

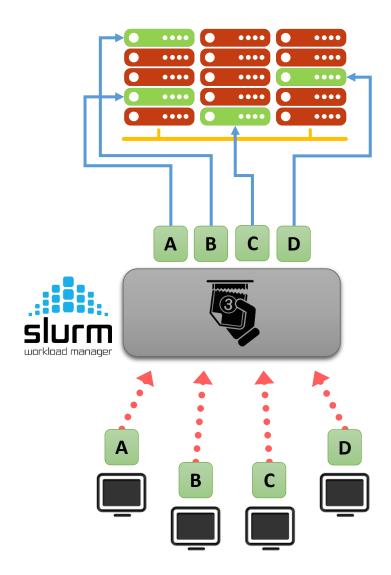




SLURM JOB SCHEDULER

WHAT IS SLURM?

Slurm is an open source cluster management and job scheduling system for Linux clusters.



- 1 Keeps track of available resources on the cluster
- Collects users resources requests for jobs
- 3 Assign priorities to jobs
- Run jobs on assigned compute nodes



PARTITIONS

Compute nodes are grouped into logical sets called **partitions** depending on their hardware characteristics or function:

| • ••• | production (default) | Standard CPU nodes |
|-----------------------------------------|-------------------------|------------------------------------------------------|
| • • • • • • • • • • • • • • • • • • • • | debug | Standard CPU nodes for debug (fast allocation times) |
| • •••• | maxwell | Nodes with Nvidia Maxwell GPUs |
| • • • • • • • • • • • • • • • • • • • • | pascal | Nodes with Nvidia Pascal GPUs |
| • • • • • • • • • • • • • • • • • • • • | mic | Nodes with Intel Xeon Phi cards |



Ask ACCRE if you would like to get access to specific partitions.



JOB EXECUTION WORKFLOW



1. DETERMINE THE RESOURCES NECESSARY FOR THE SPECIFIC JOB



2. CREATE A BATCH JOB SCRIPT



3. SUBMIT THE JOB TO THE SCHEDULER



4. CHECK JOB STATUS



5. RETRIEVE JOB INFORMATION



DETERMINE RESOURCES FOR JOB









- From 1 to the maximum allowed for your group's account.
- Default is one CPU core.





AMOUNT OF MEMORY

- Up to 246 GB per node.
- Default is 1 GB per core.

| GB per node | # nodes |
|-------------|---------|
| 20 | 90 |
| 44 | 45 |
| 58 | 55 |
| 120 | 344 |
| 246 | 44 |



Slurm will immediately kill your job if your process exceeds the requested amount of resources.





Slightly overestimate the requested job resources, but do not greatly overestimate to avoid unnecessary long wait times.







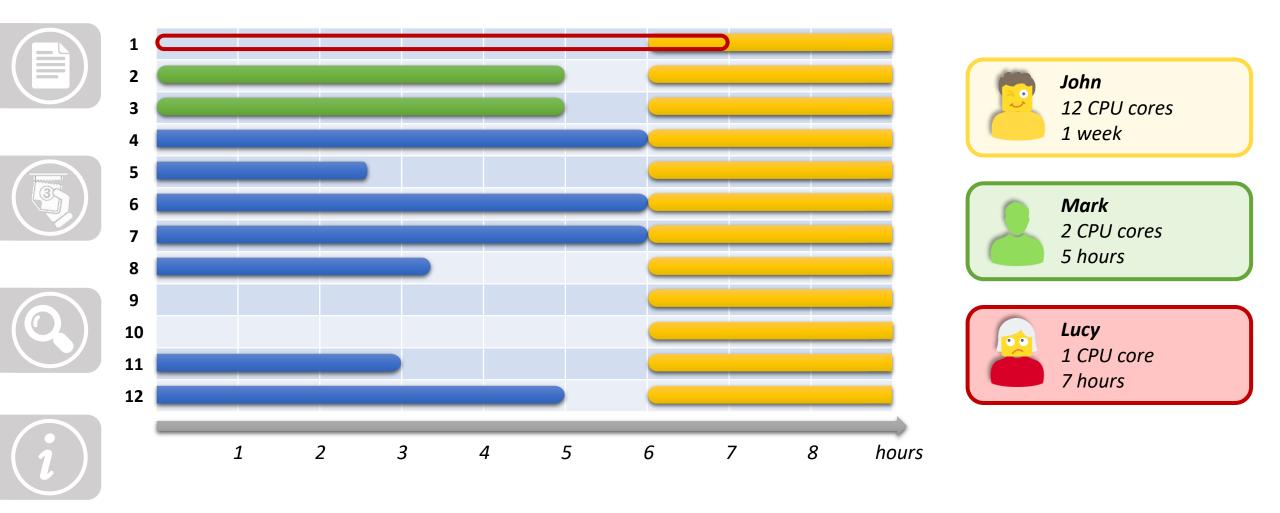
- Job duration on production can be set up to 14 days.
- Default is 15 minutes.
- **DEBUG QUEUE**: max 30 minutes



