- 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 NODELIST(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!
```

Some Complications

- For your project, you will want different options in your scripts to
  - run MD on GPUs
  - run calculation for longer
  - not overwrite previous data
  - store data on $LOCAL or $SCRATCH