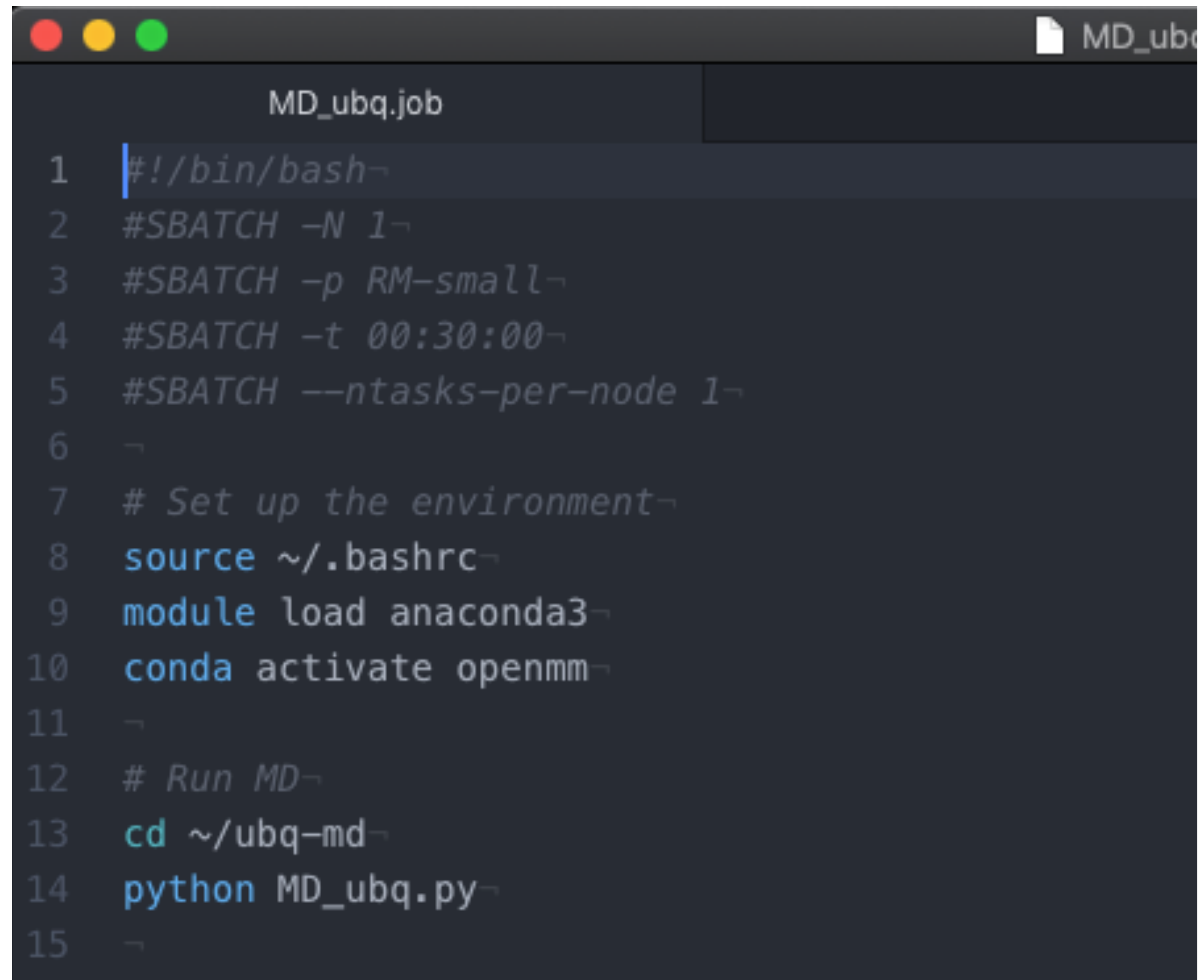


- SLURM has its own commands (<https://slurm.schedmd.com/quickstart.html>)
- Let's try two simple ones
 - sinfo - information about the Bridges partitions. We want "RM-small" for our first job. Shorter jobs can be squeezed in between longer jobs.
