# Intro to tensor compute cluster @ MEB

Robert Karlsson  Rikard Öberg

2024-10-01

# Workshop program

- **9:00** Presentation
  - What is tensor, and what can tensor do for me?
  - Using tensor
  - Other systems
  - Queue etiquette
- **9:45** Break
- **10:00** Practical: simple Slurm jobs
- **10:?? – 10:45** Q&A

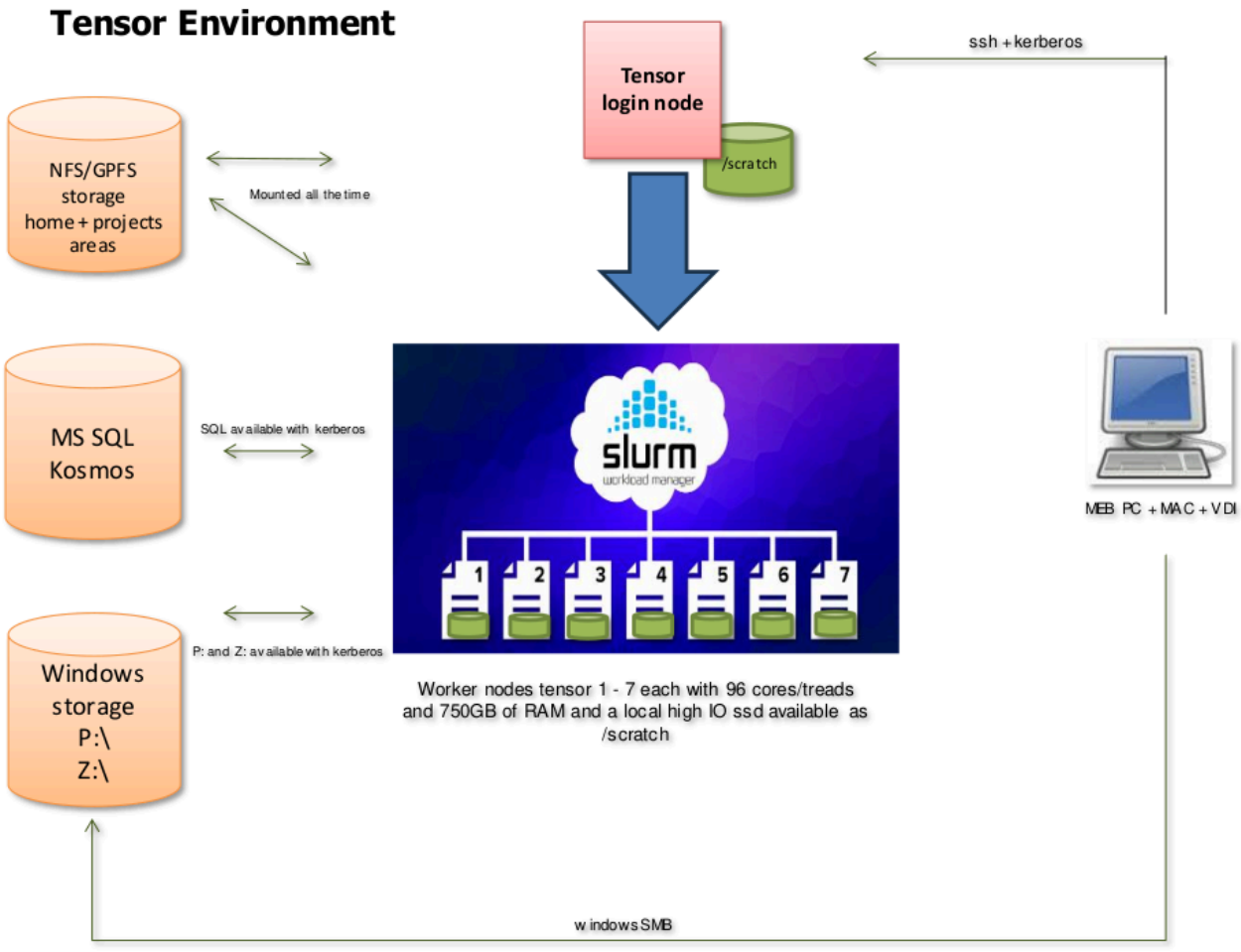
# What is tensor?

