HPC Induction

Part III: Software

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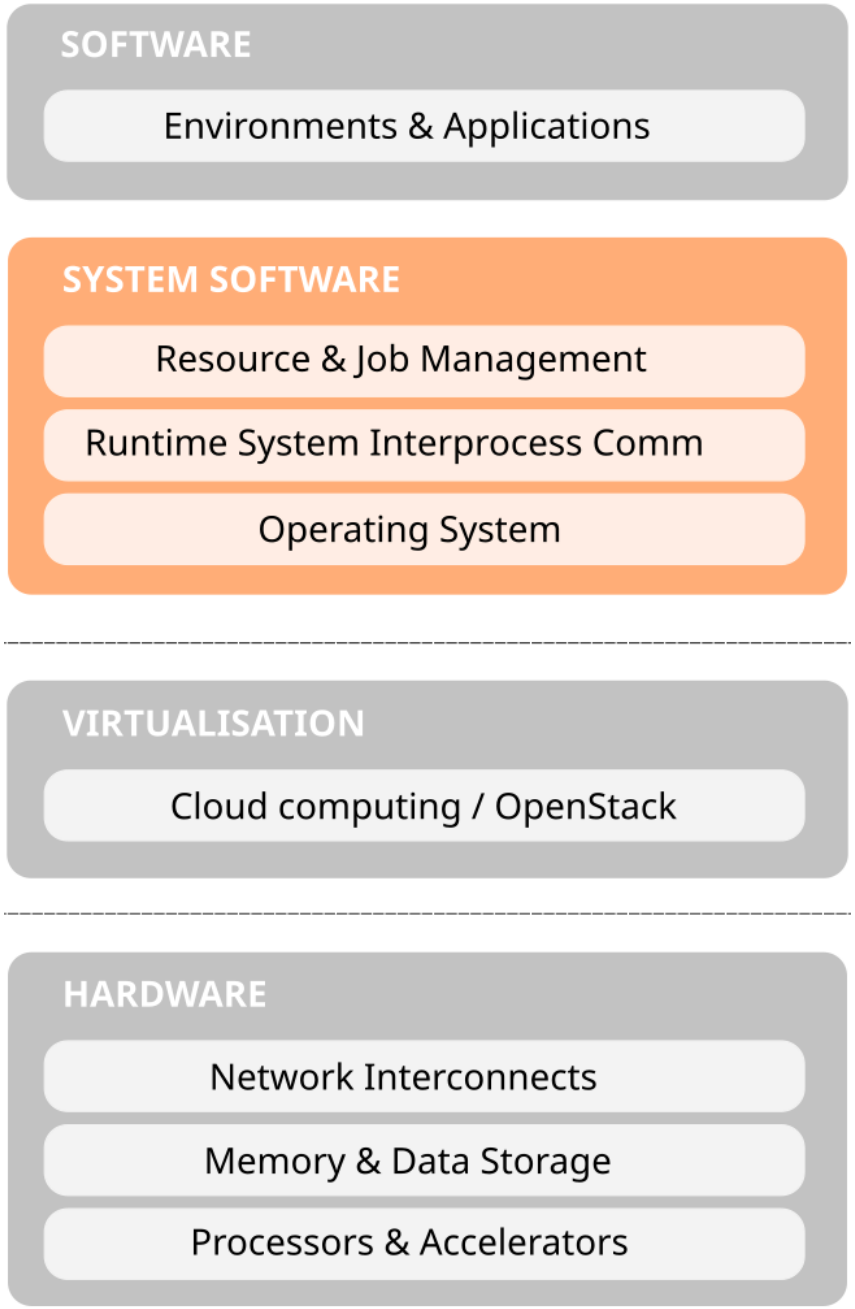
Outline

1. System Software
   - Operating System
   - Inter-Process Communication
   - Resource & Job Management
2. Software: Environments & Applications
3. Etiquette


SOFTWARE
Environments & Applications
SYSTEM SOFTWARE
Resource & Job Management
Runtime System Interprocess Comm
Operating System
VIRTUALISATION
Cloud computing / OpenStack
HARDWARE
Network Interconnects
Memory & Data Storage
Processors & Accelerators

Operating System

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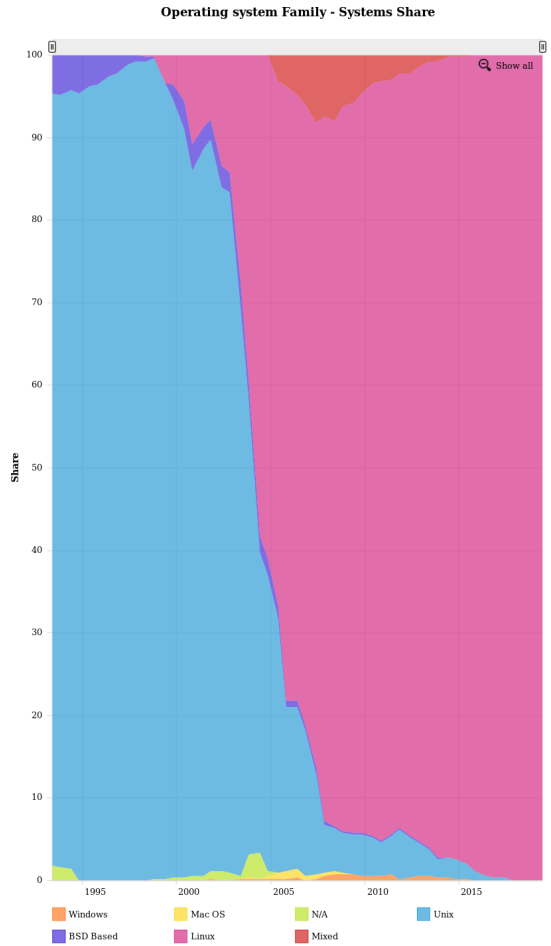

OS: Basics (cont.)

- Few distros dominate the market

Top five operating systems (November 2018)

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CentOS	139
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- For a tutorial on how to use Linux (or Unix), please see:

Linux Induction Lecture [Link]

(it is **ESSENTIAL** that you know these very few basics BEFORE you start working on the system, especially if you are using the command-line interfaces (CLI))

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- nowadays many system use SSH key authentication (e.g. RSA)

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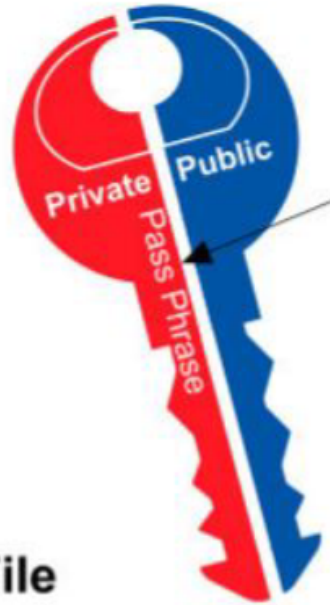

Pass Phrase

Associated with the key
is a Pass Phrase.
It is mandatory to use
a Pass Phrase.

Private Key File

Stored on your desktop
or laptop

The pass phrase
protects the
private key

Public Key File

Stored on remote server

TOP SECRET!!

NEVER share a private key !!

