SLURM @UPPMAX

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More Slurm and other advanced UPPMAX techniques

- A closer look at Slurm
- Using the GPUs on Snowy
- Job efficiency with the **`jobstats`** tool
- Advanced job submission

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From login to the first job script

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Technical summary of the UPPMAX clusters

	Rackham	**Snowy**	**Bianca**
Purpose	General-purpose	General-purpose	Sensitive
# Intel CPU Nodes	486	228	288
# GPU Nodes	-	50, Nvidia T4	10, 2x Nvidia A100 each
Cores per node	20	16	16 or 64
Memory per node	128 GB	128 GB	128 GB
Fat nodes	256 GB & 1 TB	256, 512 GB & 4 TB	256 & 512 GB
Local disk (scratch)	2/3 TB	4 TB	4 TB
Login nodes	Yes (4)	No (reached from Rackham)	Yes (2 cores and 15 GB)
"Home" storage	Domus	Domus	Castor
"Project" Storage	Crex, Lutra	Crex, Lutra	Castor

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The **Slurm** Workload Manager

- provides a framework for starting, executing, and monitoring jobs on the compute nodes

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The **Slurm** Workload Manager

- provides a framework for starting, executing, and monitoring jobs on the compute nodes
- schedules the jobs on the clusters
- allocates the required resources (compute cores or nodes, memory)

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The **Slurm** Workload Manager

- Free, popular, lightweight
- Open source:

  https://slurm.schedmd.com
- available at al SNIC centra
- UPPMAX Slurm userguide:

  https://docs.uppmax.uu.se/cluster_guides/slurm/

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Running on the login node vs. job submission

How to submit a job?

- Recap:

`sbatch`	`-A uppmax2025-2-262`	`-t 10:00`	`-p core`	`-n 10`	`my_job.sh`
Slurm batch	Project name	Maximum runtime	Partition (“job type”)	#cores	job script

Job time limits

- `-t minutes`
- `-t minutes:seconds`
- `-t hours:minutes:seconds`
- `-t days-hours`
- `-t days-hours:minutes`
- **`-t days-hours:minutes:seconds`**

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What should the wall time of a job be?

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- Q: When you have an idea of how long a program would take to run, what should you book?

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What should the wall time of a job be?

- Your first job? Testing new software or input?
  - Use a short time limit, 10 min - 1h.
- Q: When you have no idea how long a program will take to run, what should you book?
  - A: very long time, e.g. 10-00:00:00
- Q: When you have an idea of how long a program would take to run, what should you book?
  - A: overbook by 50%

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More on partitions

- **`-p core`**
  - "core" is the default partition
  - ≤ 20 cores on Rackham
  - ≤ 20 cores on Bianca
  - a script or program written without any thought on parallelism will use 1 core

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More on partitions

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  - "core" is the default partition
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  - a script or program written without any thought on parallelism will use 1 core
- **`-p node`**
  - if you wish to book full node(s)

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Getting on the fast lane

- for quick tests and development work

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Quick testing

- The “devel” partition
  - max 2 nodes per job
  - up to 1 hour in length
  - only 1 at a time
  - **`-p devcore`**, **`-p devel`**

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Quick testing

- The “devel” partition
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  - only 1 at a time
  - **`-p devcore`**, **`-p devel`**
  - Any free nodes in the devel partition? Check status with
    - `sinfo -p devel`
    - **`jobinfo -p devel`**

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Quick testing

- Any free nodes in the devel partition? Check status with
  - `sinfo -p devel`
  - **`jobinfo -p devel`**
    - more on these tools later
- High priority queue for short jobs
  - 4 nodes
  - up to 15 minutes
  - **`--qos=short`**

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- What if **1h** is not enough?
- What if the application uses a graphical user interface (GUI)?

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Debugging or complicated workflows

- Interactive jobs
  - handy for debugging a code or a script by executing it line by line or for using programs with a graphical user interface
  - `salloc -n 80 -t 03:00:00 -A uppmax2025-2-262`
  - **`interactive`** `-n 80 -t 03:00:00 -A uppmax2025-2-262`

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    or for using programs with a graphical user interface
  - `salloc -n 80 -t 03:00:00 -A uppmax2025-2-262`
  - **`interactive`** `-n 80 -t 03:00:00 -A uppmax2025-2-262`
  - up to 12 hours
  - useful together with the `--begin=<time>` flag
  - `salloc -A uppmax2025-2-262 --begin=2025-02-13T08:00:00`

    asks for an interactive job that will start

    earliest tomorrow at 08:00

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Parameters in the job script or the command line?

