Slurm

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Learning Objectives

- Using the scheduler in interactive and batch mode
- Identify the right partitions and Resources for their needs
- Choose the different file systems based on their characteristics

Section 1

Slurm

Getting started with Slurm

How to use the cluster

- Cluster divided into frontends and compute nodes
- Compute nodes to all calculations
- You cannot connect directly to the nodes
- You cannot run heavy calculations on the frontends

- So how do you use the compute nodes?

Use our scheduler: **Slurm!**

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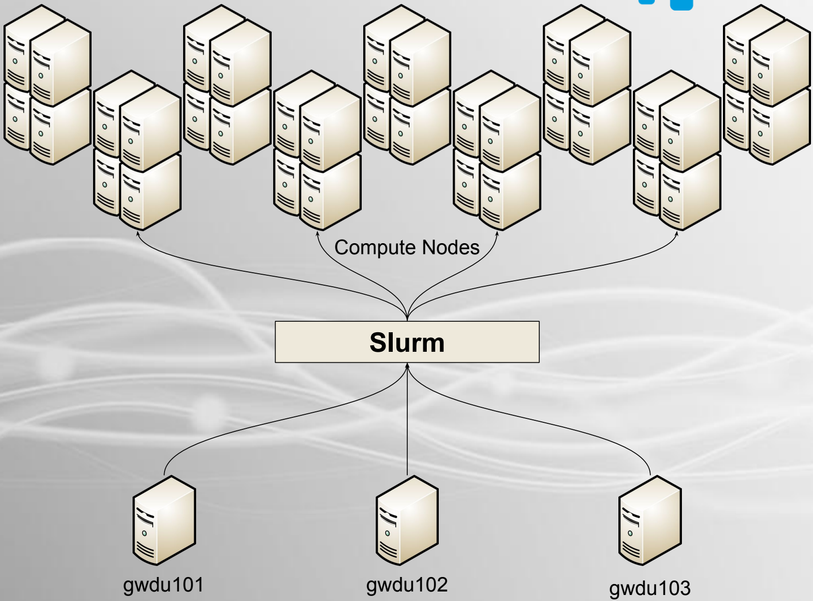
Use our scheduler: **Slurm!**

How to use the Cluster



Your first job

A job is a set of instructions for Slurm, including

- one or multiple programs to execute
- estimated runtime
- required resources (CPUs, GPUs, Memory)
- and more...

Your first job

Use srun to submit a job to Slurm

```
srun <program>
```

Example:

```
gwdu101:27 12:53:50 ~ > hostname
gwdu101
gwdu101:27 12:53:53 ~ > srun hostname
amp078
gwdu101:27 12:53:56 ~ > srun hostname -f
amp078.global.gwdg.cluster
```

Telling Slurm what to do

- `srun` submits information on your job to Slurm
  - ➥ What is to be done? (path to your program and required parameters)
  - ➥ What are its requirements? (e.g. which nodes, number of tasks, maximum runtime)
- Slurm matches the jobs requirements against the capabilities of our nodes
- When suitable free resources are found the job is started
- Slurm prioritizes the jobs based on a number of factors.

Partitions

- Different compute nodes have different features
- Slurm differentiates using **Partitions**

Available Partitions

General purpose partitions:

medium General purpose partition, well suited for most jobs. Up to 1024 cores per job.

fat Up to 512 GB in one host.

fat+ For extreme memory requirements. Up to 2048GB per host.

Special purpose partitions:

gpu For jobs using GPU acceleration.

int For interactive jobs, i.e. jobs which require a shell or a GUI.

Basic Concepts 1

Cluster A collection of networked computers intended to provide compute capabilities.

Node One of these computers, also called host or server.

Frontend Special node provided to interact with the cluster. `login-mdc|fas.hpc.gwdg.de` in our case.

Job Program consisting of one or several parallel tasks.

Partition A pool of nodes suitable for the job

Batch System Management system distributing job tasks across job slots. Slurm.

Submitting a job

```
srun <parameters> <program>
```

common parameters

-p <partition> partition.

-t <hh:mm:ss> Maximum runtime. If this is exceeded the job is killed.

-A <all> Specify account 'all'. Only necessary if you are part of a working group with access to special partitions.

Interactive Jobs

srun: Interactive jobs

--x11 Adds X11 (GUI) forwarding. This requires that you connect to the frontend with `ssh -Y` and your local machine supports X-Windows.

-p int Use the interactive partition. In `int` the nodes have no slot limit. They will take jobs until their load crosses a specified threshold, so jobs start immediately.

--pty interactive mode

Interactive X11 Job

Running Matlab

```
> ssh -Y login-mdc.gwdg.de
> module load matlab
> srun --x11 -p medium matlab
```

- The job will be dispatched and as soon as an available node is found and the Matlab interface will start.
- If you have your own license for Matlab then you need to place your `license.lic` file in `$HOME/.matlab/R2015a_licenses` directory (depending on the version you are using).

