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Running jobs on HPC cluster using SLURM: batch and interactive jobs

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Outline

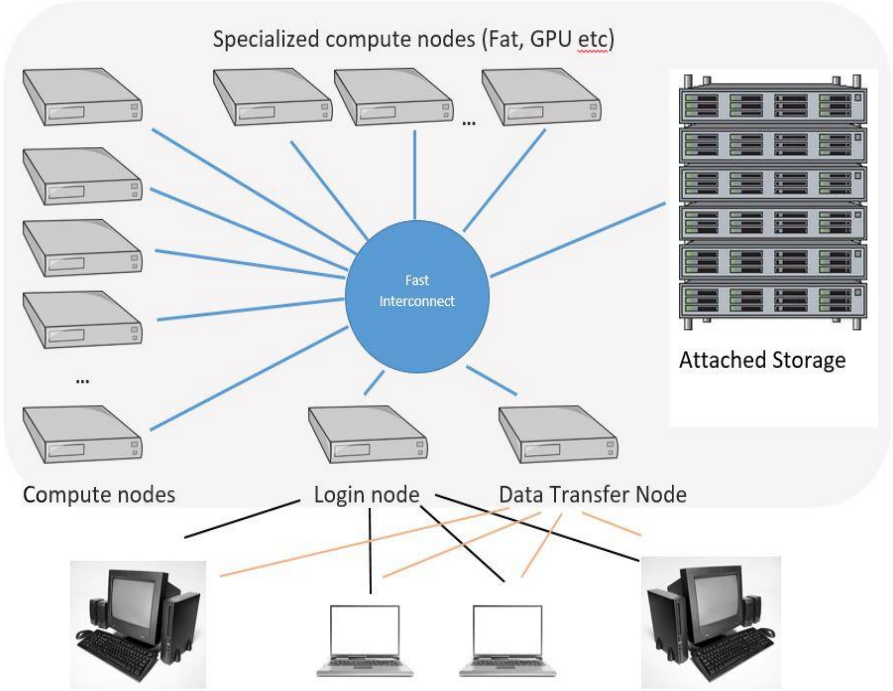
- Interactive work on the login nodes
- SLURM: a scheduler to run jobs on HPC cluster.
  - Interactive jobs via salloc
  - Batch jobs jobs via sbatch
  - What do you need to write and set a job script?
- Exercises:
  - Sleep test job; Serial Job, OpenMP job,
  - MPI Job, GPU job.
- Remarks and conclusions.

Interactive work on the login node

When you connect you get interactive session on a login node:

- Limited resources: to be used with care for basic operations
- editing files, compiling codes, download or transfer data, submit and monitor jobs, run short tests {no memory nor cpu intensive tests}
- Performance can suffer greatly from over-subscription

Recommendation: use the scheduler



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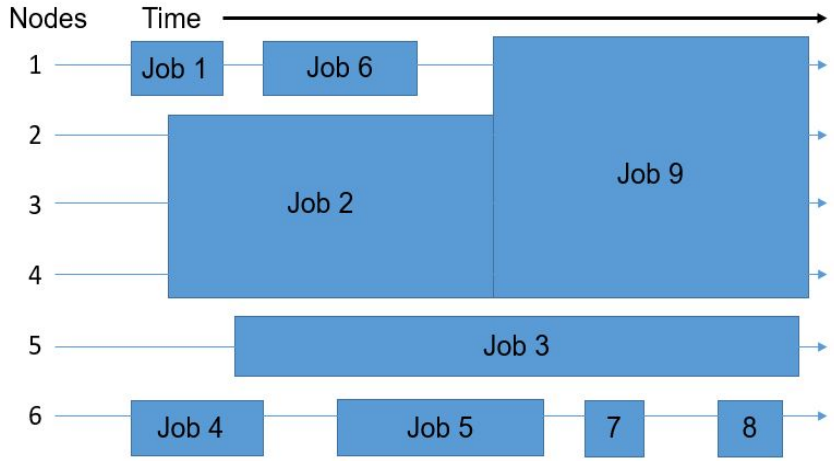
SLURM as a scheduler for HPC clusters

SLURM: Simple Linux Utility for Resource Management

- ➔ free and open-source job scheduler for Linux and Unix-like kernels
- ➔ used by many of the world's supercomputers and computer clusters.

https://slurm.schedmd.com/overview.html

sacct - sacctmgr - salloc - sattach - sbatch - sbcast - scancel - scontrol - sdiag - seff - sinfo - smail - sprio - squeue - sreport - srun - sshare - sstat - strigger - sview



