

High Performance Computing and Data Infrastructure

Recap on HPC software stack



DATA SCIENCE &
ARTIFICIAL INTELLIGENCE



SCIENTIFIC &
DATA-INTENSIVE COMPUTING

2024-2025 @ Università di Trieste

Agenda

A first look of the software stack

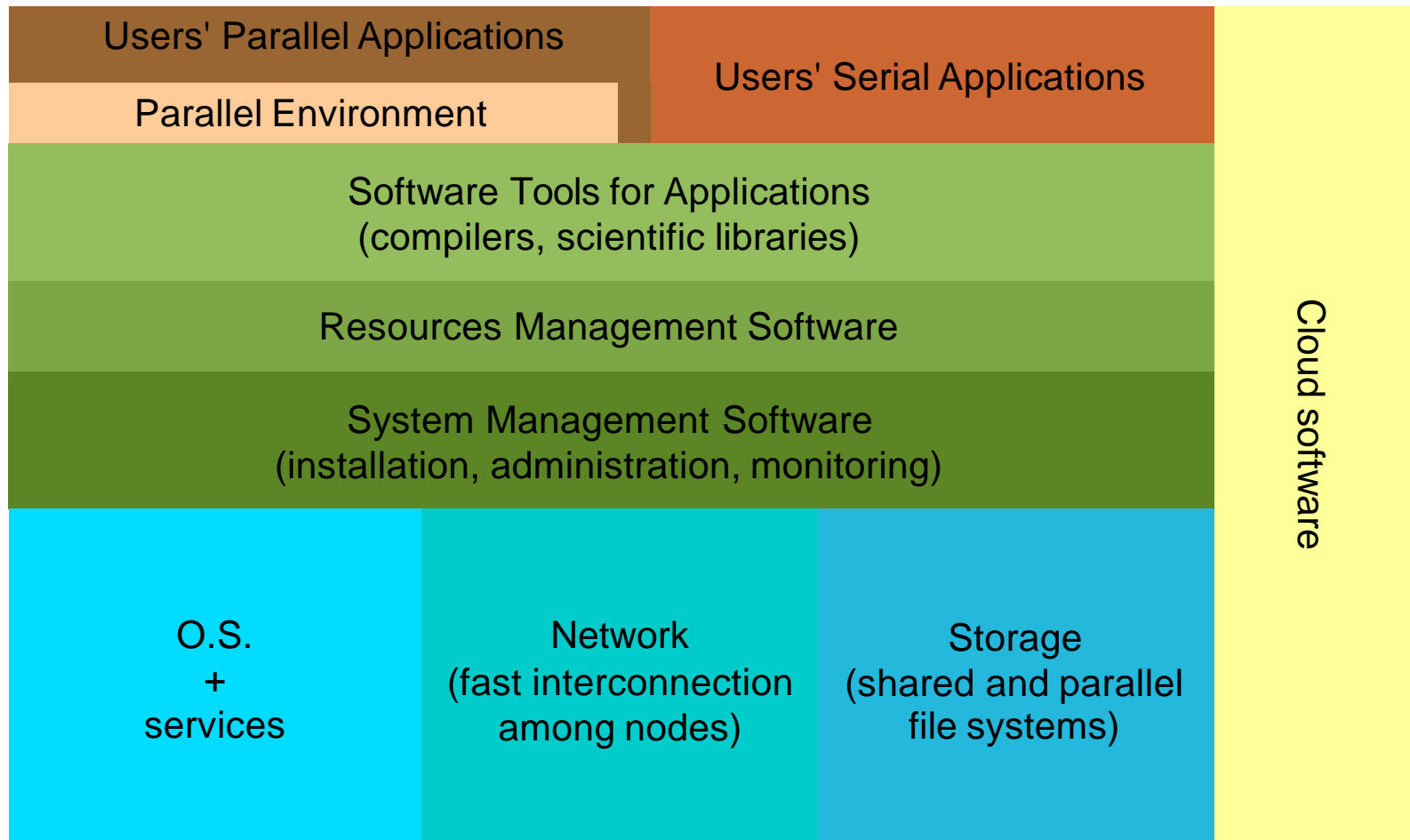
Local resource manager: queue system

Scientific software

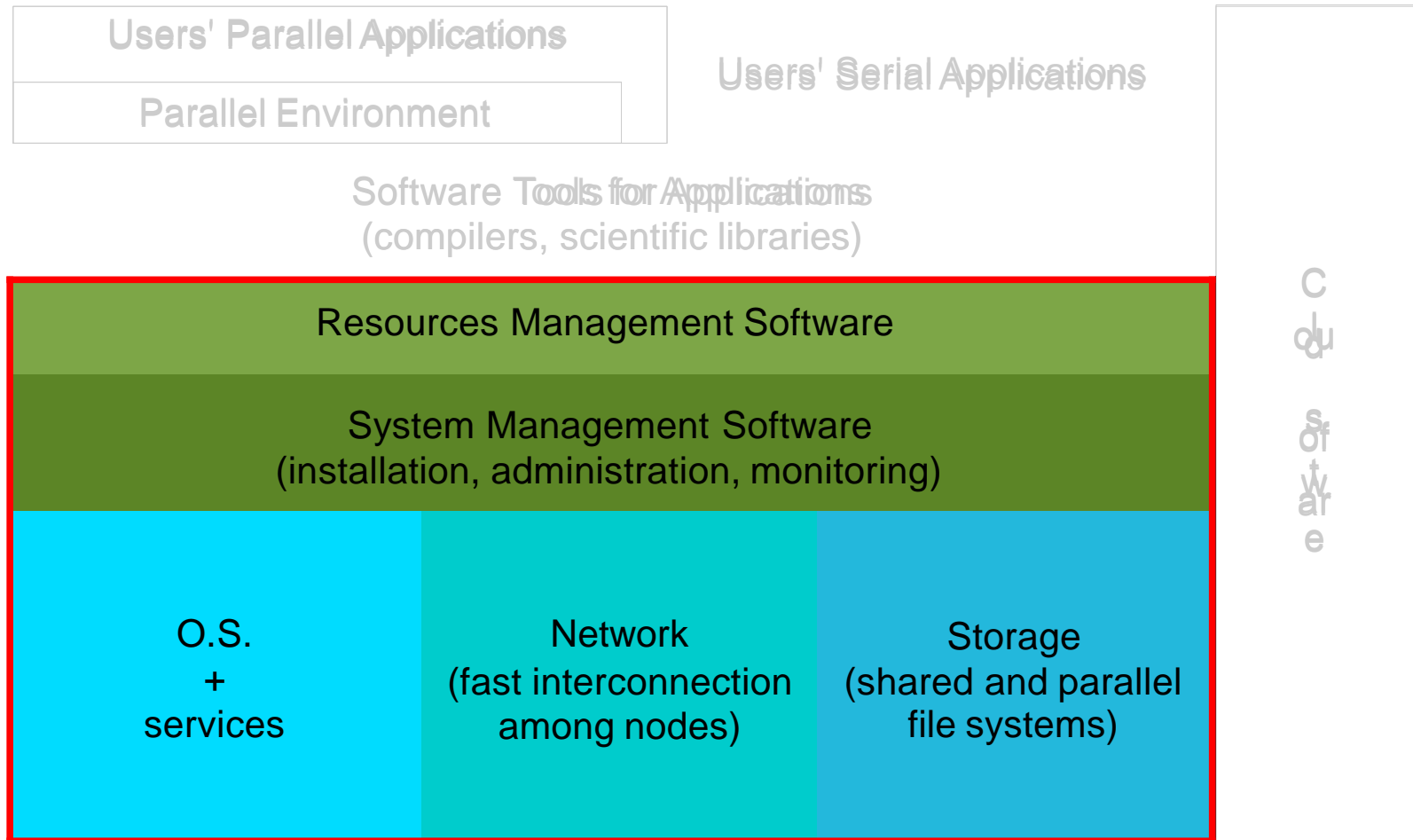
Compilers

Libraries

What we need..

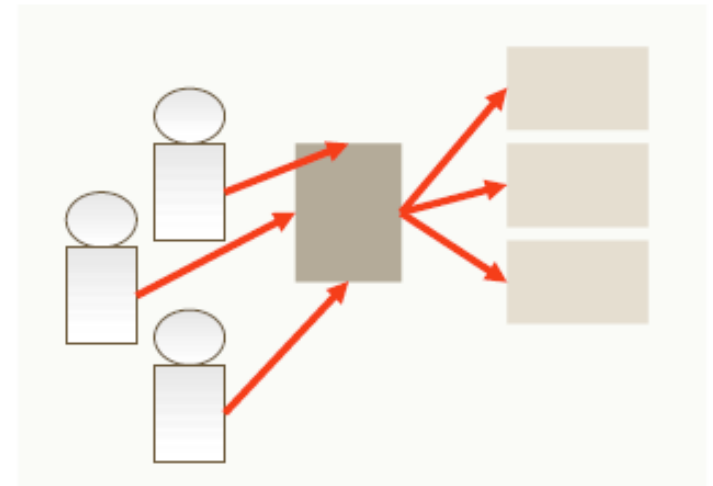
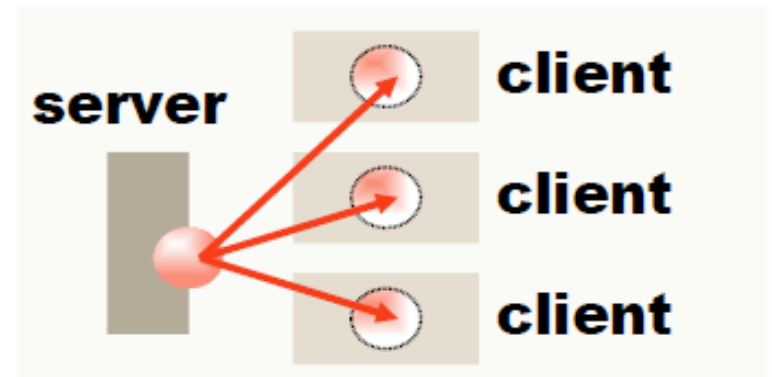


