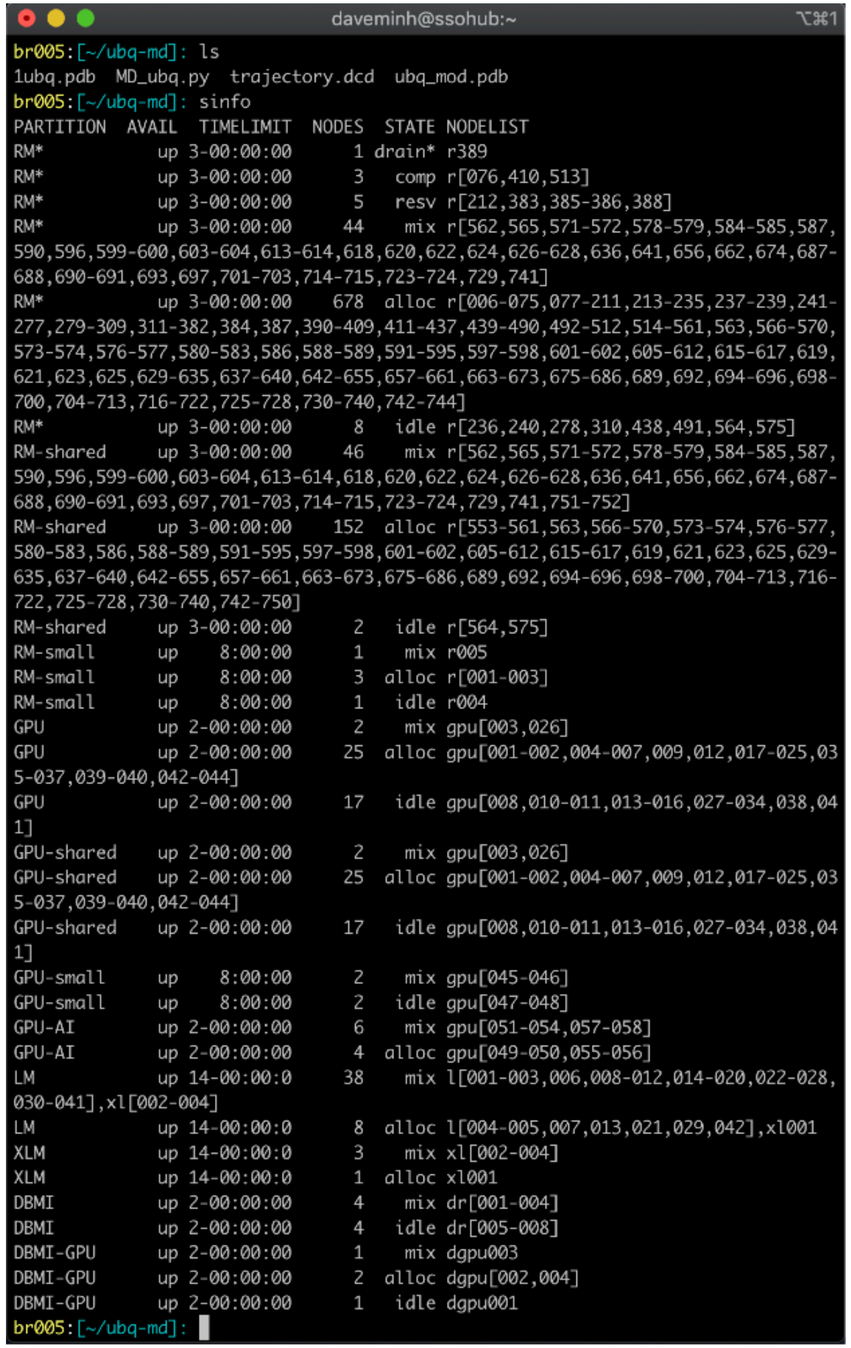
- SLURM has its own commands (https://slurm.schedmd.com/quickstart.html)
- Let's try two simple ones
  - sinfo - information about the Bridges partitions. We want "RM-small" for our first job. Shorter jobs can be squeezed in between longer jobs.
  - squeue - lists jobs currently on the queue



- Let’s write a batch script called MD_ubq.job and put it in the ~/ubq-md/ directory. You can
  - use a terminal text editor like `vi’
  - create it on your local computer and transfer it to bridges

MD_ubq.job

```
#!/bin/bash
#SBATCH -N 1
#SBATCH -p RM-small
#SBATCH -t 00:30:00
#SBATCH --ntasks-per-node 1

# Set up the environment
source ~/.bashrc
module load anaconda3
conda activate openmm

# Run MD
cd ~/ubq-md
python MD_ubq.py

```