

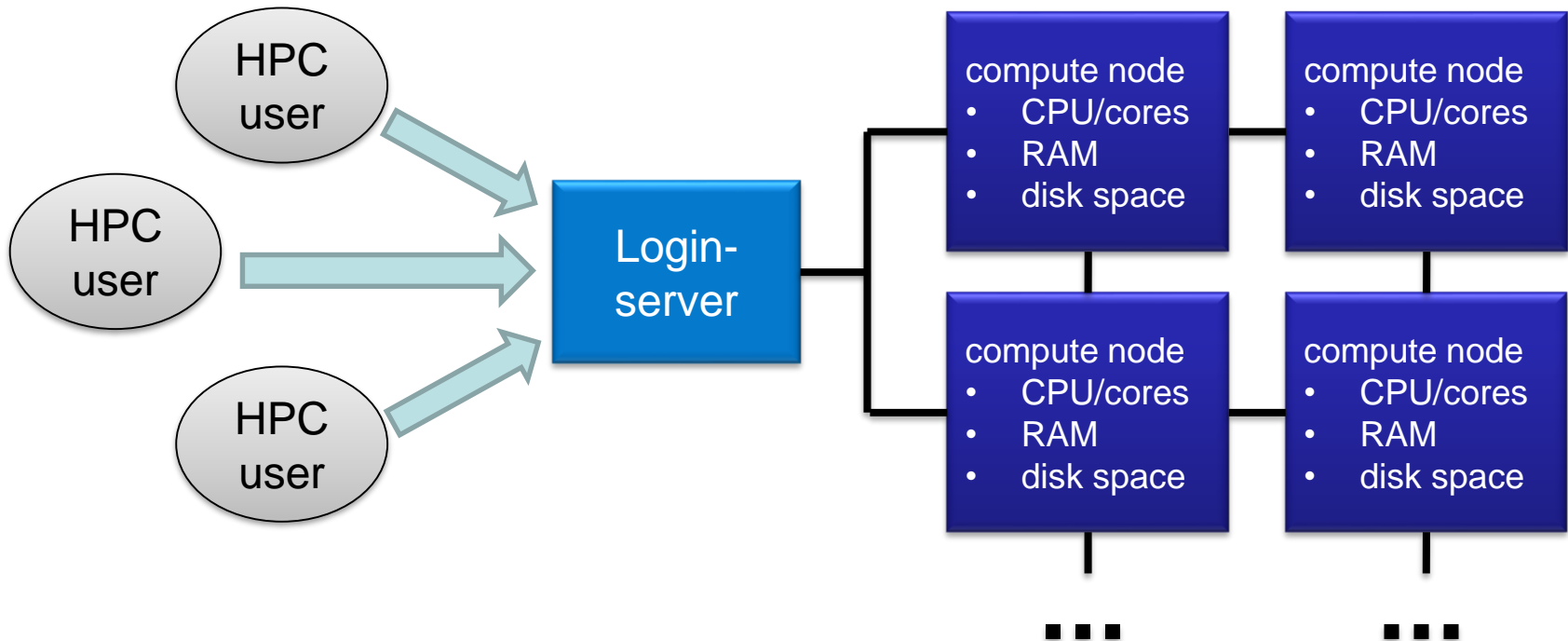
Introduction to High-Performance Computing

Session 02

Basic Cluster Usage
and Job Scheduler

Basic Usage HPC Cluster

- many users share a single HPC cluster (resource)



Basic Usage HPC Cluster

- many users share a single HPC cluster (resource)
- requires management of the resources
 - for fair sharing
 - for efficient usage
- possible strategies
 - users find free resource and use it
 - part of the resource is reserved for a (group of) user(s)
 - Resource Manager and Job Scheduler