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Interactive and batch jobs

- For interactive test, submit interactive jobs: salloc [+options]
  - SLURM uses salloc to ask for interactive jobs [compute nodes] to test and debug jobs.
  - The jobs will run on compute nodes [CPUs, GPUs]
- Submitting batch jobs for production work: sbatch
  - Wrap commands and resource requests in a "job script": myscript.sh
  - SLURM uses sbatch; submit a job using: sbatch myscript.sh
    sbatch [+options] myscript.sh
- Interactive jobs:
  - salloc [+options]
  - Load modules, run tests, debug, … etc.
  - Run "exit" to exit from the node.
- Batch jobs:
  - Add resources, commands in your script
  - sbatch myscript.sh
  - monitor jobs

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Slurm directives

Interactive jobs:

- salloc [+options]
- Load modules, run tests, debug, …

- - - account=def-sponsor
- - - nodes=1
- - - ntasks=1
- - - cpus-per-task=4
- - - mem=1000M
- - - mem-per-cpu=1000M
- - - time=1-12:30:00
- - - partition=genoa,skylake

Batch jobs:

- Add resources, commands, …
- sbatch [+options] myscript.sh

- #SBATCH - - account=def-sponsor
- #SBATCH - - nodes=1
- #SBATCH - - ntasks=1
- #SBATCH - - cpus-per-task=4
- #SBATCH - - mem=1000M
- #SBATCH - - mem-per-cpu=1000M
- #SBATCH - - time=1-12:30:00
- #SBATCH - - partition=genoa,skylake

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Interactive jobs

```
[~@bison ]$  salloc --cpus-per-task=4 --mem-per-cpu=1000M --time=1:00:00
salloc: using account: def-sponsor
salloc: No partition specified? It is recommended to set one! Will guess
salloc: selected partitions: skylake
salloc: Pending job allocation 6170818
salloc: job 6170818 queued and waiting for resources
salloc: job 6170818 has been allocated resources
salloc: Granted job allocation 6170818
salloc: Nodes n373 are ready for job
[~@n373 ~]$ {load modules, run tests, … etc}
[~@n373 ~]$  exit
exit
salloc: Relinquishing job allocation 6170818
```

Equivalent SLURM: my-script.sh

```
#!/bin/bash
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=4
#SBATCH --mem-per-cpu=1000M
#SBATCH --time=1:00:00
#SBATCH --account=def-someprof

load modules …
Run the code …
```

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Job requirements

What do you need to set your job script?

- What type of program are you going to run?
  - Serial, Threaded [OpenMP], MPI based, Hybrid [MPI+OPenMP], GPU, …
- Prepare your input files: locally or transfer from your computer.
- Test your program:
  - Interactive job via salloc: access to a compute node
  - On login node if the test is not memory nor CPU intensive.
- Prepare a script “my-job-script.sh” with the all requirements:
  - **Memory**, Number of cores, Nodes, Wall time, modules, **partition**, **accounting group**, command line to run the code.
- Submit and monitor your jobs: sbatch, squeue, sacct, seff … etc

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Scheduling jobs: exercises

Directory: jobs

- interactive: directory for interactive test via salloc.
- sleep-job: directory for a sleep job with defaults parameters.
- serial-job: directory for a serial job: 1 CPU.
- openmp-job: directory for a job with OpenMP support.
- mpi-job: directory for a job with MPI support.
- gpu-job: directory for a GPU job

- oom-kill: directory for a job killed with oom-kill event.
- time-out: directory for a job that times out.

- job-array-job: directory for an example with arrays.
- glost: directory for job farming with glost.

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Concluding remarks

The key is to know what resources are available on a given HPC machine, and how to use them efficiently [adjust resources where needed]:

- ➔ It is up to the users to go through the documentation and run tests, …
- ➔ Monitor the jobs for efficiency [seff, sacct, reportseff, …]
- ➔ Know what partitions are there, and what are their limits: sinfo, …
- ➔ Know about the hardware (how many CPUs per node, how much memory per CPU available, ….) documentation for each cluster.
- ➔ Know if your code is efficient for a given set of resources: benchmarks
- ➔ Know time limits and estimate runtime of your jobs
  - ◆ comes after some trials and errors [with experience].
- ➔ Make sure your application obeys the SLURM resource limits

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More readings

Grex:

- https://um-grex.github.io/grex-docs/start-guide/
- https://um-grex.github.io/grex-docs/running-jobs/
- https://um-grex.github.io/grex-docs/running-jobs/slurm-partitions/

Alliance clusters:

- https://docs.alliancecan.ca/wiki/Running_jobs
- https://docs.alliancecan.ca/wiki/Advanced_MPI_scheduling/en
- https://docs.alliancecan.ca/wiki/Using_GPUs_with_Slurm/en
- https://docs.alliancecan.ca/wiki/Using_node-local_storage

Thank you for your attention

Any question?