- Command line parameters override script parameters
- A typical script may be:

```
#!/bin/bash
#SBATCH -A uppmax2025-2-262
#SBATCH -p core
#SBATCH -n 1
#SBATCH -t 24:00:00
```

- Just a quick test:

```
sbatch -p devcore -t 00:15:00 jobscript.sh
```

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Hands-on #1:
`sbatch/jobinfo`

- login to Rackham
- find out which projects you're a member of using projinfo
- submit a short (10 min) test job; note the job ID
- find out if there are any free nodes in the devel partition
- submit a new job to use the devel partition
- write in the HackMD when you're done

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Memory in core or devcore jobs

- `-n X`
- on Rackham: 6.4 GB per core
- on Snowy/Bianca: 8GB per core
- Slurm reports the available memory in the prompt at the start of an interactive job

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More flags

- `-J <jobname>`
- email:
  - `--mail-type=BEGIN,END,FAIL,TIME_LIMIT_80`
  - `--mail-user` - Don't use. Set your email correctly in SUPR instead.
- out/err redirection:
  - `--output=slurm-%j.out` *and* `—error=slurm-%j.err`

    by default, where `%j` will be replaced by the job ID
  - `--output=my.output.file`
  - `--error=my.error.file`

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More flags

- Memory
  - `-C thin` / `-C 128GB`
  - `-C fat` / `-C 256GB` / `-C 1TB`
- Dependencies: `--dependency`
- Job array: `--array`
- More at https://slurm.schedmd.com/sbatch.html
  - or just `man sbatch`
  - not all options work on all systems!

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From job submission to job monitoring

- `sbatch`

- `sinfo`
- `jobinfo` (wrapper around `squeue`)

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Monitoring jobs

- **`jobinfo`** - a wrapper around **`squeue`**
  - lists running and pending jobs
  - `jobinfo -u` *`username`*
  - `jobinfo -A uppmax2025-2-262`
  - `jobinfo -u` *`username`* `--state=running`
  - `jobinfo -u` *`username`* `--state=pending`
- One may also use the **`squeue`** command.

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Monitoring and modifying jobs

- **scontrol**
  - `scontrol show job` *jobid*

Monitoring and modifying jobs

- **`scontrol`**
  - `scontrol show job` *`jobid`*
- possible to modify the job details after the job has been submitted;

  some options, like maximum runtime, may be modified (=shortened)

  even after the job started
  - `scontrol update JobID=`*`jobid`* `QOS=short`
  - `scontrol update JobID=`*`jobid`* `TimeLimit=1-00:00:00`
  - `scontrol update JobID=`*`jobid`* `NumNodes=10`
  - `scontrol update JobID=`*`jobid`* `Features=mem1TB`

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When a job goes wrong

- **`scancel`**
  - *`jobid`*
  - `-u` *`username`* - to cancel all your jobs
  - `-t` *`state`* - cancel pending or running jobs
  - `-n` *`name`* - cancel jobs with a given name
  - `-i` - ask for confirmation

Priority

- Roughly:
- The first job of the day has elevated priority
- Other normal jobs run in the order of submission (subject to scheduling)
- Projects exceeding their allocation get successively into the lower priority category
- Bonus jobs run after the jobs in the higher priority categories

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Priority

- In practice:
  - submit early = run early
  - bonus jobs always run eventually, but may need to wait until the night or weekend
- In detail:

  https://docs.uppmax.uu.se/software/jobinfo/#initial-priority-at-submit-time

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Hands-on #2:
`sbatch/squeue/scancel/scontrol/jobinfo`

- submit a new job; note the job ID
- check all your running jobs
- what is the priority or your recently-submitted job?
- submit a new job to run for 24h; note the job ID
- modify the name of the job to “wrongjob” and the maximum runtime to 7days, for example
- cancel your job with name “wrongjob”

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Determining job efficiency

- **`jostats`** - custom-made UPPMAX tool

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Job efficiency

- **`jobstats`** - a tool in the fight for productivity
  - it works only for jobs longer than 5-15 minutes
  - `-r` *`jobid`* - check running jobs
  - `-A` *`project`* - check all recent jobs of a given project
  - **`-p`** ***`jobid`*** - produce a CPU and memory usage plot
  - `-M` *`cluster`* - check jobs on other cluster
  - https://docs.uppmax.uu.se/software/jobstats/

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Hands-on #3: `jobstats`

- Generate jobstats plots for your jobs
  - Firstly, find some job IDs from this month
  - `finishedjobinfo -m` *`username`*
  - Write down the IDs from some interesting jobs.
  - Generate the images:

    ```
    $ jobstats -p ID1 ID2 ID3
    ```

- Look at the images. You may find some interesting ones in

  `/proj/introtouppmax/labs/moreslurm/jobstatsplots/`

  ```
  $ eog *png &
  ```

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Hands-on #3: `jobstats`

- Which of the plots in `/proj/introtouppmax/labs/moreslurm/jobstatsplots/`
  - Show good CPU or memory usage?
  - Indicate that the job requires a fat node?