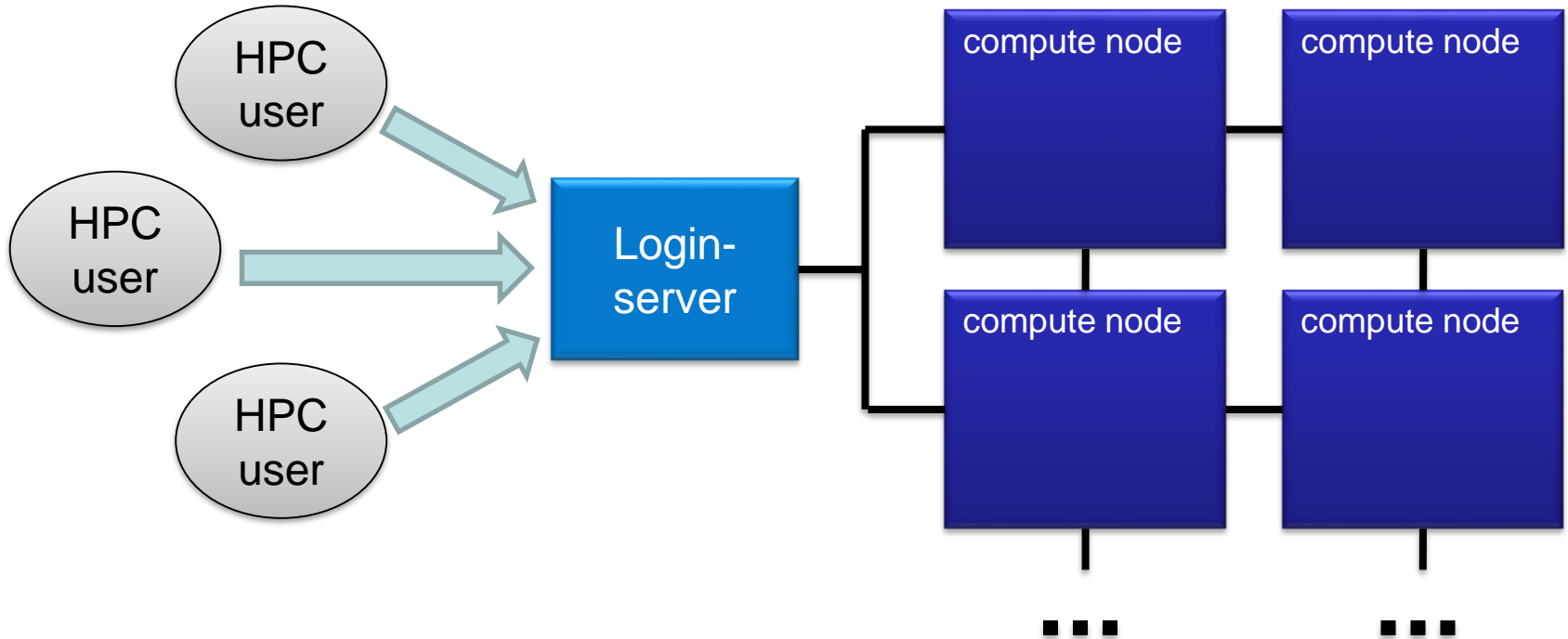
Resource Manager and Job Scheduler

- RM provides low-level functionality for managing jobs
 - start, hold, cancel, and monitor jobs
 - functionality needed by the job scheduler
- JS provides functionality to define and submit jobs
 - interface to RM functionality for the user
 - jobs are scheduled for optimal usage of resource, taking into account fair sharing and other requirements (priority)
- typically RM and JS are in one application