 - squeue - lists jobs currently on the queue

```
daveminh@ssohub:~
br005: [~/ubq-md]: ls
1ubq.pdb MD_ubq.py trajectory.dcd ubq_mod.pdb
br005: [~/ubq-md]: sinfo
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
RM*        up 3-00:00:00      1 drain* r389
RM*        up 3-00:00:00      3  comp r[076,410,513]
RM*        up 3-00:00:00      5  resv r[212,383,385-386,388]
RM*        up 3-00:00:00     44  mix  r[562,565,571-572,578-579,584-585,587,590,596,599-600,603-604,613-614,618,620,622,624,626-628,636,641,656,662,674,687-688,690-691,693,697,701-703,714-715,723-724,729,741]
RM*        up 3-00:00:00     678 alloc r[006-075,077-211,213-235,237-239,241-277,279-309,311-382,384,387,390-409,411-437,439-490,492-512,514-561,563,566-570,573-574,576-577,580-583,586,588-589,591-595,597-598,601-602,605-612,615-617,619,621,623,625,629-635,637-640,642-655,657-661,663-673,675-686,689,692,694-696,698-700,704-713,716-722,725-728,730-740,742-744]
RM*        up 3-00:00:00      8  idle r[236,240,278,310,438,491,564,575]
RM-shared  up 3-00:00:00     46  mix  r[562,565,571-572,578-579,584-585,587,590,596,599-600,603-604,613-614,618,620,622,624,626-628,636,641,656,662,674,687-688,690-691,693,697,701-703,714-715,723-724,729,741,751-752]
RM-shared  up 3-00:00:00    152 alloc r[553-561,563,566-570,573-574,576-577,580-583,586,588-589,591-595,597-598,601-602,605-612,615-617,619,621,623,625,629-635,637-640,642-655,657-661,663-673,675-686,689,692,694-696,698-700,704-713,716-722,725-728,730-740,742-750]
RM-shared  up 3-00:00:00      2  idle r[564,575]
RM-small   up    8:00:00      1  mix  r005
RM-small   up    8:00:00      3 alloc r[001-003]
RM-small   up    8:00:00      1  idle r004
GPU        up 2-00:00:00      2  mix  gpu[003,026]
GPU        up 2-00:00:00     25 alloc gpu[001-002,004-007,009,012,017-025,035-037,039-040,042-044]
GPU        up 2-00:00:00     17  idle gpu[008,010-011,013-016,027-034,038,041]
GPU-shared up 2-00:00:00      2  mix  gpu[003,026]
GPU-shared up 2-00:00:00     25 alloc gpu[001-002,004-007,009,012,017-025,035-037,039-040,042-044]
GPU-shared up 2-00:00:00     17  idle gpu[008,010-011,013-016,027-034,038,041]
GPU-small  up    8:00:00      2  mix  gpu[045-046]
GPU-small  up    8:00:00      2  idle gpu[047-048]
GPU-AI     up 2-00:00:00      6  mix  gpu[051-054,057-058]
GPU-AI     up 2-00:00:00      4 alloc gpu[049-050,055-056]
LM         up 14-00:00:0     38  mix  l[001-003,006,008-012,014-020,022-028,030-041],xl[002-004]
LM         up 14-00:00:0      8 alloc l[004-005,007,013,021,029,042],xl001
XLM        up 14-00:00:0      3  mix  xl[002-004]
XLM        up 14-00:00:0      1 alloc xl001
DBMI       up 2-00:00:00      4  mix  dr[001-004]
DBMI       up 2-00:00:00      4  idle dr[005-008]
DBMI-GPU   up 2-00:00:00      1  mix  dgpu003
DBMI-GPU   up 2-00:00:00      2 alloc dgpu[002,004]
DBMI-GPU   up 2-00:00:00      1  idle dgpu001
br005: [~/ubq-md]:
```

- 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
1  #!/bin/bash~
2  #SBATCH -N 1~
3  #SBATCH -p RM-small~
4  #SBATCH -t 00:30:00~
5  #SBATCH --ntasks-per-node 1~
6  ~
7  # Set up the environment~
8  source ~/.bashrc~
9  module load anaconda3~
10 conda activate openmm~
11 ~
12 # Run MD~
13 cd ~/ubq-md~
14 python MD_ubq.py~
15 ~
```