The cluster middleware

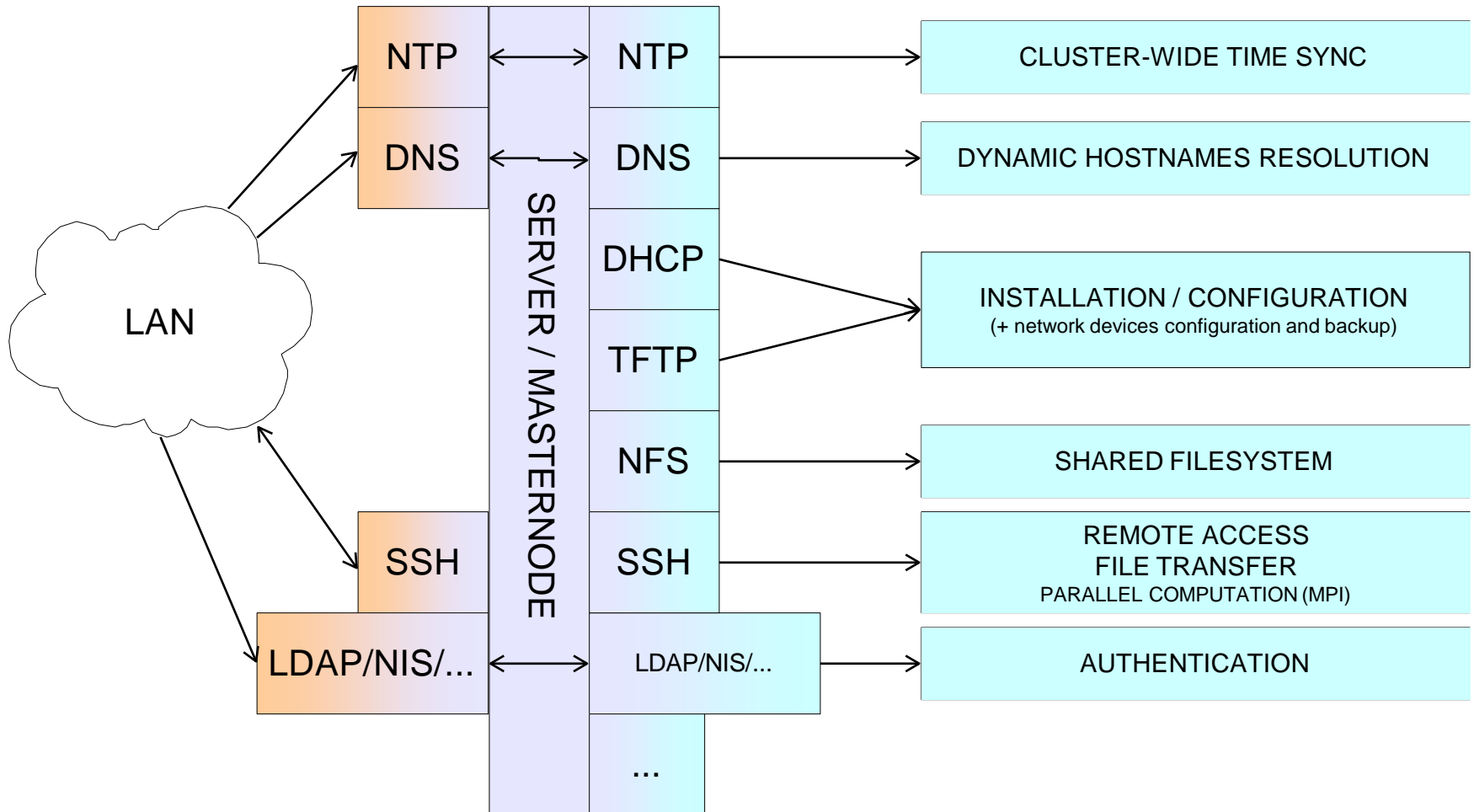


Cluster middleware

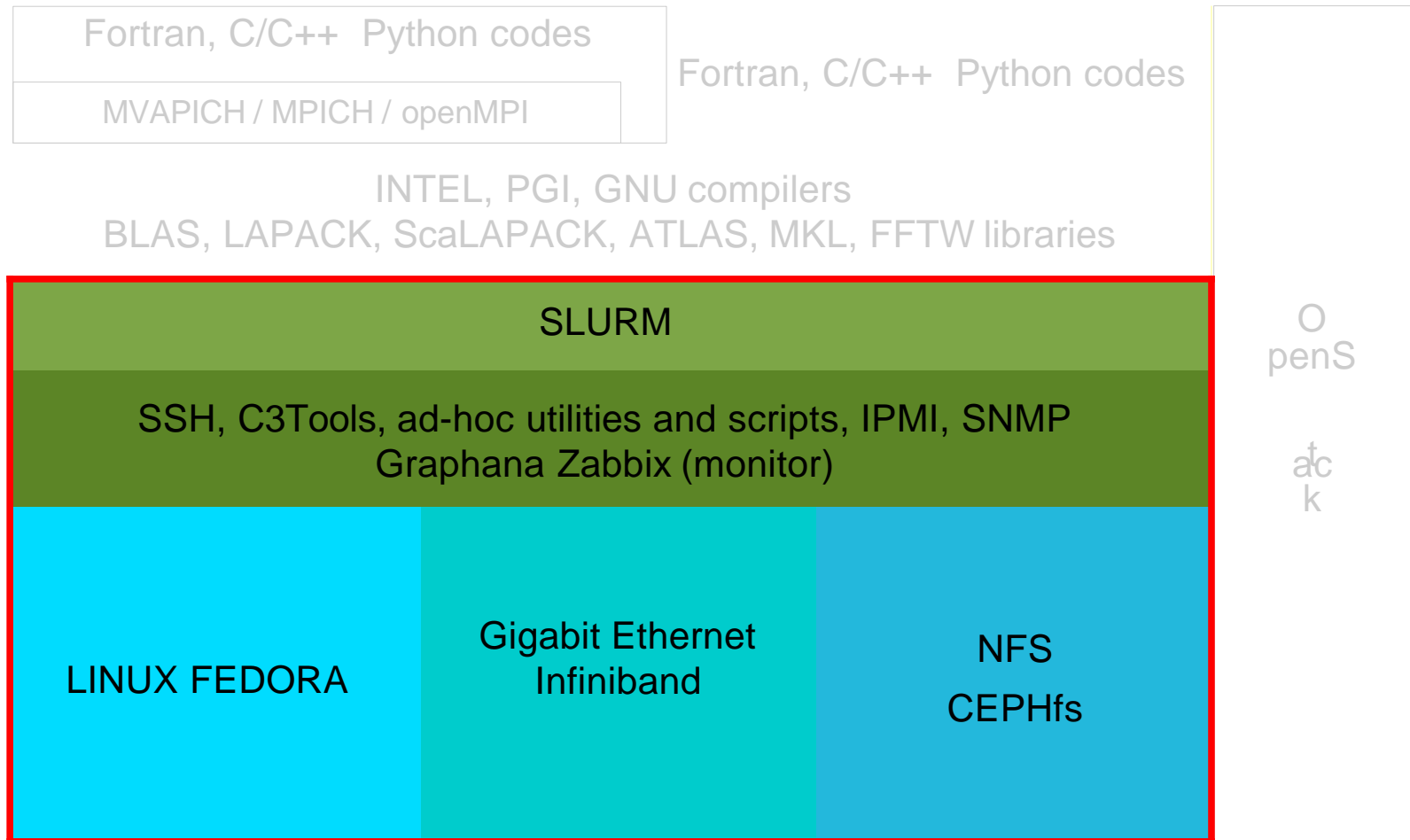
- Administration software:
 - user accounts
 - NTP/NFS/ etc...
- Resource management and scheduling software (LRMS)
 - Process distribution
 - Load balance
 - Job scheduling of multiple tasks



Cluster wide services



Middleware software used on ORFEO