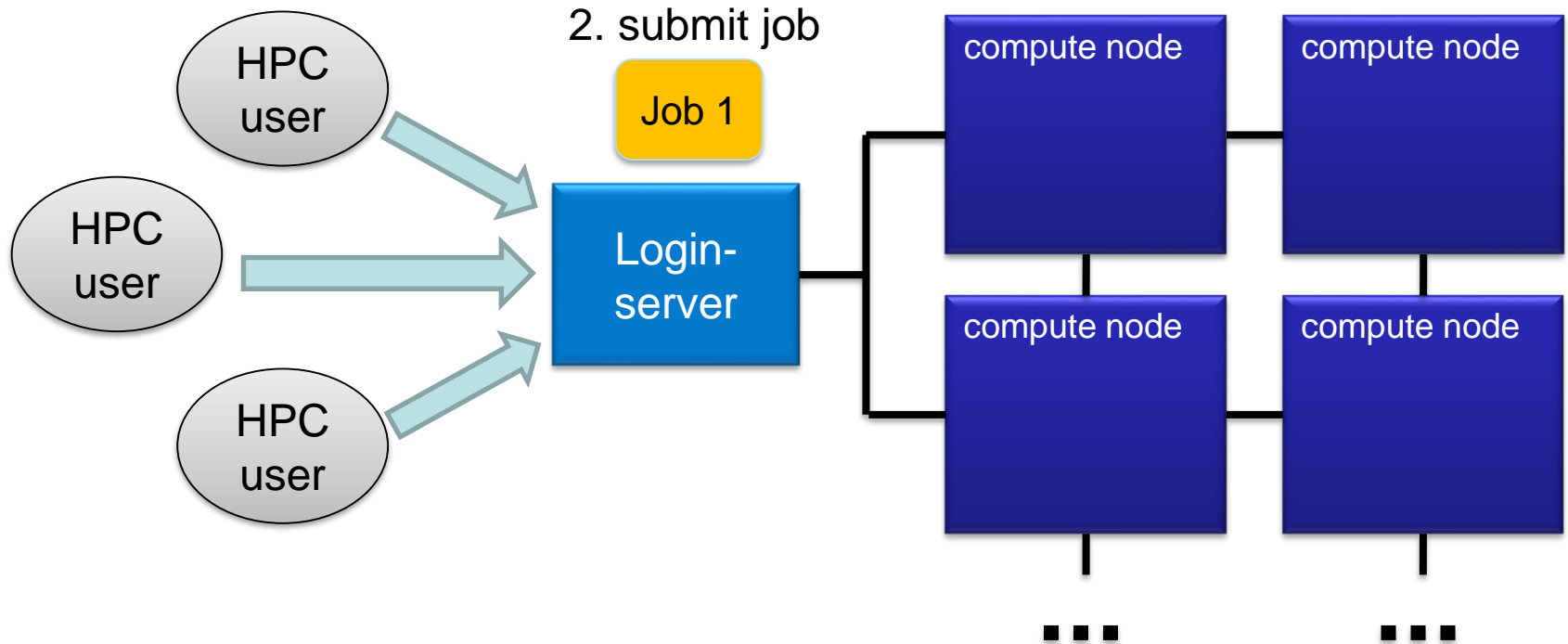
Resource Manager and Job Scheduler

1. define job

Job 1

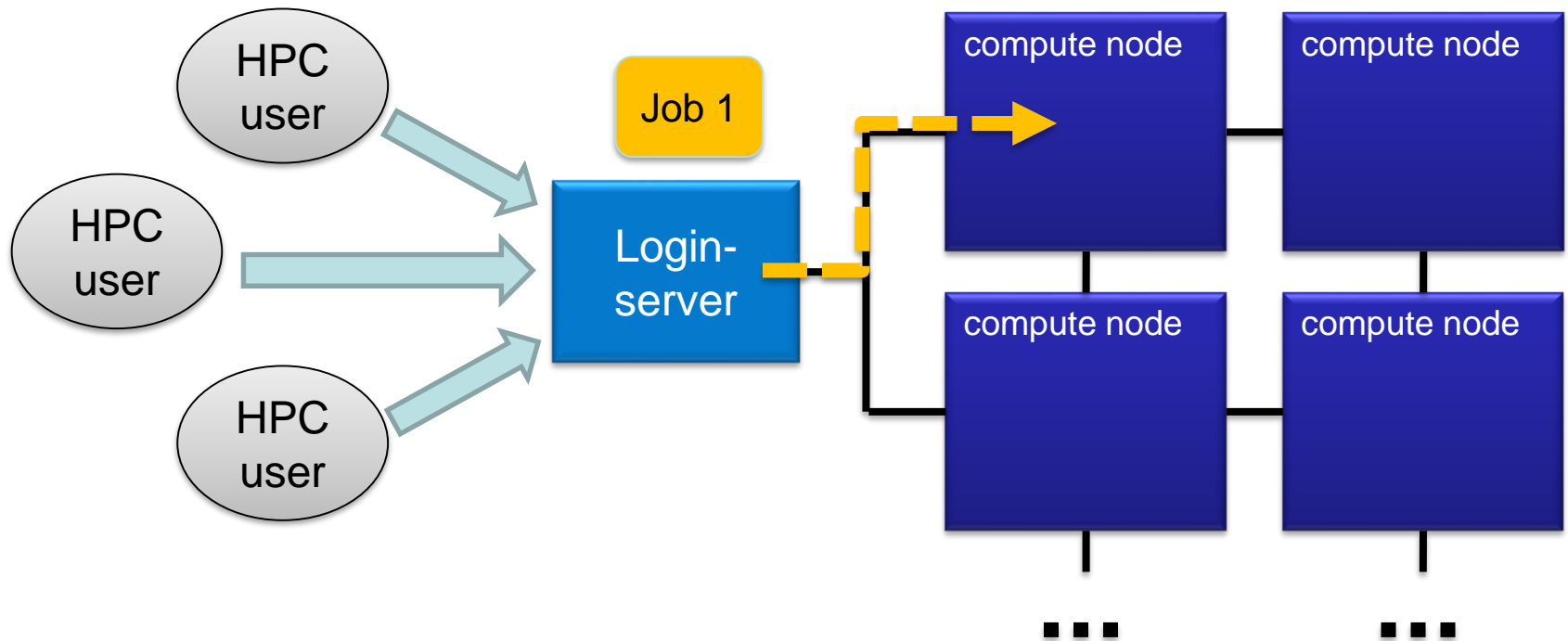


Resource Manager and Job Scheduler



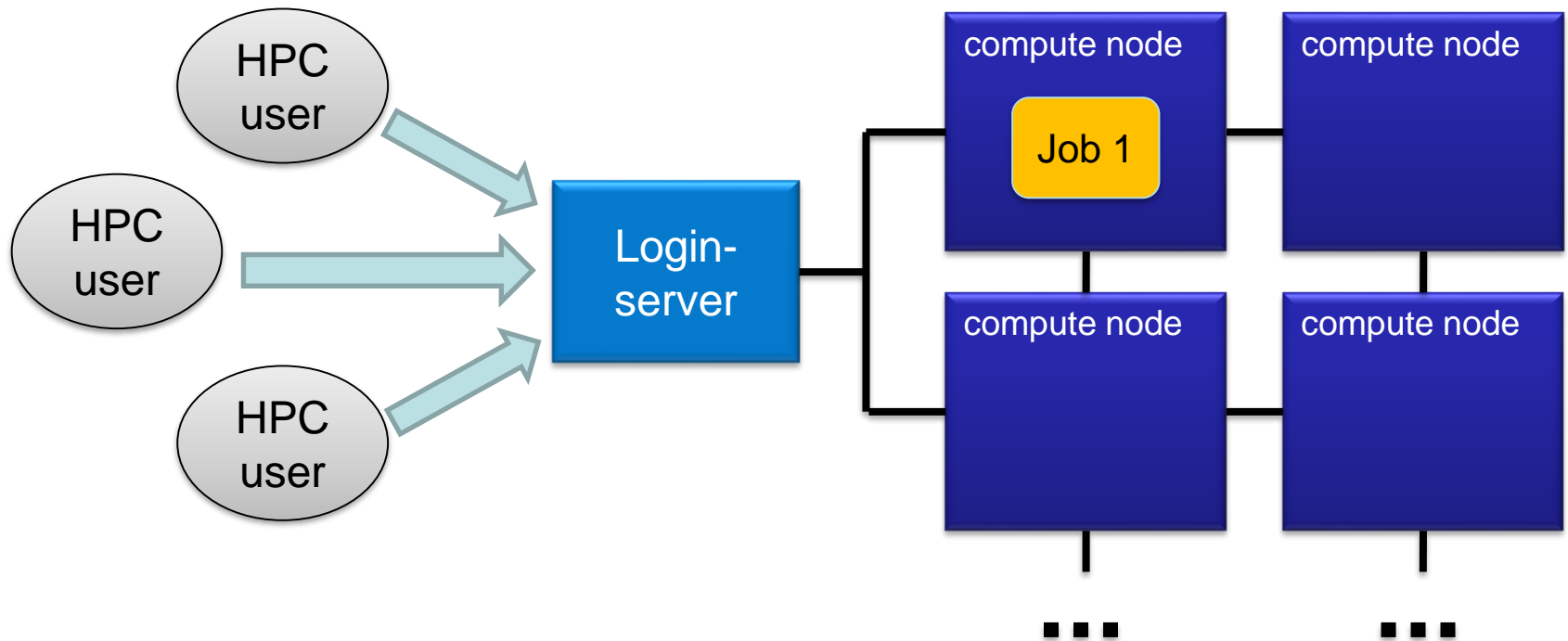
Resource Manager and Job Scheduler

3. JS checks available resources



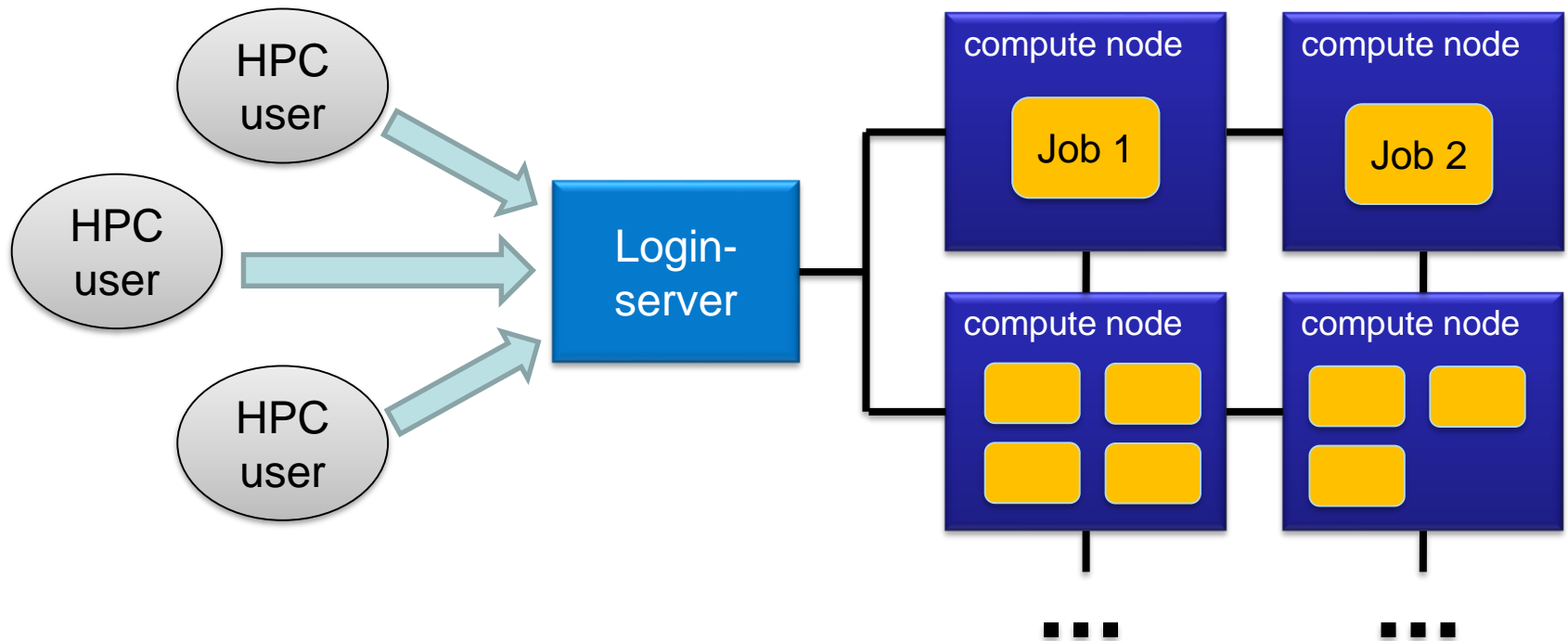
Resource Manager and Job Scheduler

4. if found job is executed



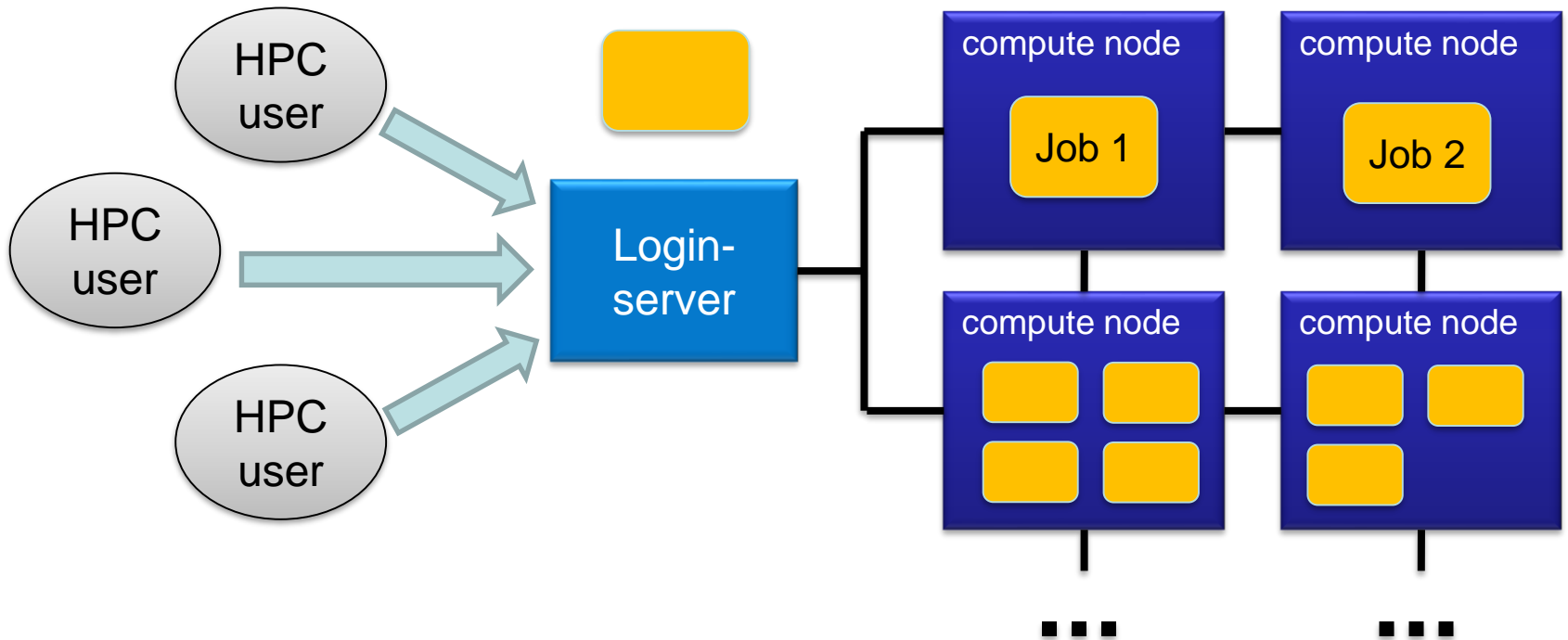