DETERMINE RESOURCES FOR JOB - BACKFILL



Backfill scheduling will start lower priority jobs if doing so does not delay the expected start time of any higher priority job.



DETERMINE RESOURCES FOR JOB - OPTIMIZATION





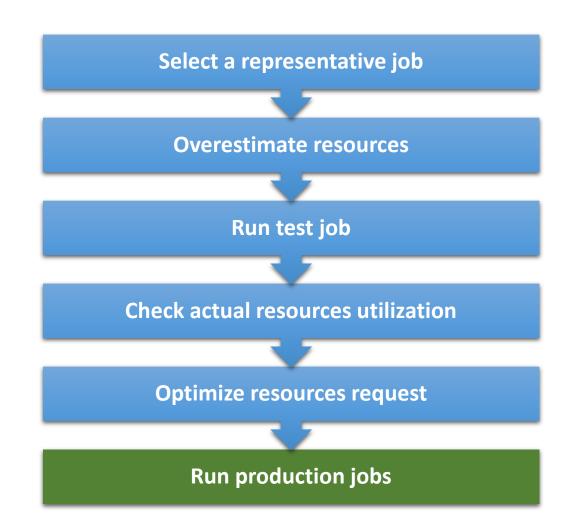
How to define the right amount of resources for my job?

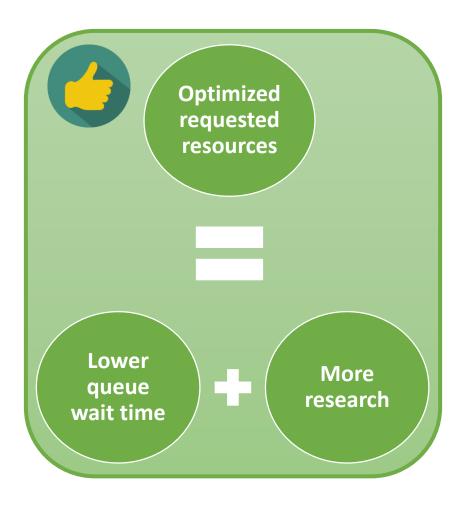












CREATE A BATCH JOB SCRIPT



A **batch job** consists of a sequence of commands listed in a file with the purpose of being executed by the OS as a single instruction.



SHEBANG

- Specify the script interpreter (Bash)
- Must be the first line!



SLURM DIRECTIVES

- Start with "#SBATCH":
 Parsed by Slurm but ignored by Bash.
- Can be separated by spaces.
- Comments between and after directives are allowed.
- Must be before actual commands!



SCRIPT COMMANDS

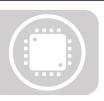
Commands you want to execute on the compute nodes.

myjob.slurm

```
#!/bin/bash
#SBATCH --nodes=1 # Nodes
#SBATCH --ntasks=1
#SBATCH --mem=1G
# Max job duration
#SBATCH --time=1-06:30:00
#SBATCH --job-name=myjob
#SBATCH --output=myjob.out
# Just a comment
setpkgs -a python
./myprogram
```



CREATE A BATCH JOB SCRIPT - THE ESSENTIALS











--nodes=**N**

Request N nodes to be allocated. (Default: N=1)

--ntasks=N

- Request N tasks to be allocated. (Default: N=1)
- Unless otherwise specified, one task maps to one CPU core.