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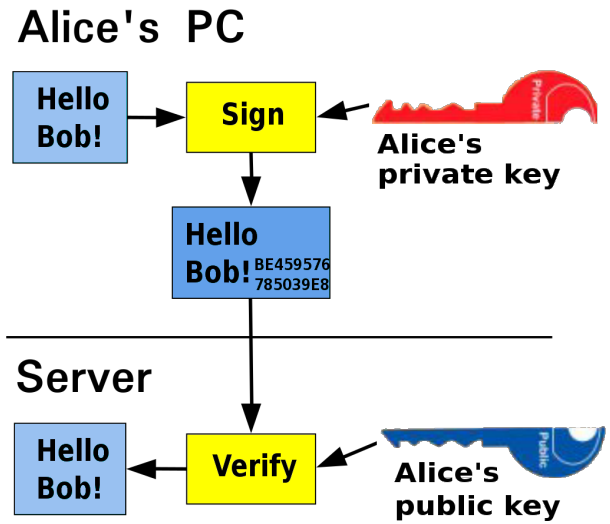

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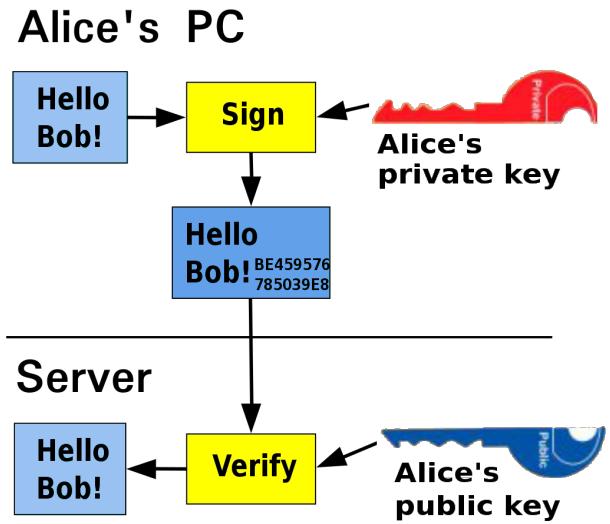

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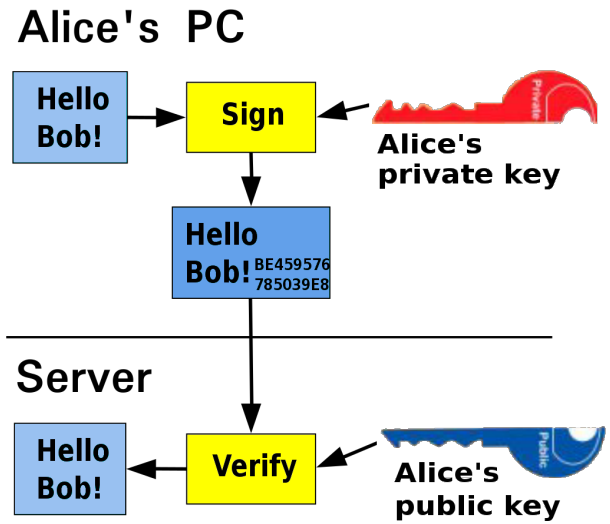
- Yet, to avoid key theft/misuse, you **MUST** protect the private key with a passphrase



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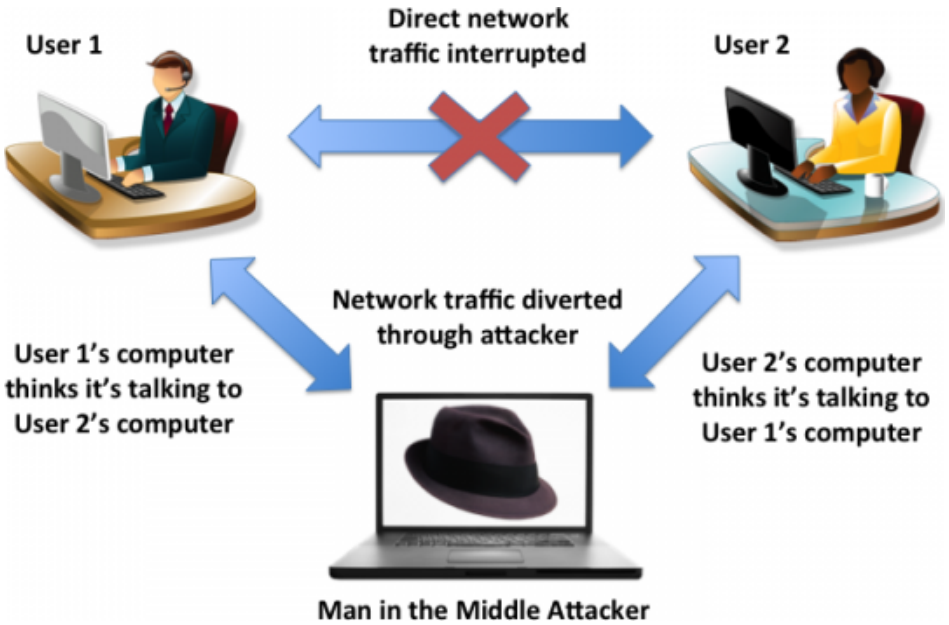

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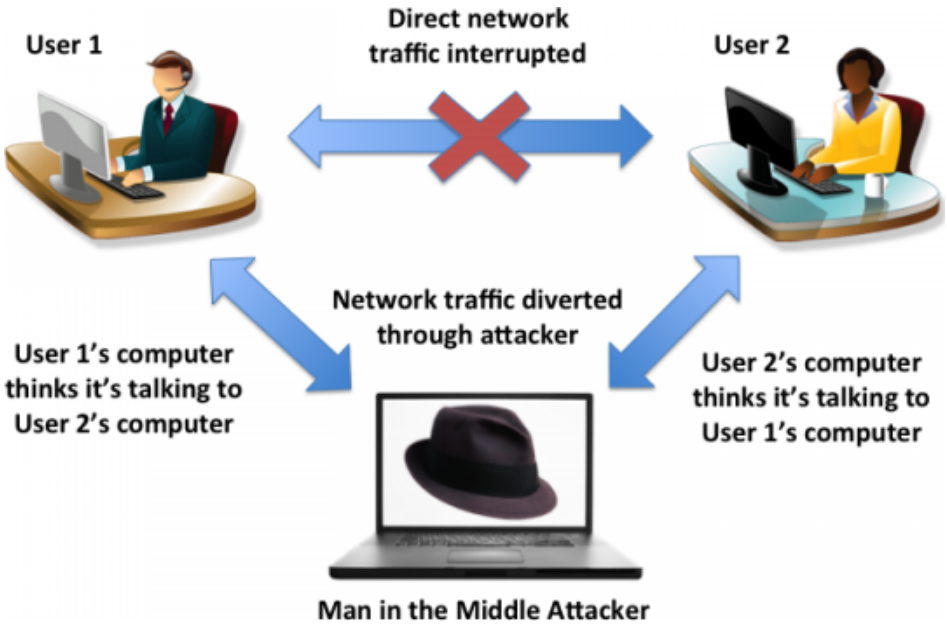

- It is a hash based on the public SSH key of the server.

OS: SSH Fingerprints (cont.)

