Foundations of High Performance Computing

Lecture 3: HPC software stack

"High performance Computing module

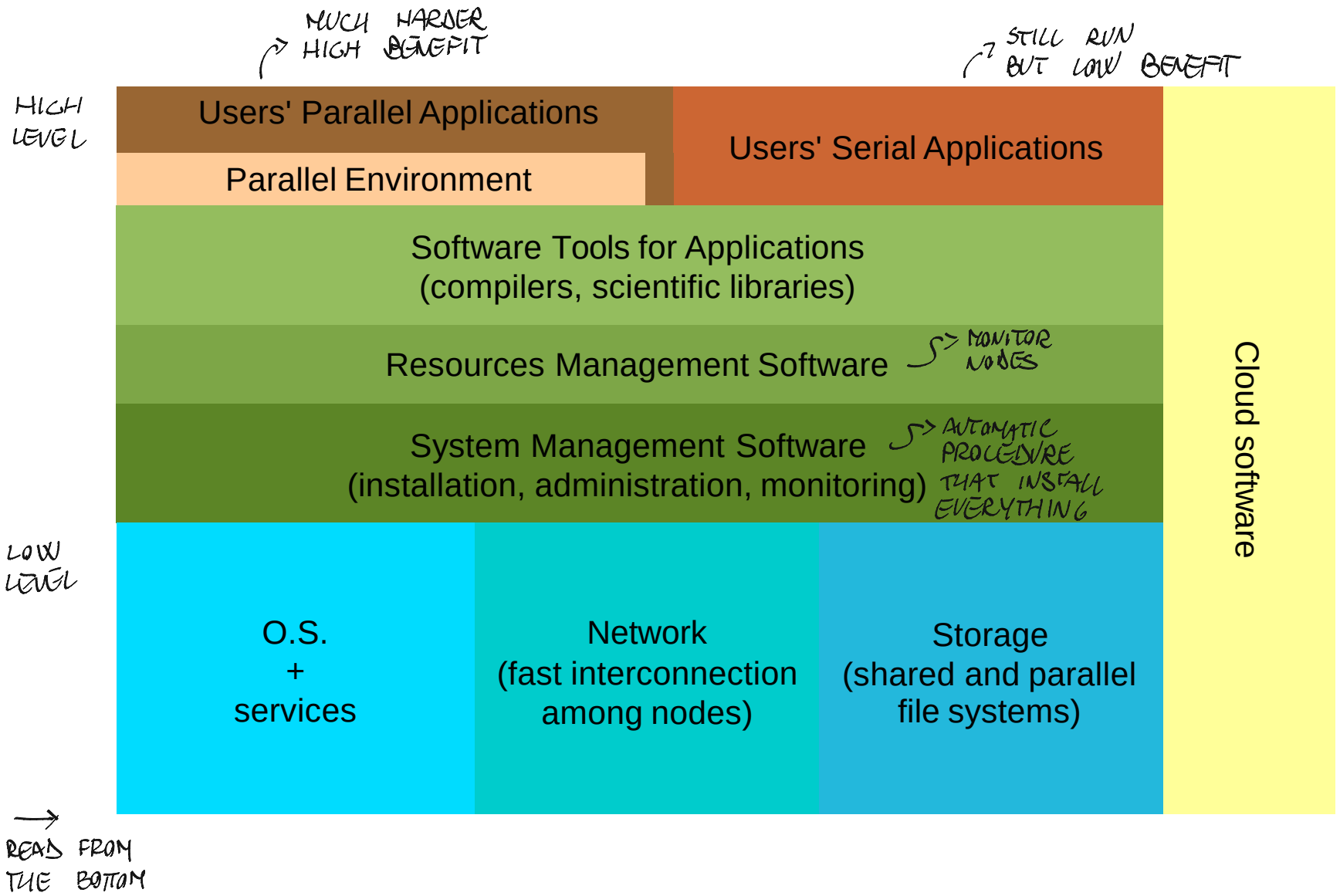
DATA SCIENCE &
ARTIFICIAL INTELLIGENCE

SCIENTIFIC &
DATA-INTENSIVE COMPUTING

Agenda

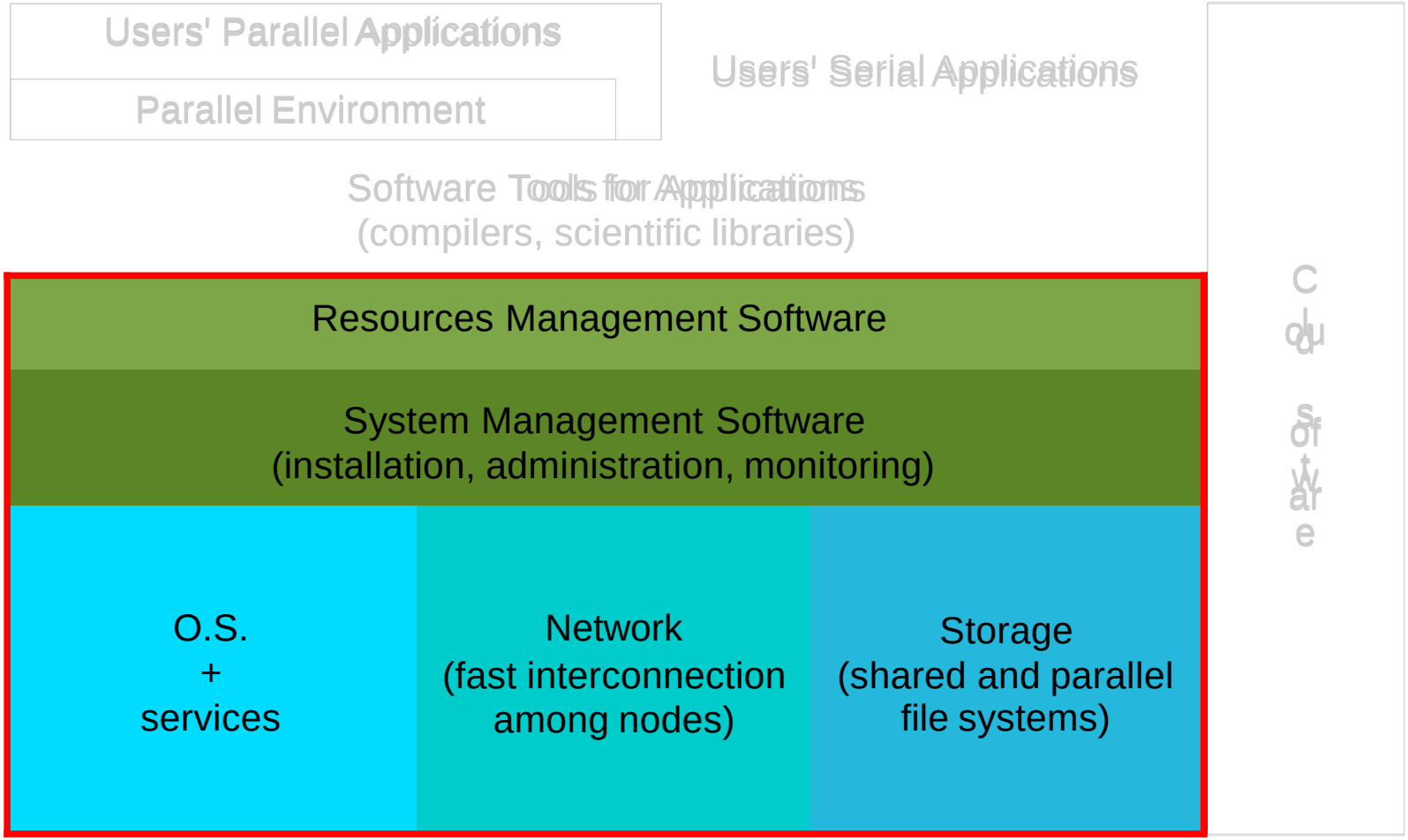
- A first look of the software stack
- Local resource manager: queue system
- Scientific software
- Compilers
- Libraries

What we need..


MUCH HARDER
HIGH BENEFIT
STILL RUN
BUT LOW BENEFIT
HIGH LEVEL
Users' Parallel Applications
Parallel Environment
Users' Serial Applications
Software Tools for Applications
(compilers, scientific libraries)
Resources Management Software
MONITOR NODES
System Management Software
(installation, administration, monitoring)
AUTOMATIC PROCEDURE THAT INSTALL EVERYTHING
Cloud software
LOW LEVEL
O.S.
+
services
Network
(fast interconnection
among nodes)
Storage
(shared and parallel
file systems)
READ FROM THE BOTTOM