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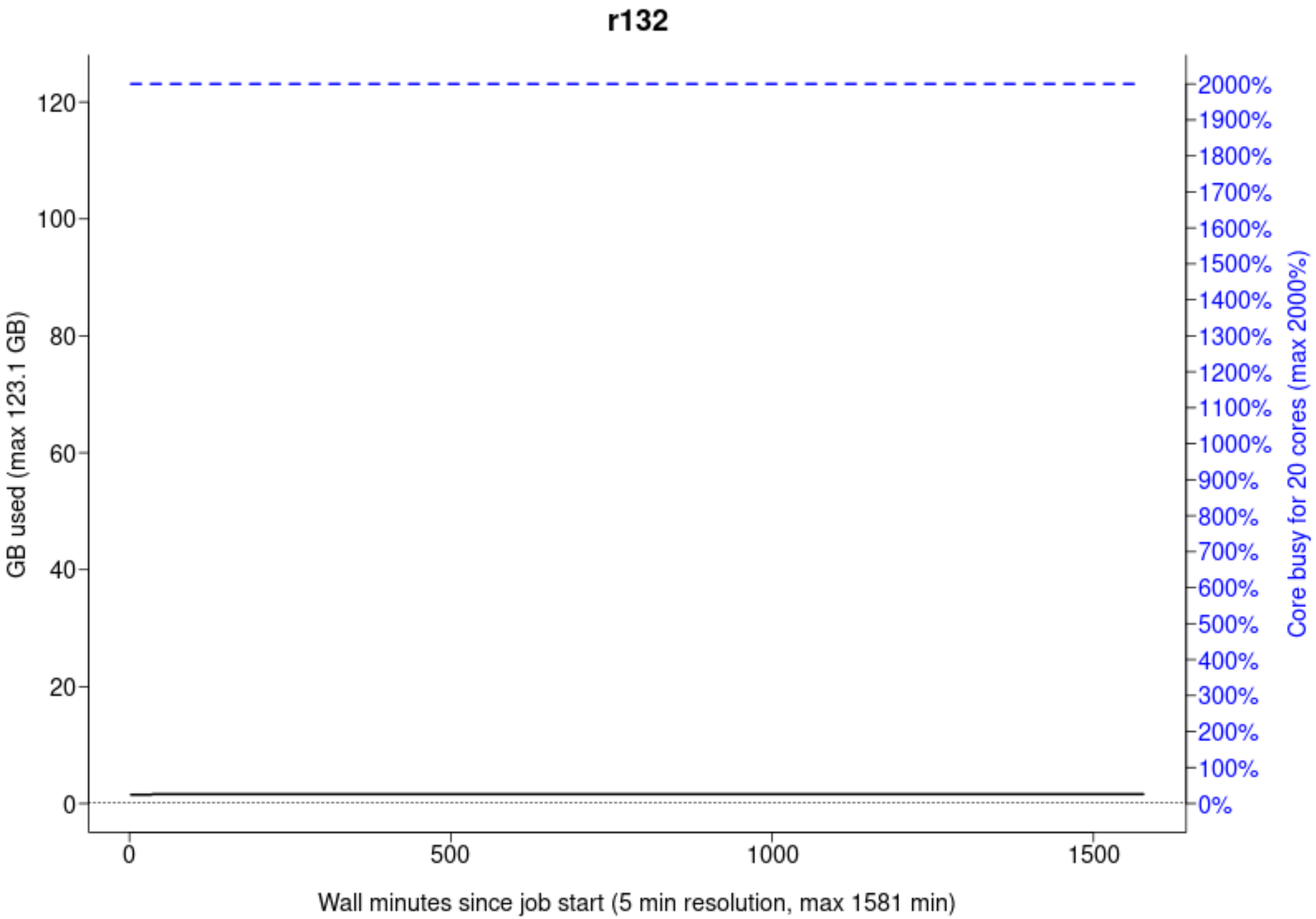
11217530 COMPLETED on rackham end: 2019-12-17T12:35:44 runtime: 1-02:16:12