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Additional Slides

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Examples of job scripts

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Slurm most used commands

- ★ salloc: submit interactive jobs.
- ★ sbatch: submit batch jobs to compute nodes.
- ★ scontrol: list and/or change parameters for jobs, partitions, ...
- ★ scancel: cancel submitted jobs
- ★ sacct: reports about jobs
- ★ seff: reports resources used about a given job.
- ★ sinfo: check the nodes (idle, drain, down), …
- ★ sprio: check the priority
- ★ squeue: list the jobs on the queue
- ★ srun: used to run MPI jobs (mpiexec, mpirun still work)
- ★ sshare: check the recent usage and LevelFS

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Slurm template

```
#!/bin/bash

#SBATCH --account=def-somegroup

{Add the resources and some options}


echo "Current working directory is `pwd`"
echo "Starting run at: `date`"

{Load appropriate modules if needed}
{Command line to run the program}


echo "Program finished with exit code $? at: `date`"
```

Script: test-job.sh

Parameters to adjust for each type of job to submit: serial, OpenMP, MPI, GPU

Default parameters:

- CPUs: 1
- Time: 0-3:00
- Memory: 256mb?

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Slurm accounting groups

```
salloc --ntasks=1 --mem=4000M --account=def-prof1
```

➔ Submit Interactive job:

```
[~yak ]$  salloc --ntasks=1 --mem=4000M
salloc: error: ----------------------------------------
salloc: error: You have more than one account:
salloc: error:  - account # 1: use sbatch/salloc --account=def-prof1
salloc: error:  - account # 2: use sbatch/salloc --account=def-prof2
salloc: error: Please pick one 'sbatch/salloc --account=_VALUE_' option from the list above ^^^
salloc: error: Or set 'export SBATCH_ACCOUNT=_VALUE_' (or 'export
SALLOC_ACCOUNT=_VALUE_') to one of the above accounts
salloc: error: Job submit/allocate failed: Invalid account or account/partition combination specified
```

➔ Accounting groups: sshare -U --user <username>

- if one accounting group, SLURM will take it by default.
- If more than one, it should be specified via: --account={your accounting group}

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Slurm: most used directives

#SBATCH --account=def-someprof	Use the accounting group def-someprof for jobs.
#SBATCH --ntasks=8	Request 8 tasks for MPI job; 1 for serial or OpenMP
#SBATCH --cpus-per-task=4	Number of threads (OpenMP); Threaded application
#SBATCH --ntasks-per-node=4	Request 4 tasks per-node for MPI job
#SBATCH --nodes=2	–nodes=<Min>-<Max> Request 2 nodes
#SBATCH --mem=1500M	Memory of 1500M for the job
#SBATCH --mem-per-cpu=2000M	Memory of 2000M per CPU
#SBATCH --partition=genoa	**GREX:** Partition name: skylake, largemem, genoa, gpu, test
#SBATCH --time=3-00:00:00	Wall time in the format: DD-HH:MM:SS

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Slurm: environment variables

SLURM_JOB_NAME	User specified job name
SLURM_JOB_ID	Unique slurm job id
SLURM_NNODES	Number of nodes allocated to the job
SLURM_NTASKS	Number of tasks allocated to the job
SLURM_ARRAY_TASK_ID	Array index for this job
SLURM_ARRAY_TASK_MAX	Total number of array indexes for this job: --array=0-999%10
SLURM_CPUS_PER_TASK	Number of threads {OpenMP: OMP_NUM_THREADS}
SLURM_JOB_NODELIST	List of nodes on which resources are allocated to a Job
SLURM_JOB_ACCOUNT	Accounting group under which this job is running.
SLURM_JOB_PARTITION	List of Partition(s) that the job is in.

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Slurm script: serial job

```
#!/bin/bash
#SBATCH --account=def-someprof
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=1
#SBATCH --mem-per-cpu=2500M
#SBATCH --time=1-00:00:00
#SBATCH --partition=genoa

# Load appropriate modules:
module load <dep> <software>/<version>
echo "Starting run at: `date`"
program.x [+options and arguments if any]
echo "Program finished with exit code $? at: `date`"
```

SLURM directives:

- Default: 1 core, 256mb, 3 hours
- **account**, tasks = 1, memory per core, wall time, **partition**, …
- Other: E-mail-notification, … etc.