Resource Manager and Job Scheduler

5. resources are filled with as many jobs as possible



Resource Manager and Job Scheduler

6. if a job is requesting more resources than available it is queued



Resource Manager and Job Scheduler

- there many Resource Manager and Job Scheduler applications available
 - PBS/Torque
 - SLURM (used on the current HPC clusters)
 - LSF
 - SGE (was used on the old HPC clusters)
 - LoadLeveler
 - ...

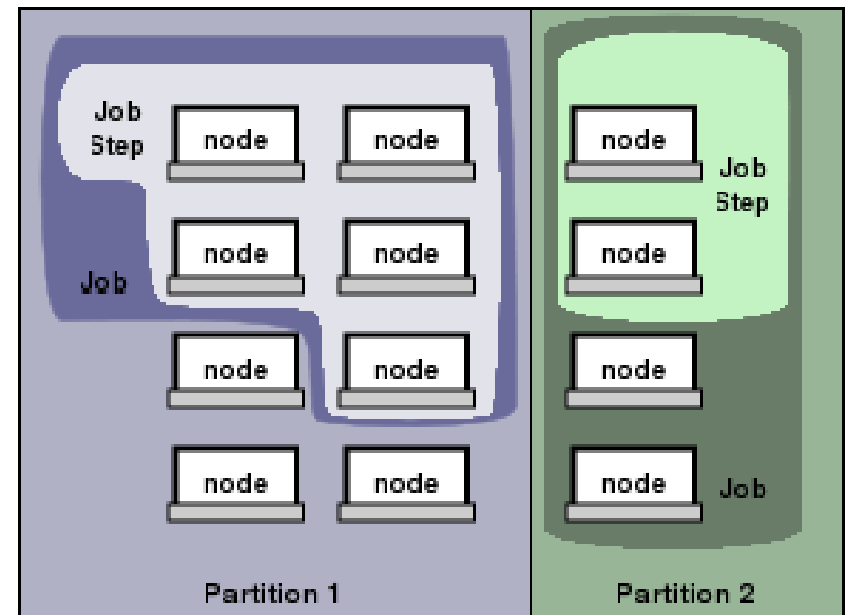
the examples in this course will use SLURM
but the principles are the same for all Job Schedulers
(see e.g. <http://slurm.schedmd.com/rosetta.pdf>)

Tasks of a Job Scheduler

- handling job requests by users (submission, deletion,...)
- prioritize jobs based on the set rules and policies
- place jobs in queue until resources become available
- organize workload on the HPC system for optimal load
- send jobs to the execution host (compute node)
- monitor running jobs
- log files
 - stdout and stderr of jobs
 - accounting information of finished jobs
- terminate job if it use more resources than requested

SLURMs System View

- compute **nodes** are the basic resource
- compute nodes are organized in **partitions**
 - logical sets
 - may overlap
- resources are allocated to **jobs**
 - jobs may contain multiple **job steps**



(see <https://slurm.schedmd.com/overview.html>)