User:
Proj: snic2019-1-12
Jobname: fesn_x

Flags: none



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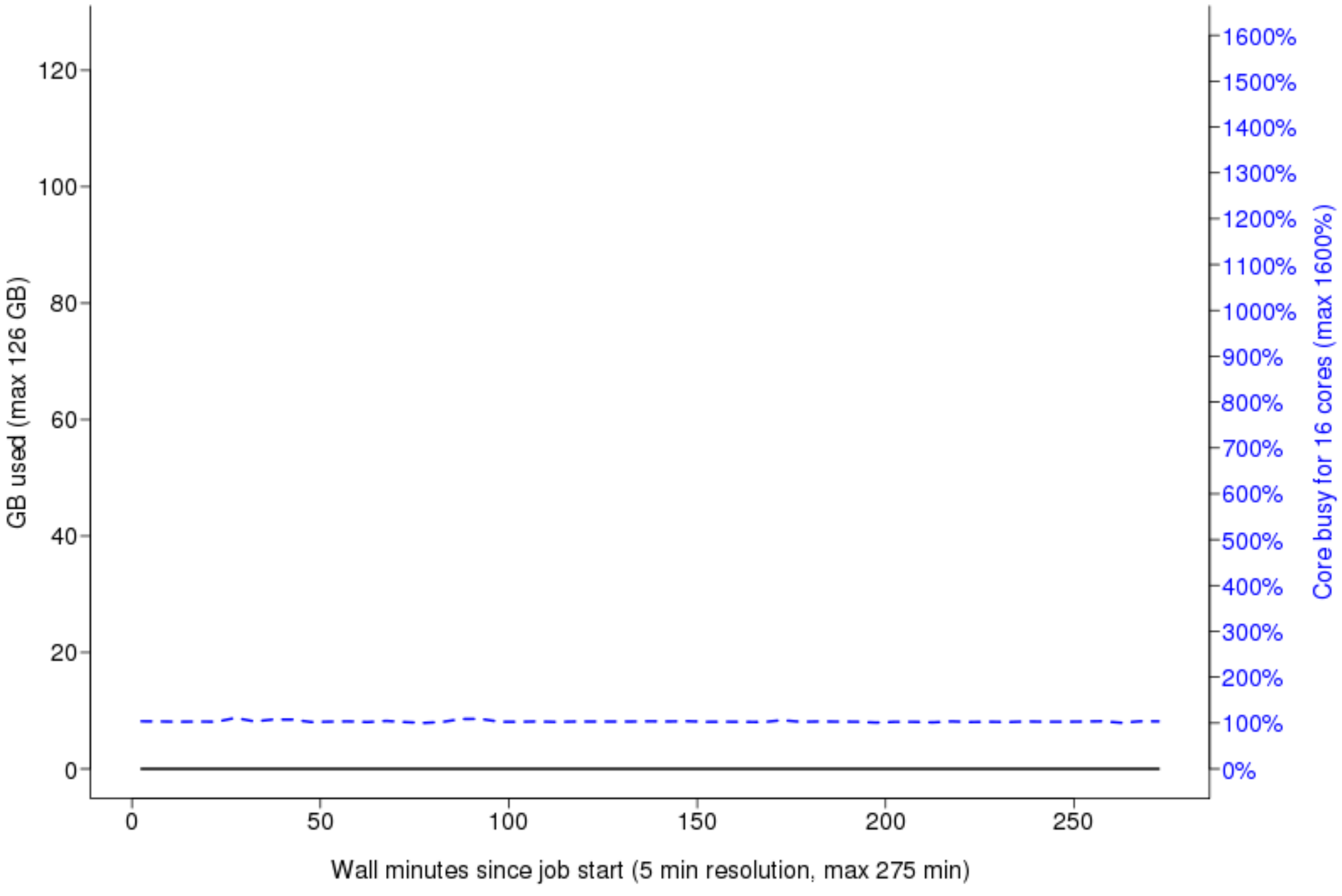
8804061 COMPLETED on milou end: 2016-10-10T20:30:26 runtime: 04:36:33