Submit and monitor the job:

- sbatch [+options] myscript.sh
- squeue -u $USER; sq; sacct -j JOB_ID

More information:

- partition-list; sinfo --format="%20P"
- Sinfo -s; sinfo -p genoa,skylake
- squeue -p genoa,skylake -t R {PD}

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Slurm script: OpenMP

```
#!/bin/bash
#SBATCH --account=def-someprof
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=4
#SBATCH --mem-per-cpu=2000M
#SBATCH --time=1-00:00:00
#SBATCH --partition=skylake
# Load appropriate modules:
module load <software>/<version>
export OMP_NUM_THREADS=${SLURM_CPUS_PER_TASK}
echo "Starting run at: `date`"
program.x [+options and arguments if any]
echo "Program finished with exit code $? at: `date`"
```

```
#!/bin/bash
#SBATCH --account=def-someprof
#SBATCH --cpus-per-task=4
#SBATCH --mem-per-cpu=2000M
#SBATCH --time=1-00:00:00
#SBATCH --partition=skylake
```

```
#SBATCH --cpus-per-task=N
#SBATCH --mem=<MEM>
```

Partitions:

- genoa: N up to 192
- skylake: N up to 52
- largemem: N up to 40

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Slurm script: MPI job

```
#!/bin/bash
#SBATCH --account=def-someprof
#SBATCH --nodes=2-4
#SBATCH --ntasks=96
#SBATCH --mem-per-cpu=1200M
#SBATCH --time=2-00:00:00
#SBATCH --partition=skylake
# Load appropriate modules:
module load arch/avx512  gcc/13.2.0  openmpi/4.1.6
lammps/2024-08-29p1
echo "Starting run at: `date`"
srun lmp -in  in.lammps
echo "Program finished with exit code $? at: `date`"
```

```
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=192
#SBATCH --mem=0
#SBATCH --partition=genoa
```

```
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=52
#SBATCH --mem=0
#SBATCH --partition=skylake
```

```
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=40
#SBATCH --mem=0
#SBATCH --partition=largemem
```

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Slurm script: MPI+OpenMP job

```
#!/bin/bash
#SBATCH --account=def-someprof
#SBATCH --nodes=4
#SBATCH --ntasks-per-node=6
#SBATCH --cpus-per-task=2
#SBATCH --mem-per-cpu=1200M
#SBATCH --time=3-00:00:00
#SBATCH --partition=skylake

# Load appropriate modules:
module load <dependencies> <software>/<version>
export OMP_NUM_THREADS=${SLURM_CPUS_PER_TASK}
echo "Starting run at: `date`"
srun program.x [+options and arguments if any]
echo "Program finished with exit code $? at: `date`"
```

```
#SBATCH --nodes=6
#SBATCH --ntasks-per-node=4
#SBATCH --cpus-per-task=2
#SBATCH --mem-per-cpu=1200M
#SBATCH --partition=genoa
```

The total memory and CPUs per node should not exceed the available resources on the nodes.

```
#SBATCH --nodes=5
#SBATCH --ntasks-per-node=8
#SBATCH --cpus-per-task=4
#SBATCH --mem-per-cpu=1000M
#SBATCH --partition=skylake
```

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Slurm script: GPU job

```
#!/bin/bash
#SBATCH --account=def-someprof
#SBATCH --gpu=1
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=6
#SBATCH --mem-per-cpu=4000M
#SBATCH --time=0-3:00:00
#SBATCH --partition=gpu
# Load appropriate modules:
module load <software>/<version>
echo "Starting run at: `date`"
program.x [+options and arguments if any]
echo "Program finished with exit code $? at: `date`"
```

SLURM directives:

- Default: 1 core, 256mb, 3 hours
- **account**, number of tasks, memory per core, wall time, **partition**, …
- Other: E-mail-notification, … etc.

Submit and monitor the job:

- sbatch [+options] myscript.sh
- squeue -u $USER

Partition:

- partition-list; sinfo --format="%20P"
- sinfo -p <partition name>

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Slurm script: Job Array

```
#!/bin/bash
#SBATCH --account=def-someprof
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=1
#SBATCH --mem-per-cpu=2500M
#SBATCH --time=3-00:00:00
#SBATCH --array=0-999%10
#SBATCH --partition=genoa
# Load appropriate modules:
module load <software>/<version>
echo "Starting run at: `date`"
./my_code test${SLURM_ARRAY_TASK_ID}
echo "Program finished with exit code $? at: `date`"
```

- ★ You have regularly named, independent datasets (test0, test1, test2, test3, …, test999) to process with a single software code
- ★ Instead of making and submitting 1000 job scripts, a single script can be used with the **--array=0-999** option to **sbatch**
- ★ Within the job script, $SLURM_ARRAY_TASK_ID can be used to pick an array element to process

  ./my_code test${SLURM_ARRAY_TASK_ID}
- ★ When submitted, once, the script will create 1000 jobs with the index added to JobID (12345_1, … , 12345_999)
- ★ You can use usual SLURM commands (scancel, scontrol, squeue) on either entire array or on its individual elements

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Bundle many jobs: Job Arrays

- Files: in.melt-0.txt, …. in.melt-9.txt; array with 10 elements; Run a maximum of 2 at a time
- All the data in one directory: use appropriate names to avoid data overlapping

```
lmp < in.melt-${SLURM_ARRAY_TASK_ID}.txt > log_lammps_array-${SLURM_ARRAY_TASK_ID}.txt
```

