How to submit a job via Slurm on an HPC cluster

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Introduction to Slurm

HPC Scheduling

Why is scheduling needed on the “Aristotle” cluster?

1. Share finite resources among multiple users
2. Manage allocation of resources in a distributed heterogeneous environment
3. Bookkeeping, efficieny monitoring, statistics

Slurm Workload Manager

- Slurm is a scheduling and workload management system for HPC environments
- Functions of Slurm
  1. Allocates and manages exclusive users access to cluster resources
  2. Provides a framework for job tracking and parallel job execution
  3. Arbitrates contention by queuing pending work

`https://slurm.schedmd.com/quickstart.html`

Using Slurm to Access HPC Resources

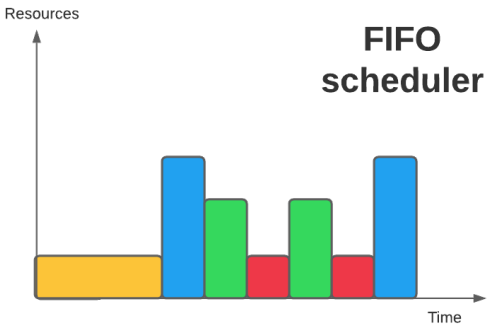
1. Users can schedule work to be executed on the cluster by submitting **jobs** to Slurm.
2. Jobs submissions include a user-defined specification of the **resources** required for the workload associated to the job.
3. Slurm will **queue** jobs and schedule them for execution when the requested resources become available.

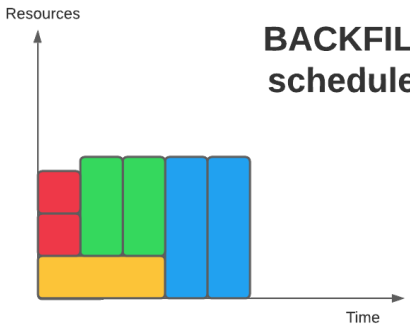
Slurm's Scheduling Algorithm

- Multifactor Priorities
  1. Age: time a job has spent in queue
  2. Size: quantity of resources requested (e.g. CPU cores, time)
  3. Fair share: decreases per user priority proportional to recently allocated resources
- Backfill Scheduling
  1. Highest Priority First Scheduling
  2. Start lower priority jobs *only* if it does not impact the *expected start time* of any higher priority jobs

  Links:
  - Fair Share `https://slurm.schedmd.com/fair_tree.html`
  - Backfill `https://slurm.schedmd.com/sched_config.html#backfill`

Slurm's Scheduling Algorithm





Slurm Examples

Getting to know Slurm

- `sinfo` Show status of available partitions
- `sinfo -N --long` Show node status
- `squeue` Show status of running and queued jobs
  - `-u <username>` Filter results for one user
  - `-p <partition>` Filter results for one partition

Example 1: A test job

Steps:

1. Create a submission script
2. Submit job to Slurm
3. Monitor job execution
4. Get job results

Related docs `https://hpc.it.auth.gr/jobs/serial-slurm/`

Example 1: A test job

Submission script

```
#!/bin/bash

#SBATCH --time=10:00
#SBATCH --partition=testing

echo "Hello from $(hostname)"
sleep 30
echo Bye
```

Example 1: A test job

Job submission

1. `sbatch <submission-script.sh>`
2. Use `man sbatch` for more options

Job monitoring

1. `squeue -j <jobid>`
2. `tail -f slurm-<jobid>.out`
3. `sacct -j <jobid>`

Cancel jobs

1. `scancel <jobid>`

Example 2A: More CPU Cores

```
#!/bin/bash

#SBATCH --partition=testing
#SBATCH --time=10:00
#SBATCH --cpus-per-task=4

stress --cpu ${SLURM_CPUS_PER_TASK} --timeout 60
```

CPU Efficiency: `seff <jobid>`

Example 2B: MPI Parallelization

- Message Passing Interface (MPI) is a system for distributed parallel application development
- Gromacs is a molecular dynamics simulation tool
- Gromacs supports MPI Parallelization and Gromacs jobs can benefit from increasing CPU core count
- For scalable use cases, increasing cpu cores reduces job walltime

`srun [...]` launch Slurm-managed MPI process Documentation

`https://hpc.it.auth.gr/applications/gromacs/`

Example 2B: MPI Parallelization

```
#!/bin/bash

#SBATCH --partition=rome
#SBATCH --time=10:00
#SBATCH --nodes=1
#SBATCH --tasks-per-node=32
#SBATCH --cpus-per-task=1

module load gcc/9.4.0-eewq4j6 openmpi/4.1.2-akxtzzl
module load gromacs/2022-47qrtrj

srun gmx_mpi mdrun -ntomp 1 -s ../benchMEM.tpr
```

Example 3: More Memory

Default memory allocation

- Proportional to number of requested cores

Example:

- `batch` partition nodes have 20 cores and 128G of RAM each
- a job for partition `batch` with 10 cores will request by default 64GB of RAM.

What happens if a job tries to use more memory than it is allocated?

Example 3: More Memory

```
#!/bin/bash

#SBATCH --partition=testing
#SBATCH --job-name=memory
#SBATCH --time=4:00


./allocate-10gb
```

Example 3: More Memory

```
#!/bin/bash

#SBATCH --partition=testing
#SBATCH --job-name=memory
#SBATCH --time=4:00
#SBATCH --mem=11G

./allocate-10gb
```

Example 4: GPU jobs

```
#!/bin/bash

#SBATCH --partition=gpu
#SBATCH --gres=gpu:1
#SBATCH --cpus-per-task=20
#SBATCH --time=10:00

nvidia-smi
```

Example 5: Allocating Licenses

- ANSYS Fluent is a computational fluid dynamics (CFD) tool
- ANSYS Fluent is one example of a licensed software available for AUTH users
- A limited number of licenses are available for HPC usage.
- A user can request that a job be scheduled only if there are enough licenses available

Documentation `https://hpc.it.auth.gr/applications/fluent/`

Example 5: Allocating Licenses

```
#!/bin/bash

#SBATCH --job-name=FLUENT-2021R1-case
#SBATCH --partition=batch
#SBATCH --ntasks-per-node=20
#SBATCH --nodes=1
#SBATCH --licenses=ansys@ansys.it.auth.gr:16
#SBATCH --time=1:00:00

module load ansys/2021R1

fluent 3ddp -g -ssh -t$SLURM_NTASKS -i elbow_journal.in
```

Documentation

More info

1. https://hpc.it.auth.gr/jobs/job-submission/
2. https://hpc.it.auth.gr/jobs/serial-slurm/
3. https://hpc.it.auth.gr/jobs/slurm/