The cluster middleware

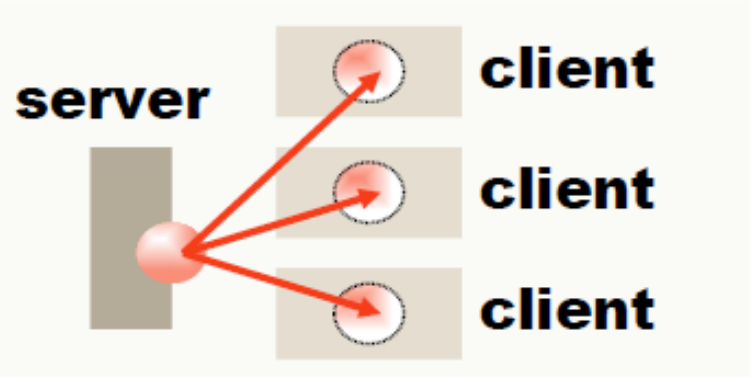
I'M NOT VERY INTRESTED IN WHAT IS HAPPENING BUT IS BETTER TO KNOW

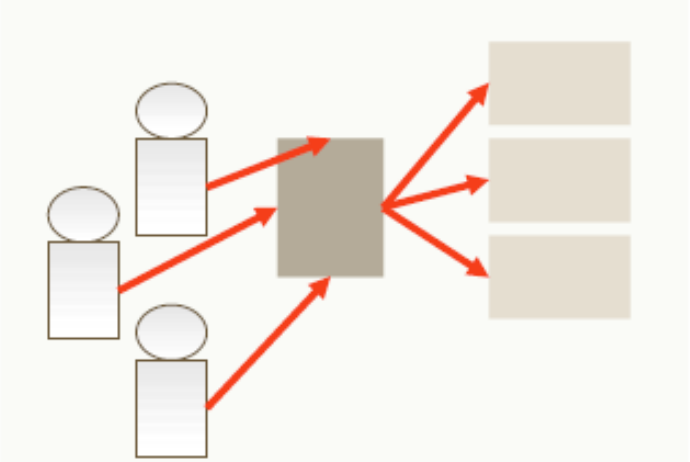


Cluster middleware

Cluster middleware refers to software that manages the administration, resource management, and scheduling of tasks in a cluster computing environment.

- Administration software:
  - user accounts
  - NTP/NFS/ etc…
- Resource management and scheduling software (LRMS)
  - Process distribution
  - Load balance
  - Job scheduling of multiple tasks





This includes tasks like setting up user accounts, managing network time protocol (NTP) and network file system (NFS), as well as distributing processes, load balancing, and scheduling jobs multiple nodes in the cluster. The middleware plays a key role in optimizing the performance and efficiency of the cluster by coordinating the execution of various tasks and resources.

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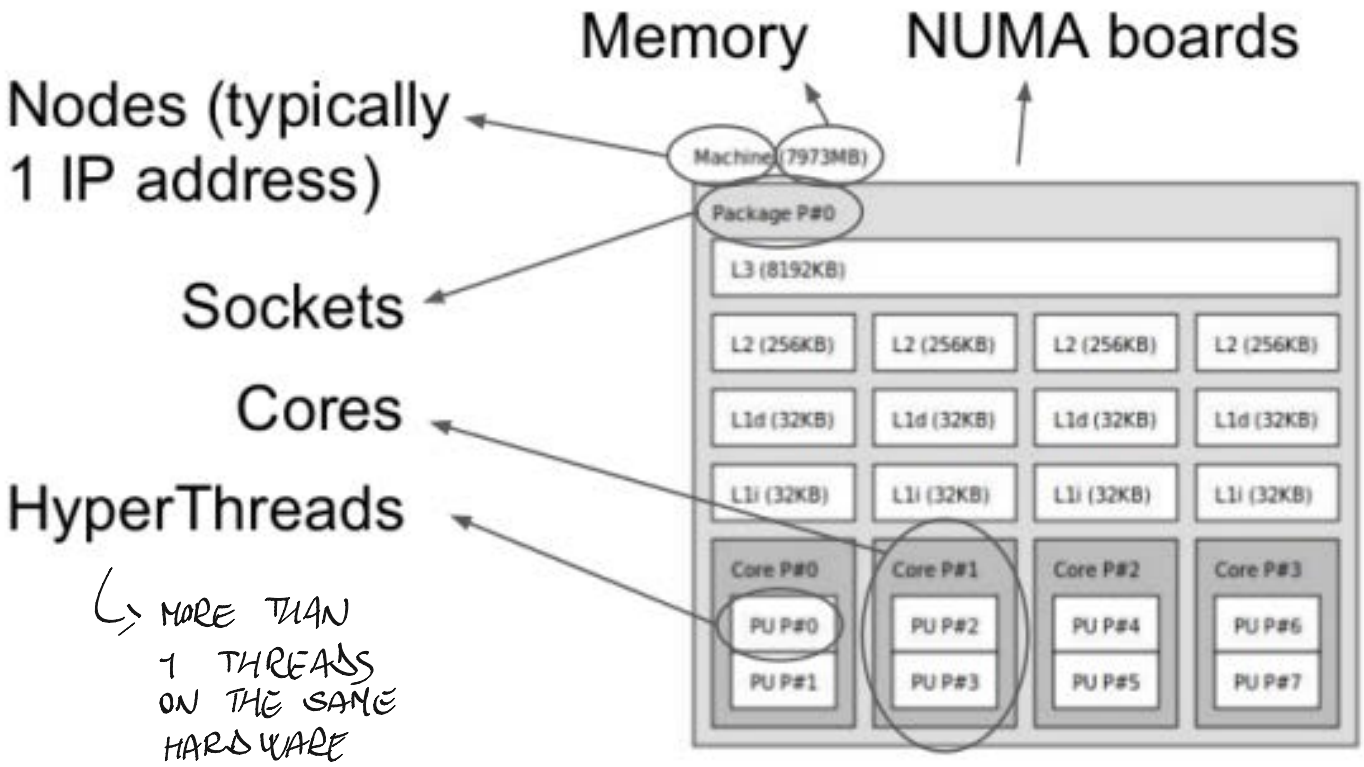
Resource Management Problem