Interactive Console Job

Running R interactively

```
> ssh login-fas.hpc.gwdg.de
> srun --pty -p medium R
```

Exercises

Exercise

- Run a command on a compute node (e.g. `hostname`)
- Get an interactive shell on a compute node
- Try X11 forwarding

5 Minutes

Basic Concepts 2

Serial job Job consisting of one task using one job slot.

SMP job Job with shared memory parallelization (often realized with OpenMP), meaning that all processes need access to the memory of the same node. Therefore uses several job slots **on the same node**.

MPI job Job with distributed memory parallelization, realized with MPI. Can use several job slots on several nodes and needs to be started with a helper program, e.g., `mpirun` or `srun`.

Single node vs. MPI

- MPI jobs are a lot of independent tasks that (usually) use one core each
  - started with `srun` or `mpirun`
  - Slurm calls these `tasks`
- Single node jobs are usually just one task with many cores
- Both can be combined into hybrid jobs: multiple tasks using multiple cores each

Resource selection: CPU

`srun` options for parallel (SMP or MPI) jobs.

-N <min>-<max>, --nodes=<min>-<max>	Minimum and maximum node count. You can also specify the exact number.
-n,--ntasks=<n>	Number of tasks (not equally distributed!)
--tasks-per-node=<n>	Tasks per node. If used with `-n` it denotes the maximum number of tasks per node.
-c,--cpus-per-task=<n>	CPUs per tasks.

Rule of thumb

- `-c` for single node jobs
- `-n` for MPI jobs

Resource Selection: Memory

srun options

`--mem` <size[K|M|G|T] > Memory per node.

`--mem-per-cpu` <size[K|M|G|T] > Memory per core.

- without options:
  - ➥ each partition has a `DefMemPerCPU` option
  - ➥ can be retrieved via `scontrol show partition <name>`

How to avoid waiting

Reservation: `pchpc-course`

Usage

Either: `--reservation=pchpc-course` for each job
Or: `export SBATCH_RESERVATION=pchpc-course`
The latter has to be unset, if you want to submit to a partition besides medium.

Exercises

Exercise

- Try these job configurations:
  1. 10 tasks
  2. 10 tasks distributed over 3 nodes
  3. 3 nodes with 3 tasks each
  4. 1 task with 5 cores
  5. 2 tasks per node on 2 nodes with 4 cores per task
- Play with the combination of number of cores or tasks, nodes and their effect on your available memory:
  1. 1 core and `--mem` 4G
  2. 3 tasks and 2 nodes, see effect of `--mem` and `--mem-per-cpu`
  3. 20 tasks, see distribution of memory over hosts.
- use `slurm_resources` script to get see the resources of your job

Time: 20 Minutes

Non interactive Jobs

Problem

- if you have big jobs, your queue time will be long
- `srun` needs you to stay logged in
- jobs can run for days

Solution

Batch Jobs!

Non interactive Jobs

Problem

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- jobs can run for days

Solution

Batch Jobs!

A job script is a shell script with a special comment section.
The #SBATCH lines have to come first!

sbatch: Basic job script example

```
#!/bin/bash
#SBATCH -p medium
#SBATCH -t 10:00
#SBATCH -o job-%J.out

slurm_resources
```

Submit with:

```
sbatch <script name>
```

Jobscripts

- A job script is essentially a normal script
- usually bash/shell, but can be any scripting language (R, python, perl)
- `#SBATCH` lines need to be at the top!
- you can copy files, load modules, and do any scripting you want
- for MPI, use `srun` or `mpirun` to start your program

sbatch: Using Job Scripts

More Options

```
sbatch <slurm options> jobscript
```

--mail-type=<TYPE>	get mail notifications (type: BEGIN, END, etc.)
--mail-user=<address>	Default: ${USER}@gwdg.de
-o/-e <file>	Store job output in file (slurm-<jobid>.out by default). %J in the filename stands for the jobid.

Slurm Commands

sinfo Info about the system and partitions.

```
-p <partition>, -t <state>
```

squeue Show the job queue.

```
-p <partition>, --me
```

scancel Cancel Job

```
scancel <JobID>
scancel -p <partition>|-u $USER
```

Exercises

Exercise

Write your own Job script.

- Use `echo`, `hostname`, and `sleep X` (sleep for X seconds) to generate output or have it running for a longer time.
- Have the job send you an email. Advanced: Take a look at the different mail-type options. What do they do?
- Write the output to a different file. Redirect output and error into different files. Advanced: Take a look at the filename pattern options. Include node and job name in the output file.

Time: 20 Minutes

Task Distribution

Distributing tasks in the medium partition

```
#SBATCH -p medium
#SBATCH -n 240
#SBATCH -o job-%J.out

module purge
module load intel/compiler intel/mkl intel/mpi namd

srun namd2 +setcpuaffinity apoa1.namd
```

This will spread tasks among many nodes.

Task Distribution fixed

Distributing tasks in the `medium` partition

```
#SBATCH -p medium
#SBATCH -N 10
#SBATCH --ntasks-per-node 24
#SBATCH -o job-%J.out

module purge
module load intel/compiler intel/mkl intel/mpi namd

srun namd2 +setcpuaffinity apoa1.namd
```

Memory is faster then network!
Try to spread your tasks to as little nodes as possible.