- When you log in for the first time to a server (e.g. login node), you will be notified that the server is not known yet to your system and this fingerprint will be shown

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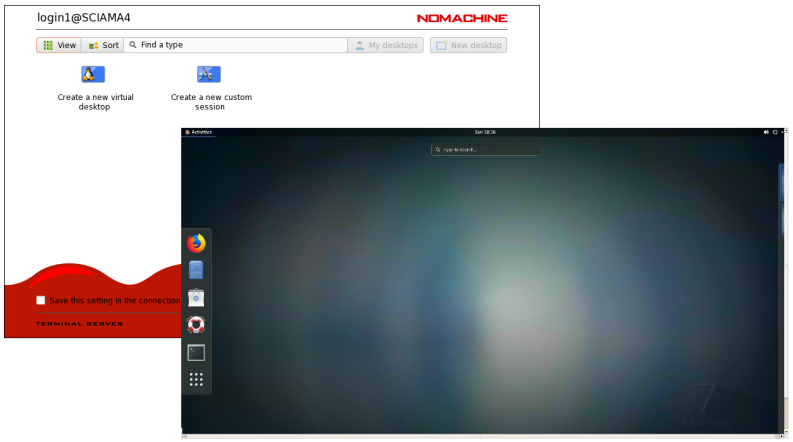


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- Anything else **MUST** be run on the compute nodes (via `slurm`)

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- Additionally, many data centres also provide the possibility to do long-term backups on data tapes

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- Alternatively, you can use the SFTP protocol, either via CLI tools or using GUI-based tools (e.g. many Linux file managers support it natively, FileZilla on Windows)

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- A convenient way to do this is to use cloud storage e.g. GoogleDrive storage

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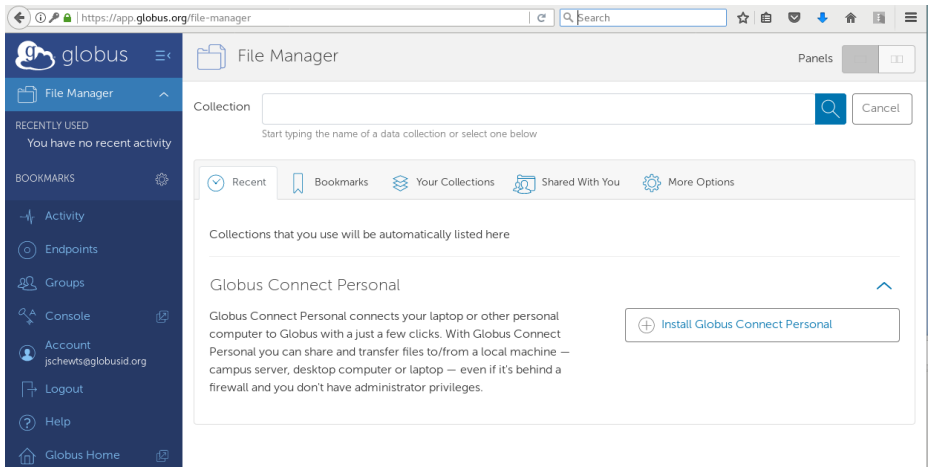
- Uses a web interface to manage transfers (works as a download/upload manager)



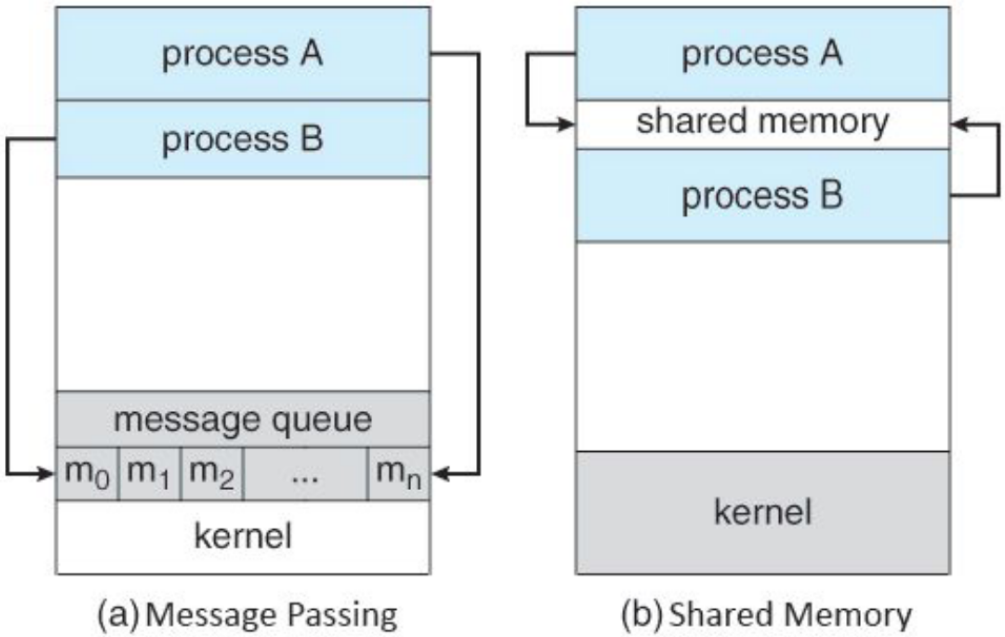
Inter-Process Communication

Inter-Process Communication

Two models of IPC

Message Passing - communication takes place by means of messages exchanged between the cooperating process.

Shared Memory - a region of memory that is shared by cooperating processes is established then exchange information takes place by reading and writing data to the shared area



MUCH more on this on Day 2 & 3 !!

Resource & Job Management

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- If resources required for jobs exceed available resources at the moment, a scheduling strategy is needed

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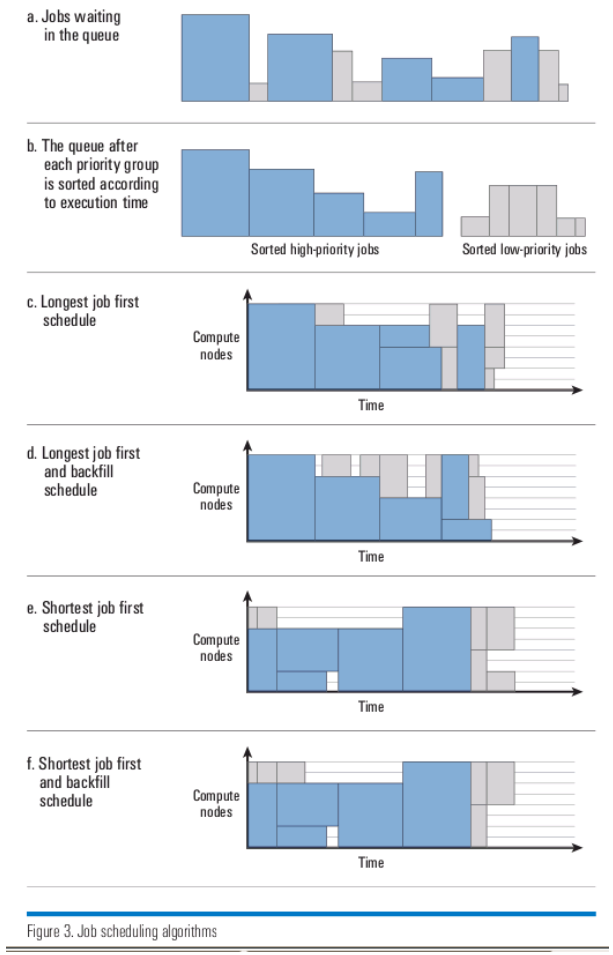