- 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

HPC resources..



↳ MORE THAN 1 THREADS ON THE SAME HARDWARE

PLUS:

- network resources
- GPU/Accelerator
- Software resources

Some definition

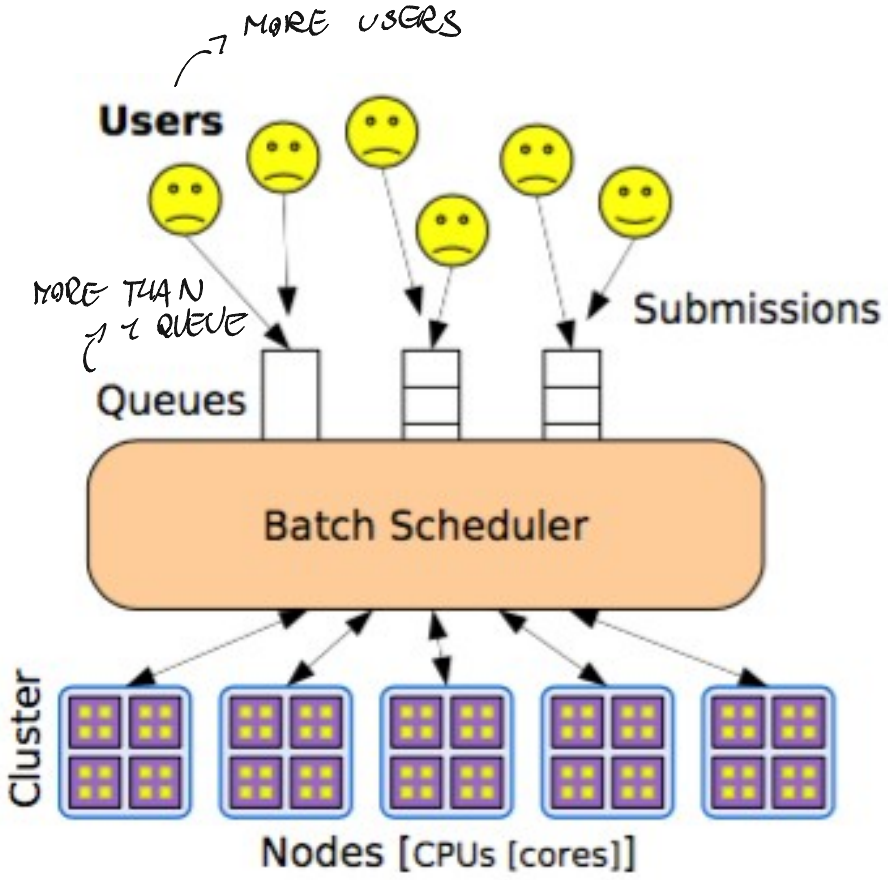
LIKE A PROCESS SCHEDULER

- **Batch Schedule**r: 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 Manage**r: software that enable the jobs to connect the nodes and run.
- **Node** (aka **Computing Node**): computer used for its computational power.
- **Login/Master node**: it's through this node that the users will submit/launch/manage jobs.