--mem=NG

Request N gigabytes of memory per node. (Default: N=1)

--time=d-hh:mm:ss

• Request d days, hh hours, mm minutes and ss seconds. (Default: 00:15:00)

• Specify a name for the job allocation. (*Default*: batch file name)

- Write the batch script's standard output in the specified file.
- If not specified the output will be saved in the file: slurm-<jobid>.out

CREATE A BATCH JOB SCRIPT - EMAIL NOTIFICATION











- --mail-user=<address>
 - Send email to address.
 - It accepts multiple comma separated addresses.
- --mail-type=<event>

• Define the events for which you want to be notified:

| BEGIN | Job begins |
|---------------|--------------------------------------------|
| END | Job ends |
| FAIL | Job fails |
| ALL | BEGIN+END+FAIL |
| TIME_LIMIT_50 | Elapsed time reaches 50% of allocated time |
| TIME_LIMIT_80 | Elapsed time reaches 80% of allocated time |
| TIME_LIMIT_90 | Elapsed time reaches 90% of allocated time |

SUBMIT JOB TO THE SCHEDULER



sbatch batch_file

- Submit *batch_file* to Slurm.
- If successful, it returns the job ID of the submitted job.



SUBMISSION

Job is added to the queue

PRIORITY

A priority value is assigned to the job.

WAIT

Job waits in queue until:

- Resources are available
- There are no jobs with higher priority in queue

ALLOCATION AND EXECUTION







How do I remove a job from the queue?

scancel jobid

Cancel the job corresponding to the given jobid from the queue.

SUBMIT JOB TO THE SCHEDULER





How is my job's priority calculated?

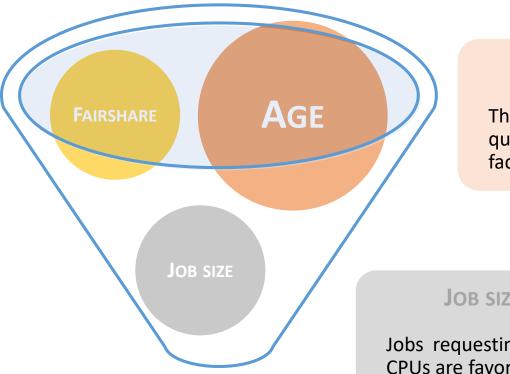


FAIRSHARE

Prioritizes jobs belonging to underserviced accounts.

It reflects:

- 1. The share of resources contributed by your research group.
- historical amount of 2. The computing resources consumed by your account.



PRIORITY

AGE

The longer the job waits in queue, the larger its age factor becomes.

JOB SIZE

Jobs requesting more CPUs are favored.



CHECK JOB STATUS



squeue -u *vunetid*

• Show the queued jobs for user *vunetid*.



| [vanzod@vmps10 ~]\$ squeue -u vanzod | | | | | | | | |
|--------------------------------------|------------|--------------------|--------|----|------------|-------|--------------------|--|
| JOBID | PARTITION | NAME | USER | ST | TIME | NODES | NODELIST(REASON) | |
| 9528424 | production | mdrun 1 | vanzod | R | 1-03:53:33 | 1 | vmp825 | |
| 9528421 | production | mdrun ² | vanzod | PD | 0:00 | 2 | (Priority) | |
| 9528398 | production | mdrun_3 | vanzod | PD | 0:00 | 3 | (AssocGrpCpuLimit) | |



STATUS

R = Running

PD = Pending

CA = Cancelled





NODELIST (REASON)

- For running jobs shows the allocated nodes.
- For pending jobs shows the wait reason:

| Priority | Other jobs in queue have higher priority. | | |
|-------------------|-----------------------------------------------------------------------------------------|--|--|
| Resources | Insufficient resources available on the cluster. | | |
| AssocGrpCpuLimit | Reached maximum number of allocated CPUs by all jobs belonging to the user's account. | | |
| AssocGrpMemLimit | Reached maximum amount of allocated memory by all jobs belonging to the user's account. | | |
| AssocGrpTimeLimit | Reached maximum amount of allocated time by all jobs belonging to the user's account. | | |

