SLURM @BIANCA

Diana Iuşan

Application expert and

training coordinator UPPMAX

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More Slurm and other advanced UPPMAX techniques

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

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The **Slurm** Workload Manager

- Free, popular, lightweight
- Open source:

  https://slurm.schedmd.com
- available at all NAISS centra
- UPPMAX Slurm userguide:

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

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More on **`sbatch`**

- Recap:

`sbatch`	**`-A sens2023598`**	**`-t 10:00`**	**`-p core`**	**`-n 10`**	**`my_job.sh`**
Slurm batch	Project name	Maximum runtime	Partition (“job type”)	#cores	job script

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More on time limits

- **`-t dd-hh:mm:ss`**
- `0-00:10:00 = 00:10:00 = 10:00 = 10`
- `0-12:00:00 = 12:00:00`
- `3-00:00:00 =` `3-0`
- `3-12:10:15`

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Job walltime

- Q: When you have no idea how long a program will take to run, what should you book?

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

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Job wall time

- 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%

More on partitions

- **`-p core`**
  - “core” is the default partition
  - ≤ 16 cores on Bianca
  - a script or program written without any thought on parallelism will use 1 core

More on partitions

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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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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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  - **`-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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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 sens2023598`
  - **`interactive`** `-n 80 -t 03:00:00 -A sens2023598`

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Debugging or complicated workflows

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  - 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 sens2023598`
  - **`interactive`** `-n 80 -t 03:00:00 -A sens2023598`
  - up to 12 hours
  - useful together with the `--begin=<time>` flag
  - `salloc -A sens2023598 --begin=2022-02-17T08:00:00`

    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 sens2023598
#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 Bianca
- 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`
- 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 512GB`
- 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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Monitoring jobs

- **`jobinfo`** - a wrapper around **`squeue`**
  - lists running and pending jobs
  - `jobinfo -u` *`username`*
  - `jobinfo -A sens2023598`
  - `jobinfo -u` *`username`* `--state=running`
  - `jobinfo -u` *`username`* `--state=pending`
- One may also use the **`squeue`** command.

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Monitoring jobs

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  - `jobinfo -u` *`username`*
  - `jobinfo -A sens2023598`
  - `jobinfo -u` *`username`* `--state=running`
  - `jobinfo -u` *`username`* `--state=pending`
- One may also use the **`squeue`** command.
- **`bianca_combined_jobinfo`** (queued jobs of all projects)

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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`

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:

  http://docs.uppmax.uu.se/cluster_guides/running_jobs/jobinfo_reason/

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
  - http://docs.uppmax.uu.se/software/jobstats/

