Liquid Water equilibration problem

PROCEDURE

1. **Initialize atoms on a bcc lattice at a specified density**

```
# Define the lattice
variable        lattice_constant equal 3.90859
lattice         bcc ${lattice_constant}

# Define region
# multiples of lattice spacing
region          simbox block 0 5 0 5 0 5

# Create Atoms
create_box              1 simbox
create_atoms            1 box
mass                    1 18.015
```

2. **Set their velocities to have a temperature of 300 K**

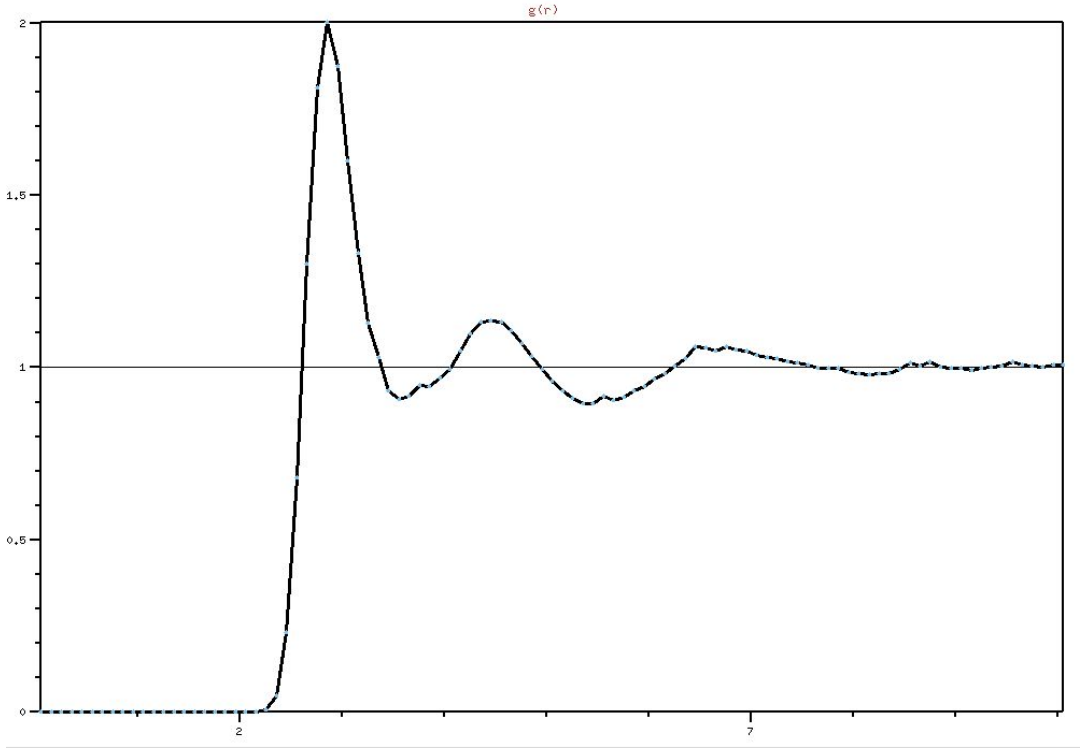
```
velocity    all create 300.0 97287

fix             1 all nve
timestep        0.0005
run             5000
```

3. **They are in an unfavorable configuration so a lot of potential energy gets converted to KE, and temperature explodes**
4. **Freeze the atoms after a while**
5. **Re-set their velocities to have 300 K**