# What is tensor?

- MEB's new(ish)[1] local High Performance Computing system
- For medium-size computing, data management, statistical analysis, bioinformatics, ...
- Replaces previous servers vector, matrix[2]
- Runs Red Hat Enterprise Linux 9.4 and Slurm 23.11.1

1. online since April 2024
2. but keep using matrix for SAS, for now

# What is tensor?



# What can tensor do for me?

- run analyses that take *longer time* than I'd like to keep my own computer running
  - "I usually start the analysis, then leave the laptop open over the weekend..."
- run analyses that use *more resources* than my computer has (CPU cores and/or memory)
  - "My analysis data consists of approximately 500 million rows..."

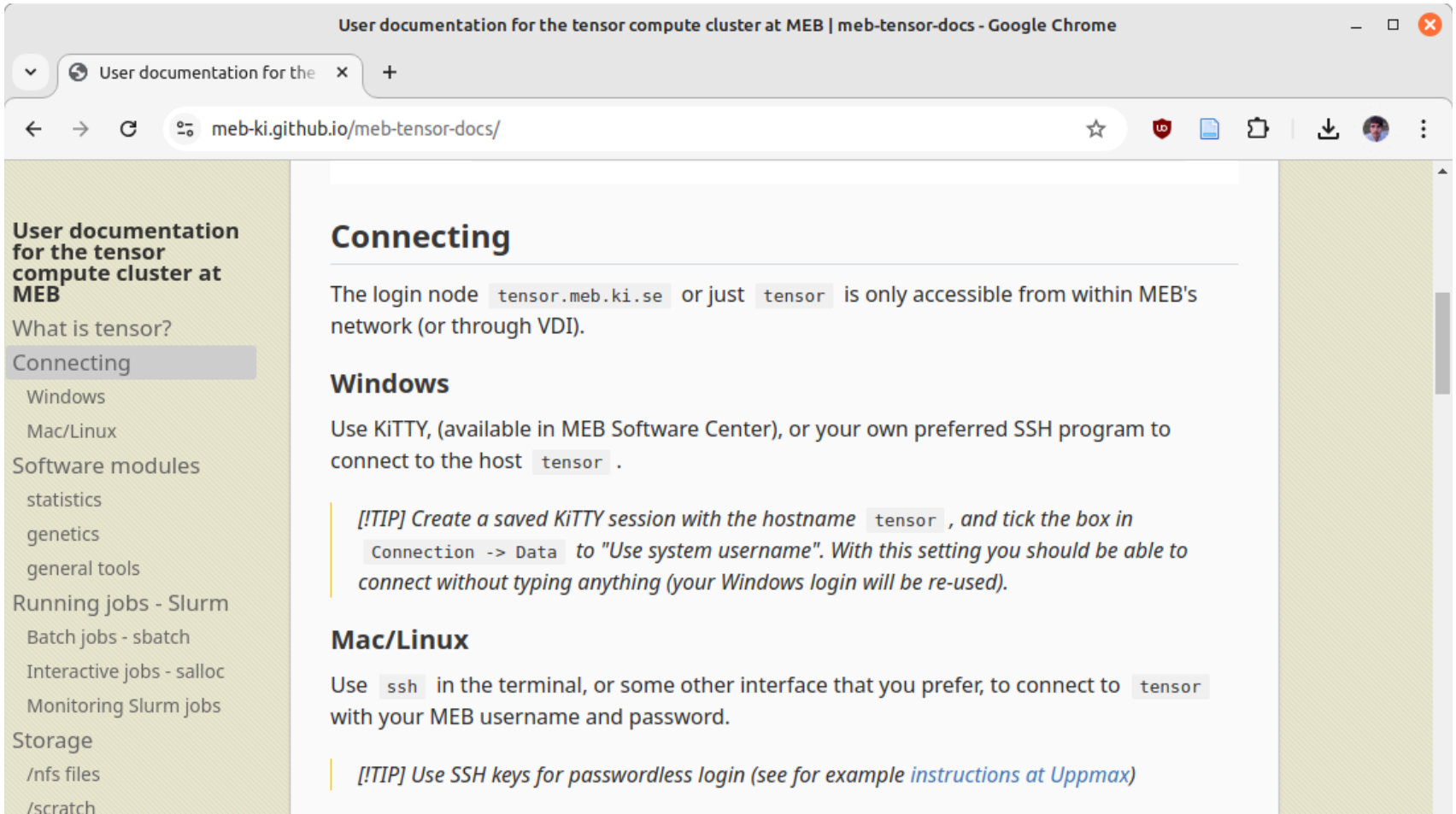
# What can tensor do for me (continued)?