RETRIEVE JOB INFORMATION



rtracejob jobid

• Print requested and utilized resources (and more) for the given jobid.









| User: vanzod | JobID: 9837216 |
|------------------|-------------------------|
| Account | l accre |
| Job Name | test job |
| State | Completed |
| Exit Code | 0:0 |
| Wall Time | 3-00:00:00 |
| Requested Memory | 40Gn |
| Memory Used | 40333256K |
| CPUs Requested | 8 |
| CPUs Used | 8 |
| Nodes | j 1 |
| Node List | vmp372 |
| Wait Time | 5.2 minutes |
| Run Time | 452.0 |
| Submit Time | Mon Aug 8 09:14:53 2016 |
| Start Time | Mon Aug |
| End Time | Mon Aug |
| | + |
| Today's Date | Mon Aug |



The used memory may not be an exact value.

Take it with reservations.

JOB ARRAYS

Submit multiple similar jobs with a single job batch script.

To each job within the array is assigned a unique task ID.

--array=start-end[:step][%limit]

- Define task ID interval from *start* to *end* as unsigned integer values.
- The *step* between successive values can be set after colon sign.
- Set the *limit* to the number of simultaneously running jobs with "%".
- Individual task IDs can be specified as a comma separated values list.

$$--array=2,3,6,15 \longrightarrow 2,3,6,15$$



All jobs in a job array must have the same resource requirements.



The maximum array size is **30,000** jobs.



Significantly shorter submission times than submitting jobs individually.

JOB ARRAYS



How to select different input/output for each job in the array?

Use Slurm environment variable:

SLURM_ARRAY_TASK_ID

The task ID for the specific job in the array.

EXECUTED COMMAND

OUTPUT FILE

#!/bin/bash #SBATCH --ntasks=1 #SBATCH --time=00:05:00 #SBATCH --job-name=job_array #SBATCH --array=1-4 #SBATCH --output=job_%A_task_%a.out my_program file_3 my_program file_3 my_program file_3 job_1234567_task_1.out my_program file_1 my_program file_3 my_program file_3 my_program file_4 my_program file_4 my_program file_4

JOB ARRAYS



What if my input files do not have a numerical index?

```
#!/bin/bash
#SBATCH
...

myfile=$( ls DataDir | awk -v line=${SLURM_ARRAY_TASK_ID} '{if (NR==line) print $0}')

my_program ${myfile}
```



- ① Get the list of files names in the data directory in alphabetical order
- Send the list to awk
- Pass the value of the bash variable SLURM_ARRAY_TASK_ID to the awk variable "line"
- Print only the NRth line in the list of files names for which NR corresponds to the job task ID
- Pass the file name in the myfile variable to the main program

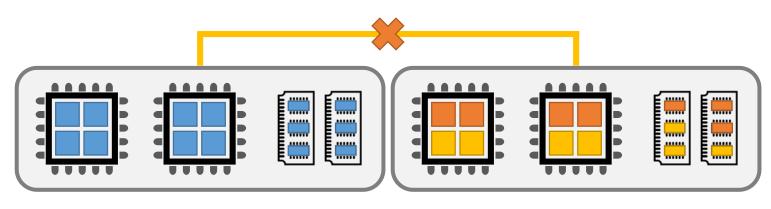
MULTITHREADED JOBS



POSIX THREADS

- Single task with multiple concurrent execution threads.
- Each thread uses a single CPU core.
- All threads share the same allocated memory.

Single node only!



1 node 1 task 8 CPUs per task 1 node 2 tasks 4 CPUs per task

MULTITHREADED JOBS

Request N CPU cores to be allocated <u>for each task</u>.