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
  - `$ eog *png &`

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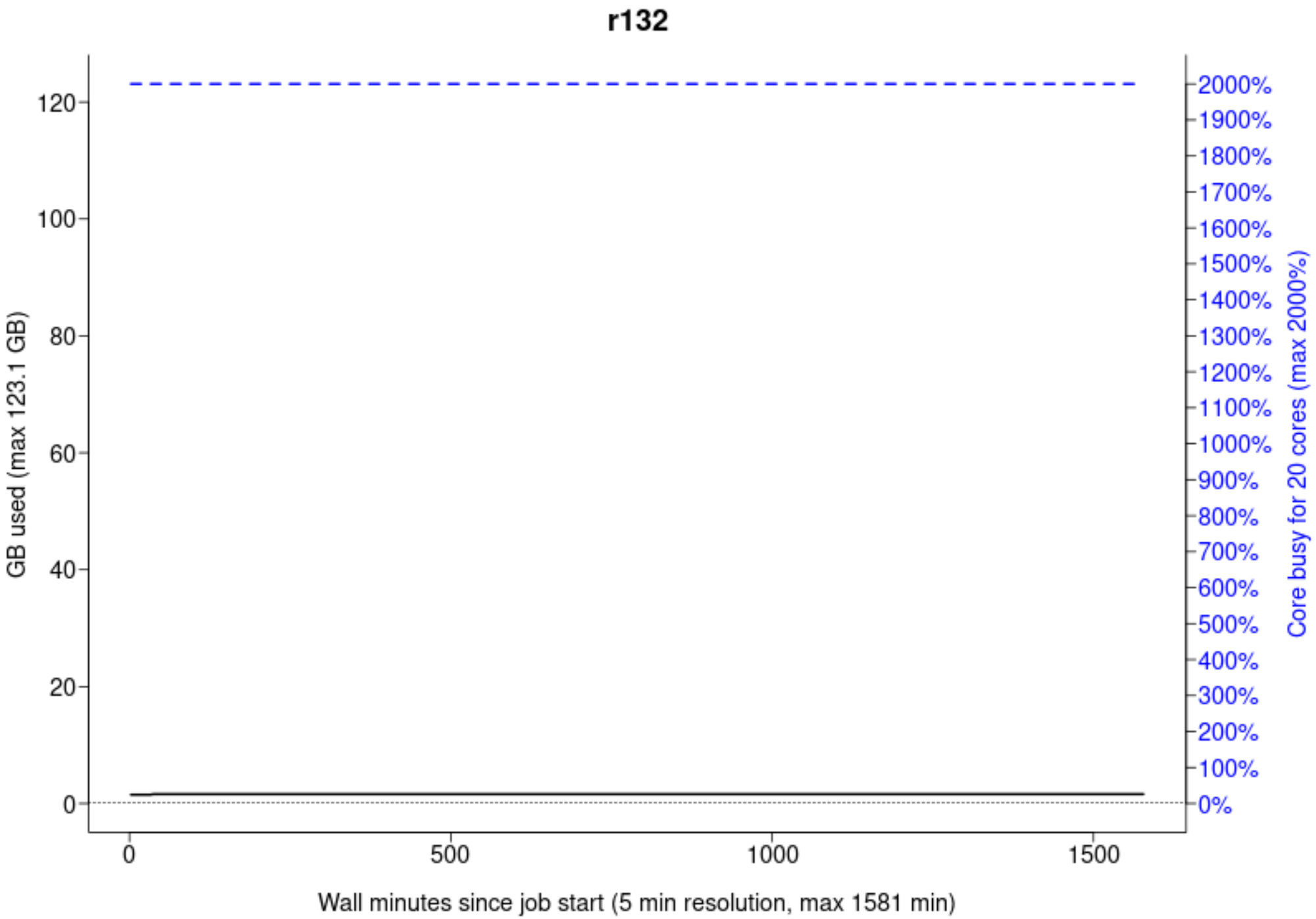
Hands-on #3: `jobstats`

- Which of the plots
  - Show good CPU or memory usage?
  - Indicate that the job requires a fat node?