- ➔ Directories: 0, …. 9; each directory has a an input file: in.melt
- ➔ Job array with 10 elements
- ➔ Run a maximum of 2 at a time
- ➔ Output in different directories: the data may have the same name.

```
cd ${SLURM_ARRAY_TASK_ID}
lmp < in.melt > log_lammps_array-${SLURM_ARRAY_TASK_ID}.txt
```

https://docs.alliancecan.ca/wiki/Job_arrays/en
https://um-grex.github.io/grex-docs/running-jobs/batch-jobs/#job-arrays

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Bundle many jobs: GLOST

```
#!/bin/bash
#SBATCH --account=def-someprof
#SBATCH --ntasks=4
#SBATCH --mem-per-cpu=2500M
#SBATCH --time=1-00:00:00
#SBATCH --partition=genoa

# Load appropriate modules + glost:
module load arch/avx512  gcc/13.2.0
openmpi/4.1.6 glost/0.3.1
echo "Starting run at: `date`"
srun glost_launch list_glost_tasks.txt
echo "Program finished with exit code $? at: `date`"
```

- You have many short independent jobs (job1, job2, job3, …) to process with a single software code.
- Instead of submitting and running many jobs, a single script can be used to run these jobs as MPI job.

- List of tasks: list_glost_tasks.txt

```
job1
job2
job3
job4
–
–
job199
job200
```

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Estimating resources

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What resources to ask for?

- CPUs:
  - How many CPUs are required to run a particular job?
- Memory
  - How much memory is needed to run a particular job?
- Time
  - How to estimate the run time for run a particular job?
- GPUs
  - Could I run my job on a GPU?

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Jobs optimization

Estimate the resources for your jobs:

- Number of CPUs: serial, OpenMP, MPI
- Memory: total memory or memory per core
- Run time

➔ Use interactive jobs

➔ Submit test jobs:

  ❖ Run a benchmark if needed {OpenMP; MPI jobs, Hybrid}

➔ Collect the stats about memory usage, wall time, .. etc.

➔ Adjust your scripts for similar jobs

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Estimating the resources: CPU

- How to estimate the CPU resources?
  - No direct answer: it depends on the code
  - Serial code: 1 core [--ntasks=1 --mem=2500M]
  - Threaded and OpenMP: no more than available cores on a node [--cpus-per-task=X]
  - MPI jobs: can run across the nodes [--nodes=2 --ntasks-per-node=52 --mem=0].
- Are threaded jobs very efficient?
  - Depends on how the code is written
  - Does not scale very well

  Run a benchmark and compare the performance and efficiency.
- Are MPI jobs very efficient?
  - Scale very well with the problem size.
  - Limited number of cores for small size: when using domain decomposition

  Run a benchmark and compare the efficiency.

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Estimating the resources: Memory

- How to estimate the memory for my job?
  - No direct answer: it depends on the code
  - Java applications require more memory in general
  - Hard to estimate the memory when running R, Python, Perl, …
- To estimate the memory, run tests:
  - Interactive job, ssh to the node and run top -u $USER {-H}
  - Start smaller and increase the memory
  - Use whole memory of the node; seff <JOBID>; then adjust for similar jobs
  - MPI jobs can aggregate more memory when increasing the number of cores
- What are the best practices for evaluation the memory:
  - Run tests and see how much memory is used for your jobs {seff; sacct}
  - **Do not oversubscribe the memory** since it will affect the usage and the waiting time: accounting group charged for resources reserved and not used properly.

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Estimating the resources: Wall Time

```
[~@bison ]$  seff 5080534
Job ID: 5080534
Cluster: grex
User/Group: someuser/someuser
State: COMPLETED (exit code 0)
Cores: 1
CPU Utilized: 01:28:33
CPU Efficiency: 99.87% of 01:28:40
core-walltime
Job Wall-clock time: 01:28:40
Memory Utilized: 274.48 MB
Memory Efficiency: 3.43% of 7.81 GB
```

- ➔ Job completed
- ➔ CPU Efficiency: 99.87%
- ➔ Wall time: 01:28:40
- ➔ Memory Utilized: 274.48 MB

Steps: 10000 (iterations)
Wall time: 1:30 to 2:00
Memory: 300 mb to 400 mb

Steps: 10000 x 10
Wall time: {1:30 to 2:00} x 10
Memory: 300 mb to 400 mb

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Optimizing jobs: Memory and CPU

- How to estimate the run time for my job?
  - No direct answer: it depends on the job and the problem size
  - See if the code can use checkpoints
  - For linear problems: use a small set; then estimate the run time accordingly if you use more steps (extrapolate).
- To estimate the time, run tests:
  - Over-estimate the time for the first tests and adjust for similar jobs and problem size.
- What are the best practices for time used to run jobs?
  - Have a good estimation of the run time after multiple tests.
  - Analyse the time used for previous successful jobs.
  - Add a margin of 15 to 20 % of that time to be sure that the jobs will finish.
  - Do not overestimate the wall time since it will affect the start time depending on the limits sets on the cluster: partition, GrpTRESRunMins, …

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Monitor and get more information about jobs, partitions, … etc

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Scheduling policies

- There is a policing engine, the Scheduler, in SLURM that will enforce priorities, allocations, and limits {per user, group, partitions, …}.
- Limits can be per User or Group, in the form of Maximum Walltime, Max number of jobs per User, … etc.