- run many independent analyses in parallel
  - Simulation over a range of parameters, data analysis in batches, ...
- run analyses that require software that is only available for, or runs better on, Linux
- all of the above with access to the MEB network file storage and databases
  - `P:`, `Z:`, `kosmos`, ...

# Using tensor

# The user guide

- Available at https://meb-ki.github.io/meb-tensor-docs/
- Holds answers to many common questions (continuously updated)



# Slurm workload manager

- To use tensor, you must use Slurm[1]
- Why Slurm?
  - allocates resources efficiently
  - keeps jobs separated while running

1. “Simple Linux Utility for Resource Management”

# Slurm in practice

# Slurm (batch jobs)

- `sbatch` – submits batch jobs
  - You already have a script: send it to the job queue

```
# instead of
./run_analyses.sh
# or
Rscript simulate_something.R

# send jobs to the Slurm queue
sbatch -c 2 -t 0-8 --memory=10G run_analyses.sh
sbatch -c 2 -t 0-8 --memory=10G --wrap='Rscript simulate_something.R'
```

- Tell Slurm:
  - resources needed (cpu cores, memory)
  - for how long (roughly)?
- Slurm will run your job as soon as possible

# Slurm (batch jobs)

- Manage batch jobs: `squeue`, `scancel`

```
[robkar@tensor ~]$ squeue
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
             98108      core BT_K60_H   hamkha  R    6:16:46      1 tensor4
             95475      core interact   robkar  R 1-19:57:08      1 tensor7
             98123      core DCSM_bmi   pegler  R    3:36:49      1 tensor3
```

- See also `squeue -l`, `squeue -O ...`, `squeue --me`

- When you change your mind:

```
scancel 95475 # cancel a specific job
scancel --me  # cancel all my jobs
```

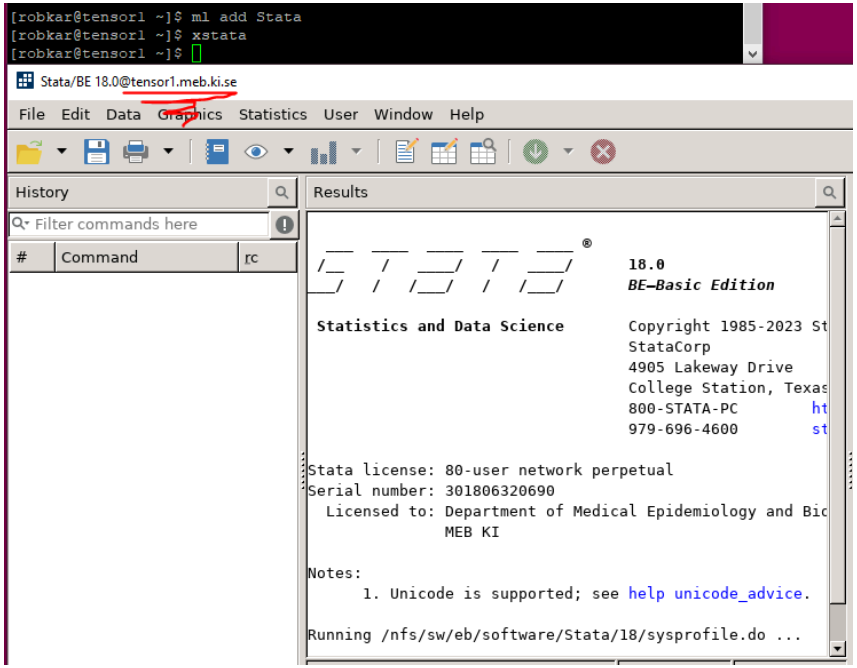
# Slurm (interactive)

