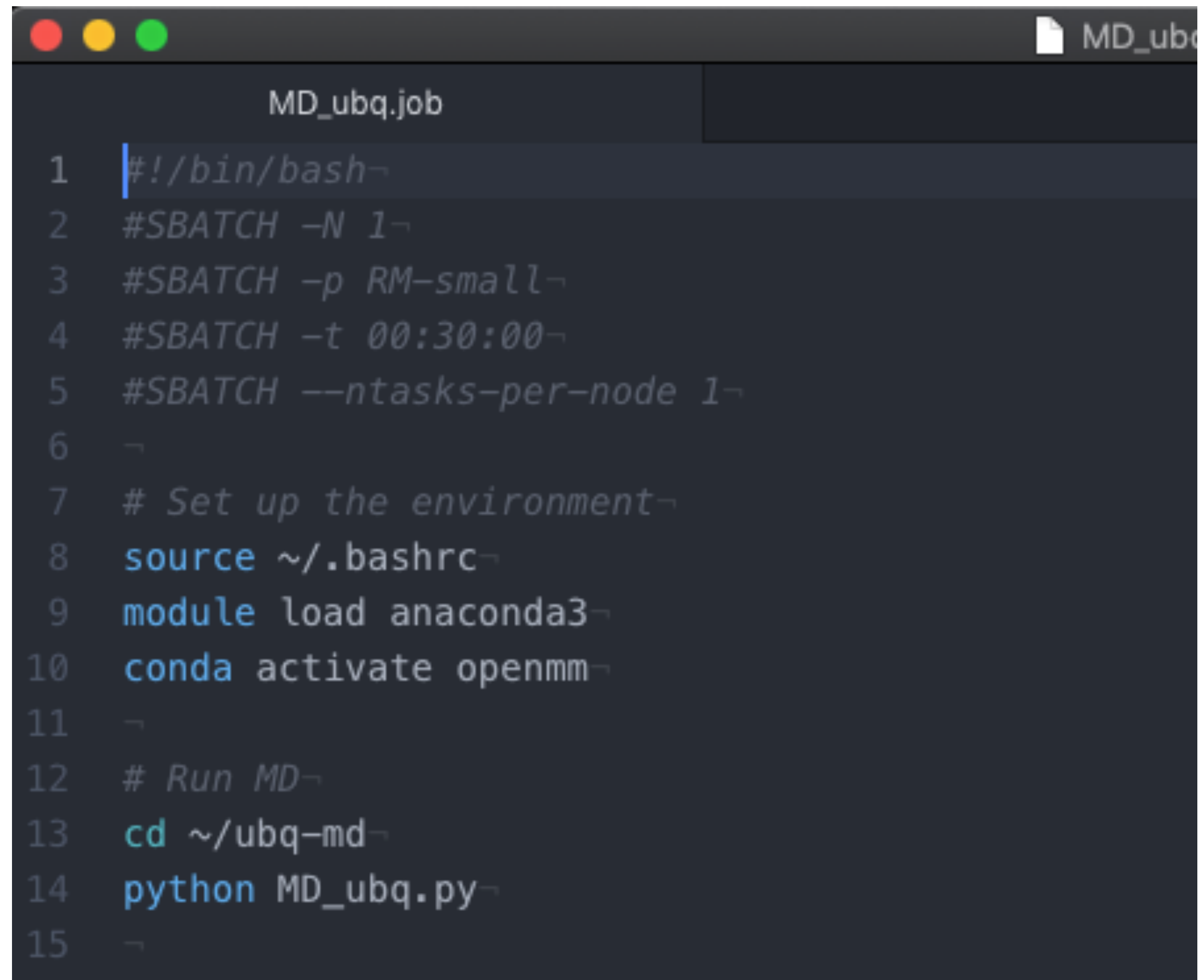


- Let's write a batch script called MD_ubq.job and put it in the ~/ubq-md/ directory. You can
 - use a terminal text editor like 'vi'
 - create it on your local computer and transfer it to bridges



```
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 ~
```

- Once you have created the job file, you can submit it to the queue using `sbatch MD_ubq.job`
- After submitting the job you can log out or be disconnected from the server and it will still run
- You can use `squeue -u *user_name*` to check the status of your job(s)
- The calculation will complete the same way as an interactive job
- The output that would be sent to the terminal in an interactive job is sent to a file

```
br006:[~/ubq-md]: sbatch MD_ubq.job
Submitted batch job 7589729
br006:[~/ubq-md]: squeue -u dminh
```

JOBID	PARTITION	NAME	USER	ST	TIME	NODES	ODELIST(REA SON)
7589729	RM-small	MD_ubq.j	dminh	R	0:06	1	r005

```
br006:[~/ubq-md]: ls -ltr
total 312
-rw-r--r-- 1 dminh mc4s8bp 50895 Jan 31 18:44 1ubq.pdb
-rw-r--r-- 1 dminh mc4s8bp 1678 Jan 31 18:50 MD_ubq.py
-rw-r--r-- 1 dminh mc4s8bp 221 Feb 5 17:17 MD_ubq.job
-rw-r--r-- 1 dminh mc4s8bp 99863 Feb 5 17:23 ubq_mod.pdb
-rw-r--r-- 1 dminh mc4s8bp 148796 Feb 5 17:23 trajectory.dcd
-rw-r--r-- 1 dminh mc4s8bp 727 Feb 5 17:23 slurm-7589729.out
br006:[~/ubq-md]: more slurm-7589729.out
Minimizing...
Running Production...
#"Progress (%)" "Step" "Potential Energy (kJ/mole)" "Temperature (K)"
"Speed (ns/day)" "Time Remaining"
10.0% 100 -12891.608289052907 182.75168707244657 0 --
20.0% 200 -12679.091283728229 208.12074466763545 8.22 0:16
30.0% 300 -12544.950513910171 222.9911557564418 8.27 0:14
40.0% 400 -12417.294668972278 241.63949664412493 8.29 0:12
50.0% 500 -12182.148295443869 250.84879213741047 8.31 0:10
60.0% 600 -12086.427954357983 250.25410151752132 8.31 0:08
70.0% 700 -12201.427649847661 275.4539256800823 8.3 0:06
80.0% 800 -12071.165875336525 278.7590849918891 8.29 0:04
90.0% 900 -11779.891281989974 278.2551306095054 8.28 0:02
100.0% 1000 -11804.03142004821 289.69894096208446 8.27 0:00
Done!
```