User:
Proj: b2015110
Jobname: nf-MergeBam_(2)

overbooked:12%, !!half_overbooked, !!severely_overbooked,
cores_overbooked:16:2, mem_overbooked:126:0, core_mem_overbooked:15.8:0

m102



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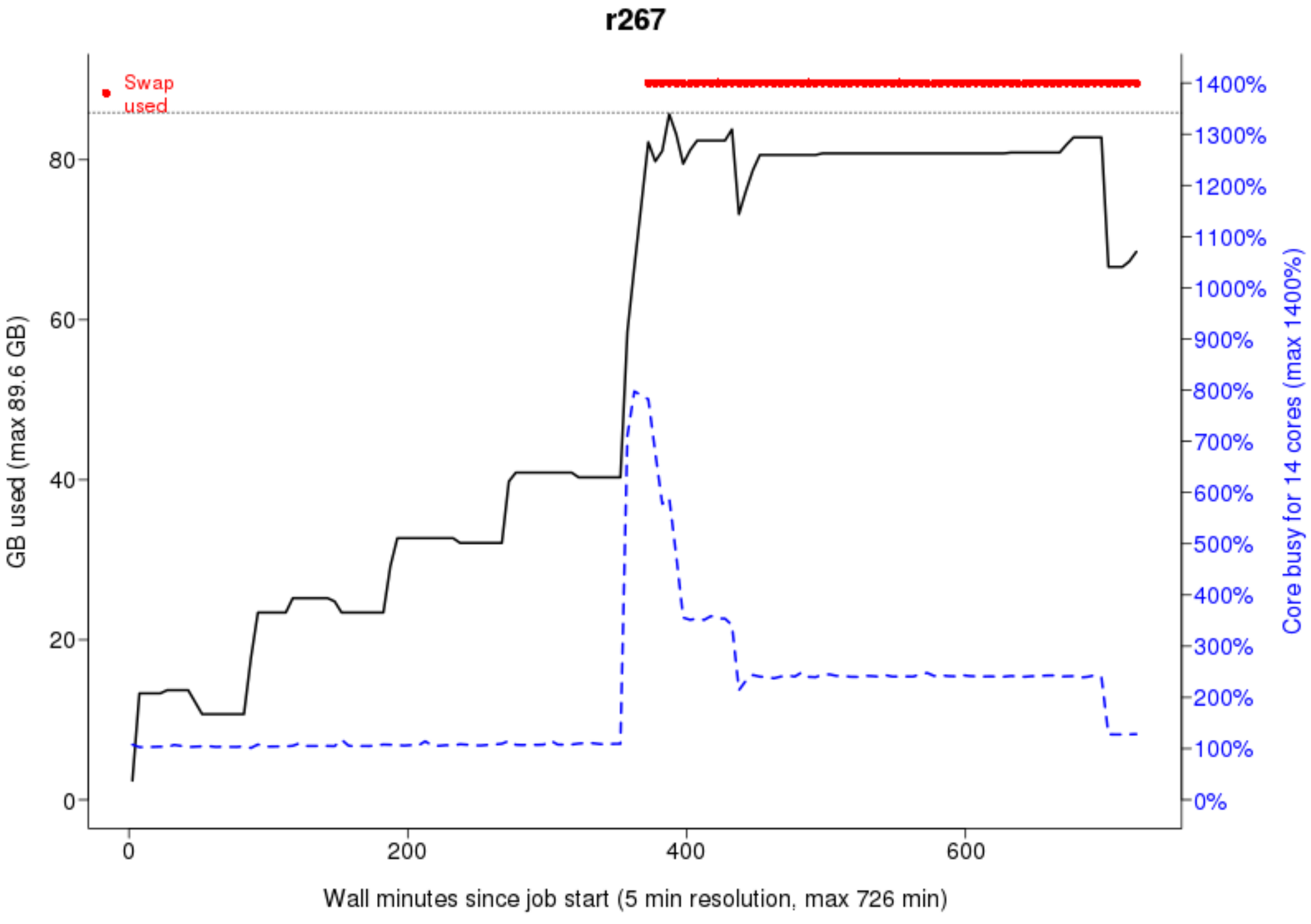
607031 OUT_OF_MEMORY on rackham end: 2018-08-25T07:29:39 runtime: 12:08:5

User:
Proj: snic2017-1-355
Jobname: pgd.apps

!!swap_used, cores_overbooked:14:11



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Different flavours of Slurm

Job script examples and workflows

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Simple workflow

```
#!/bin/bash
#SBATCH -J jobname
#SBATCH -A uppmax2025-2-262
#SBATCH -p core
#SBATCH -n 10
#SBATCH -t 10:00:00

module load software/version
module load python/3.9.5

./my-script.sh
./another-script.sh
./myprogram.exe
```

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Why do we need to load modules in the job script?

or in other words:

What does module load do?