- Limits can be per Partition {for example max WallTime}.
- Limits can be per QoS policy (not used on Grex or CC)

- Priorities are set based on allocation values and recent usage and waiting time in the queue. Priorities is what determines which job can run first (if not blocked by a given limit).

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Monitor and control jobs

```
squeue -u $USER [-t RUNNING] [-t PENDING]                    # list all current jobs.
squeue -p PartitionName [genoa, skylake, largemem]           # list all jobs in a partition.
sinfo --format="%P"                                          # view information about Slurm partitions.
sacct -j jobID --format=JobID,MaxRSS,Elapsed                 # resources used by completed job.
sacct -u $USER --format=JobID,JobName,AveCPU,MaxRSS,MaxVMSize,Elapsed
seff  -d jobID                                               # produce a detailed usage/efficiency report for the job.
sprio [-j jobID1,jobID2] [-u $USER]                          # list job priority information.
sshare -U --user $USER                                       # show usage info for user.
sinfo --state=idle; -s; -p <partition>                       # show idle nodes; more about partitions.
scancel [-t PENDING] [-u $USER] [jobID]                      # kill/cancel jobs.
scontrol show job -dd jobID                                  #show more information about the job.
```

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Memory and CPU efficiencies: seff

Output from seff command for a job {OpenMP} that asked for 24 CPUs and 187 GB of memory on cedar:

Job ID: 123456789
Cluster: cedar
User/Group: someuser/someuser
State: COMPLETED (exit code 0)
Nodes: 1
Cores per node: 24
CPU Utilized: 38-14:26:22
CPU Efficiency: 38.46% of 100-08:45:36 core-walltime
Job Wall-clock time: 4-04:21:54
Memory Utilized: 26.86 GB
Memory Efficiency: 14.37% of 187.00 GB

Successful job

Low CPU efficiency: 40 %
Better performance with 8 CPU

Used less memory: 15 %

billing=46,cpu=24,mem=187G,node=1

Optimization:
Better performance with 8 CPU
Memory: 4000 M per core [32 GB]

```
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=8
#SBATCH --mem-per-cpu=4000M
```

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Memory and CPU efficiencies: reportseff

```
[~@yak ~]$  reportseff -u someuser -s COMPLETED
   JobID    State                Elapsed  TimeEff   CPUEff   MemEff
 6865022  COMPLETED             00:01:26     0.0%     9.9%     0.9%
 6866046  COMPLETED           1-17:11:47     8.2%     8.8%     3.4%
 6866067  COMPLETED             22:12:02     4.4%    11.0%     3.8%
 6866070  COMPLETED           1-18:06:54     8.4%    10.9%     3.8%
 6866074  COMPLETED           2-16:58:29    12.9%    10.9%     3.8%
 6866078  COMPLETED           3-14:49:23    17.2%    10.9%     2.7%
 6866082  COMPLETED           2-17:31:19    13.0%    10.9%     2.7%
 6868344  COMPLETED           1-14:49:19     7.7%     8.7%     4.3%
```

```
[~@yak ~]$ reportseff -u someuser -s COMPLETED
[~@yak ~]$ reportseff -u someuser --partition skylake -s COMPLETED
[~@yak ~]$ reportseff <JOB_ID>
[~@yak ~]$ reportseff --help
```

https://github.com/troycomi/reportseff

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SLURM messages

- None: the job is running (ST=R)
- PartitionDown: one or more partitions are down (the scheduler is paused)
- Resources: the resources are not available for this job at this time
- Nodes required for job are DOWN, DRAINED or RESERVED for jobs in higher priority partitions: similar to Resources.
- Priority: the job did not start because of the low priority due to a recent usage.
- Dependency: the job did not start because it depends on another job that is not done yet.
- JobArrayTaskLimit: the user exceeded the maximum size of array jobs
  - [~@yak ~]$ scontrol show config | grep MaxArraySize
    MaxArraySize = 2000
- ReqNodeNotAvail, UnavailableNodes: n410: node not available