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Resource Management Problem

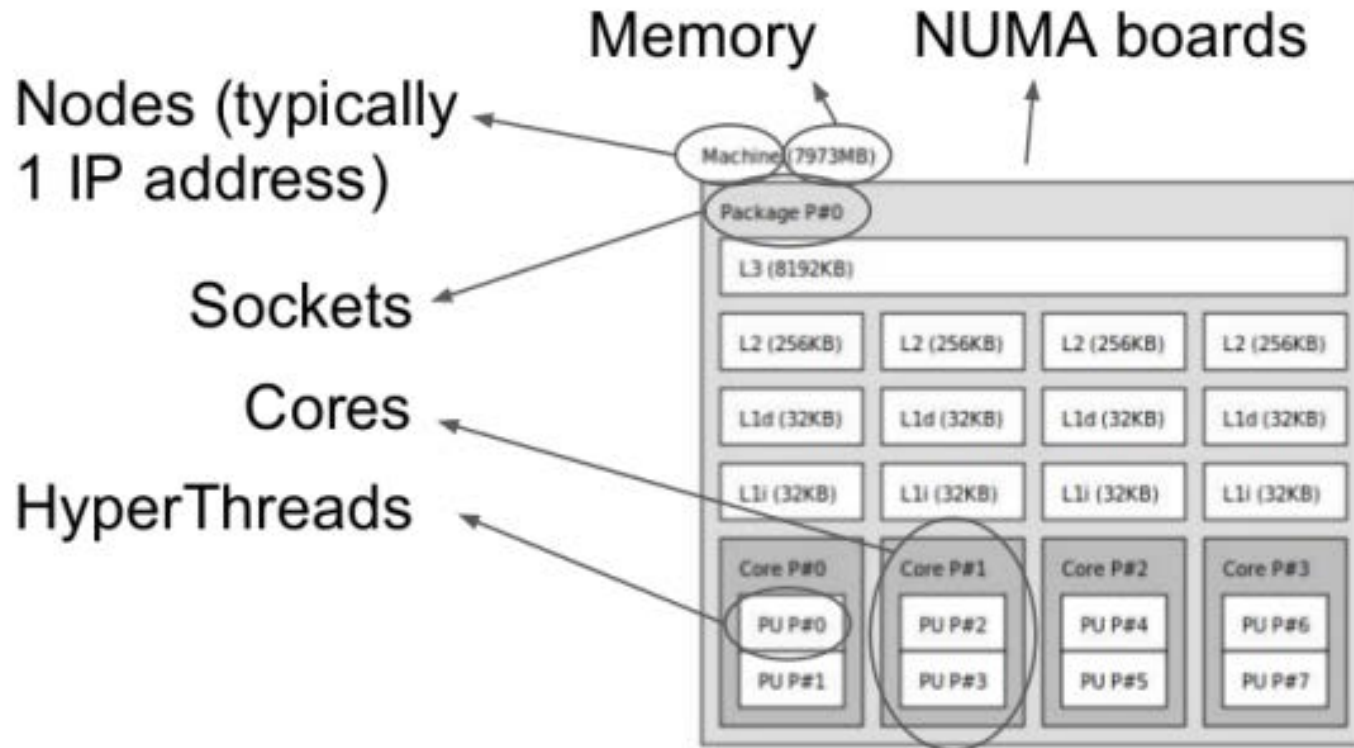
- We have a pool of users and a pool of resources, then what?
 - some software that controls available resources
 - some other software that decides which application to execute based on available resources
 - some other software devoted to actually execute applications

