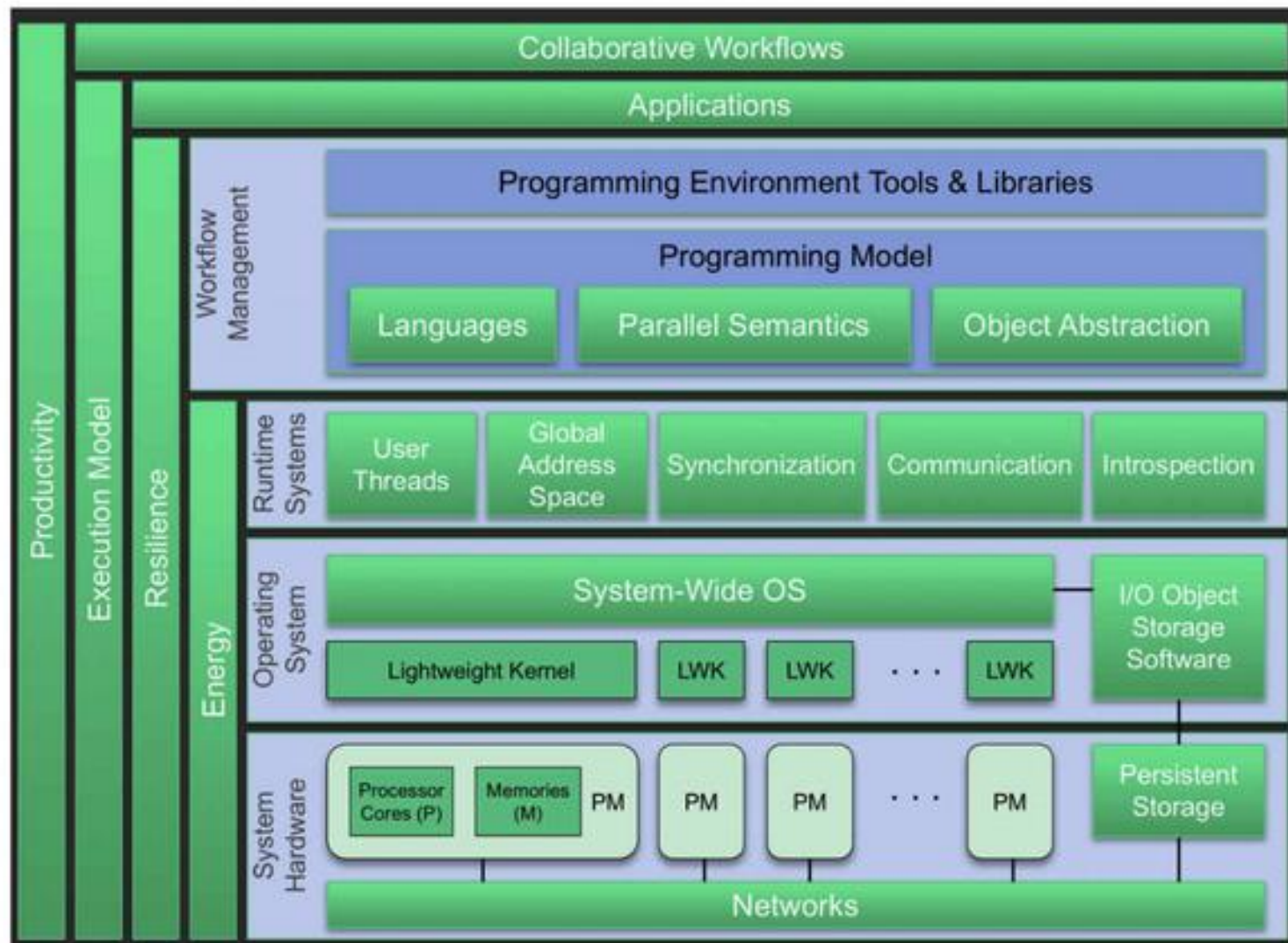
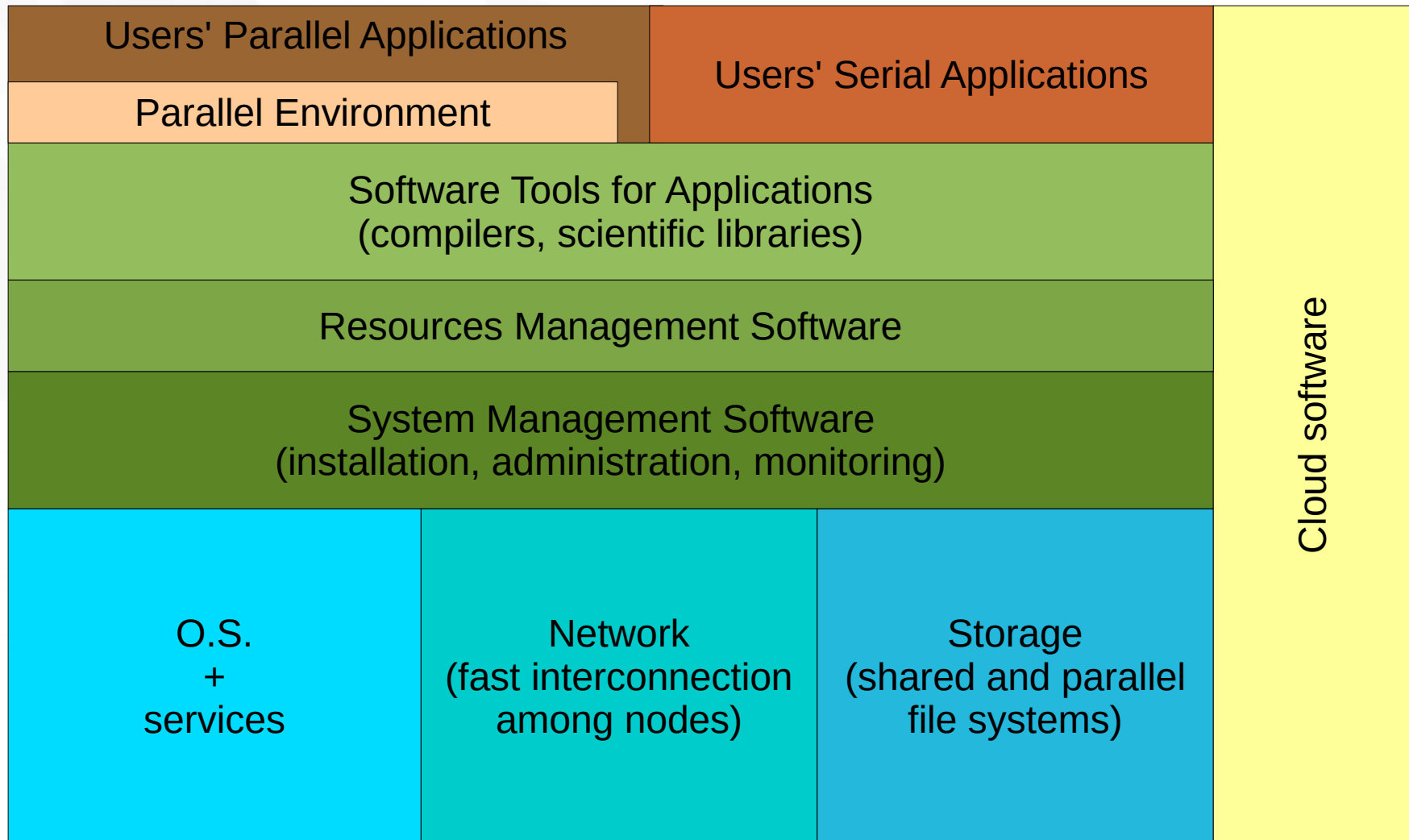
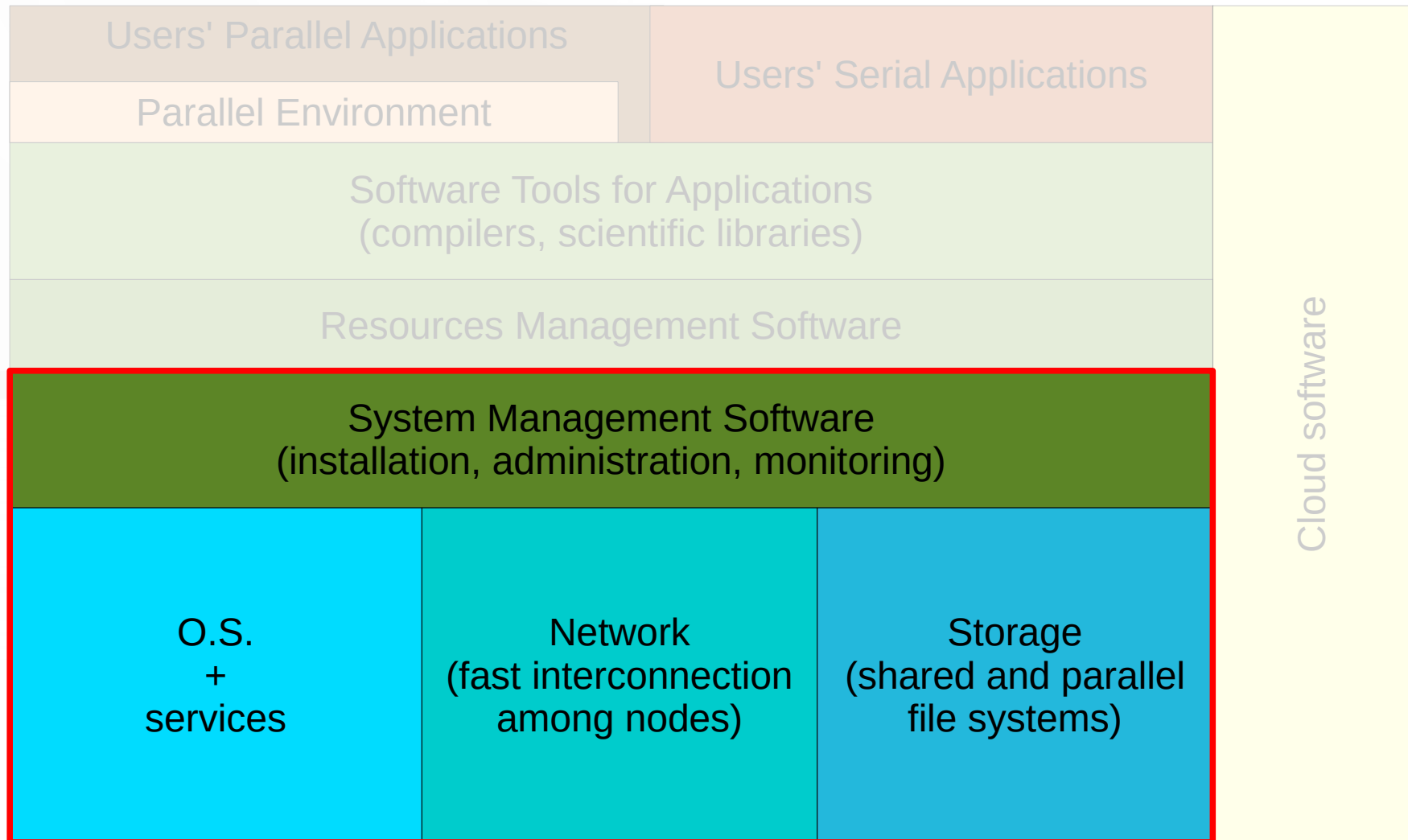