Basic Usage of SLURM

Important SLURM Commands

Command	Used for
<code>squeue</code>	overview of jobs in the scheduler queue
<code>sinfo</code>	information about SLURM nodes and partitions
<code>sacct</code>	accounting information about jobs
<code>sbatch</code>	submit jobs to the scheduler
<code>srun</code>	allocate resources if needed and launch a job step within an job allocation
<code>scancel</code>	delete queued or running jobs
<code>scontrol</code>	manage jobs (limited) and more

to get information about commands visit <https://slurm.schedmd.com/documentation.html> or use

```
$ man <command>
```

squeue

- get information about jobs in the scheduler queue

```
$ squeue
  JOBID PARTITION      NAME      USER ST      TIME  NODES NODELIST (REASON)
2580499_ all_nodes ofparamt hoga9120 PD      0:00     16 (ArrayTaskLimit)
 1196528   eddy.p   300ren  guab0721  R 18-21:40:13     1 cfd1054
 1229276   carl.p  crystal_ wexo7212  R 16-03:57:31     1 mpcs023
 1229277   carl.p  crystal_ wexo7212  R 16-03:56:11     1 mpcs093
 1229278   carl.p  crystal_ wexo7212  R 16-03:54:47     1 mpcs016
...
```

- use the option **-u \$USER** to only show your own jobs
- the option **-l** gives additional information, output can also be adjusted as needed
- jobs can be shown depending on partition, state, ...

sacct

- accounting information about jobs

```
$ sacct -j 2303252
      JobID      JobName      Partition      Account      AllocCPUS      State      ExitCode
-----
2303252      HelloClus+      mpcs.p          hrz           8      COMPLETED      0:0
2303252.bat+      batch          hrz            2      COMPLETED      0:0
2303252.0          orted          hrz            3      COMPLETED      0:0
```

- option `-l` for long format, or `--format=` to specify output
- use `sacct -e` to see possible output formats
- per default `sacct` shows all jobs of user on the current day

sinfo

- information about nodes and partitions

```
$ sinfo -p mpcs.p
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
mpcs.p      up 21-00:00:0      1  drain mpcs025
mpcs.p      up 21-00:00:0     61   mix mpcs[002,004,007,009,015,018-
019,022,024,026-027,029-031,034,036-038,041,044,046-050,052-
053,069,072,075,078-082,084-087,089-092,099-102,104-107,110-112,114-
116,119,123,149,152]
mpcs.p      up 21-00:00:0     76  alloc mpcs[001,005-006,011-014,016-
017,020-021,023,032-033,039-040,042-043,045,051,054-068,071,073-
074,083,088,093-098,108-109,113,117,120-122,133-148,151,153-158]
mpcs.p      up 21-00:00:0     20   idle mpcs[003,008,010,028,035,070,076-
077,103,118,124-132,150]
```

- give idea about used and free resources on cluster

sbatch

- allows to submit a job with
sbatch [options] <job-script>
 - one mandatory option is **-p** to set the partition

```
$ cat HelloWorld_v1.job
#/bin/bash

# execute these commands
sleep 10
echo "Hello World from `hostname`"
$ . HelloWorld_v1.job
Hello World from hpc1001
$ sbatch -p carl.p HelloWorld_v1.job
Submitted batch job 2582937
$ squeue -u $USER
$ ls
... slurm-2582937.out ...
```

sbatch

- options allow to specify requested resources and other settings
 - options have long formation and sometimes short format as well

```
$ sbatch -p carl.p --time=0:10:00 -o HelloWorld.o%j
HelloWorld_v1.job
Submitted batch job 2582942
$ squeue -u $USER
  JOBID PARTITION      NAME          USER  ST  TIME  NODES NODELIST
  2582942      carl.p HelloWorld lees4820  R  0:03      1 mpcs019
$ ls
. . . HelloWorld.o2582942
$ cat HelloWorld.o2582942
Hello World from mpcs019
$
```

sbatch

- alternatively, sbatch options are specified in job script
 - SLURM options begin with **#SBATCH** (a special comment)
 - then similar to cmd-line option, e.g **#SBATCH -p carl.p**
 - cmd-line options overwrite specifications in script

```
$ sbatch HelloWorld_v2.job  
Submitted batch job 2583091  
$
```

HelloWorld_v2.sge

```
$ cat HelloWorld_v2.job
#!/bin/bash

##### SLURM options begin

### general settings
#SBATCH --partition=carl.p
#SBATCH --job-name=HelloWorld
#SBATCH --output=HelloWorld.o%j

### requested resources
#SBATCH --time=0:10:00      # max runtime
#SBATCH --mem=1G           # max memory

##### SLURM options end

# execute these commands
sleep 10
echo "Hello World from `hostname`"
```