What are we speaking about ?



REPLACE THE CAKE WITH HPC RESOURCE

HPC resources..



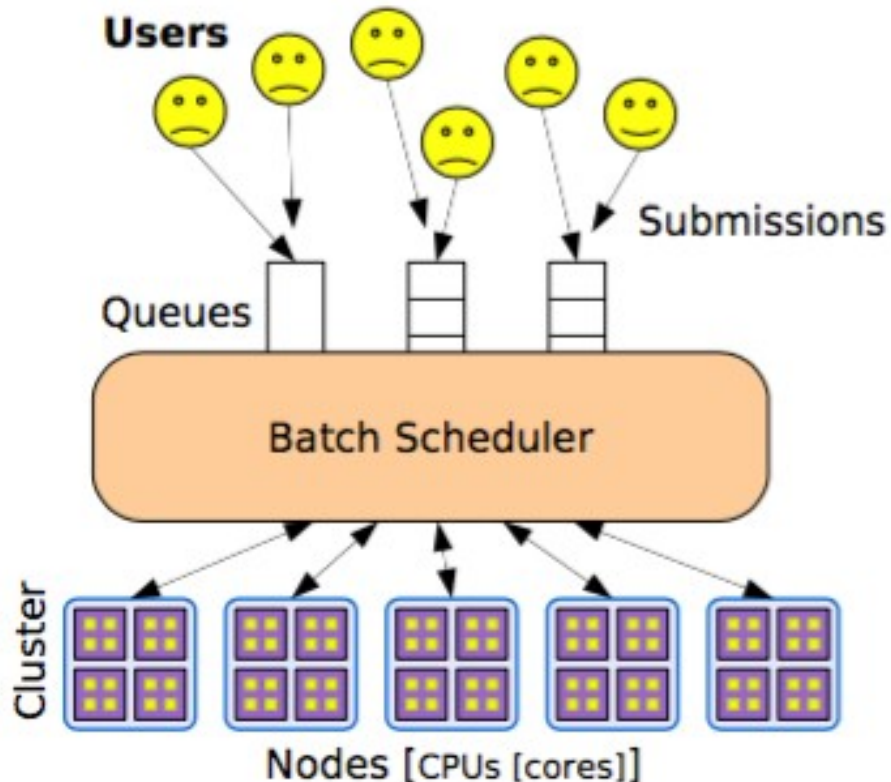
PLUS:

- network resources
- GPU/Accelerator
- Software resources

Some definition

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

Batch scheduler

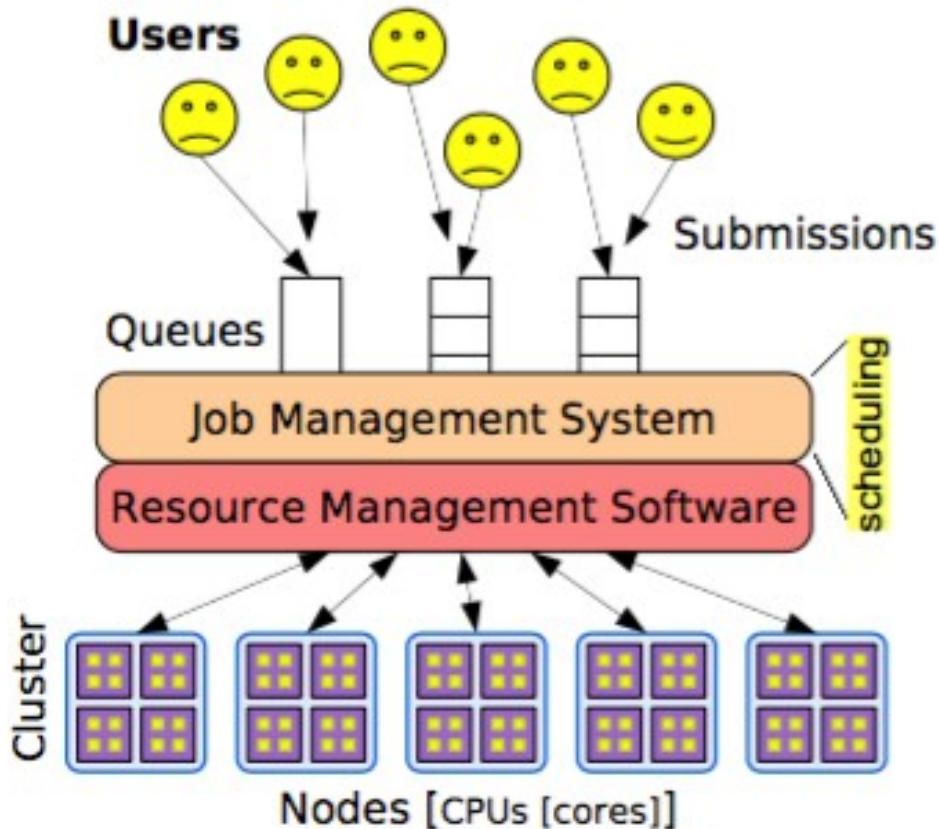


- Allocate resources for each applications with respect of their requirements and users' rights.