Figure 1.9 The system stack of a general supercomputer consists of a system hardware layer and several software layers. The first software layer is the operating system, encompassing both resource management and middleware to access input/output (I/O) channels. Higher software layers include runtime systems and workflow management.

HPC software stack: Overview



HPC cluster middleware: Overview



Cluster middleware: Middleware Design Goals

- Complete Transparency (Manageability):
 - Lets us see a single cluster system..
 - Single entry point, ftp, ssh, software loading...
- Scalable Performance:
 - Easy growth of cluster
 - no change of API & automatic load distribution.
- Enhanced Availability:
 - Automatic Recovery from failures
 - Employ checkpointing & fault tolerant technologies

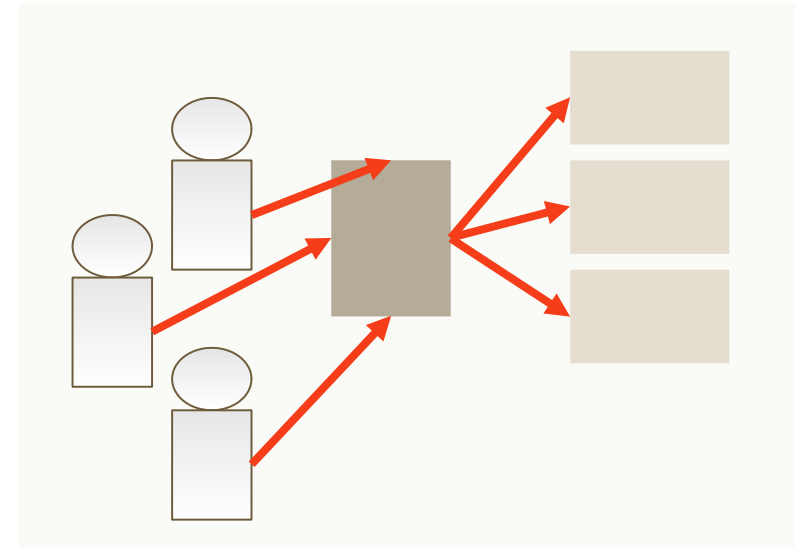
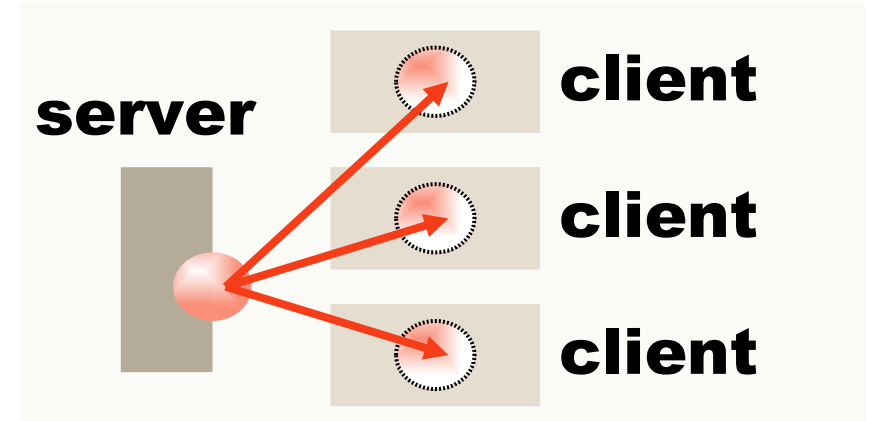
Cluster middleware