Options for SBATCH

<https://slurm.schedmd.com/sbatch.html>

Option	Short Form	Description
<code>--job-name=JobName</code>	<code>-J JobName</code>	sets a name for job which is display in the queue
<code>--partition=<partition></code>	<code>-p <partition></code>	(comma-separated list of) partition(s) where the job should run, no default
<code>--output=<filename></code> <code>--error=<filename></code>	<code>-o <filename></code> <code>-e <filename></code>	output files for STDOUT and STDERR, default is join in slurm-%j.out
<code>--ntasks=<n></code>	<code>-n <n></code>	number of tasks (e.g. for MPI parallel jobs)
<code>--mem-per-cpu=<m></code>		memory per core/task, optional
<code>--mem=<m></code>		memory per node, exclusive with above
<code>--mail-type=<MT></code> <code>--mail-user=...</code>		mail settings

sbatch

what happens when a job is submitted?

- during the execution of sbatch
 - SLURM makes a copy of your job script (changes after submission have no effect)
 - if SLURM accepts job a job ID is returned
 - SLURM may also reject a job, should return error message
- after execution of sbatch
 - SLURM computes job priority (many factors are counted)
 - places the job in the queue
 - executes the job script when resources become available

Partitions

- in SLURM job limits are defined for each partition
 - partitions know about and manage available resource of the compute nodes
 - other limits (e.g. maximum run time) can be imposed
 - jobs are placed in a partition only if the requested resources fit
 - jobs can be placed in more than one partition (different partitions may have access to different resources)
 - you need to specify at least one partition
 - if you do not specify resources defaults will be used
 - information about partitions (for experts) with scontrol

scontrol

```
$ scontrol show part mpcs.p
PartitionName=mpcs.p AllowGroups=carl,hrz AllowAccounts=ALL
AllowQos=ALL AllocNodes=ALL Default=NO QoS=N/A
DefaultTime=02:00:00 DisableRootJobs=YES ExclusiveUser=NO
TraceTime=0 Hidden=NO MaxNodes=UNLIMITED MaxTime=21-00:00:00
MinNodes=1 LLN=NO MaxCPUsPerNode=24 Nodes=mpcs[001-158]
PriorityJobFactor=1 PriorityTier=1 RootOnly=NO ReqResv=NO
OverSubscribe=NO PreemptMode=OFF State=UP TotalCPUs=3792
TotalNodes=158 SelectTypeParameters=NONE DefMemPerCPU=10375
MaxMemPerNode=249000
```

Partitions

- partitions can be considered job queues
 - each node type has its own partition
 - partitions define the available resources and set defaults

Partition	NodeType	CPUs	Default RunTime	Default Memory	Misc
mpcs.p	MPC-STD	24	2h	10 375M	
mpcl.p	MPC-LOM	24		5 000M	
mpcb.p	MPC-BIG	16		30G	2x GTX 1080 in mpcb[001-4]
mpcp.p	MPC-PP	40		50G	
mpcg.p	MPC-GPU	24		10 375M	1-2x Tesla P100 GPU
carl.p	combines mpcl.p and mpcs.p				

Information about Finished Jobs

- output from job script is written to SLURM output file
 - per default **STDOUT** and **STDERR** are written to the same file
 - default name of output file is **slurm-`<jobid>`.out**
 - behavior can be modified with options **--output** and **--error**
- running and finished jobs can also be analyzed with **sacct**
 - get information about runtime, CPU time, memory usage
 - see https://wiki.hpcuser.uni-oldenburg.de/index.php?title=Information_on_used_Resources

Job Control

- delete a job
 - use `scancel <jobID>`
- change job details
 - in principle e.g. with `scontrol update jobid=<jobid> TimeLimit=0:05:00`
 - limitations on what can be changed, also dependent on state of job
 - examples for possible (and useful) changes:
 - reduce `TimeLimit` (only admins can increase)
 - change `Partition` while job is pending

Practical Part

Practical Part

1. Try the **HelloWorld** Example
2. Use the **sacct** command to analyse job
 - a. Use the job with id **22407526**
 - b. How long was the job running? On which nodes?
 - c. How much memory was used?
 - d. What else can you say about the job?
3. Use the **squeue** and **sinfo** commands to get information about the cluster
 - a. How many jobs are running? How many are pending?
 - b. What is the status of the nodes in the partition **mpc1.p**?