→ Satisfy users:
response time, reliability

→ Satisfy admins
high resource utilization
efficiency, energy
management

Batch scheduler (2)

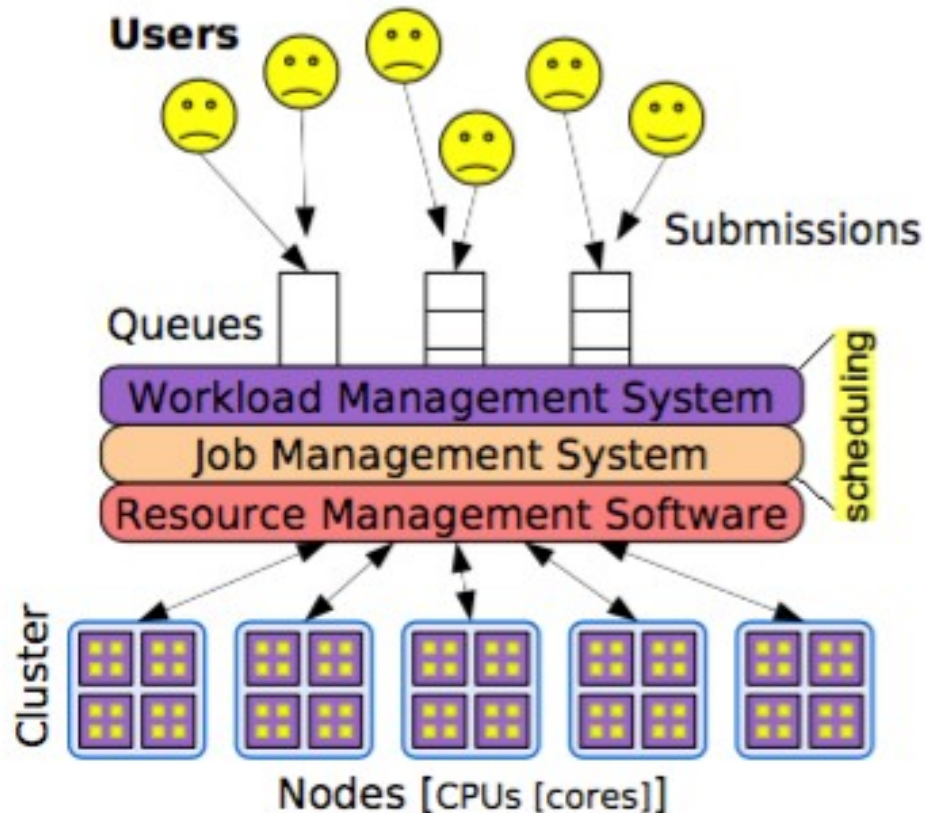


Resource Management Layer
→ launching, cleaning,
monitoring

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

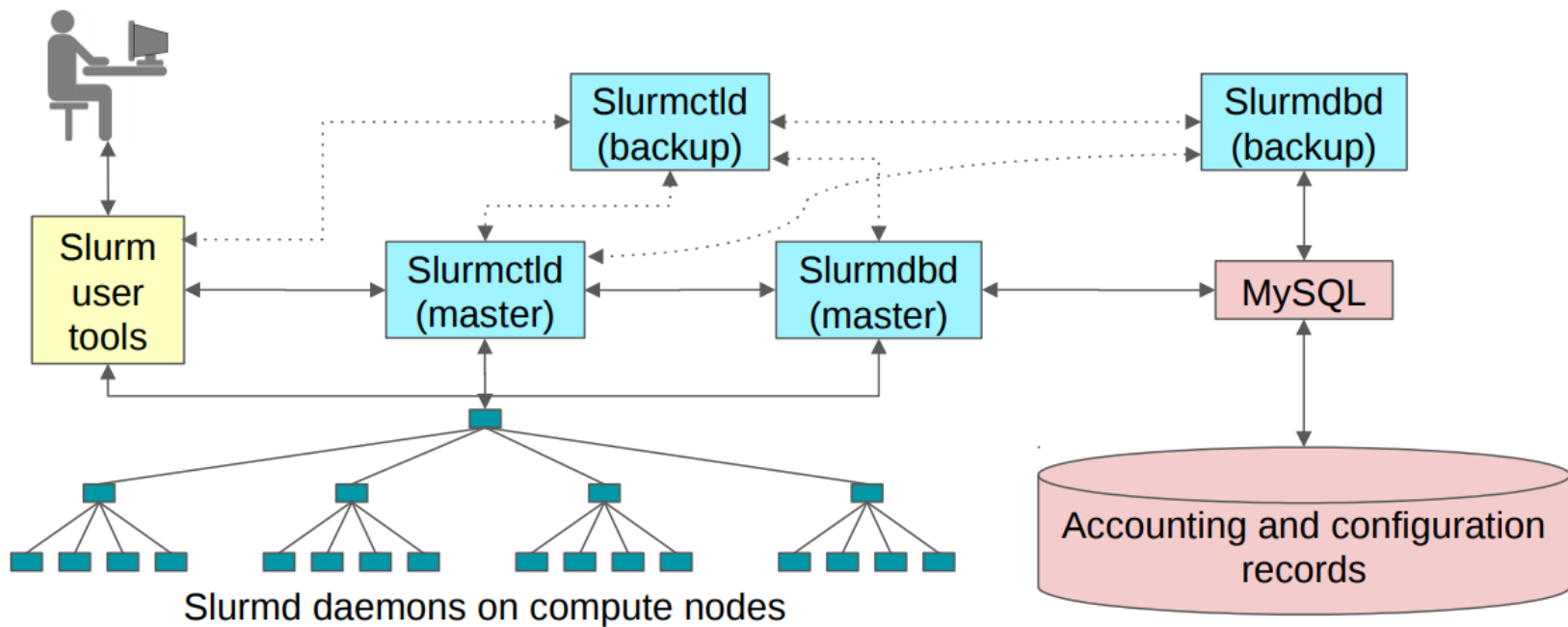
What is SLURM ?