Administration software:

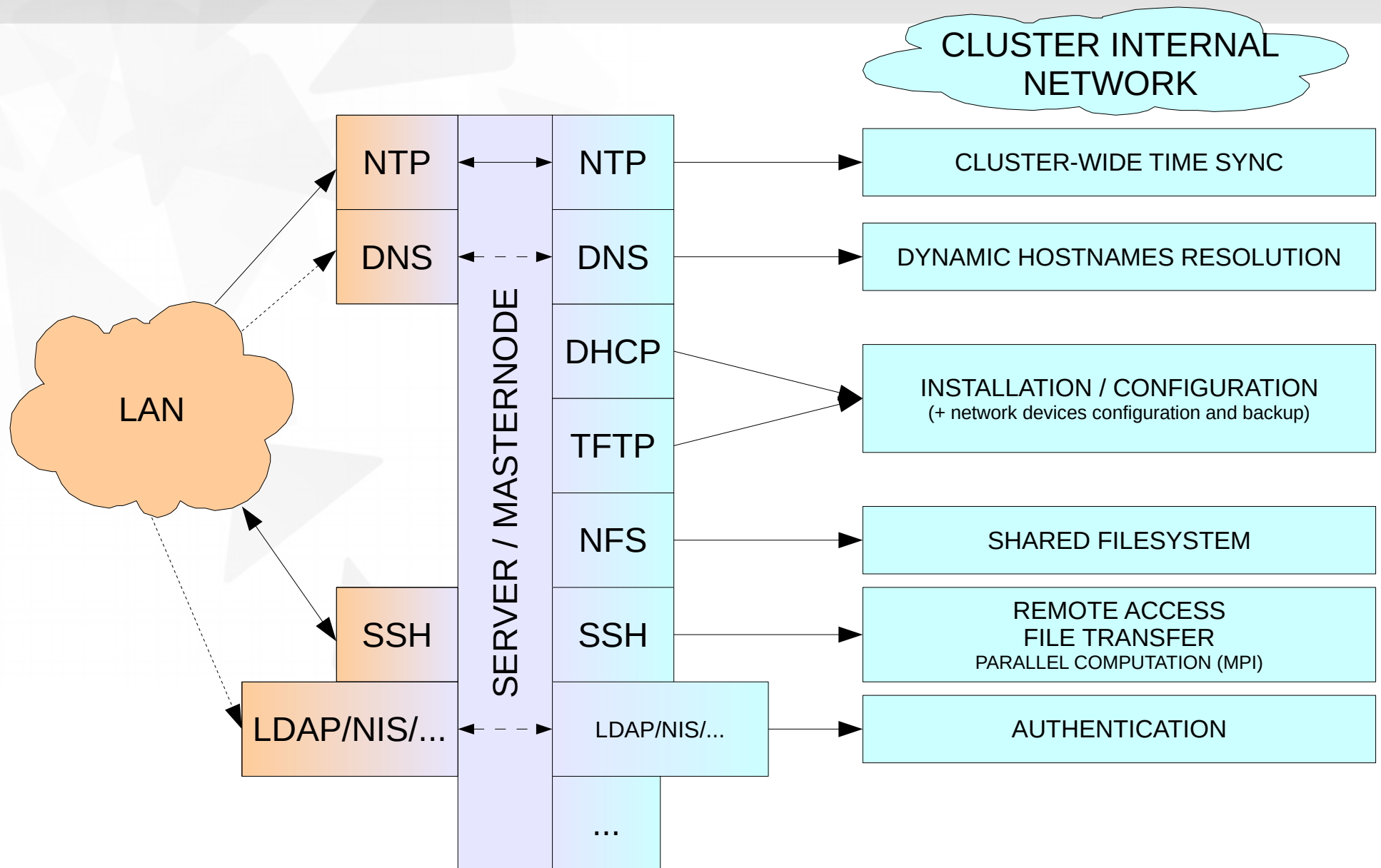
- user accounts
- NTP/NFS/ etc...

Resource management and scheduling software (LRMS)

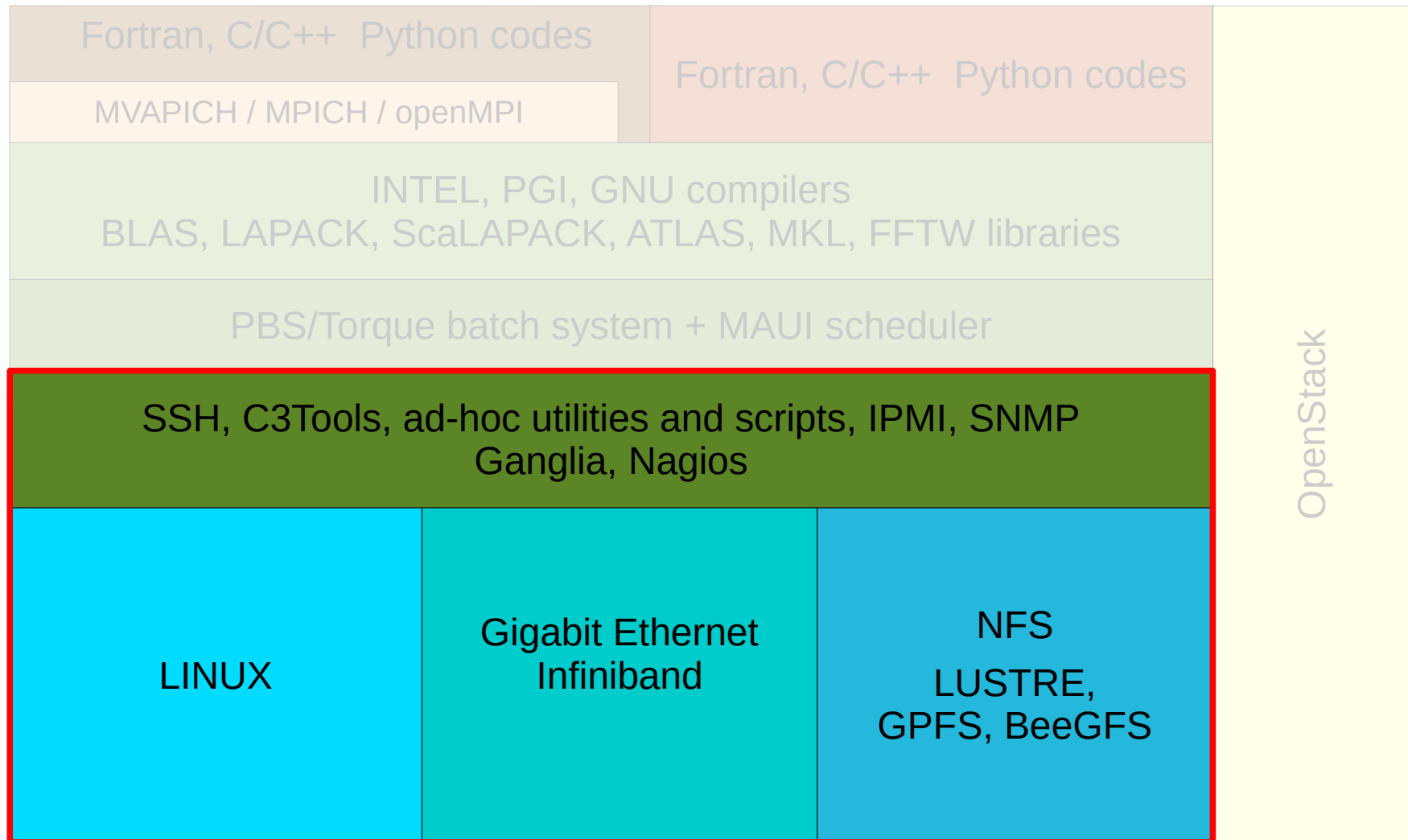
- Process distribution
- Load balance
- Job scheduling of multiple tasks



CLUSTER SERVICES



Cluster middleware tools used by us



Resource Management Problem

We have a pool of users and a pool of resources, then what?