Batch scheduler



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

→ Satisfy users:

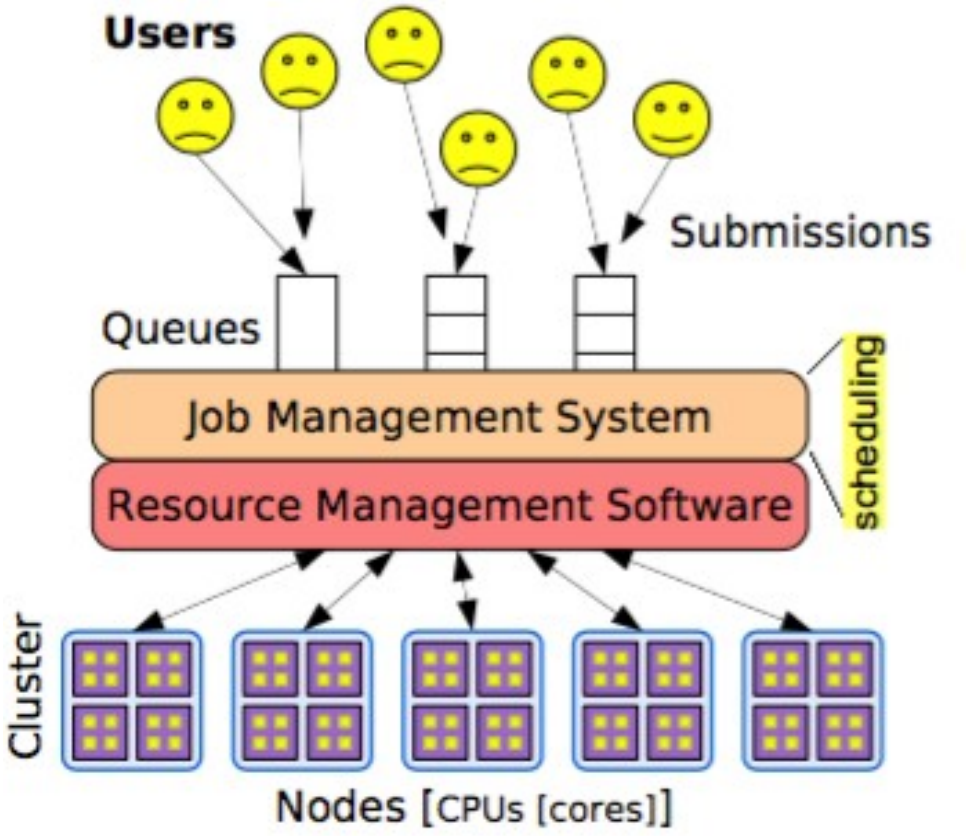
response time,reliability

↳ A RESONABLE AMOUNT OF TIME

→ Satisfy admins (HAVE TO MAINTAIN THE SYSTEM)

high resource utilization efficiency,energy management

Batch scheduler (2)