Figure 3. Job scheduling algorithms

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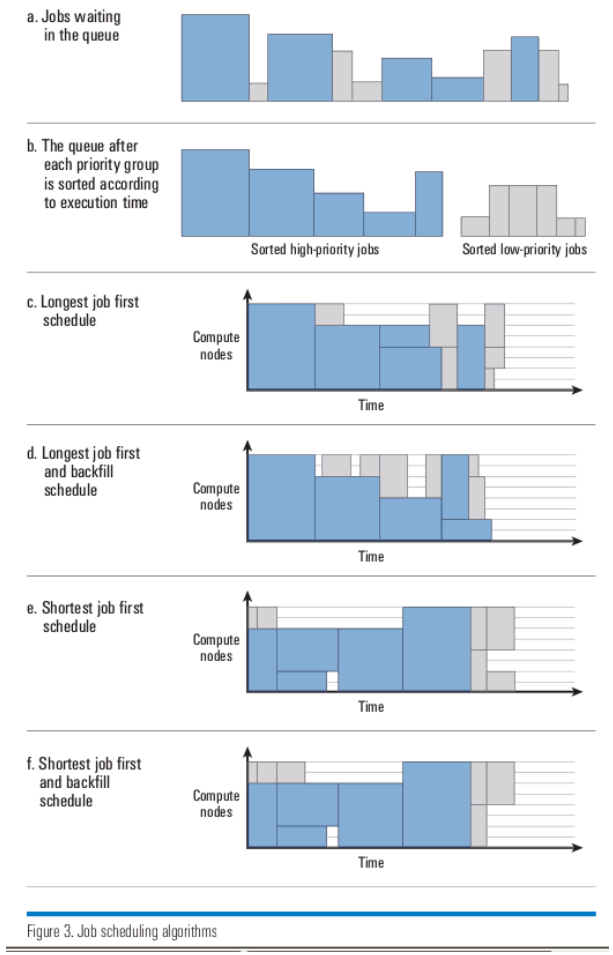

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  - Job can be prioritized by e.g. job age, job partition, job size, etc.
- Supports resource limits (by queue, user, group/project, etc.)

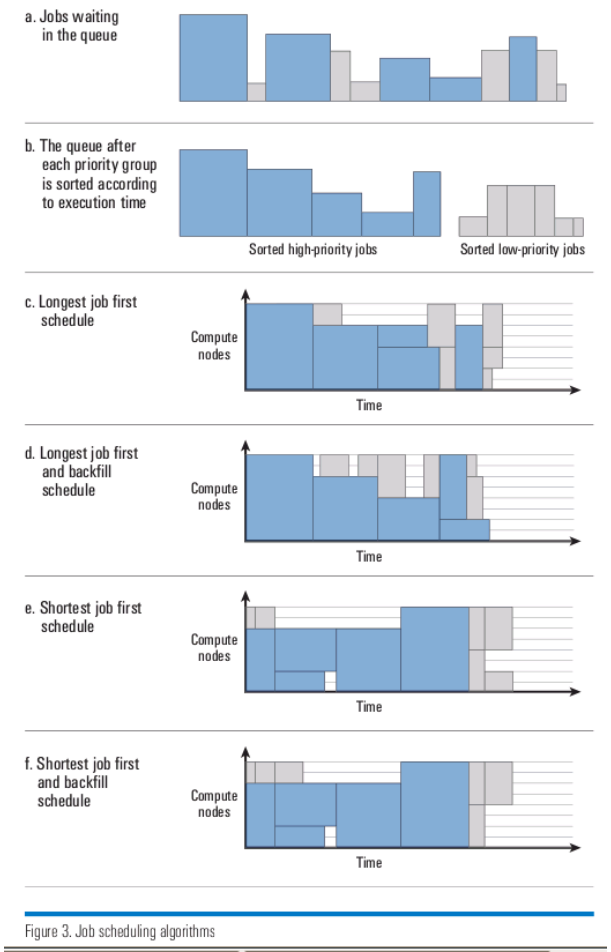

Figure 3. Job scheduling algorithms

Resource Management / Scheduling Software

- There is a variety of software packages for HPC resource management and Job scheduling:

Resource Managers	Schedulers
ALPS (Cray)	Maui
Torque	Moab
LoadLeveler (IBM)	
Slurm	
LSF	
PBS Pro	

Many packages cover both roles.

Resource Management / Scheduling Software

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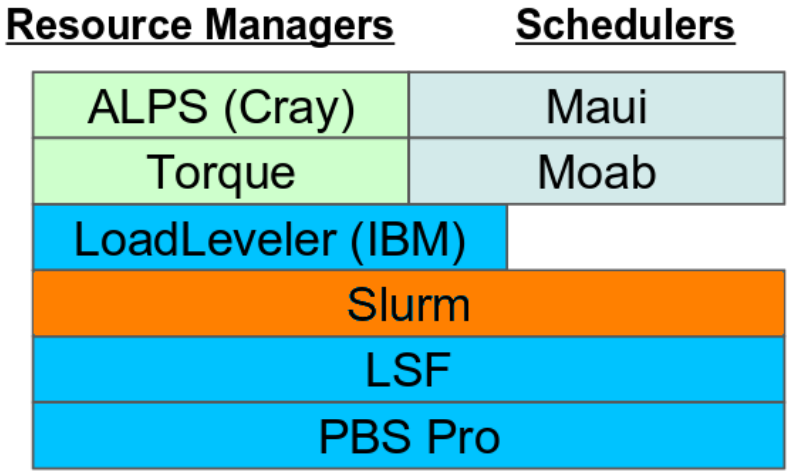

  Many packages cover both roles.

- While you can encounter any of them out there on HPC systems, we focus here on open-source software `slurm` in particular as it is used by Artemis.

slurm: General

- Historically Slurm was an acronym standing for **S**imple **L**inux **U**tility for **R**esource **M**anagement

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DISCnet

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- Development started in 2002 at Lawrence Livermore National Laboratory as a resource manager for Linux clusters
- Sophisticated scheduling plugins added in 2008
- Used on many of the world's largest computers (e.g. managing 3.1 million core Tianhe-2)
- Plugins for various MPI libraries available (i.e. MPI "talks" to `slurm` to determine number of tasks)

`slurm`: Terminology

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Step A job may or may not consist of one or more steps started with `srun` which run sequentially, but each step may have multiple tasks running in parallel. If started from CLI, there will be one step, in a new job. If included in a batch script, each `srun` will be a new step. Useful to attach different input (cf. `sattach`).

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CPU here used as a synonym for core (e.g. in `--cpus-per-task`)

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slurm: Job Submission / Interactive Jobs

- You can execute programs on the resources interactively by using srun e.g.

  ```
  $ srun --pty bash
  ```

  If you run it without salloc, this will try to allocate a single slot on the cluster. Otherwise, it will use on of the slots requested by salloc. You will then have to wait until the resources are available.