- 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
- Supports Linux and limited support for other Unix variants
- Used on many of the world's largest computers
- Active global user community

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

<p>SLURM directives using the tag #SLURM, describe the job requirements in terms of execution queue, number of nodes and cores, job name, walltime, etc.</p>	<pre>#!/bin/bash #SLURM --ntasks=128 #SLURM --cpus-per-task=2 #SLURM --mem-per-cpu=20 #SLURM --time=60</pre>
<p>The rest of the job is a standard shell script</p> <p>SLURM "lands" user's home directory: it is important to change the directory to the one in which we want to run the job</p>	<pre>cd \$HOME/MyJobDir hostname pwd</pre>

Advanced SLURM tutorial by Niccolo'.

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)

Resource sharing policies is not at all a technical problem !

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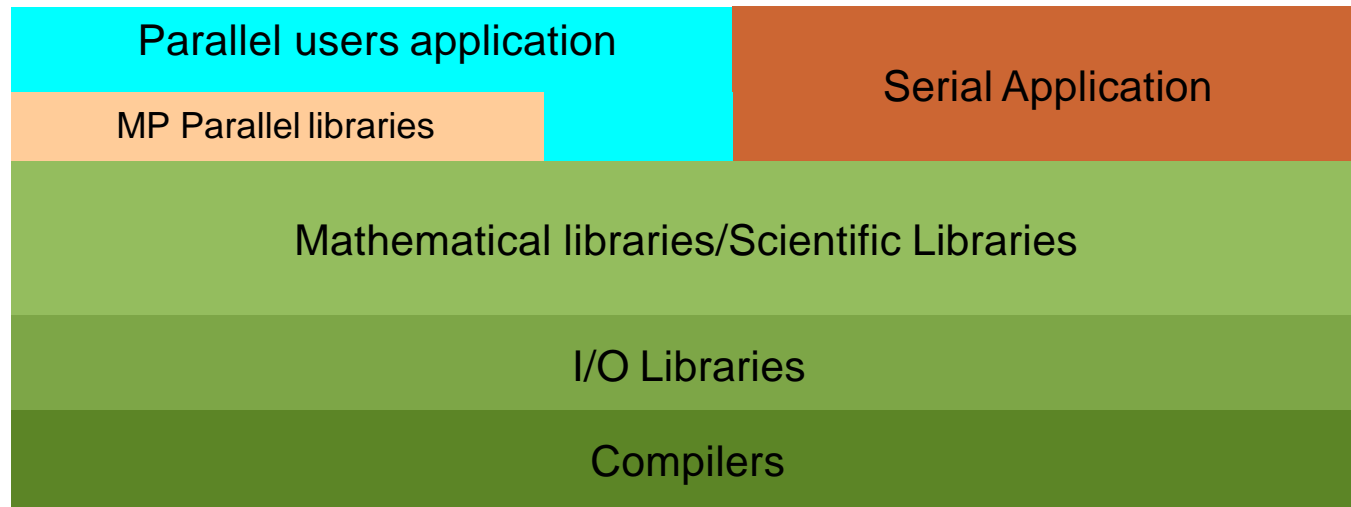
Scientific software

Compilers

Libraries

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

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 ENVIRONMENT VARIABLE for you
 - PATH
 - LD_LIBRARY_PATH