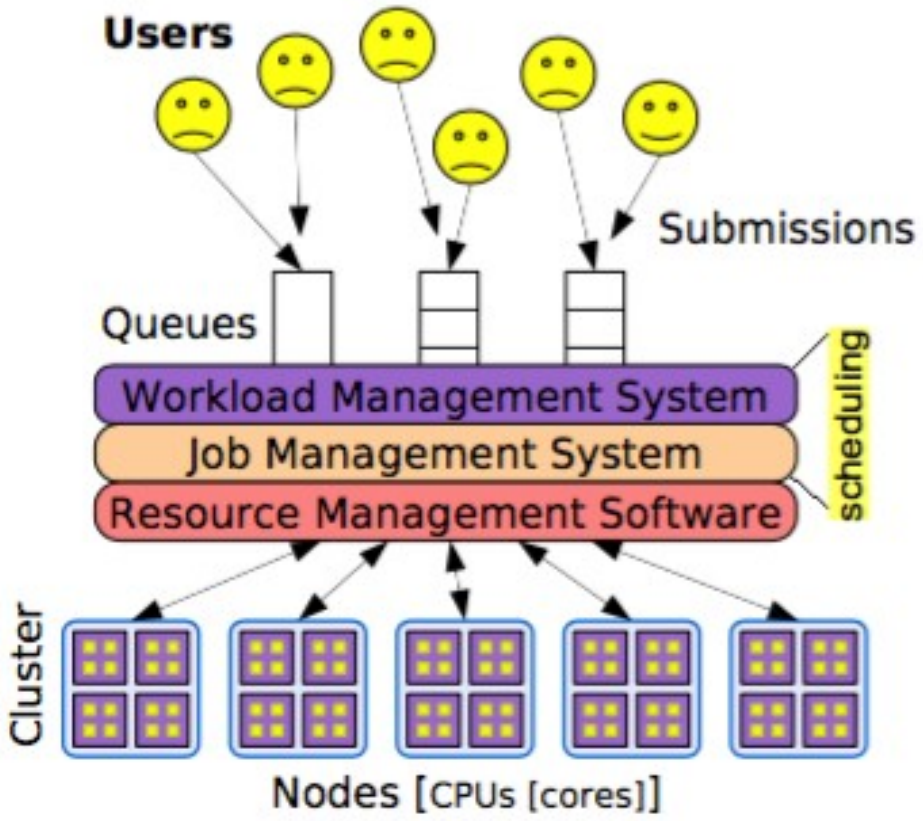


Resource Management Layer
→ launching, cleaning, monitoring

Job Management Layer

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

Batch scheduler (3)



Workload/Job Management

→ more complete job scheduling policies

→ Fairsharing, Quality of Service (QoS), SLA (Service Level Agreement), Energy Saving

→ Sometime a dedicated software

Main LRMS packages

↳ A LOT OF THEME

- IBM LSF
  - commercial
- Univa Grid Engine (UGE)
  - Commercial originates from SGE
- PBSPRO
  - Portable Batch System Professional once commercial now open
  - Support is commercial
  - **no longer Available on ORFEO**
- SLURM
  - Open source
  - Support is commercial
  - **Available on ORFEO just for you**

What is SLURM ? ONE OF THE MOST USED

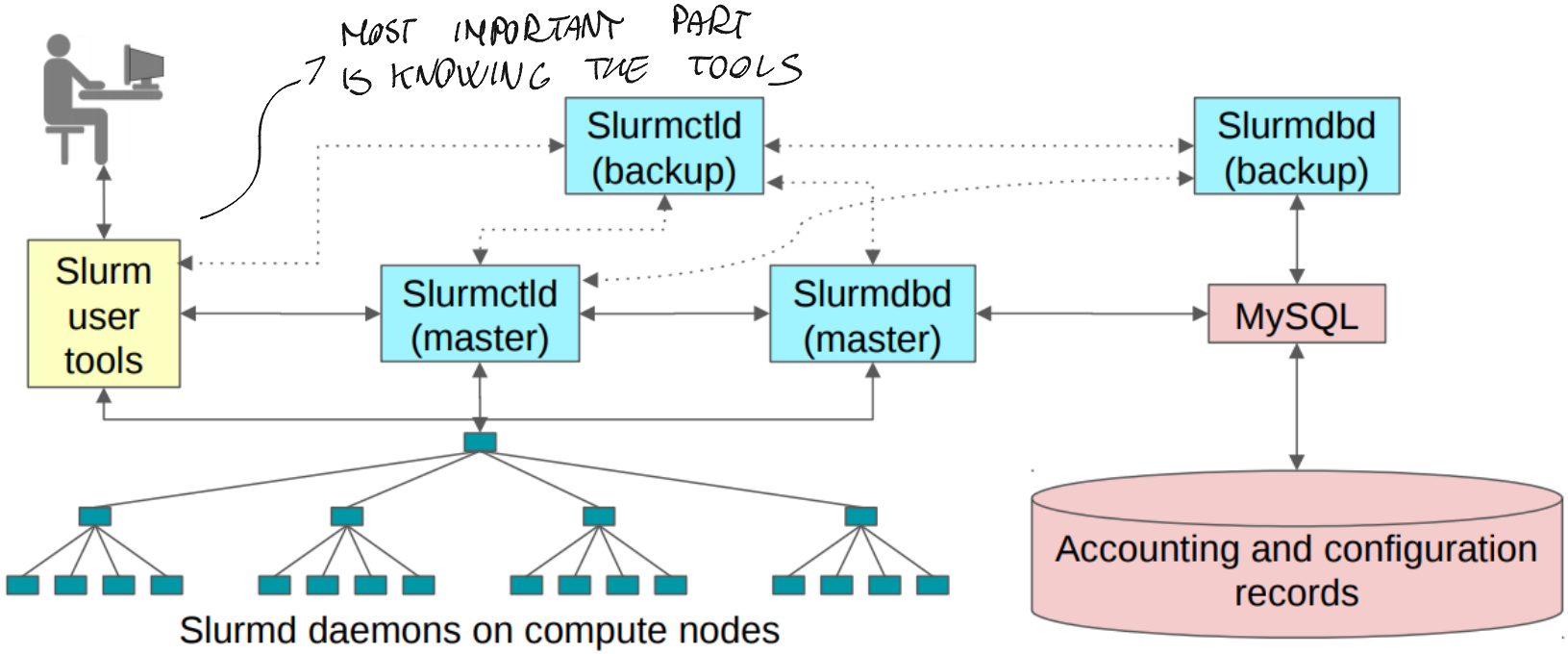
- Historically, Slurm was an acronym of:
- – Simple Linux Utility for Resource Management
- Dev. started in 2002 @ Lawrence Livermore National Lab as a resource manager for Linux clusters
- Sophisticated scheduling plugins added in 2008
- About 550,000 lines of C code today
- Used on many of the world's largest computers
- Active global user community