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  If you run it without salloc, this will try to allocate a single slot on the cluster. Otherwise, it will use on of the slots requested by salloc. You will then have to wait until the resources are available.
- Once the resources are allocated, a new shell on a compute node opens. The resources stay allocated until you close this shell (or when you hit your defined time limit).
- The waiting time can be substantial and any loss of your ssh connection to the login node would results in loss of the allocation (request). You can use e.g. screen to prevent that (see exercises).

  ```
  $ screen -S my_useful_name
  [user@artemis-login-0 ~]$ srun --pty bash
  ```

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- `sbatch` requires a batch script to specify the request of resources and commands to be run on these resources

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- example script for a simple single-threaded, single-process program:

```
#!/bin/bash
#SBATCH --job-name=test_simple
#SBATCH --output=test_simple.log
#SBATCH --partition=discnet
#SBATCH --nodes=4
#SBATCH --ntasks=4
#SBATCH --time=1:00

echo "$SLURM_JOB_NODELIST #:$SLURM_NTASKS"
hostname
echo "== srun"
srun hostname
echo "== srun -n1 -N1"
srun -n1 -N1 hostname
echo "== srun -n$SLURM_NTASKS"
srun -n$SLURM_NTASKS hostname
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echo "== srun -n$SLURM_NTASKS"
srun -n$SLURM_NTASKS hostname
```

Content of test_simple.log:

```
node[111,114,172,194] #:4
==
node111.pri.sciama3.alces.network
== srun
node111.pri.sciama3.alces.network
node114.pri.sciama3.alces.network
node172.pri.sciama3.alces.network
node194.pri.sciama3.alces.network
== srun -n1 -N1
node111.pri.sciama3.alces.network
== srun -n4
node111.pri.sciama3.alces.network
node114.pri.sciama3.alces.network
node172.pri.sciama3.alces.network
node194.pri.sciama3.alces.network
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== srun -n1 -N1
node111.pri.sciama3.alces.network
== srun -n4
node111.pri.sciama3.alces.network
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node111.pri.sciama3.alces.network
node114.pri.sciama3.alces.network
node172.pri.sciama3.alces.network
node194.pri.sciama3.alces.network
```

- there is a login (here running on node111) for bootstraping
- Make sure to wrap your commands into srun if you want them to run on any other than the login node (actually, nothing but VERY light-weight tasks should be run without srun)

slurm: Job Submission / Batch job (multi-threading)

- example script for a multi-threaded, single-process program:

```
#!/bin/bash
#
#SBATCH --job-name=test_threading
#SBATCH --output=test_threading.log.%j
#
#SBATCH --partition=discnet
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=4
#SBATCH --time=1:00

module purge
module load intel/2022a

echo "#:$SLURM_NTASKS *:$SLURM_CPUS_PER_TASK"
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

echo "=="
./test_threading
echo "== srun"
srun ./test_threading
```

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export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

echo "=="
./test_threading
echo "== srun"
srun ./test_threading
```

- The %j in the output file pattern will be substituted by the JOB_ID (i.e. make it easier to manage output file from multiple submissions of the same script)

slurm: Job Submission / Batch job (multi-processing)

- example script for a multi-threaded, single-process program:

```
#!/bin/bash
#
#SBATCH --job-name=test_mpi
#SBATCH --output=test_mpi.log.%j.%t
#
#SBATCH --partition=discnet
#SBATCH --ntasks=4
#SBATCH --time=1:00

module purge
module load intel/2022a
module load OpenMPI/4.1.4-GCC-11.3.0

echo $SLURM_JOB_NODELIST
echo "#:$SLURM_NTASKS *: $SLURM_NTASKS"

echo "=="
mpirun ./test_mpi
echo "== srun"
srun --mpi=pmi2 ./test_mpi
```

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#SBATCH --ntasks=4
#SBATCH --time=1:00

module purge
module load intel/2022a
module load OpenMPI/4.1.4-GCC-11.3.0

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echo "=="
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echo "== srun"
srun --mpi=pmi2 ./test_mpi
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- both methods work without explicitly passing on the number of tasks (MPI "talks" to slurm)

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srun --mpi=pmi2 ./test_mpi
```

- both methods work without explicitly passing on the number of tasks (MPI "talks" to `slurm`)
- it is preferable to use `srun` rather than `mpirun` for bootstrapping (but skip the `--mpi=pmi2` for Intel MPI as it is not supported)

slurm: Job Submission / Batch job (Arrays)

- To submit a lot of similar tasks efficiently, you can use job arrays:

```
# Submit a job array with index values between 0 and 31
$ sbatch --array=0-31  <batch file>

# Submit a job array with index values of 1, 3, 5 and 7
$ sbatch --array=1,3,5,7 <batch file>

# Submit a job array with index values between 1 and 7
# with a step size of 2 (i.e. 1, 3, 5 and 7)
$ sbatch --array=1-7:2  <batch file>

# Submit a job array with index values between 1 and 7
# but limit the number of simultaniously running tasks to 4
$ sbatch --array=1-7%4  <batch file>
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- you can then use e.g. the env variable SLURM_ARRAY_JOB_ID to assign the right data to each of the jobs inside the array's batch script or your program

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- you can then use e.g. the env variable SLURM_ARRAY_JOB_ID to assign the right data to each of the jobs inside the array's batch script or your program
- it also helps to keep the scheduler/queues not being overwhelmed by 100s of single submissions/job requests

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- Sometimes, jobs may require other jobs to run, their results or are only required to run if another job fails

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```
# Wait for specific job to be started
sbatch --depend=after:123 my.job

# Wait for jobs to complete
sbatch --depend=afterany:123:126 my.job

# Wait for jobs to complete successfully
sbatch --depend=afterok:123 my.job

# Wait for job / entire job array to complete and at least one task fails
sbatch --depend=afternotok:123 my.job
```

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# Wait for jobs to complete successfully
sbatch --depend=afterok:123 my.job

# Wait for job / entire job array to complete and at least one task fails
sbatch --depend=afternotok:123 my.job
```

- You can create complex dependencies by combining conditions e.g.

```
# Wait for specific jobs to be started and another to fail
sbatch --depend=after:123:126,afternotok:125 my.job
```

`slurm`: Additional arguments

There are many additional arguments that can be passed to the resource manager:

- Scheduling/resource allocation:

  `--nodes=<N>` / `--nodes=<N-M>` Request that a minimum of N (and a maximum of M) nodes be allocated to this job

  `--tasks-per-node=<N>` Requests that (a maximum of) N tasks be invoked on each node

  `--mem=<size>` / `--mem-per-cpu=<size>` Specify the real memory required per node / allocated core

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  - `--exclusive` Requests, that nodes must ont be shared with other running jobs
- Logging:
  - `--error=<filename>` Instruct Slurm to connect stderr directly to the file specified (by default same as `--output`)
  - `--mail-type=<type>` Requests notifications by email to user (email address stored in system)

slurm: Resources/Accounting (sinfo)

- The command `sinfo` lists the nodes and their states belonging to the various partitions (aka queues) of the computational resources.