- some software that controls available resources
- some other software that decides which application to execute based on available resources
- some other software devoted to actually execute applications

What are we speaking about ?



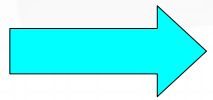
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REPLACE THE CAKE WITH HPC
RESOURCE

Resource management

The resource manager allows

- better **resource control**
- better **access control**



better resource utilization

Some definitions

Batch Scheduler: software responsible for scheduling the users' jobs on the cluster.

scheduling is the method by which work specified by some means is assigned to resources that complete the work

Resources Manager: software that enable the jobs to connect the nodes and run.

Node (aka Computing Node): computer used for its computational power.

Frontend/Master node: it's through this node that the users will submit/launch/manage jobs.

Management of job and resources

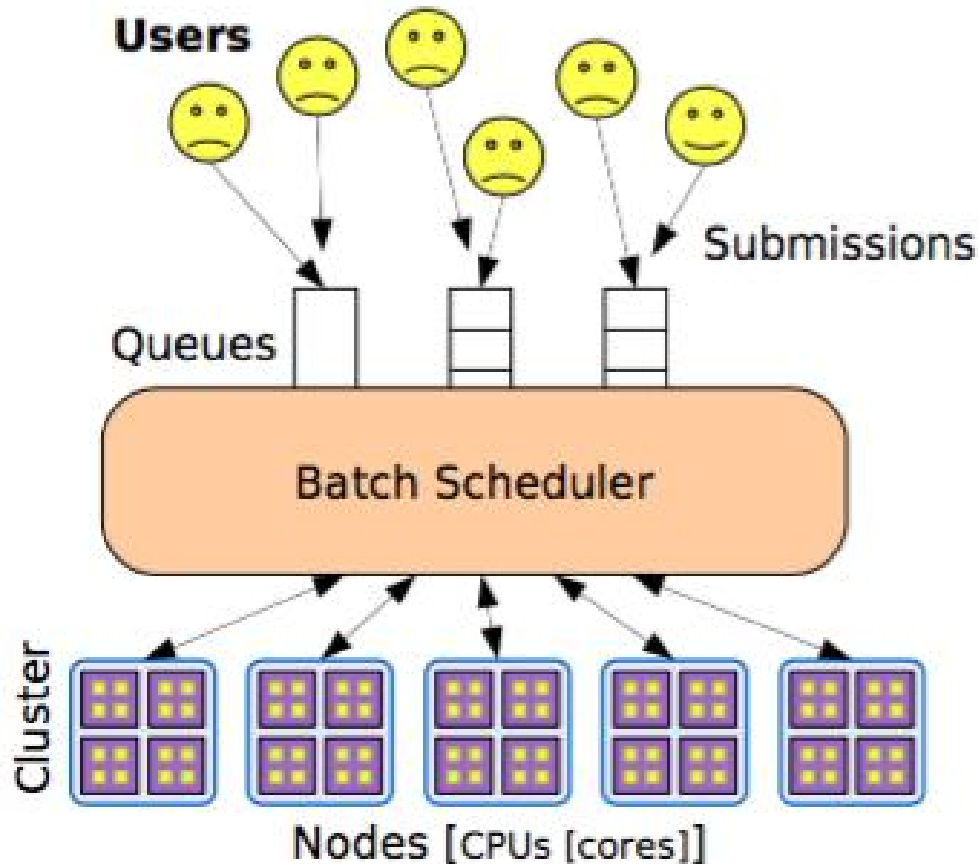
- **Management: Batch Scheduler and Resource Manager**

- Submission
- Scheduling
- Resources Allocation
- Job Launch
- Monitoring, logging...

2 layers

- Resource Management Layer: launching, cleaning, monitoring...
- Job Management Layer: batch/interactive job, Scheduling, Suspend/Resume, Preemption, Dependencies, Resubmission, Advance Reservation...

Batch scheduler: a global picture (1)

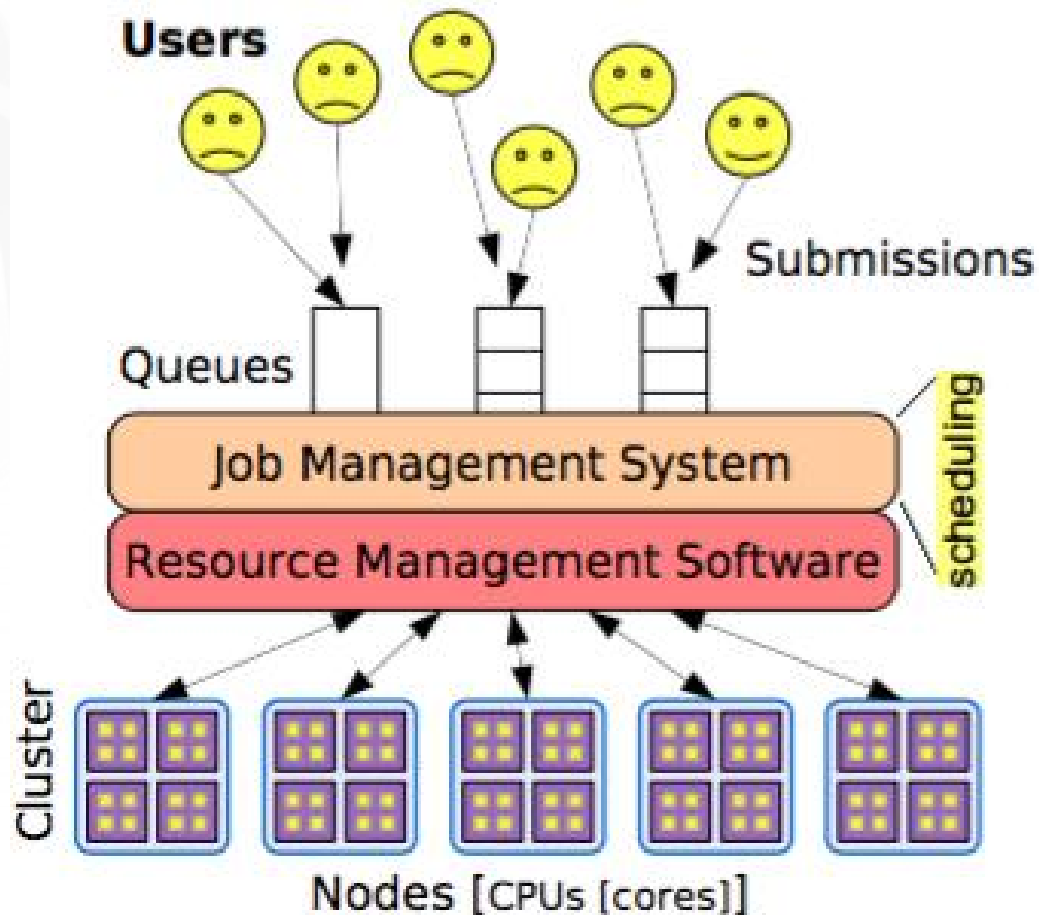


Allocate resources for each applications with respect of their requirements and users' rights.