Is it needed to specify the version of the software when loading the module? Why?

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Job dependencies

- `sbatch jobscript.sh` submitted job with *`jobid1`*
- `sbatch anotherjobscript.sh` submitted job with *`jobid2`*
- `--dependency=afterok:`*`jobid1`*`:`*`jobid2`* job will only start running after the successful end of jobs *`jobid1`*`:`*`jobid2`*
- very handy for clearly defined workflows
- One may also use `--dependency=afternotok:`*`jobid`* in case you'd like to resubmit a failed job, OOM for example, to a node with a higher memory: `-C mem215GB` or `-C mem1TB`

I/O intensive jobs: $SNIC_TMP

```
#!/bin/bash
#SBATCH -J jobname
#SBATCH -A uppmax2025-2-262
#SBATCH -p core
#SBATCH -n 1
#SBATCH -t 10:00:00

module load bioinfotools
module load bwa/0.7.17 samtools/1.14

export SRCDIR=$HOME/path-to-input

cp $SRCDIR/foo.pl $SRCDIR/bar.txt $SNIC_TMP/.
cd $SNIC_TMP

./foo.pl bar.txt

cp *.out $SRCDIR/path-to-output/.
```

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OpenMP or multi-threaded job

```
#!/bin/bash
#SBATCH -A uppmax2025-2-262
#SBATCH --exclusive
#SBATCH -p node
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=20
#SBATCH -t 01:00:00

module load uppasd
export OMP_NUM_THREADS=20

sd > out.log
```

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GPU nodes on Snowy

- Nodes with 1 Nvidia T4
- Available to everyone, priority to groups that paid for them

```
#SBATCH -M snowy
#SBATCH -C gpu
#SBATCH –gres=gpu:1
#SBATCH –gpus-per-node=1
```

- Further documentation:

https://slurm.schedmd.com/gres.html#Running_Jobs

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Running on several nodes: MPI jobs

```
#!/bin/bash -l
#SBATCH -J rsptjob
#SBATCH —mail-type=FAIL
#SBATCH -A uppmax2025-2-262
#SBATCH -t 00-07:00:00
#SBATCH -p node
#SBATCH -N 4
### for jobs shorter than 15 min (max 4 nodes):
###SBATCH --qos=short

module load RSPt/2021-10-04
export RSPT_SCRATCH=$SNIC_TMP

srun -n 80 rspt

rm -f apts dmft_lock_file e_entropy efgArray.dat.0 efgData.out.0
energy_matrices eparm_last interstitialenergy jacob1 jacob2
locust.* out_last pot_last rspt_fft_wisdom.* runs.a symcof_new
```

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Job arrays

- Submit many jobs at once with the same or similar parameters
- Use `$SLURM_ARRAY_TASK_ID` in the script in order to find the correct path

```
#!/bin/bash
#SBATCH -A uppmax2025-2-262
#SBATCH -p node
#SBATCH -N 2
#SBATCH -t 01:00:00
#SBATCH -J jobarray
#SBATCH --array=0-19
#SBATCH --mail-type=ALL,ARRAY_TASKS

# SLURM_ARRAY_TASK_ID tells the script which iteration to run
echo $SLURM_ARRAY_TASK_ID

cd /pathtomydirectory/dir_$SLURM_ARRAY_TASK_ID/

srun -n 40 my-program
env
```

- You may use `scontrol` to modify some of the job arrays.

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Snakemake and Nextflow

- Conceptually similar, but with different flavours
- First define steps, each with an input, an output, and a command that transforms the input into output
- Then just ask for the desired output and the system will handle the rest

Hands-on #4: make it your own

- use 2 or 3 of the sample job scripts as a starting point for your own job script
- tweak them so that you run something closer to your research; or just feel free to experiment
- paste at least one of the examples in the HackMD
- great if you could add a comment what the job script is about

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Feedback on Slurm

- what did you find useful?
- not so useful?
- what is most challenging while editing your job script / workflow?
- something that was not covered that you'd like to know about?
- please provide your feedback in the HackMD

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Where to go from here?

Code documentation

NAISS training newsletter or https://www.naiss.se/events/ - software-specific training events included

https://coderefinery.org/workshops/upcoming/ (Git, Jupyter, code testing, writing code documentation, …)

https://nbis.se/training/events.html (bio)

https://enccs.se/events

https://supr.naiss.se/support/ or email support@uppmax.uu.se

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