HPC Workflows using Slurm

Introduction to Slurm Scheduling
Working with Python on Aristotle

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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.

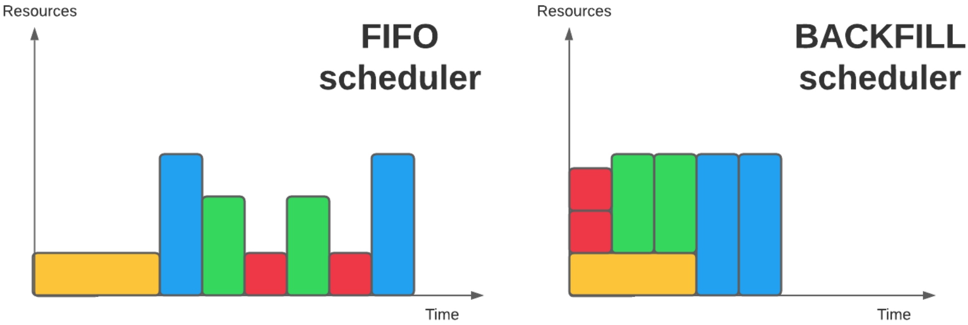
Slurm's Scheduling Algorithm

- 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

```bash
#!/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

```bash
#!/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

```bash
#!/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/`

Working with Python on Aristotle

In this session

- Create a conda environment with PyTorch
- Add the environment to Jupyter server
- Submit a test PyTorch job on a GPU node

Conda environment

- Conda is an open-source package management system and environment management system.
- Miniconda is a free minimal installer for conda.
- Miniconda3 is available on Aristotle.
  `module spider miniconda3` See available versions.

Environment setup 1/4

```bash
#!/bin/bash

#SBATCH --partition=gpu
#SBATCH --gres=gpu:1
#SBATCH --cpus-per-task=20
#SBATCH --time=1:30:00

# Load Miniconda
module load gcc/9.4.0-eewq4j6 miniconda3
source "${CONDA_PROFILE}/conda.sh"
```

Environment setup 2/4

```
# Create pytorch environment
conda create -p ./test.env pytorch==1.12.0 torchvision==0.13.0 \
    torchaudio==0.12.0 cudatoolkit=11.3 \
    -c pytorch
```

Also see `https://pytorch.org/get-started/previous-versions/`

Environment setup 3/4

```
# Check if CUDA is installed properly
conda activate ./test.env

cat <<EOF | python -
import torch
print(torch.cuda.is_available())
print(torch.cuda.device_count())
EOF
```

Environment setup 4/4

```
# Install additional libraries
conda install -c conda-forge jupyter matplotlib tqdm
```

What is Jupyter

- Jupyter is an open-source web application that allows you to create and share notebooks
- Notebooks are documents that contain live code, equations, visualizations and narrative text
- Jupyter is available on Aristotle via Open OnDemand (`https://hpc.auth.gr`)

Setup environment in Jupyter

- Jupyter was installed in environment
- To add the new environment to Jupyter:

```
conda activate ./test.env
python -m ipykernel install \
    --user --name torch-env \
    --display "Torch Test Environment"
```

- Also see `https://hpc.it.auth.gr/applications/jupyter/#custom-python-virtual-environments`

A demo

- PyTorch is a deep learning framework
- The MNIST dataset contains 60,000 training images of *handwritten digits* from zero to nine and 10,000 images for testing.
- The MNIST digit classification problem is almost the *Hello, world!* of deep learning.

This demo is from `https://github.com/jiuntian/pytorch-mnist-example`

A demo

```bash
#!/bin/bash

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

module load gcc/9.4.0-eewq4j6 miniconda3
source "${CONDA_PROFILE}/conda.sh"
conda activate ../test.env

python pytorch-mnist.py
```

Thank you!