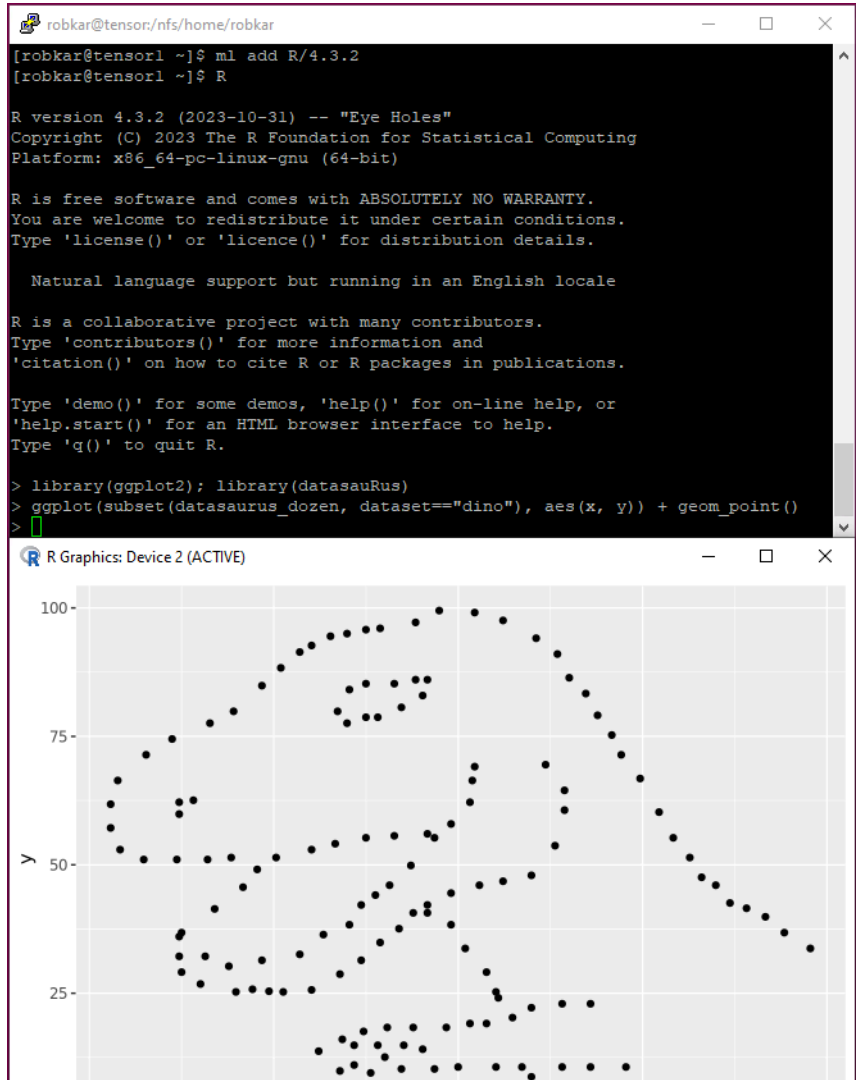
- When developing your analysis code, ask for an interactive session with `salloc`
- Like sbatch, specify time, cpu cores (memory)
- Exit when done to free up resources

```
# interactive job using 4 cores for 8 hours
salloc -t 0-8 -c 4
```

# Slurm (interactive)

- X11 graphics available (see user guide for details)



# Slurm job parameters

- Specify in job script *or* on sbatch command line
  - on command line: `sbatch -c 4 -t 0-4 ...`
  - in job script (must come before any commands):

```
#SBATCH -c 4
#SBATCH -t 0-4
...
```

# Slurm job parameters

- Time: `-t` or `--time`
  - format: `days-hours` or `hours:minutes:seconds` or `minutes`
- CPU threads: `-c N`, `--cpus-per-task N` for N threads
- Memory: `--mem`
  - format: `nnn` for nnn megabytes, or use suffixes `[K|M|G|T]`
- Defaults if left unspecified: 4 hours, 2 threads, 7 GB memory per thread

# Asking for the right amount of time/memory/CPU

- Think first (for a rough estimate)
- Test run(s) - interactive or batch

- Checking on resource usage:
  - `seff [jobid]` (after the test job finishes)
  - `/usr/bin/time -v [your command...]` (see results in slurm-$JOBID.out)
  - `srun --jobid=[jobid] --overlap --pty htop` (monitor the job while it runs)
    - replace “htop” with “bash” for a shell to examine files in job-specific /scratch