With OpenMP in your batch script don't forget to set:

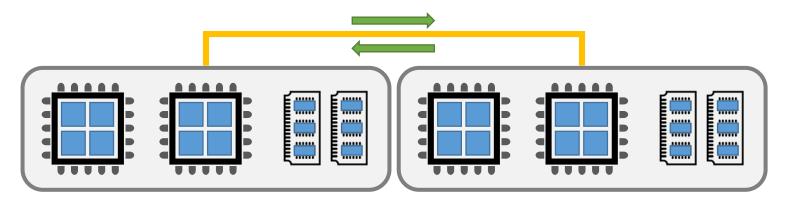
export OMP_NUM_THREADS = \$SLURM_CPUS_PER_TASK

DISTRIBUTED MEMORY JOBS

MESSAGE PASSING INTERFACE (MPI)

- Multiple tasks with private memory allocations.
- Tasks exchange data through communications.
- Tasks can reside on the same node or on multiple nodes.

Single or multiple nodes



2 nodes 8 tasks per node 1 CPU per task

DISTRIBUTED MEMORY JOBS

```
--nodes=N
```

Request N nodes to be allocated.

```
--tasks-per-node=N
```

- Request N tasks per node.
- Unless otherwise specified, one task maps to one CPU core.

In the batch script, run the MPI program with:

```
srun ./program_name
```

Run MPI program called program_name.



Do not use **mpirun** or **mpiexec**! srun will use the correct launcher for the MPI library you selected via setpkgs.



For **OpenMPI** only, add the following flag to srun:

srun --mpi=pmi2 ./program_name

INTERACTIVE SHELL JOB

salloc options

- Obtain job allocation with shell access.
- Accepts all the same *options* previously seen for sbatch.

Gateway

[vanzod@vmps10 ~]\$ salloc --nodes=1 --ntasks=4 --mem=16G --time=1:00:00

Compute node



Recommended for debugging and benchmarking sessions.



Why is my job still pending?

Check overall cluster utilization

Check you account's resources use

Check your account limits

SlurmActive -m mem

- Show the overall cluster utilization.
- Count as available cores only the ones with at least mem amount of memory (in GB). <u>Default</u>: 1GB

| [vanzod@vmps08 ~]\$ SlurmActive -m 10 | | | | | |
|---------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------|--|--|--|
| Standard Nodes Info: | 554 of 567 nodes active 4664 of 5912 processors in use by local jobs 945 of 5912 processors are memory-starved 303 of 5912 available processors | (97.71%) (78.89%) (15.98%) (5.13%) | | | |
| GPU Nodes Info: | Fermi: 40 of 52 GPUs in use Maxwell: 9 of 48 GPUs in use | (76.92%) (18.75%) | | | |
| Phi Nodes Info: | <pre>0 of 2 nodes active 0 of 32 processors in use by local jobs 8 of 32 processors are memory-starved</pre> | | | | |
| ACCRE Cluster Totals: | 567 of 594 nodes active 4769 of 6192 processors in use by local jobs 966 of 6192 processors are memory-starved 457 of 6192 available processors | | | | |
| 3041 running jobs, <u>2</u> 069 | pending jobs, 1 jobs in unrecognized state | | | | |



Why is my job still pending?

Check overall cluster utilization

Check you account's resources use

Check your account limits

qSummary -g group

• Show the total number of jobs and CPU cores allocated or waiting for allocation for the selected *group*.

| [vanzod@vmps09 ~]\$ qSummary -g capra lab GROUP USER ACTIVE_JOBS ACTIVE_CORES PENDING_JOBS PENDING_CORES | | | | | | | |
|-------------------------------------------------------------------------------------------------------------|-----|-----|-----|-----|--|--|--|
| capra_lab | 148 | 203 | 156 | 156 | | | |
| chenl11 | 3 | 10 | 0 | 0 | | | |
| colbrall | 1 | 1 | 0 | 0 | | | |
| fishae | 3 | 3 | 0 | 0 | | | |
| sivleyrm | 125 | 125 | 156 | 156 | | | |
| zhanj10 | 16 | 64 | 0 | 0 | | | |



Why is my job still pending?

Check overall cluster utilization

Check you account's resources use

Check your account limits

showLimits -g group

• Show the cluster resources limits for a specific *group*.



Users in the same group share the same amount of resources.

?

Why did my job fail?

Check the job's output file for error messages.

1

Check with **rtracejob**:

State Exit Code Failed 11:0

A non-zero exit code means your application failed.

Check your Slurm batch job script for syntax or logic errors.