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SLURM messages: Reason

None: the job is running (ST=R)
PartitionDown: one or more partitions are down (the scheduler is paused)
Resources: the resources are not available for this job at this time
Nodes required for job are DOWN, DRAINED or RESERVED for jobs in higher priority partitions: similar to Resources.
Priority: the job did not start because of the low priority
Dependency: the job did not start because it depends on another job that is not done yet.
JobArrayTaskLimit: the user exceeded the maximum size of array jobs

[~@fir]$ cat /etc/slurm/slurm.conf | grep MaxArraySize
MaxArraySize=10000 (not the same on other clusters)
ReqNodeNotAvail, UnavailableNodes:fc931: node not available

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Information about the cluster

- sinfo: check the nodes (idle, drain, down), …
  - sinfo --state=idle {shows idle nodes on the cluster}
  - sinfo --R {shows down, drained and draining nodes and their reason}
  - sinfo --Node --long {shows more detailed information}
  - sinfo --p largemem {shows more detailed information}
- scontrol: to see reservations and more

```
[~@narval2: ~]$ scontrol show res
ReservationName=MAINT20251021 StartTime=2025-10-21T08:00:00 EndTime=2025-10-28T08:00:00
Duration=7-00:00:00

Nodes=nc[10101-10156,31401-31433],ng[10101-10104,,20401-20404,20501-20504,20601-20604,30801-30811,,31
301-31305,31401-31402],nl[1001-11003,31001-31002,31101-31103,31201] NodeCnt=1442 CoreCnt=89760
Features=(null) PartitionName=(null) Flags=MAINT,IGNORE_JOBS,SPEC_NODES,ALL_NODES
   TRES=cpu=89760
   Users=root Groups=(null) Accounts=(null) Licenses=(null) State=INACTIVE BurstBuffer=(null) Watts=n/a
   MaxStartDelay=(null)
```

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Information about a partition

```
[~@bison ~]$  sinfo -p largemem
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
largemem       up 14-00:00:0  5      mix n[328-331,333]
largemem       up 14-00:00:0  6  alloc n[326-327,334-337]
largemem       up 14-00:00:0  1   idle n332
```

```
[~@bison ~]$  scontrol show partition largemem --oneliner
PartitionName=largemem AllowGroups=ALL AllowAccounts=ALL AllowQos=normal,high
AllocNodes=aurochs,tatanka,bison,wisent,yak,n[001-316],g32[1-5],g338,g383,n[326-337],n[33
9-381] Default=NO QoS=N/A DefaultTime=03:00:00 DisableRootJobs=NO ExclusiveUser=NO
GraceTime=0 Hidden=NO MaxNodes=UNLIMITED MaxTime=14-00:00:00 MinNodes=0
LLN=NO MaxCPUsPerNode=UNLIMITED Nodes=n[326-337] PriorityJobFactor=0
PriorityTier=1 RootOnly=NO ReqResv=NO OverSubscribe=NO OverTimeLimit=NONE
PreemptMode=OFF State=UP TotalCPUs=480 TotalNodes=12 SelectTypeParameters=NONE
JobDefaults=(null) DefMemPerCPU=7000 MaxMemPerNode=UNLIMITED
TRESBillingWeights=CPU=2.0,Mem=0
```

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Information about queued jobs

```
[~@bison ~]$ squeue

[~@bison ~]$ squeue -u $USER

[~@bison ~]$ sq

[~@bison ~]$ squeue -u <someuser>

[~@bison ~]$ squeue -t R

[~@bison ~]$ squeue -t PD

[~@bison ~]$ squeue -p genoa,skylake -t R

[~@bison ~]$ squeue -j <jobid>
```

Monitor queued jobs:

- Per user
- Job ID
- Per partition
- Running jobs
- Pending job
- Combine two or more from the above.
- .. etc.

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Information about queued jobs: scontrol

```
[~@bison ~]$ scontrol show job 1234567 --oneliner
JobId=1234567 JobName=run-lmp-serial.sh UserId=someuser(3333333)
GroupId=someuser(3333333) MCS_label=N/A Priority=491351 Nice=0 Account=def-someprof
QOS=normal JobState=RUNNING Reason=None Dependency=(null) Requeue=0 Restarts=0
BatchFlag=1 Reboot=0 ExitCode=0:0 RunTime=01:23:18 TimeLimit=12:00:00 TimeMin=N/A
SubmitTime=2023-11-03T09:26:35 EligibleTime=2023-11-03T09:26:35
AccrueTime=2023-11-03T09:26:35 StartTime=2023-11-03T09:26:51 EndTime=2023-11-03T21:26:51
Deadline=N/A SuspendTime=None SecsPreSuspend=0 LastSchedEval=2023-11-03T09:26:51
Scheduler=Backfill Partition=compute AllocNode:Sid=yak:174565 ReqNodeList=(null)
ExcNodeList=(null) NodeList=n204 BatchHost=n204 NumNodes=1 NumCPUs=1 NumTasks=1
CPUs/Task=1 ReqB:S:C:T=0:0:*:* TRES=cpu=1,mem=4000M,node=1 Socks/Node=*
NtasksPerN:B:S:C=0:0:*:* CoreSpec=* MinCPUsNode=1 MinMemoryCPU=4000M
MinTmpDiskNode=0 Features=(null) DelayBoot=00:00:00 OverSubscribe=OK Contiguous=0
Licenses=(null) Network=(null) Command=/home/someuser/Workshop/Serial_Job/run-lmp-serial.sh
WorkDir=/home/someuser/Serial_Job StdErr=/home/someuser/Serial_Job/slurm-1234567.out
StdIn=/dev/null StdOut=/home/someuser/Serial_Job/slurm-1234567.out Power=
```