- Satisfy users
response time, reliability
- Satisfy admins
high resource utilization
efficiency
energy management

...

Batch scheduler: a global picture (2)



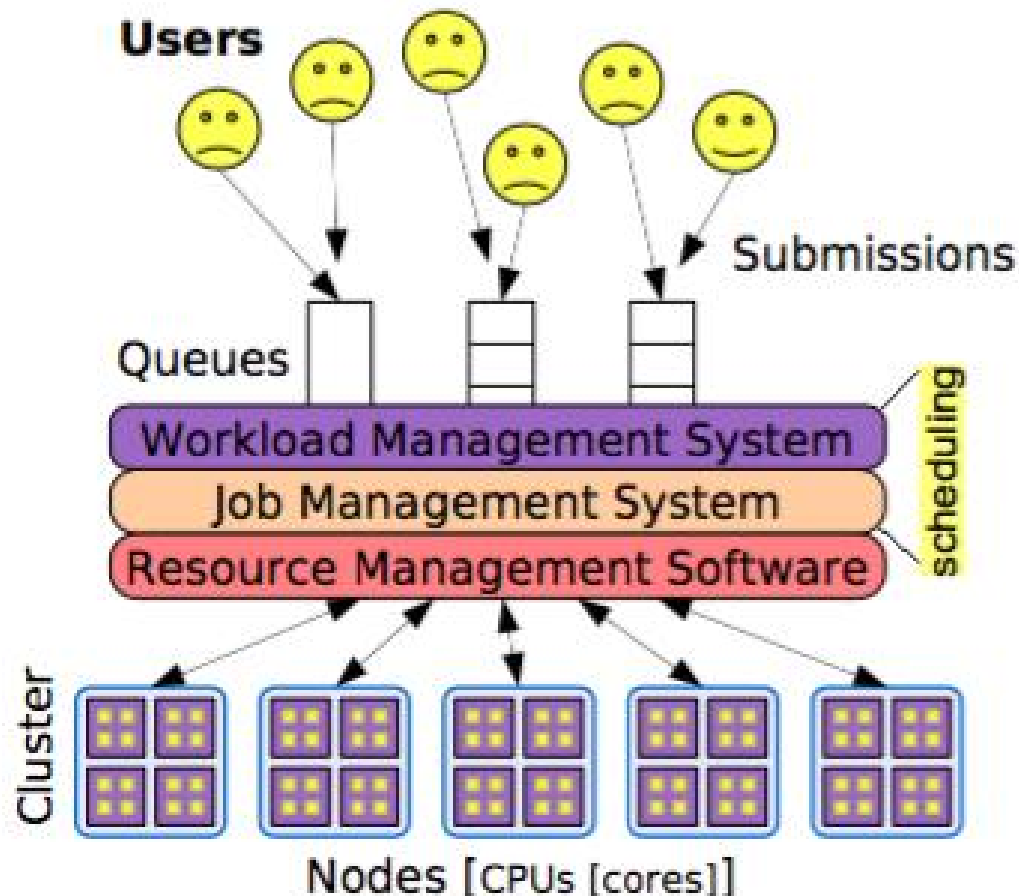
Resource Management Layer

→ launching, cleaning, monitoring

Job Management Layer

→ batch/interactive job
→ backfilling
→ scheduling
→ suspend/Resume
→ preemption
→ dependencies
→ resubmission
→ advance reservation

Batch scheduler: a global picture (3)



Workload/Job Management
→ more complete job scheduling policies
→ Fairsharing, Quality of Service (QoS), SLA (Service Level Agreement), Energy Saving
→ Dedicated software: MAUI

Mainly adopted schedulers

- GridEngine (SGE)
 - Sun of Grid Engine (SoGE)
 - Open Grid Scheduler (OGS)
 - Univa Grid Engine (UGE) – Commercial
- LoadLeveler – IBM
- LSF
 - expensive, but free in OpenLava edition
- PBSPRO
 - commercial or community edition
- SLURM
 - free, new, commercial support
- Torque resource manager +
 - MOAB scheduler, commercial
 - Maui scheduler, open source

PBSPRO/ Torque queue system

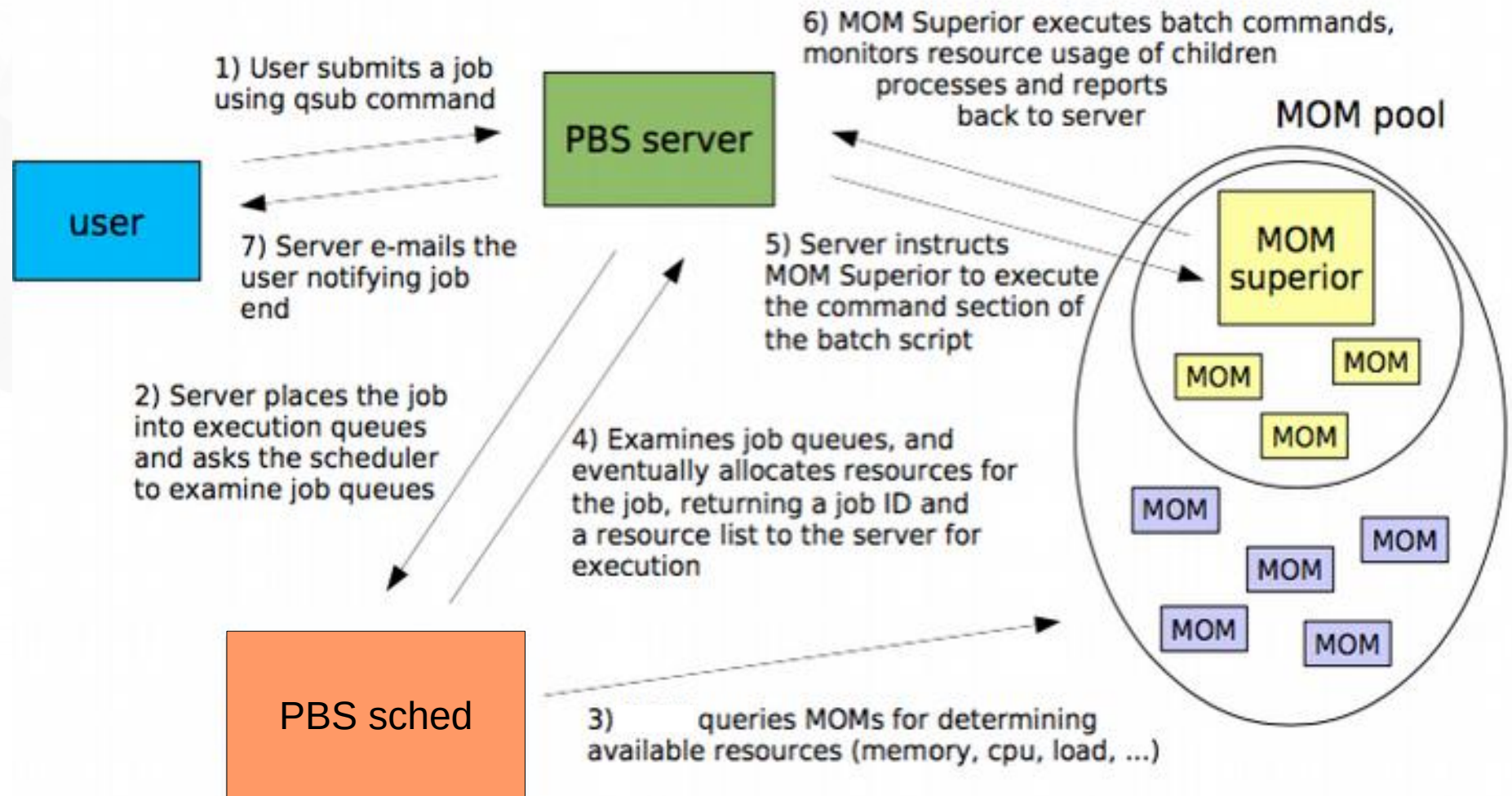
- General components
 - LM-X license server (if commercial edition)
 - resource manager *pbs_server*
 - scheduler *pbs_sched* / *maui* in case of Torque
 - executors *pbs_mom*

