Introduction to SLURM and modules

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1. SLURM: introduction

Limited resources

- Cluster has many users wanting to run jobs, which limits:
  - CPU
  - Working memory
  - Time
- How to assign which resources to which job?

Job scheduling

Job (computing)

From Wikipedia, the free encyclopedia

In computing, a **job** is a unit of work or unit of execution (that performs said work).

Job scheduler

From Wikipedia, the free encyclopedia

A **job scheduler** is a computer application for controlling unattended background program execution of jobs.[1]

SLURM

- **S**imple **L**inux **U**tility for **R**esource **M**anagement
- Job scheduler on:
  - UBELIX
  - IBU cluster
  - and many more

Resource allocation commands

- sbatch
- srun
- salloc

script.sh

```
#!/usr/bin/env bash

my_program \
--cpu 32 \
--memory 128G
```

```
sbatch [options] script
```

```
$ sbatch --cpus-per-task=32 --mem-per-cpu=4G ./script.sh
```

script.sh

```
#!/usr/bin/env bash

#SBATCH --cpus-per-task=32
#SBATCH --mem-per-cpu=4G

my_program \
--cpu 32 \
--memory 128G
```

```
$ sbatch ./script.sh
```

```
$ sbatch ./script.sh
Submitted batch job 6245994
$ squeue --job 6245994
JOBID   PARTITION NAME      USER      ST TIME  NODES NODELIST(REASON)
6245995 pall      script.sh gvangees  R  0:07  1      binfservas01
$ squeue –A gvangeest
JOBID   PARTITION NAME      USER      ST TIME  NODES NODELIST(REASON)
6245995 pall      script.sh gvangees  R  0:07  1      binfservas01
```

2. Frequently used sbatch options

2.1 Required resources

- CPU
  - `--cpus-per-task=2`
- Working memory
  - `--mem-per-cpu=4G`
- Time (days-hours:minutes:seconds)
  - `--time=1-05:00:00`

Low values could cause your job to start earlier
But: job will fail if resources are overrequested!

2.2 user specific

- Job name:
  - `--job-name=my_job_name`
- e-mail
  - `--mail-user=user@students.unibe.ch`
  - `--mail-type=begin,end,fail`

2.3 output & error

- `--output=existing/path/output_%j.o`
- `--error=existing/path/error_%j.e`

Path should exist!
Job will fail otherwise
(without error message)

3. Interactive jobs

Why submit interactive job?

- **Interactive job:** allocated resources that are approachable with shell
- Head (login) node is not for computation
- Debugging and testing can be much more convenient if interactive

srun

- Versatile command
- Used for job steps within sbatch (not treated in this course)
- Also for allocation of interactive job with `pty` (pseudo-terminal mode)

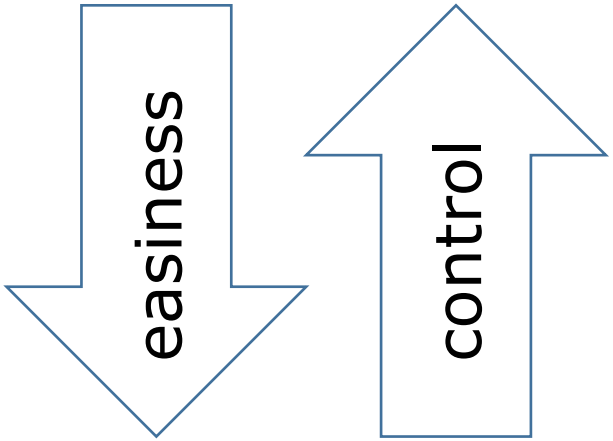
```
$ srun --cpus-per-task=1 --mem-per-cpu=4000 \
> --time=00:05:00 --pty bash
```

Exit the interactive job with `exit`

4. Modules

Software

- Install it yourself (at ~)
- Use a container
- Install with conda
- Use modules