```
[jschewts@login1(sciama) ~]$ sinfo
PARTITION    AVAIL  TIMELIMIT  NODES  STATE NODELIST
sciama4.q       up   infinite      1    mix node304
sciama4.q       up   infinite      8  alloc node[300-303,308-311]
sciama4.q       up   infinite      3   idle node[305-307]
sciama4-12.q    up   infinite      1  drain node312
sciama4-12.q    up   infinite      1    mix node315
sciama4-12.q    up   infinite      2  alloc node[313-314]
sciama4-12.q    up   infinite     12   idle node[316-327]
sciama2.q*      up   infinite      1 drain* node125
sciama2.q*      up   infinite      2  down* node[100,194]
sciama2.q*      up   infinite      1  drain node137
sciama2.q*      up   infinite     17    mix node[101-105,127-129,158,162,169,172,178-180,190-191]
sciama2.q*      up   infinite     73  alloc node[106-124,126,130-136,138-157,159-161,163-168,170-171,173-177,181-189,192]
sciama2.q*      up   infinite      1   idle node193
sciama3.q       up   infinite      1  drain node200
sciama3.q       up   infinite     16    mix node[201-212,225-228]
sciama3.q       up   infinite     16  alloc node[213-224,229-232]
sciama3.q       up   infinite     15   idle node[233-247]
himem.q         up   infinite      1   idle vhmem01
rsm1.q          up   infinite      2    mix node[190-191]
rsm1.q          up   infinite      5  alloc node[186-189,192]
rsm1.q          up   infinite      1   idle node193
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sciama4-12.q    up   infinite      2  alloc node[313-314]
sciama4-12.q    up   infinite     12   idle node[316-327]
sciama2.q*      up   infinite      1 drain* node125
sciama2.q*      up   infinite      2  down* node[100,194]
sciama2.q*      up   infinite      1  drain node137
sciama2.q*      up   infinite     17    mix node[101-105,127-129,158,162,169,172,178-180,190-191]
sciama2.q*      up   infinite     73  alloc node[106-124,126,130-136,138-157,159-161,163-168,170-171,173-177,181-189,192]
sciama2.q*      up   infinite      1   idle node193
sciama3.q       up   infinite      1  drain node200
sciama3.q       up   infinite     16    mix node[201-212,225-228]
sciama3.q       up   infinite     16  alloc node[213-224,229-232]
sciama3.q       up   infinite     15   idle node[233-247]
himem.q         up   infinite      1   idle vhmem01
rsm1.q          up   infinite      2    mix node[190-191]
rsm1.q          up   infinite      5  alloc node[186-189,192]
rsm1.q          up   infinite      1   idle node193
```

- There are various states, nodes can be in: e.g. `alloc`/`mixed`/`idle`, `drng`/`drain`/`down`; For the latter, reasons are provided

```
[jschewts@login1(sciama) ~]$ sinfo -R
REASON               USER      TIMESTAMP           NODELIST
Investigation        jschewts  2019-10-01T20:39:31 node312
Infiniband fault     root      2019-07-30T14:56:26 node125
Not responding       nobody    2019-08-23T19:36:50 node100
Not responding       nobody    2019-10-11T14:44:56 node194
batch job complete f nobody    2019-08-28T07:20:28 node137
investigation lustre jschewts  2019-10-19T12:44:19 node200
```

slurm: Resources/Accounting (sacct)

- There is a record of each job a user submits/runs

```
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     User        JobID    JobName  Partition      State  Timelimit               Start                 End    Elapsed     MaxRSS  MaxVMSize   NNodes      NCPUS        NodeList
--------- ------------ ---------- ---------- ---------- ---------- ------------------- ------------------- ---------- ---------- ---------- -------- ---------- ---------------
   [user] 1135959         starccm  sciama4.q    RUNNING 2-00:00:00 2019-10-22T15:17:11             Unknown 1-02:14:01                             1          8         node300
          1135959.0          bash               RUNNING            2019-10-22T15:17:40             Unknown 1-02:13:32                             1          8         node300
   [user] 1153763         starccm  sciama4.q CANCELLED+ 2-00:00:00 2019-10-23T14:44:31 2019-10-23T14:47:47   00:03:16                             1          8         node308
          1153763.bat+      batch             CANCELLED            2019-10-23T14:44:31 2019-10-23T14:47:48   00:03:17      7492K    414804K        1          8         node308
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   [user] 1153770         starccm  sciama4.q CANCELLED+ 2-00:00:00 2019-10-23T14:47:31 2019-10-23T14:49:59   00:02:28                             1          8         node308
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   [user] 1153805         starccm  sciama4.q  COMPLETED 2-00:00:00 2019-10-23T14:53:02 2019-10-23T14:53:24   00:00:22                             1          8         node308
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   [user] 1153825         starccm  sciama4.q  COMPLETED 2-00:00:00 2019-10-23T15:08:04 2019-10-23T15:08:30   00:00:26                             1          8         node309
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```

- on public HPC framework, this accounting is used to keep track/limit resource usage for charging users/project
- on Artemis, it can be used for debugging or obtaining useful statistics to optimize your resource requests (e.g. `MaxRSS` size tells you about your actual memory requirements)

Resource Management / Scheduling: Controlling

- Once you submitted a job, you can keep track of its process using the command `squeue` (e.g. use `squeue -u <username>` to list all of the active (i.e. queued or running) jobs of a specific user

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- Furthermore, `scontrol` allows you to make changes to your submitted jobs (e.g. holding them in the queue)

`slurm`: Man Pages / Cheat Sheet

- For more details on all the presented commands, please check their man pages (e.g. `man sbatch`)

slurm: Man Pages / Cheat Sheet

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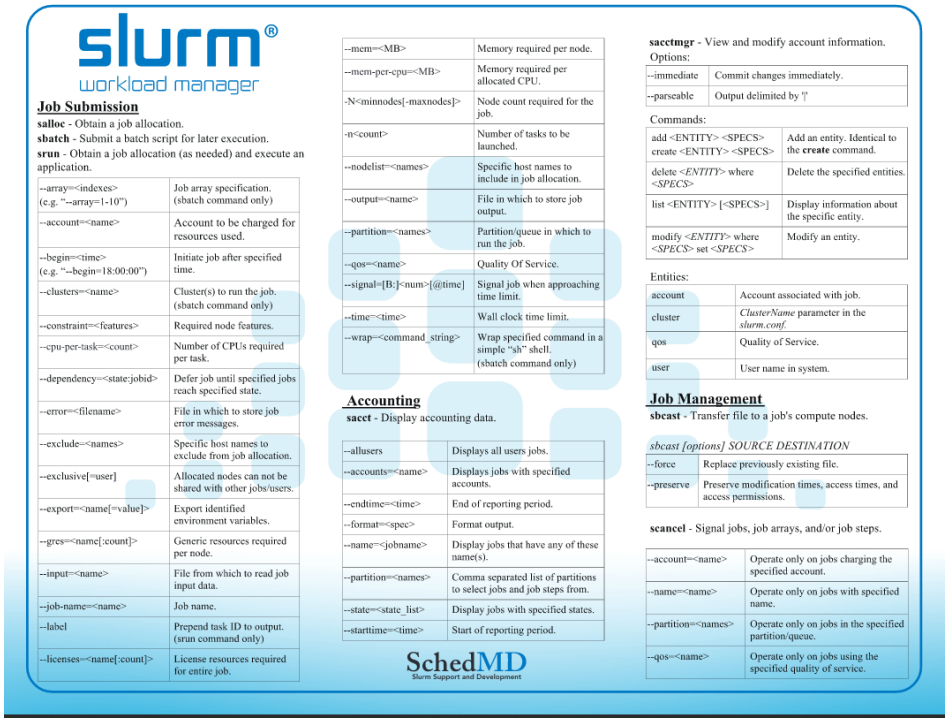
- There is a also handy slurm cheat sheet which you can download from e.g.