Job Disk Space Usage Options

/local Local hard disk of the node. SSD based and therefore a very fast option for storing temporary data. Automatic file deletion. A temporary directory is created on all nodes at `$TMP_LOCAL`.

/scratch Shared scratch space, available on most nodes, but there are two instances (use `-C scratch` or `-C scratch2`). Very fast, no automatic file deletion, but also no backup! Files may have to be deleted manually when we run out of space.

/scratch/ssd special extra fast scratch file system only on scratch1. Ideal for temporary data in jobs spanninh multiple nodes. Automatic file deletion. A per-job directory is created at `$TMP_SCRATCH`.

$HOME Available everywhere, permanent, with backup. Personal disk space can be increased. Comparably slow.

Recipe: Using /scratch

```
#!/bin/bash
#SBATCH -p medium
#SBATCH -n 24
#SBATCH -N 1
#SBATCH -C scratch
#SBATCH -t 1-00:00:00

export g09root="/usr/product/gaussian/g09/d01"
source $g09root/g09/bsd/g09.profile

if [ ${TMP_SCRATCH} -a -d ${TMP_SCRATCH} ]; then
  export GAUSS_SCRDIR=${TMP_SCRATCH}
else
  export GAUSS_SCRDIR=$TMP_LOCAL
fi

g09 myjob.com myjob.log
```

Exercises

Exercise

Write a job script, where you

- create a scratch directory
- copy data from your home file system to the scratch directory
- run a job with the data
- copy the results back
- delete the scratch directory

If you do not have a program/data to try this on, there is a small python program in `/scratch1/projects/scc-course/` and a bit of input data.

The fat+ partition

The `fat+` partition contains:

- 5 nodes with 1.5Tb Memory
- 1 node with 2Tb Memory

Usage recommendations:

- Work your way up. Start in `fat` and only use `fat+` if your jobs runs out of memory.
- Use `sacct` or `profit-hpc`, see if your job really is memory bound
- When unsure, ask us!
- `--mem`or `--mem-per-cpu` is mandatory
- You might get angry mails from me, if you waste resources here

Recipe: Combine shared memory and MPI

Running hybrid jobs

```
#SBATCH -p medium
#SBATCH -N 5
#SBATCH --ntasks-per-node=4
#SBATCH --cpus-per-task=6
#SBATCH -o job-%J.out

module purge
module load openmpi/gcc

export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

srun hybrid_job
```

Longer or shorter jobs

The --qos parameter

- Default maximum runtime: 2 days
- --qos= <qos> can select a QoS
- Two extra QoS available:

short for shorter jobs (max. 2h), has higher priority, limited job slots

long longer jobs (max. 5d), limited job slots.

But my job is even longer

- try parallelizing more
- break it down into smaller steps
- check, if your software supports checkpoints
- check again!
- contact us

More Slurm Commands

scontrol show [partition|node|job] <x> where x should be a node name, JobID or partition name.

sprio Priority information about pending jobs

sacct Get information about a job after it finished

```
-j <jobid>
--format=JobID,User,JobName,MaxRSS,Elapsed,Timelimit
```

Using the gpu partition

GPU parameters

-G | --gpus=[type:]<n> requests `n` GPUs of `type`

--gpus-per-task=[type:]<n> requests `n` GPUs of `type` per task

--gpus-per-node=[type:]<n> requests `n` GPUs of `type` per node

- CPUs are evenly distributed for every GPU
- Available types are:
  - ➥ rtx5000
  - ➥ v100
  - ➥ k40
  - ➥ gtx1080
  - ➥ gtx980
- See: `sinfo -p gpu --format=%N,%G`

Debugging

- take a look at your output files, while the job is running:
  - ➥ tail -f /path/to/output
- take a look at the jobs, while it is running
  - ➥ you can `ssh` into every node that currently calculates your job
  - ➥ use `htop` to see the processor and ram usage

Debugging

Read the extra job information

```
======================================================================
JobID = 4383174
User = mboden, Account = admin
Partition = gpu, Nodelist = dge[001,006]
======================================================================
[job output]
============ Job Information =========================================
Submitted: 2020-04-24T17:35:41
Started: 2020-04-24T17:35:41
Ended: 2020-04-24T17:45:45
Elapsed: 10 min, Limit: 60 min, Difference: 50 min
CPUs: 2, Nodes: 2
============= ProfiT-HPC =============================================
To generate the ProfiT-HPC text report, run the following command
profit-hpc 4383174
======================================================================
```

Take a look at all the information. Is it as expected?

Debugging

Read your errors!

```
slurmstepd: error: Detected 1064 oom-kill event(s) in step XXXXXX.0 cgroup.
Some of your processes may have been killed by the cgroup out-of-memory handler.
srun: error: gwda024: task 3: Out Of Memory
```

Might have something to do with memory!
Have a look at your jobs memory with:

```
sacct -j JOBID -o jobid,MaxRSS,MaxRSSNode
```

And for more advanced job statistics, use profit-hpc