# When you asked for too little:

## Not enough time

```
[robkar@tensor ~]$ salloc -t 1:00
salloc: Granted job allocation 113359
salloc: Nodes tensor4 are ready for job

[robkar@tensor4 ~]$ salloc: Job 113359 has exceeded its time limit and its allocation has been
revoked.
slurmstepd: error: *** STEP 113359.interactive ON tensor4 CANCELLED AT 2024-09-25T12:00:52 DUE TO
TIME LIMIT ***
srun: Job step aborted: Waiting up to 32 seconds for job step to finish.
srun: error: tensor4: task 0: Killed

[robkar@tensor ~]$ seff 113359
Job ID: 113359
...
State: TIMEOUT (exit code 0)
...
```

# When you asked for too little:

## Not enough memory

```
[robkar@tensor ~]$ sbatch -t 0-1 -c 2 --mem=4G --wrap='ml add R; Rscript -e "x <- rnorm(1e9)"'
Submitted batch job 113367

[robkar@tensor ~]$ cat slurm-113367.out
/var/spool/slurm/d/job113367/slurm_script: line 4: 2590672 Killed                  Rscript -e "x <-
rnorm(1e9)"
slurmstepd: error: Detected 1 oom_kill event in StepId=113367.batch. Some of the step tasks have been
OOM Killed.

[robkar@tensor ~]$ seff 113367
Job ID: 113367
...
State: OUT_OF_MEMORY (exit code 0)
...
Memory Utilized: 3.00 MB
Memory Efficiency: 0.07% of 4.00 GB
```

Note that `seff` memory statistics do not always capture spikes in memory usage (but the system OOM killer will)

# More Slurm job parameters

- Job name: `-J` or `--job-name`
  - give your job a nice label in squeue
- Job output files: `-e` and `-o`
  - save your job's error messages and output in named files (`-e` and `-o` can point to the same file, by default `"slurm-$JOBID.out"`)
- Advanced: job arrays `--array=1-N`
- Advanced: job dependencies `--dependency=...`

# Login vs compute nodes

- Please don't use the login node for computing
  - Impolite: can interfere with others' work
  - Slow: login node tasks are confined to a single core per login and 12G memory
- Instead use `salloc` or `sbatch`
- OK to stay on login node for text editing, file management, other small tasks

# Software modules

- Growing collection of preinstalled software, but must enable packages before using
- Show what's currently available: `ml avail` (or user guide)
- Enable a package: `ml load package/version`
- When a package you need is not in modules:
  - *and only you need it*: /nfs/home/$USER installation
  - *and many others need it too*: ask for /nfs/sw central installation
- apptainer (previously Singularity) is installed for containerized workflows

# Storage folders

- tensor-specific network folders:
  - /nfs/home/$USER
  - /projects/$PROJECT
- Regular MEB network folders
  - /cifs/Z/$USER “Windows Z:”
  - /cifs/P/$PROJECT “Windows P:”
  - `ml add mebauth` for P/Z access
- tensor node-local storage /scratch/tmp - use it! It is fast! But:
  - **/scratch is machine-(and job-)specific**

    tensor1:/scratch ≠ tensor2:/scratch
  - **/scratch is cleared when the job ends**

# What tensor is not set up to do

- GPU
- Multi-node parallel jobs (MPI)
- Windows-only software
- Really big jobs (N = 7 will be quickly saturated)

# When tensor is not big enough

- NAISS (previously SNIC) national resources
- Clusters Bianca (UU) for sensitive data, Dardel (KTH) for non-sensitive data

# Queue/tensor etiquette

- Do read the manual
- Don’t run analyses on the login node
- Don’t reserve resources you don’t need
- Release interactive sessions when done

**Running a long command as the last thing in an interactive session**

```
some_command --param 1 --param 2 && exit
```

- Rules and limits for heavy use still under development – your input most welcome!
- When there is a queue, jobs from heavy users get lower priority
  - `sprio` to see the priority for jobs in queue

# part 2: tensor practical

# Practical: simple slurm jobs

- Use VDI (to ensure we all have the same environment) to
  - log in to tensor
  - create a small job script using a specific R version (or Stata)
  - submit to queue (sbatch)
  - check status (squeue)
  - examine output (cat slurm-$JOBID.out)
- Example scripts available from https://github.com/robkar/meb-tensor-intro/

# part 3: general Q&A, help with specific tasks