`https://slurm.schedmd.com/pdfs/summary.pdf`



slurm®
workload manager

Job Submission

salloc - Obtain a job allocation.
sbatch - Submit a batch script for later execution.
srun - Obtain a job allocation (as needed) and execute an application.

--array=<indexes> (e.g. "--array=1-10")	Job array specification. (sbatch command only)
--account=<name>	Account to be charged for resources used.
--begin=<time> (e.g. "--begin=18:00:00")	Initiate job after specified time.
--clusters=<name>	Cluster(s) to run the job. (sbatch command only)
--constraint=<features>	Required node features.
--cpu-per-task=<count>	Number of CPUs required per task.
--dependency=<state:jobid>	Defer job until specified jobs reach specified state.
--error=<filename>	File in which to store job error messages.
--exclude=<names>	Specific host names to exclude from job allocation.
--exclusive[=user]	Allocated nodes can not be shared with other jobs/users.
--export=<name[=value]>	Export identified environment variables.
--gres=<name[:count]>	Generic resources required per node.
--input=<name>	File from which to read job input data.
--job-name=<name>	Job name.
--label	Prepend task ID to output. (srun command only)
--licenses=<name[:count]>	License resources required for entire job.
--mem=<MB>	Memory required per node.
--mem-per-cpu=<MB>	Memory required per allocated CPU.
-N<minnodes[-maxnodes]>	Node count required for the job.
-n<count>	Number of tasks to be launched.
--nodelist=<names>	Specific host names to include in job allocation.
--output=<name>	File in which to store job output.
--partition=<names>	Partition/queue in which to run the job.
--qos=<name>	Quality Of Service.
--signal=[B:]<num>[@time]	Signal job when approaching time limit.
--time=<time>	Wall clock time limit.
--wrap=<command_string>	Wrap specified command in a simple "sh" shell. (sbatch command only)

Accounting

sacct - Display accounting data.

--allusers	Displays all users jobs.
--accounts=<name>	Displays jobs with specified accounts.
--endtime=<time>	End of reporting period.
--format=<spec>	Format output.
--name=<jobname>	Display jobs that have any of these name(s).
--partition=<names>	Comma separated list of partitions to select jobs and job steps from.
--state=<state_list>	Display jobs with specified states.
--starttime=<time>	Start of reporting period.

SchedMD
Slurm Support and Development

sacctmgr - View and modify account information.
Options:

--immediate	Commit changes immediately.
--parseable	Output delimited by |

Commands:

add <ENTITY> <SPECS> create <ENTITY> <SPECS>	Add an entity. Identical to the **create** command.
delete <*ENTITY*> where <*SPECS*>	Delete the specified entities.
list <ENTITY> [<SPECS>]	Display information about the specific entity.
modify <*ENTITY*> where <*SPECS*> set <*SPECS*>	Modify an entity.

Entities:

account	Account associated with job.
cluster	*ClusterName* parameter in the *slurm.conf*.
qos	Quality of Service.
user	User name in system.

Job Management

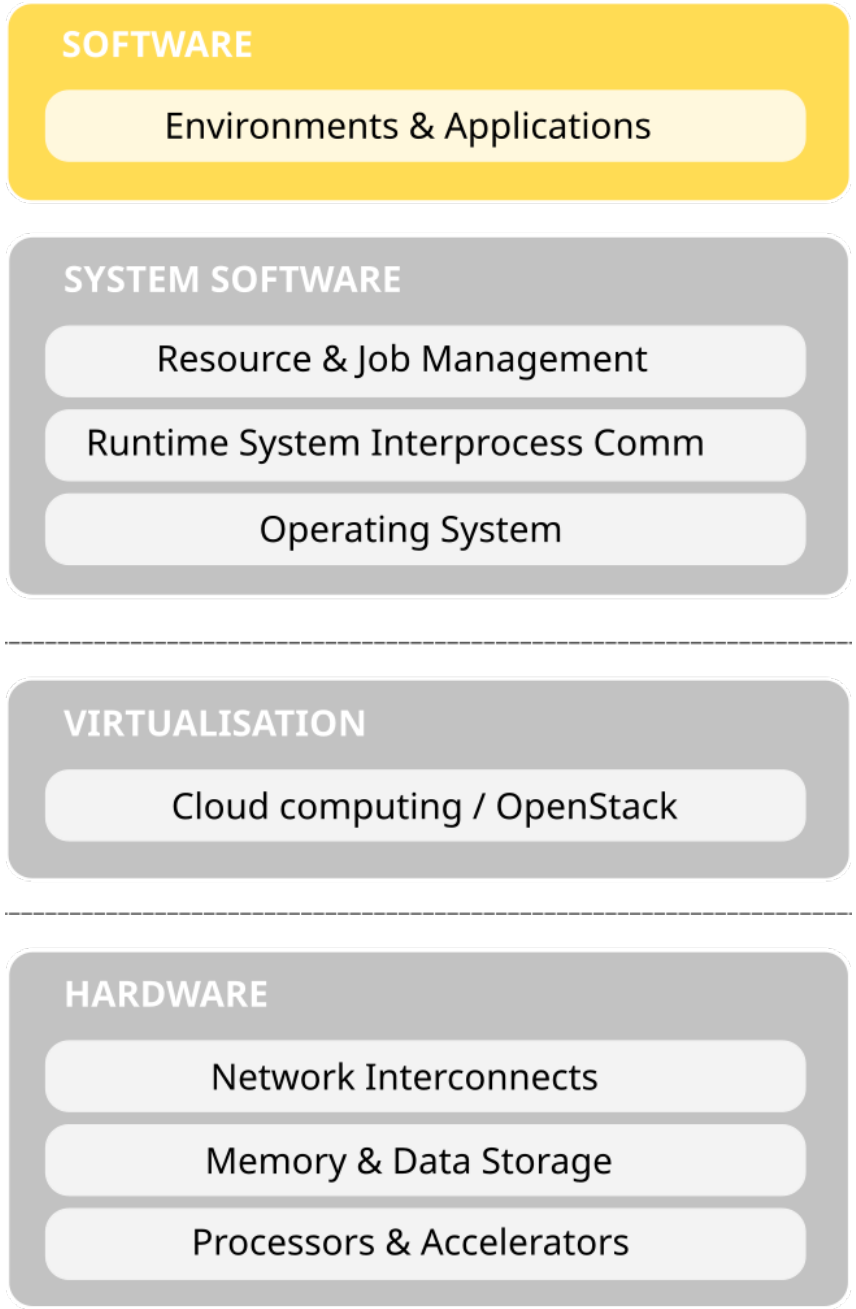
sbcast - Transfer file to a job's compute nodes.

sbcast [options] SOURCE DESTINATION

--force	Replace previously existing file.
--preserve	Preserve modification times, access times, and access permissions.

scancel - Signal jobs, job arrays, and/or job steps.