Modules

- Check for available modules:
  - `module avail`
- Add a module to environment:
  - `module add`
- Unload a module:
  - `module rm`
- Available modules:
  - https://www.vital-it.ch/services

5. Job arrays

5.1 Jobs in parallel

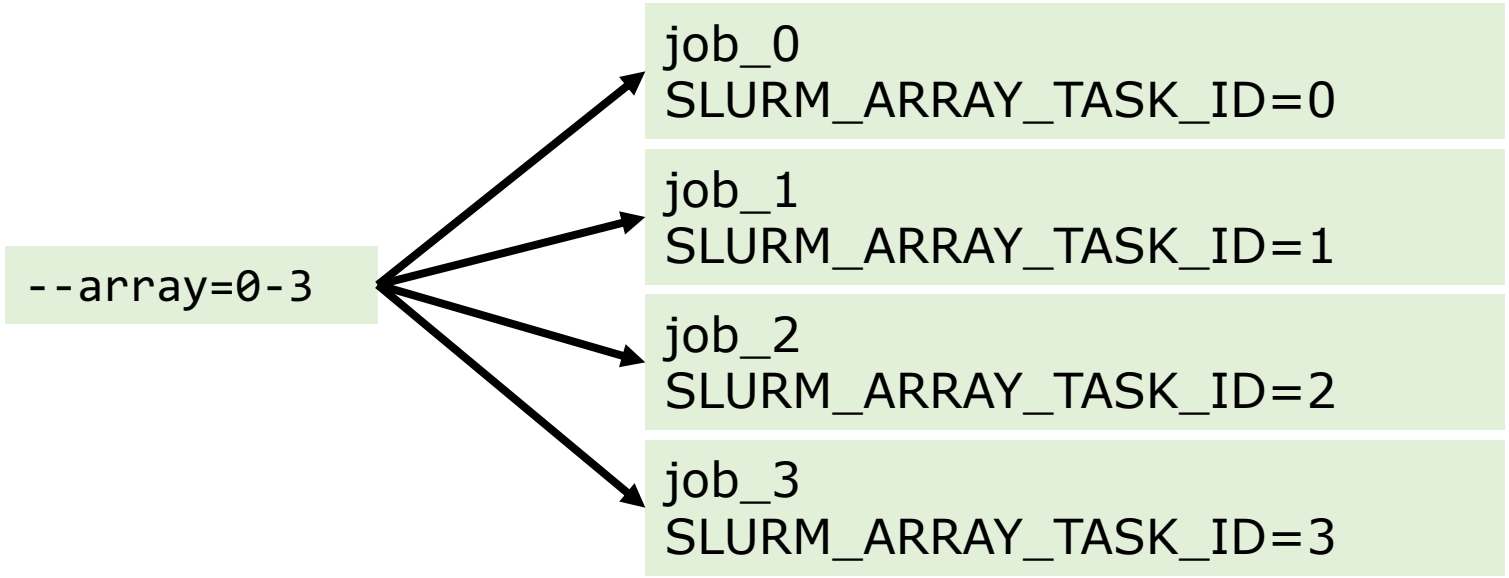
- Run similar command with different parameters: parameter sweep
- E.g. alignment (e.g. with `minimap2`) on several files.

script.sh

```
#!/usr/bin/env bash

#SBATCH --array=0-3
#SBATCH --cpus-per-task=32
#SBATCH --mem-per-cpu=4G

my_program \
$SLURM_ARRAY_TASK_ID
```



5.2 Using UNIX arrays

```
$ ls
file1.txt file2.txt file3.txt
$ FILES=(./*)
$ echo ${FILES[0]}
file1.txt
$ echo ${FILES[1]}
file2.txt
$ echo ${FILES[2]}
file3.txt
```

UNIX uses zero-based indexing

script.sh

```
#!/bin/bash

#SBATCH --cpus-per-task=32
#SBATCH --mem-per-cpu=4G
#SBATCH --array=0-7

FILES=(/path/to/input_data/*)

my_program ${FILES[$SLURM_ARRAY_TASK_ID]}
```