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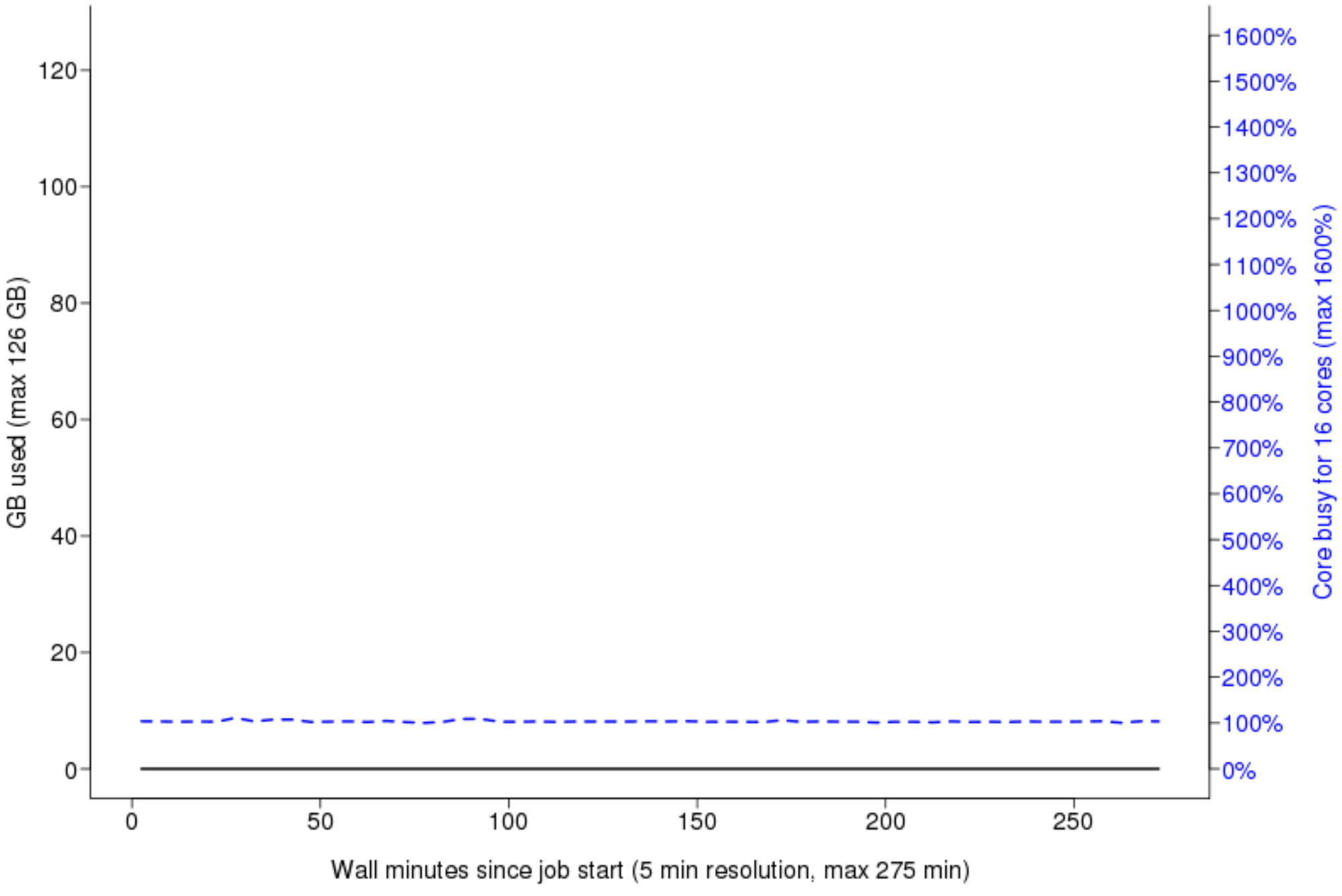
8804061 COMPLETED on milou end: 2016-10-10T20:30:26 runtime: 04:36:33