--account=<name>	Operate only on jobs charging the specified account.
--name=<name>	Operate only on jobs with specified name.
--partition=<names>	Operate only on jobs in the specified partition/queue.
--qos=<name>	Operate only on jobs using the specified quality of service.


SOFTWARE
Environments & Applications
SYSTEM SOFTWARE
Resource & Job Management
Runtime System Interprocess Comm
Operating System
VIRTUALISATION
Cloud computing / OpenStack
HARDWARE
Network Interconnects
Memory & Data Storage
Processors & Accelerators

Environments & Applications

System Environment & Multi-user systems

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- Thus, it requires a way to adapt a system environment for each user/purpose: Environment variables / modules

Environment variables: General

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- `env` prints all environmental variables

Environment variables: `PATH`

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- the first occurence found in `PATH` is used

```
export PATH=<INSTALL PATH>/bin:$PATH
```

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- Similar to `PATH`, if you want to make custom-installed libraries available to the compiler, the resp. `include`, `lib`, etc. folders have to be added to the variables e.g.

```
export CFLAGS="-I<INSTALL PATH>/include $CFLAGS"
```

or

```
export LDFLAGS="-L<LIB PATH> -Wl,-rpath=<LIB PATH> $LDFLAGS"
```

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- `MODULESPATH` is a list of folders checked for modules (similar to `PATH` for commands). You can append it to add custom modules

Modules: Usage

- There are a few important commands:

  `module av` lists available modules
  `module load <modulename>` loads a module
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  `module list` lists all currently loaded modules
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- if you want to have certain modules loaded by default, simply modify the `.bashrc` and/or `.bash_profile` in your home directory accordingly

Modules: Artemis

- Artemis uses LMod (i.e. Lua-based reimplementation of original TCL/L-based module system)

```
[js2347@artemis-login-0 ~]$ module av

------------------------------------------------------------------------------ /opt/ohpc/pub/modulefiles -------------------------------------------------------------
   gnu12/12.2.0    hwloc/2.11.1 (D)    libfabric/1.18.0    os    papi/6.0.0    pmix/4.2.9    prun/2.2    ucx/1.17.0

---------------------------------------------------------------------------- /mnt/shared/easybuild/modules/all ----------------------------------------------------------
   ANSYS/2023R1                                 OpenMPI/4.0.6-GCC-10.3.0                     groff/1.22.4-GCCcore-11.2.0
   ATK/2.36.0-GCCcore-11.2.0                    OpenMPI/4.0.7-GCC-10.3.0                     groff/1.22.4-GCCcore-11.3.0
   ATK/2.38.0-GCCcore-11.3.0                    OpenMPI/4.1.1-GCC-10.3.0                     groff/1.22.4-GCCcore-12.2.0
   ATK/2.38.0-GCCcore-12.2.0                    OpenMPI/4.1.1-GCC-11.2.0                     groff/1.22.4-GCCcore-12.3.0
   ATK/2.38.0-GCCcore-12.3.0                    OpenMPI/4.1.4-GCC-11.3.0                     groff/1.23.0-GCCcore-13.2.0                (D)
   ATK/2.38.0-GCCcore-13.2.0             (D)    OpenMPI/4.1.4-GCC-12.2.0                     grpcio/1.57.0-GCCcore-12.3.0
   Abseil/20230125.2-GCCcore-12.2.0             OpenMPI/4.1.5-GCC-12.3.0                     gzip/1.10-GCCcore-10.2.0
   Abseil/20230125.3-GCCcore-12.3.0      (D)    OpenMPI/4.1.6-GCC-13.2.0                     gzip/1.10-GCCcore-10.3.0
   Anaconda3/2022.10                            OpenMPI/5.0.3-GCC-13.3.0              (D)    gzip/1.10-GCCcore-11.2.0
   Armadillo/11.4.3-foss-2022b                  OpenMolcas/22.10-foss-2021b                  gzip/1.12-GCCcore-11.3.0
   Armadillo/12.6.2-foss-2023a                  OpenPGM/5.2.122-GCCcore-12.3.0               gzip/1.12-GCCcore-12.2.0
   Armadillo/12.8.0-foss-2023b           (D)    OpenSSL/1.1                           (L)    gzip/1.12-GCCcore-12.3.0
   Autoconf/2.69-GCCcore-9.3.0                  OpenSSL/1.1.1e-GCCcore-9.3.0                 gzip/1.13-GCCcore-13.2.0                   (L)
   Autoconf/2.69-GCCcore-10.2.0                 OpenSSL/1.1.1h-GCCcore-10.2.0                gzip/1.13-GCCcore-13.3.0                   (D)
   Autoconf/2.71-GCCcore-10.3.0                 OpenSSL/1.1.1k-GCCcore-10.3.0                h5py/3.2.1-foss-2021a
   Autoconf/2.71-GCCcore-11.2.0                 OpenSSL/1.1.1n-GCCcore-11.3.0                h5py/3.9.0-foss-2023a                      (D)
   Autoconf/2.71-GCCcore-11.3.0                 OpenSSL/1.1.1q-GCCcore-12.2.0                hatchling/1.18.0-GCCcore-12.3.0
   Autoconf/2.71-GCCcore-12.2.0                 OpenSSL/3                             (D)    hatchling/1.18.0-GCCcore-13.2.0            (D)
   Autoconf/2.71-GCCcore-12.3.0                 PBZIP2/1.1.13-GCCcore-12.3.0                 help2man/1.47.12-GCCcore-9.3.0
   Autoconf/2.71-GCCcore-13.2.0                 PCRE/8.44-GCCcore-10.3.0                     help2man/1.47.16-GCCcore-10.2.0
   Autoconf/2.71                                PCRE/8.45-GCCcore-11.2.0                     help2man/1.48.3-GCCcore-10.3.0
   Autoconf/2.72-GCCcore-13.3.0          (D)    PCRE/8.45-GCCcore-11.3.0                     help2man/1.48.3-GCCcore-11.2.0
   Automake/1.16.1-GCCcore-9.3.0                PCRE/8.45-GCCcore-12.2.0                     help2man/1.49.2-GCCcore-11.3.0
   Automake/1.16.2-GCCcore-10.2.0               PCRE/8.45-GCCcore-12.3.0                     help2man/1.49.2-GCCcore-12.2.0
   Automake/1.16.3-GCCcore-10.3.0               PCRE/8.45-GCCcore-13.2.0              (D)    help2man/1.49.3-GCCcore-12.3.0
```

- Modules resolve dependencies automatically, **BUT** loading a new module with conflicts (e.g. dependency with different version) replaces already loaded(!)

```
[js2347@artemis-login-0 ~]$ module load intel
[js2347@artemis-login-0 ~]$ module load GCC

The following have been reloaded with a version change:
  1) GCCcore/11.3.0 => GCCcore/13.3.0     2) binutils/2.38-GCCcore-11.3.0 => binutils/2.42-GCCcore-13.3.0     3) zlib/1.2.12-GCCcore-11.3.0 => zlib/1.3.1-GCCcore-13.3.0
```

Containers: Singularity/Apptainer

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- popular software:

  Docker (requires root privileges)
  Singularity/Apptainer (supported on Artemis)

DISCnet

Etiquette

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Recap: HPC as a service