Recap on LRMS

- LRMS is a fundamental tool in the HPC management:
 - User: know it well and you will almost run !
 - Sys. Adm.: know it well and you will keep your system busy..
- Many possible choices
 - Concepts are similar /commands sometime also (to help survive: <http://www.schedmd.com/slurmdocs/rosetta.pdf>) .
 - Key point is THE scheduler
- Theoretically is **almost all possible** in resource scheduling with modern LRMS software to accommodate requests from users
- Practically is almost impossible satisfy all your users (and/or communities)

Resource sharing policies is not at all a technical problem !

Typical job session



Fair sharing

Fairshare is a mechanism which allows historical resource utilization information to be incorporated into job feasibility and priority decisions.

Fairshare information only affects the job's priority relative to other jobs.

Using the standard fairshare target

- the priority of jobs of a particular group which has used too many resources over the specified fairshare window is lowered
- the priority of jobs which have not received enough resources will be increased

Backfill 1/2

Backfill is a scheduling optimization which allows a scheduler to make better use of available resources by running jobs out of order.

Consider this example with a 10 CPUs machine:

Job1 (priority=20 walltime=10 nodes=6)
Job2 (priority=50 walltime=30 nodes=4)
Job3 (priority=40 walltime=20 nodes=4)
Job4 (priority=10 walltime=10 nodes=1)

- 1)The scheduler prioritizes the jobs in the queue according to a number of factors and then re-orders the jobs into a 'highest priority first' sorted list.

Sorted list:

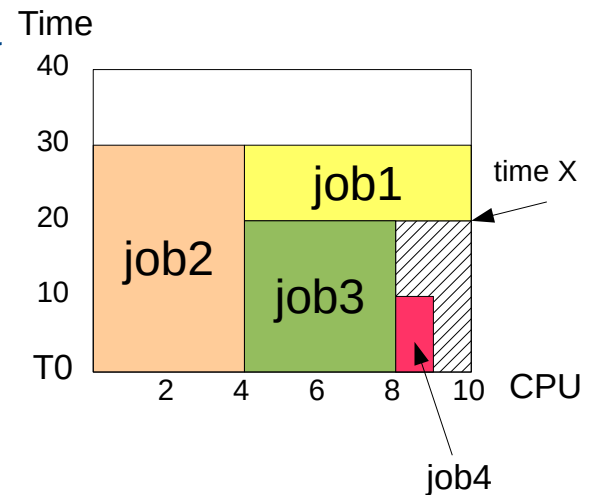
Job2 (priority=50 walltime=30 nodes=4)
Job3 (priority=40 walltime=20 nodes=4)
Job1 (priority=20 walltime=10 nodes=6)
Job4 (priority=10 walltime=10 nodes=1)

Backfill 2/2

2) It starts the jobs one by one stepping through the priority list until it reaches a job which it cannot start.

3) All jobs and reservations have a start time and a walltime limit, so the scheduler can determine:

- the completion time of all jobs in the queue
- the earliest the needed resources will become available for the highest priority job to start (time X)
- which jobs can be started without delaying this job (job4)



- Enabling backfill allows the scheduler to start other, lower-priority jobs so long as they do not delay the highest priority job, essentially filling in holes in node space.
- Backfill offers significant scheduler performance improvement:
 - increased system utilization by around 20% and improved turnaround time by an even greater amount in a typical large system
 - backfill tends to favor smaller and shorter running jobs more than larger and longer running ones: It is common to see over 90% of these small and short jobs backfilled.

Job2 (priority=50 walltime=30 nodes=4)
Job3 (priority=40 walltime=20 nodes=4)
Job1 (priority=20 walltime=10 nodes=6)
Job4 (priority=10 walltime=10 nodes=1)

A job's life

- The user describes the resources he he needs in a shell script, the **job** file
 - From the login node, the user **submits** the job to the queue system
 - The system sends the job to the **execution queue**
 - The job is executed on the compute node, without user intervention
 - The **results** of the job are written in the folder specified by the user
- The queue system free the resources to get ready for the next excution

A job file (PBS pro and torque)

PBS directives, using the tag **#PBS**, describe the job requirements in terms of execution queue, number of nodes and cores, job name, walltime, etc.

```
#!/bin/bash
# This is an example script
#PBS -q blade
#PBS -l nodes=1:ppn=2
#PBS -N myjob
#PBS -l walltime=2:00:00
```

The rest of the job is a standard shell script

Load Octave module, version 3.6.4

```
module load octave/3.6.4
```

PBS "lands" user's home directory: it is important to change the directory to the one in which we want to run the job

```
cd $HOME/MyJobDir
octave MyOctaveScript
```

Job submission

Jobs are submitted using **qsub**

- `qsub myJob.sh`
- The resource, queue, etc., can be specified in the job file or from command line
 - `qsub -l nodes=8:ppn=4 myJob.sh`
 - `qsub -l select=8:ncpus=4:mpiprocs=8 -l place=scatter myJob.sh`
- If the job is accepted, a JOBID is given
 - JOBID is necessary to monitor the job status

```
[degiorgi@grid0 ~]$ qsub -l nodes=2:ppn=4 script.sh
2715.grid0.mercuriofvg.it
[degiorgi@grid0 ~]$
```

Job submission


- You can be more specific about the resources needed
 - `#PBS -l nodes=m001:ppn=4`
 - Requests **four cores** on node **m001**
 - `#PBS -l select=m001:ncpus=4:mpiprocs=4`
 - Requests node **m001 and** node **m048**
 - `#PBS -l nodes=2:ppn=4+m010`
 - Requests **two nodes** with 4 cores **and** node **m010**

Queues

- The user can use different **queues**
 - Each queue can be configured to accept jobs
 - From a certain user groups
 - Requesting resources between certain limits
 - The proper needs to be selected
 - In the job script using `#PBS -q <queue name>`
 - From command line using `-q <queue name>`

Interactive jobs

- It is possible to have **interactive jobs**
 - `qsub -l nodes=2:ppn=2 -I`
 - `qsub -l select=2:ncpus=2:mpiprocs=2 -l place=scatter -I`
- If resources are available, the users gets a prompt on the first node reserved



```
[brandino@master ~]$ qsub -l nodes=2:ppn=2 -I -q gpu
qsub: waiting for job 138510.master to start
qsub: job 138510.master ready

[brandino@b21 ~]$ cat $PBS_NODEFILE
b21
b21
b22
b22
[brandino@b21 ~]$
```

Not the best way to use cluster resources.