SLURM slides taken and slightly adapted from: slurm_overview.pdf (schedmd.com)

SLURM entities

- **Jobs:** Resource allocation requests
- **Job steps:** Set of (typically parallel) tasks
  - Typically an MPI and/or multi-threaded application program
  - Allocated resources from the job's allocation
  - A job can contain multiple job steps which can execute sequentially or concurrently
  - Lighter weight than jobs
- **Partitions:** Job queues with limits and access controls
- **Qos:** Limits and policies

SLURM architecture



A slurm jobfile

SLURM directives using the tag **#SLURM**, describe the job requirments in terms of execution queue, number of nodes and cores, job name, walltime, etc.	#!bin/bash #SLURM --ntasks=128 #SLURM --cpus-per-task=2 #SLURM --mem-per-cpu=20 #SLURM --time=60
The rest of the job is a standard shell script SLURM "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 hostname pwd

SLURM tutorial on march 24th..

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 different choices
- Concepts are similar /commands sometime also (to help survive: http://www.schedmd.com/slurmdocs/rosetta.pdf, available on our repo)
- 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)

MORE AN IDEOLOGY

Resource sharing policies is not at all a technical problem !

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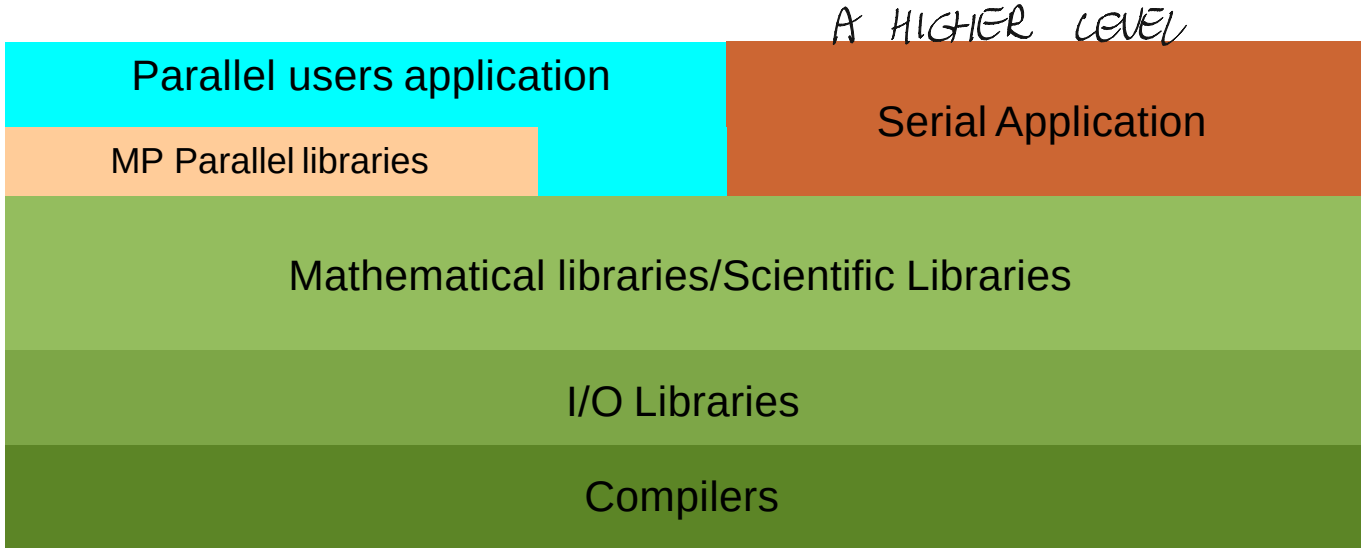
HPC scientific Software layers (interleaved..)