ORFEO situation

```
[cozzini@login02 ~] > module avail
```

```
----- /orfeo/opt/modules/tools -----
cutadapt/4.2          java/1.8.0          picard/3.0.0
STAR/2.7.9a          fastp/0.23.4       java/18.0.2.1      plink/1.9
bcftools/1.17        fastqc/0.12.1      java/19.0.1        sambamba/1.0
bcl2fastq2/2.20      foldseek/5-53465f0 ont-guppy-cpu/6.2.1 samtools/1.17
bedtools2/2.21.0     foldseek/7-04e0ec8 (D) ont-guppy-cpu/6.5.7 (D) singularity/3.10.4
bwa-mem2/2.2.1       gatk/4.3.0         ont-guppy-gpu/6.2.1 trim_galore/0.6.10
conda/23.3.1         hwloc/2.8.0        (L) ont-guppy-gpu/6.5.7 (D)
```

```
----- /orfeo/opt/modules/profiles -----
architecture/AMD      architecture/Intel (L)  architecture/x86 (D)
```

```
----- /orfeo/opt/modules/oneAPI -----
latest               dnnl-cpu-gomp/2022.2.1 (D)  intel_ipp_intel64/latest
advisor/2022.3.1     (D)      dnnl-cpu-iomp/latest       intel_ipp_intel64/2021.6.2 (D)
ccl/latest           dnnl-cpu-iomp/2022.2.1 (D)  intel_ippcp_ia32/latest
ccl/2021.7.1         (D)      dnnl-cpu-tbb/latest        intel_ippcp_ia32/2021.6.2 (D)
clk/latest           dnnl-cpu-tbb/2022.2.1 (D)  intel_ippcp_intel64/latest
clk/2021.7.1         (D)      dnnl/latest                intel_ippcp_intel64/2021.6.2 (D)
compiler-rt/latest   dnnl/2022.2.1 (D)      itac/latest
compiler-rt/2022.2.1 (L,D)    dpct/latest               itac/2021.7.1 (D)
compiler-rt32/latest dpct/2022.2.1 (D)      mkl32/latest
compiler-rt32/2022.2.1 (D)    dpl/latest               mkl32/2022.2.1 (D)
```

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What does mean compiling ?

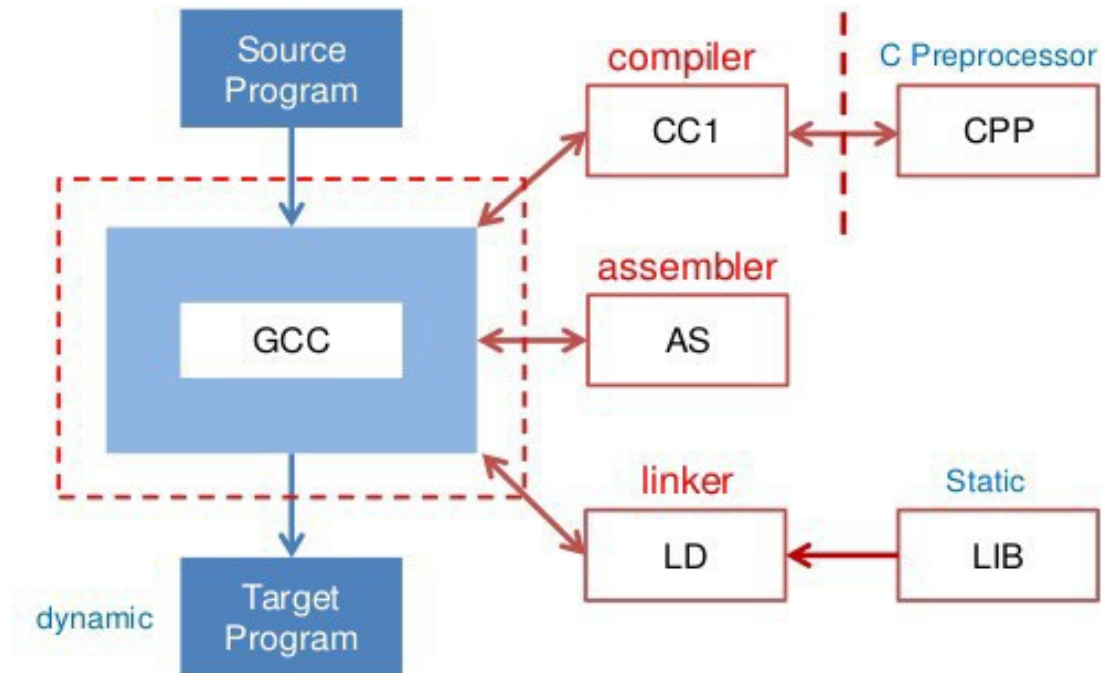
- A complex translation from high level language (C/Fortran...)to a stream of instructions..

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

Compiling with gcc..

GCC compiler



GCC is a collection that invokes compiler, assembler and linker...

What is available on ORFEO ?

```
[cozzini@login ~]$ module avail
```

```
----- /opt/area/shared/modules/mpi -----  
openmpi/4.0.3/gnu/4.8.5 (D)    openmpi/4.0.3/gnu/9.3.0
```

```
----- /opt/area/shared/modules/applications -----  
python/3.7.7/gnu/4.8.5    python/3.8.2/gnu/4.8.5
```

```
----- /opt/area/shared/modules/utilities -----  
hwloc/2.2.0    numactl/2.0.13
```

```
----- /opt/area/shared/modules/compilers -----  
cuda/11.0.3    gnu/9.3.0    intel/20.1
```

Where:

D: Default Module

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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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