Humans are slow:

- Waste of resources
 - CPU/RAM, ... , energy
- Job terminates only when
 - The user closes the session
 - It hits the walltime



Accessing compute nodes

- Normally, you cannot ssh to a compute node

```
[degiorgi@grid0 ~]$ ssh m001  
Connection closed by 10.2.12.1
```

- If a user has a job running on some nodes, ssh is allowed on those nodes

```
[degiorgi@grid0 ~]$ echo "sleep 30" | qsub -l nodes=m001  
2702.grid0.mercuriofvg.it  
[degiorgi@grid0 ~]$ ssh m001  
[degiorgi@m001 ~]$
```

- After job completion, the permission is revoked

Queue status

- `qstat / qstat -a`
 - Status of the jobs in queue
- `qstat -q / qstat -Q`
 - Status of the execution queue
- `qstat -rn`
 - Status of the running jobs with indicated which nodes they are running on
- `qstat -u username`
 - Status of the job for a specific user

Job tracking

- `tracejob` ID
 - Job lifetime: from queuing, to execution, to completion
 - Useful to understand where a job is failing

```
[degiorgi@grid0 ~]$ tracejob 2699.grid0.mercu 2> /dev/null  
  
Job: 2699.grid0.mercuriofv.it  
  
09/25/2013 22:33:13 S   enqueueing into blade, state 1 hop 1  
09/25/2013 22:33:14 S   Job Run at request of maui@grid0.mercuriofv.it  
09/25/2013 22:33:14 S   Not sending email: User does not want mail of this type.  
09/25/2013 22:33:49 S   Exit_status=0 resources_used.cput=00:00:00 resources_used.mem=2820kb  
resources_used.vmem=26656kb resources_used.walltime=00:00:36  
09/25/2013 22:33:49 S   Not sending email: User does not want mail of this type.  
09/25/2013 22:33:49 S   on_job_exit valid pjob: 2699.grid0.mercuriofv.it (substate=50)  
09/25/2013 22:43:53 S   dequeuing from blade, state COMPLETE  
[degiorgi@grid0 ~]$
```

Job status

- A job can be in several states

Status	Meaning
Q	Job <u>Queued</u> , waiting for execution
R	Job is <u>Running</u>
E	Job is <u>Ending</u>
H	Job is on <u>Hold</u> (set by the user or by the system)

Useful commands (i)

- `qdel ID`
 - Job receives signal TERM and KILL and quits

```
[degiorgi@grid0 ~]$ qsub -t 0-4 script.sh
2719[.grid0.mercuriofvg.it
[degiorgi@grid0 ~]$ qstat -r
```

```
grid0.mercuriofvg.it:
```

Job ID	Username	Queue	Jobname	SessID	NDS	TSK	Req'd Memory	Req'd Time	S	Elap Time
2718[.grid0.mer	degiorgi	blade	script.sh	--	1	4	--	01:00:00	R	00:00:00

std error, std output

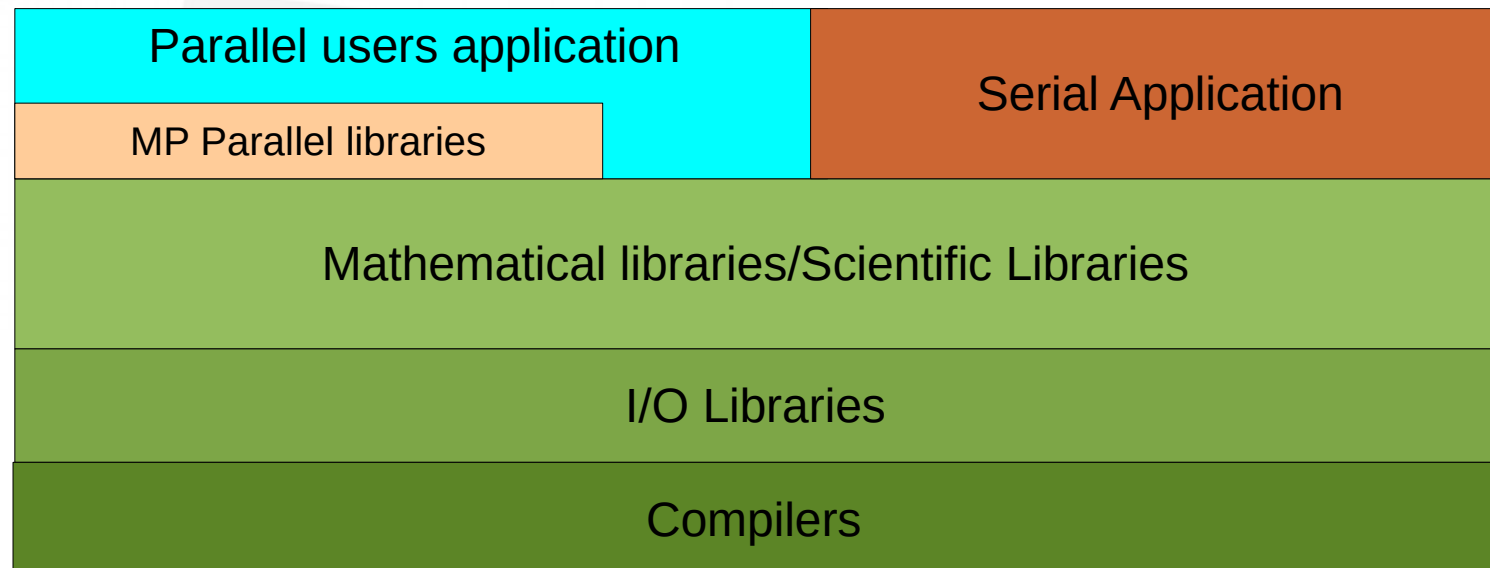
- Every submission produces a standard error and a standard output files
 - By default the file are called
 - `<jobname>.e<jobid>`
 - `<jobname>.o<jobid>`
 - Custom file names can be defined
 - `#PBS -o myPath/jobScript.out`
 - `#PBS -e myPath/jobScript.err`

Execution environment

- When a job is executed, the resource manager creates several environment variables
 - Those variables can be used to set filenames/folder, take decision, etc..
 - Some variables:
 - PBS_JOBNAME
 - PBS_O_WORKDIR → **directory** in which the job runs
 - PBS_NODEFILE → list of nodes on which the job runs
 - PBS_QUEUE
 - PBS_ARRAYID

HPC scientific Software layers (interleaved..)

- User's applications (both parallel and serial)
- Message Passing Libraries
- Mathematical/Scientific Libraries
- I/O libraries
- Compilers



Who cares about scientific HPC software ?