- User's applications (both parallel and serial)
- Parallel Libraries&Tools
- Mathematical/Scientific Libraries
- I/O libraries
- Compilers



HPC software

- 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..

Scientific software: where is ?

- Generally 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

IN THIS WAY YOU CAN EASLY DOWNLOAD AND RELOAD DIFFERENT VERSION OF SOFTWARE

Module package (1)

- Modules allow to dynamically modify user environment
- Useful tool to track different version of installed software

Module package (2)

- 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 and environment

- Module command change on the fly the most important ENVIROMENT VARIABLE for you
  - PATH
  - LD_LIBRARY_PATH

ORFEO situation

```
cozzini@login02 ~] > module avail

------------------------------------------------------ /orfeo/opt/modules/tools -------------------------------------------------------
  IGV/2.18.0              bwa-mem2/2.2.1       gromacs/2022.6      (D)    ont-guppy-cpu/6.5.7 (D)    singularity/3.10.4
  R/4.3.3                 cmake/3.28.1         hwloc/2.10.0               ont-guppy-gpu/6.2.1        singularity/3.11.5 (D)
  R/4.4.1           (D)   cutadapt/4.2         java/8-8u402b06            ont-guppy-gpu/6.5.7 (D)    trim_galore/0.6.10
  STAR/2.7.11b            fastp/0.23.4         java/11.0.22               picard/3.2.0
  bcftools/1.17           fastqc/0.12.1        java/17.0.10               plink/1.90
  bcl2fastq2/2.20.0       foldseek/8-ef4e960   java/21.0.2         (D)    sambamba/1.0
  bedtools2/2.31.1        gromacs/2018.4       ont-guppy-cpu/6.2.1        samtools/1.17

------------------------------------------------------ /orfeo/opt/modules/mpi ---------------------------------------------------------
  openMPI/4.1.6/gnu/14.2.1

---------------------------------------------------- /orfeo/opt/modules/libraries -----------------------------------------------------
  cuda/11.7    cuda/12.0       cuda/12.6.3         openBLAS/0.3.26-omp
  cuda/11.8    cuda/12.1 (D)   cutensor/2.0.2.5    openBLAS/0.3.26     (D)
```

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What does mean compiling ?

- A complex translation from high level language (C/Fortran…)to a stream of instructions..

FORGET PYTHON, TOO SLOW
(UNLESS THE GOOD LIBRARY)

Compiler

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

What is available on ORFEO ?

```
cozzini@login02 ~] > module avail

------------------------------------------------- /orfeo/opt/modules/tools -------------------------------------------------
  IGV/2.18.0              bwa-mem2/2.2.1       gromacs/2022.6      (D)    ont-guppy-cpu/6.5.7 (D)    singularity/3.10.4
  R/4.3.3                 cmake/3.28.1         hwloc/2.10.0               ont-guppy-gpu/6.2.1        singularity/3.11.5 (D)
  R/4.4.1           (D)   cutadapt/4.2         java/8-8u402b06            ont-guppy-gpu/6.5.7 (D)    trim_galore/0.6.10
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  bcftools/1.17           fastqc/0.12.1        java/17.0.10               plink/1.90
  bcl2fastq2/2.20.0       foldseek/8-ef4e960   java/21.0.2         (D)    sambamba/1.0
  bedtools2/2.31.1        gromacs/2018.4       ont-guppy-cpu/6.2.1        samtools/1.17

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```

IF SOMEBODY REQUIRES A DIFFERENT VERSION
IT NEED TO BE INSTALLED WITH ALL THE REQUIRED LIBRARY

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Scientific Libraries

- Plenty of them for many different tasks
- Dedicated lecture later during the course
- Today let us just focus on static vs dynamic libraries on basic system libraries

Static libraries: libfoo.o

- .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
- 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.

All done !

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