Introduction to SLURM and modules

1. SLURM: introduction

Limited resources

- Cluster has many users wanting to run jobs, which limits: **1. CPU 2. Working memory 3. Time**
- How to assign which resources to which job?

Job scheduling

- Job(computing) In **computing**, a **job** is a unit of work or unit of execution(that performs said work).
- Job scheduler: A **job scheduler** is a computer application for controlling unattended background program execution of jobs.

SLURM

- Simple Linux Utility for Resource Management
- Job scheduler on: UBELIX, IBU cluster, and many more

Resource allocation commands

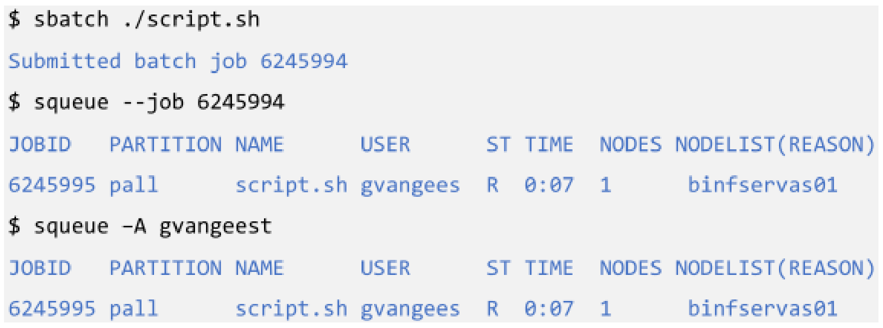
- `sbatch`, `srun`, `salloc`
- **sbatch [options] script**
- `$ sbatch --cpus-per-task=32 --mem-per-cpu=4G ./script.sh`

  ```
  #!/usr/bin/env bash
  my_program \
  --cpu 32 \
  --memory 128G
  ```

- `$ sbatch ./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
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

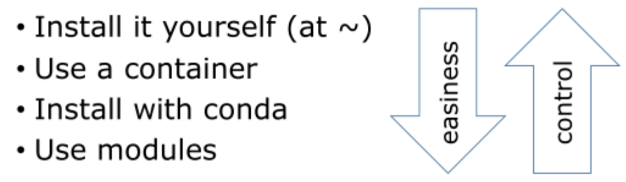
- Versatile command
- Used for job steps within sbatch (not treated in this course)
- Also for allocation of interactive job with pty (pseudo-terminal mode)

```
$ 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

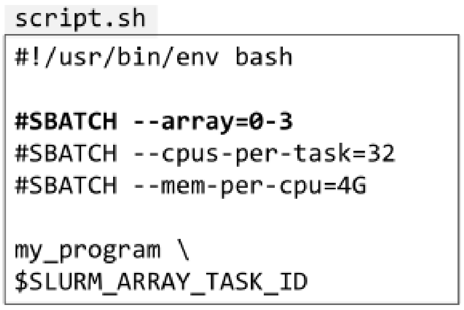
Modules

- 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

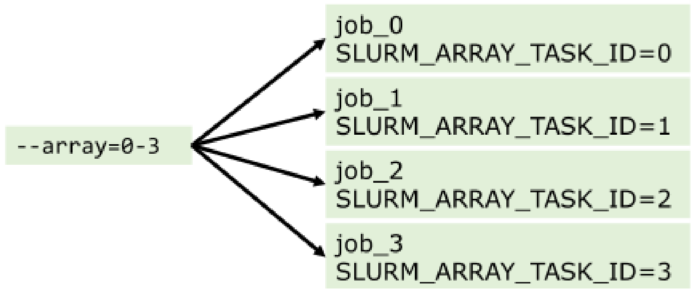
- Run similar command with different parameters: parameter sweep
- E.g. alignment (e.g. with minimap2) on several files



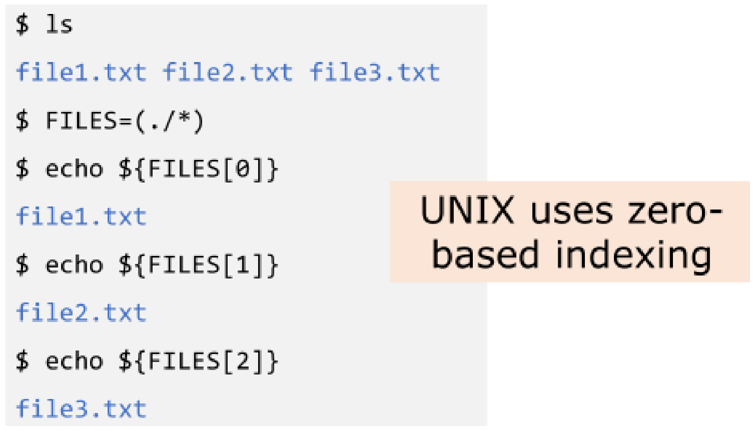
script.sh
```
#!/usr/bin/env bash

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

my_program \
$SLURM_ARRAY_TASK_ID
```

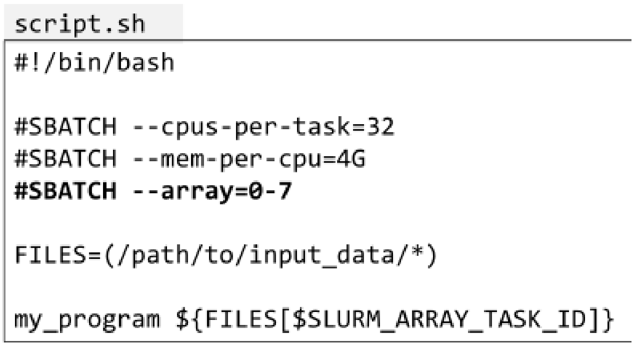


5.2 Using UNIX arrays



```
$ 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]}
```