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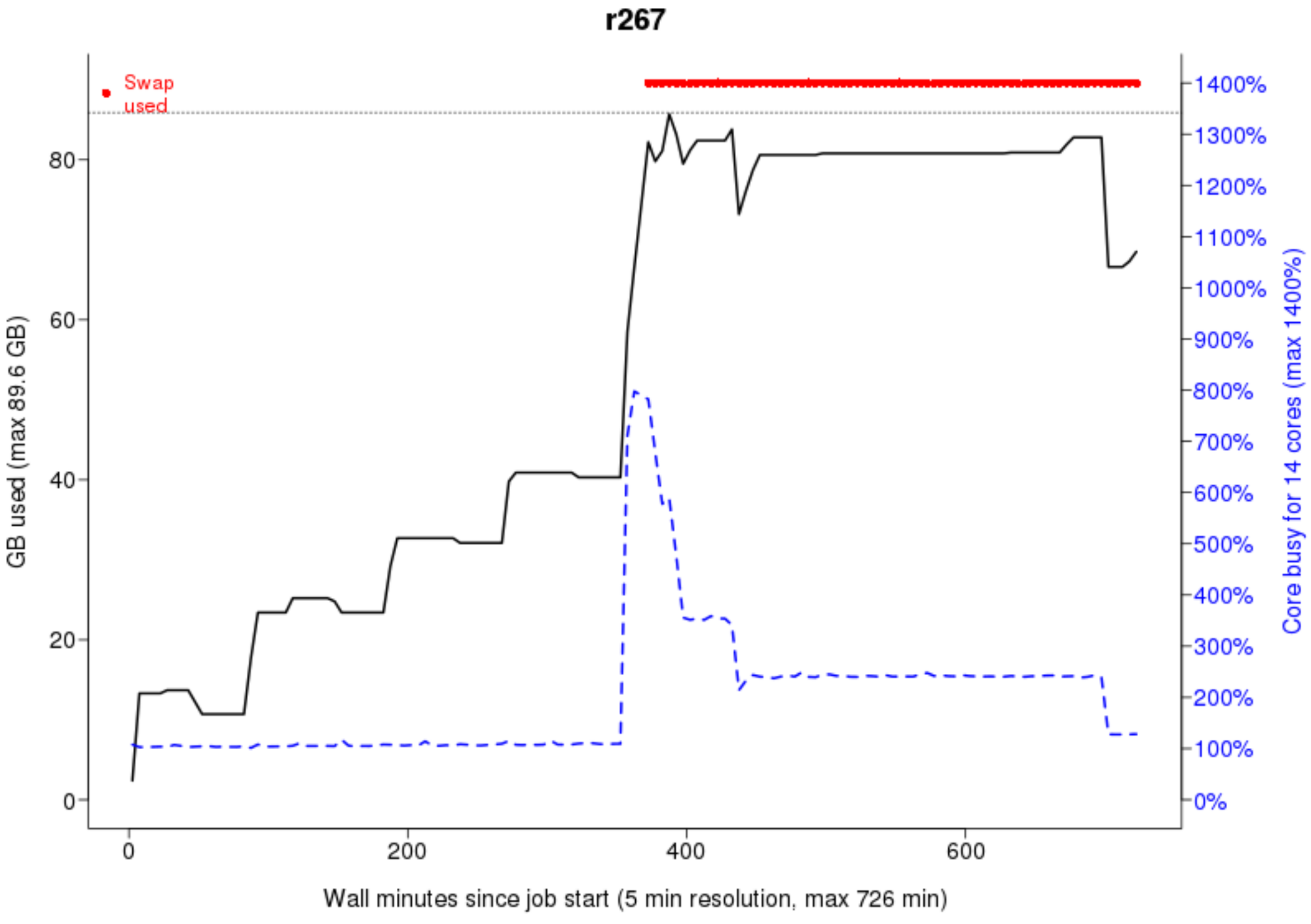
607031 OUT_OF_MEMORY on rackham end: 2018-08-25T07:29:39 runtime: 12:08:5

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 sens2023598
#SBATCH -p core
#SBATCH -n 10
#SBATCH -t 10:00:00

module load software/version
module load python/3.11.8

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

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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 mem512GB`

I/O intensive jobs: $SNIC_TMP

```
#!/bin/bash
#SBATCH -J jobname
#SBATCH -A sens2023598
#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 sens2023598
#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 Bianca

- Nodes with Nvidia A100 40 GB
- All GPU nodes have at least 256 GB RAM (fat nodes) with 16 CPU cores and 2 GPUs per node

GPU nodes on Bianca

- Nodes with Nvidia A100 40 GB
- All GPU nodes have at least 256 GB RAM (fat nodes) with 16 CPU cores and 2 GPUs per node
- SBATCH options:

```
#SBATCH -C gpu
#SBATCH --gpus=2                #number of GPUs requested
#SBATCH --gpus-per-node=2 #number of GPUs per node
nvidia-smi
```

- 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 sens2023598
#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
```

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 sens2023598
#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

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- 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
- Snakemake hackathon: https://www.naiss.se/event/online-training-snakemake-hackathon-2024-05/
- Nextflow training: https://training.nextflow.io/

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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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Where to go from here?

Code documentation

NAISS training newsletter - software-specific training events included

https://coderefinery.org/workshops/upcoming/

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

contact UPPMAX support via https://supr.naiss.se/support/

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