- End Users of HPC Software
 - Install and run HPC applications and tools
- HPC Application Teams
 - Manage third-party dependency libraries
- Package Developers
 - People who want to package their own software for distribution
- User support teams at HPC Centers
 - People who deploy software for users at large HPC sites

HPC Software Complexity

- Not much standardization in HPC: every machine/app has a different software stack
 - This is done to get the best performance
- HPC frequently trades reuse and usability for performance
 - Reusing a piece of software frequently requires you to port it to many new platforms
- List of packages/combination can diverge...

Dependency nightmare !

Software for HPC

- Scientific packages requires generally:
 - A compiler
 - Some libraries
 - Some parallel tool (MPI libraries but not only)
- Different code may require different sets of the above..
- The same package can require different sets of the above software
 - A compiler could be needed for performance another for portability.
- Different compilers/libraries/mpi need different **environment variables**

Scientific software: which is the production version ?

- Someone's home directory?
- Which MPI implementation?
- Which compiler?
- Which dependencies?
- Which versions of dependencies?
- Many applications require specific dependency versions.

Real answer: there isn't a single production environment or a standard way to build. Reusing someone else's software is HARD.

Software should be available cluster-wide

- installed in /opt/cluster/software (or similar) and mounted read-only on the nodes via nfs
- Generally managed by modules package
- Several versions managed by some agreement
 - Software/version/compiler/version
 - Netcdf/4.4.3/gnu/4.9.2

Environment modules

- Modules allow to dynamically modify user environment
- Useful tool to track different version of installed software
- **A few useful commands**
 - `module avail` – lists all available modules
 - `module list` – lists all loaded modules
 - `module load` – adds a module to your environment
 - `module unload` – removes a module from your environment

Module example

```
##Modules
proc ModulesHelp { } {
    puts stderr "\tThis module provides the path for the \n";
    puts stderr "\tOpen64 Compiler Suite by AMD\n";
    puts stderr "\tVersion 4.5.2.1\n";
}

prepend-path PATH          "/opt/amd/x86_open64-4.5.2.1/bin"
prepend-path LD_LIBRARY_PATH "/opt/amd/x86_open64-4.5.2.1/lib/gcc-lib/x86_64-open64-linux/4.5.2.1/"
#EOF
```

- Allows the dynamic modification of user environment
 - avoid the shell reconfiguration
 - PATH and LD_LIBRARY_PATH
 - MANPATH, etc.
- every user can create her/his own personal module

Installed modules on example cluster: C3HPC

Main categories

- compilers
- applications
- libraries
- MPI

```
netcdf/4.3.2/gnu/4.8.3
```

```
^^^^^^  ^^^^^  ^^^  ^^^^^
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```

```
+--> version of the compiler used to compile that software
```

```
+--> compiler used to compile that software
```

```
+--> Software version
```

```
+--> Software name
```

3 major build systems to be aware of...

- Make (usually GNU Make)
 - <https://www.gnu.org/software/make/>
 - (see openblas library)
- GNU Autotools
 - Automake: <https://www.gnu.org/software/automake/>
 - Autoconf: <https://www.gnu.org/software/autoconf/>
 - Libtool: <https://www.gnu.org/software/libtool/>
 - (see hdf5 library)
- CMAKE
 - <https://cmake.org>
 - (See geotop package)

Make

- Many projects opt to write their own Makefiles.
 - Can range from simple to very complicated
- Make declares some standard variables for various compilers
 - Many HPC projects don't respect them
 - No standard install prefix convention
 - Makefiles may not have install target
- Automating builds with Make usually requires editing files
 - Typical to use sed/awk/some other regular expression tool on Makefile
 - Can also use patches

Typical build incantation

```
<edit Makefile>  
make PREFIX=/path/to/prefix
```

Configure options

```
None. Typically must edit Makefiles.
```

Environment variables

CC	CFLAGS	LDFLAGS
CXX	CXXFLAGS	LIBS
FC	FFLAGS	CPP
F77	F77FLAGS	

autotools

- Three parts of autotools:
 - autoconf: generates a portable configure script to inspect build host
 - automake: high-level syntax for generating lower-level Makefiles.
 - libtool: abstraction for shared libraries
- Typical variables are similar to make
- Much more consistency among autotools projects
 - Wide use of standard variables and configure options
 - Standard install target, staging conventions.

Typical build incantation

```
./configure --prefix=/path/to/install_dir  
make  
make install
```

Configure options

```
./configure \  
  --prefix=/path/to/install_dir \  
  --with-package=/path/to/dependency \  
  --enable-foo \  
  --disable-bar
```

Environment variables

CC	CFLAGS	LDLAGS
CXX	CXXFLAGS	LIBS
FC	FFLAGS	CPP
F77	F77FLAGS	

cmake

- increasingly popularity
- Easier (?) to use (for developers) than autotools
- Similar standard options to autotools
 - different variable names
 - More configuration options
 - Abstracts platform-specific details of shared libraries
- Most CMake projects should be built “out of source”
 - Separate build directory from source directory

Typical build incantation

```
mkdir BUILD && cd BUILD
cmake -DCMAKE_INSTALL_PREFIX=/path/to/install_dir ..
make
make install
```

Configure options

```
cmake \  
  -D CMAKE_INSTALL_PREFIX=/path/to/install_dir \  
  -D ENABLE_FOO=yes \  
  -D ENABLE_BAR=no \  
  ..
```

Common -D options

CMAKE_C_COMPILER	CMAKE_C_FLAGS
CMAKE_CXX_COMPILER	CMAKE_CXX_FLAGS
CMAKE_Fortran_COMPILER	CMAKE_Fortran_FLAGS
CMAKE_SHARED_LINKER_FLAGS	CMAKE_EXE_LINKER_FLAGS
CMAKE_STATIC_LINKER_FLAGS	

Compilers

- Free : Gnu suite
 - Always available
 - Many different version
 - Fundamental but some time lacks performance
- Commercial compilers
 - Intel suite :
 - A full software stack (includes libraries/ profiling /benchmariking tools MPI libraries)
 - Expensive but highly optimized
 - PGI
 - Good compiler
 - Comes with some nice extension (openACC /Cuda Fortran)
 - Community edition available for free

Static/dynamic library

- Static libraries: libfoo.a
 - .a files are archives of .o files (object files)
 - Linker includes needed parts of a static library in the output executable
 - No need to find dependencies at runtime – only at build time.
 - Can lead to large executables
 - Often hard to build a completely static executable on modern systems.
- Shared libraries: libfoo.so (Linux)
 - More complex build semantics, typically handled by the build system
 - Must be found by ld.so and loaded at runtime
 - Can cause lots of headaches with multiple versions
 - 2 main ways:
 - **LD_LIBRARY_PATH**: environment variable configured by user and/or module system
 - **RPATH**: paths embedded in executables and libraries, so that they know where to find their own dependencies.

TAKE HOME MESSAGE:=> Comment code

Communication libraries for HPC

- MPI is a standard
- Several Libraries implement the standard
 - OpenMPI: widely adopted very portable and available for all networks/cluster
 - MPICH: historical one
 - MVAPICH: MPI over InfiniBand, Omni-Path, Ethernet/iWARP, and RoCE

Container: a solution to the HPC software ?

- Software systems are often complex and installation can be error prone
- When multiple packages need to interact conflicts arise:
 - Different software libraries
 - Different operating system
- Containerization allows systems to be packaged with everything they need so they can run anywhere.
- Many containers can run on a single system