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Jobs and nodes by partition

```
[~@bison ~]$  squeue -p skylake
[~@bison ~]$  squeue -p skylake -t PD
[~@bison ~]$  squeue -p skylake -t R

[~@biison ~]$  sinfo -p skylake
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
skylake    up 21-00:00:0  1  inval n349
skylake    up 21-00:00:0  3  down* n[352,359-360]
skylake    up 21-00:00:0  1  drain n375
skylake    up 21-00:00:0  26    mix n[339-342,346-347,350-351,356-358,366-374,376-381]
skylake    up 21-00:00:0  12  alloc n[343-345,348,353-355,361-365

[~@bison ~]$  sinfo -p skylake --state=down
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
skylake    up 21-00:00:0  3  down* n[352,359-360]
```

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How to get most of the scheduler?

The key is to know what resources are available on a given HPC machine, and to adjust your requests accordingly.

- ➔ It is up to the users to go through the documentation and run tests, …
- ➔ Know what partitions are there, and what are their limits: sinfo, …
- ➔ Know about the hardware (how many CPUs per node, how much memory per CPU available, …. documentation for each cluster
- ➔ Know if your code is efficient for a given set of resources: benchmarks
- ➔ Know time limits and estimate runtime of your jobs
  - ◆ comes after some trials and errors, with experience
- ➔ Make sure your application obeys the SLURM resource limits

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Custom script: partition-list

sinfo -se --format=" %10P %.10A %.12l %.6a %.17C %.8m [%.18G]"

```
PARTITION  NODES(A/I)    TIMELIMIT  AVAIL     CPUS(A/I/O/T)   MEMORY [              GRES]
skylake*       22/20  21-00:00:00     up  650/1534/52/2236   186000 [            (null)]
chrim            4/0  21-00:00:00     up      80/688/0/768   750000 [            (null)]
chrimlm          1/0  21-00:00:00     up      144/48/0/192  1500000 [            (null)]
genlm            3/0  21-00:00:00     up      19/557/0/576  1500000 [            (null)]
genoa            9/18 21-00:00:00     up   326/4858/0/5184   750000 [            (null)]
genoacpu-b       4/0   7-00:00:00     up      80/688/0/768   750000 [            (null)]
genoacpu-b       1/0   7-00:00:00     up      144/48/0/192  1500000 [            (null)]
genoacpu-b       1/4   7-00:00:00     up     160/680/0/840  1500000 [            (null)]
largemem        11/0   21-00:00:00    up    147/293/40/480   381500 [            (null)]
mcordcpu         1/4   21-00:00:00    up     160/680/0/840  1500000 [            (null)]
agro             0/2   21-00:00:00    up         0/48/0/48   248000 [    gpu:a30:2(S:0)]
agro-b           0/2   7-00:00:00     up         0/48/0/48   248000 [    gpu:a30:2(S:0)]
gpu              1/1   7-00:00:00     up        32/32/0/64   191000 [ gpu:v100:4(S:0-1)]
lgpu             0/1   3-00:00:00     up         0/64/0/64   381500 [ gpu:l40s:2(S:0-1)]
livi             0/1   21-00:00:00    up         0/48/0/48  1500000 [gpu:v100:16(S:0-1)]
livi-b           0/1   7-00:00:00     up         0/48/0/48  1500000 [gpu:v100:16(S:0-1)]
mcordgpu         0/2   21-00:00:00    up         0/64/0/64   495000 [    gpu:a30:4(S:0)]
mcordgpu-b       0/2   7-00:00:00     up         0/64/0/64   495000 [    gpu:a30:4(S:0)]
stamps           1/2   21-00:00:00    up         8/88/0/96   191000 [ gpu:v100:4(S:0-1)]
stamps-b         1/2   7-00:00:00     up         8/88/0/96   191000 [ gpu:v100:4(S:0-1)]
test             0/1     23:00:00     up         0/18/0/18   509000 [            (null)]
```