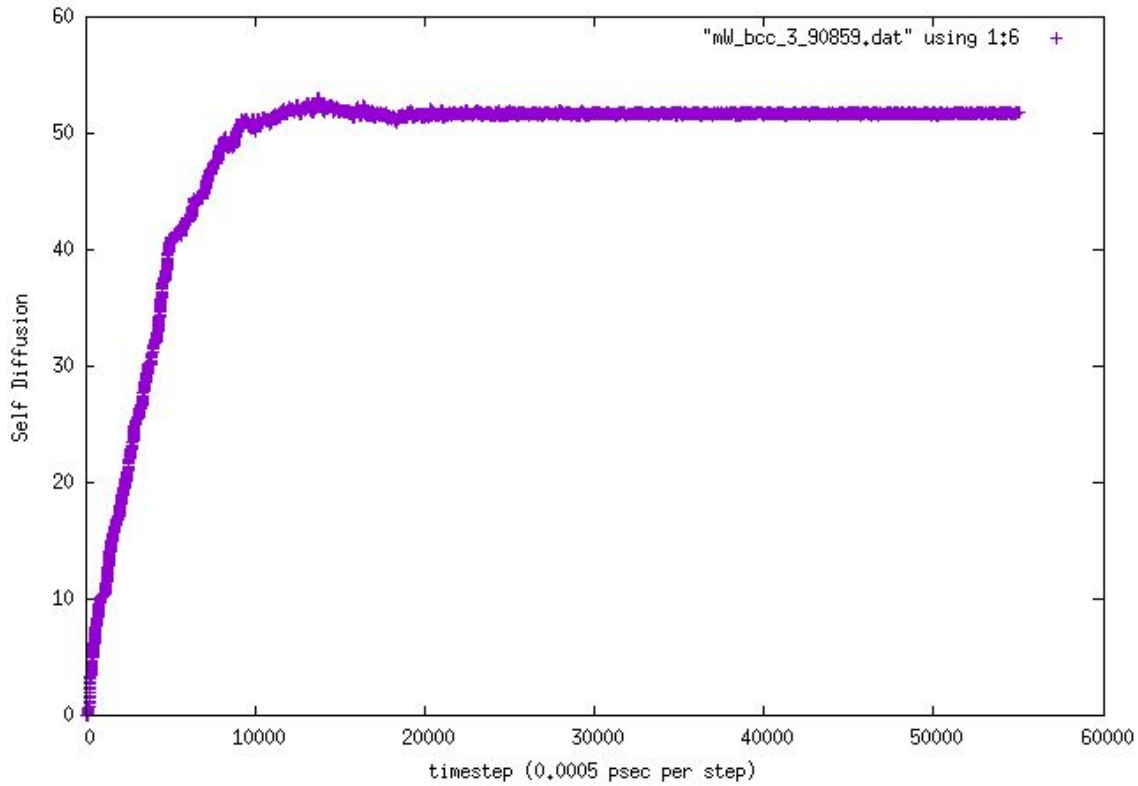
```
unfix 1
velocity      all create 300.0 97287
fix           2 all nve
timestep    0.0005
run           5000
```

6. **This time there is not as much PE to be converted, but there is still a lot and the temperature explodes**
7. **Freeze atoms and reset velocities to 300 K**
8. **After about 8 of these cycles the atoms are in a liquid-like configuration and will maintain the temperature given during the velocity set**

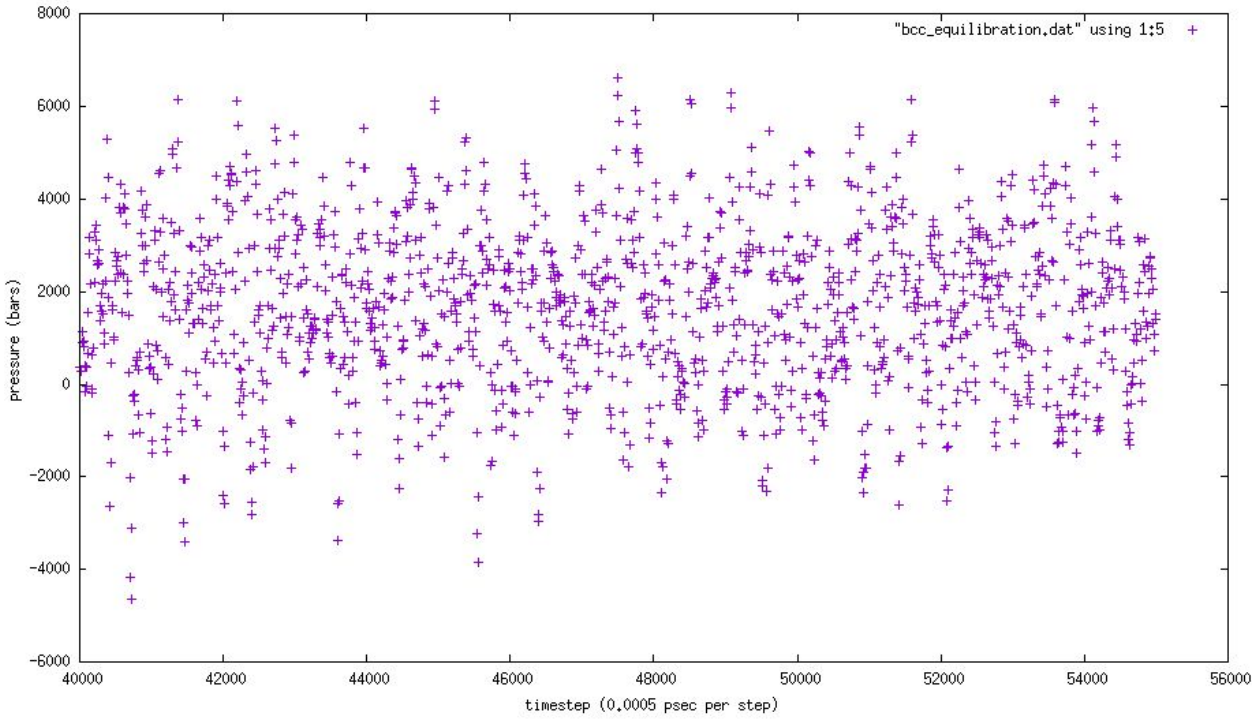
Resulting System has a liquid-like configuration:



But non-liquid-like behavior in terms of self diffusion (Mean Square Diffusion) of the molecules:



And I don’t know if this is the expected pressure behavior (starting at 40000 timestep):



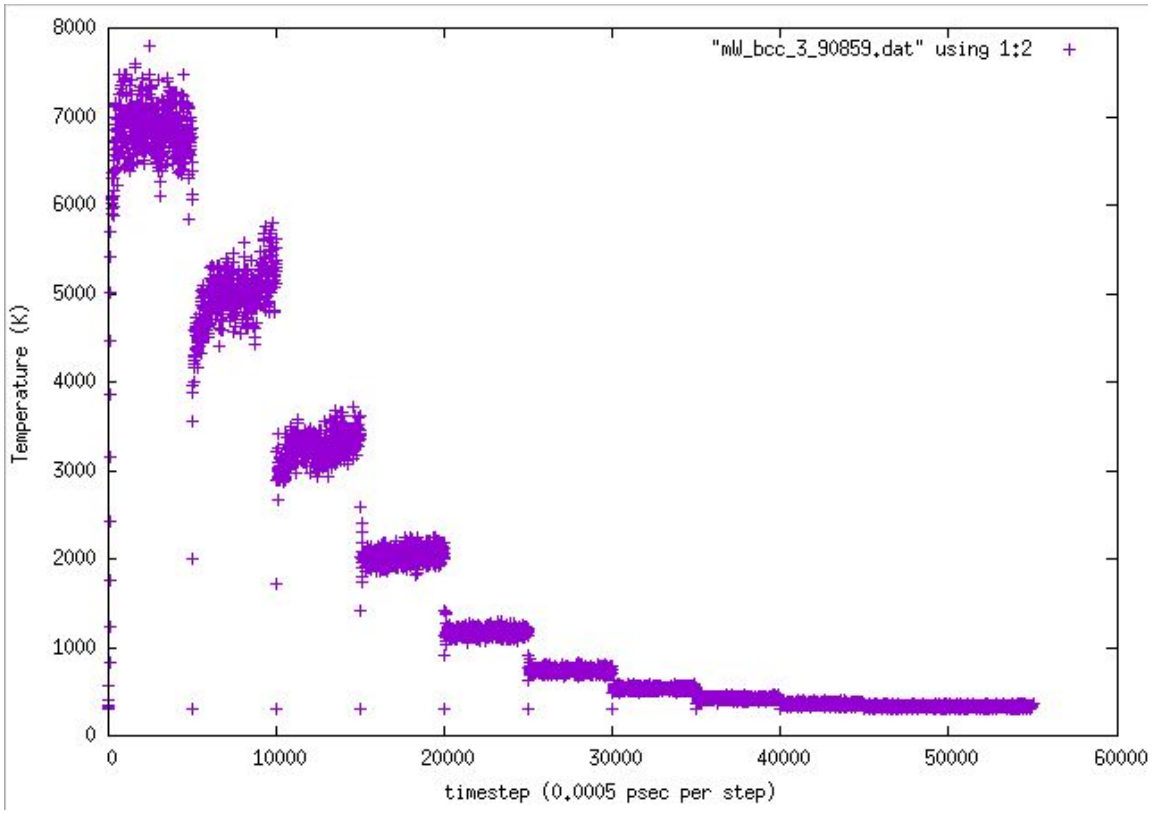
Ideas:
Why do the mW water molecules tend to freeze up and sit at a fixed position?

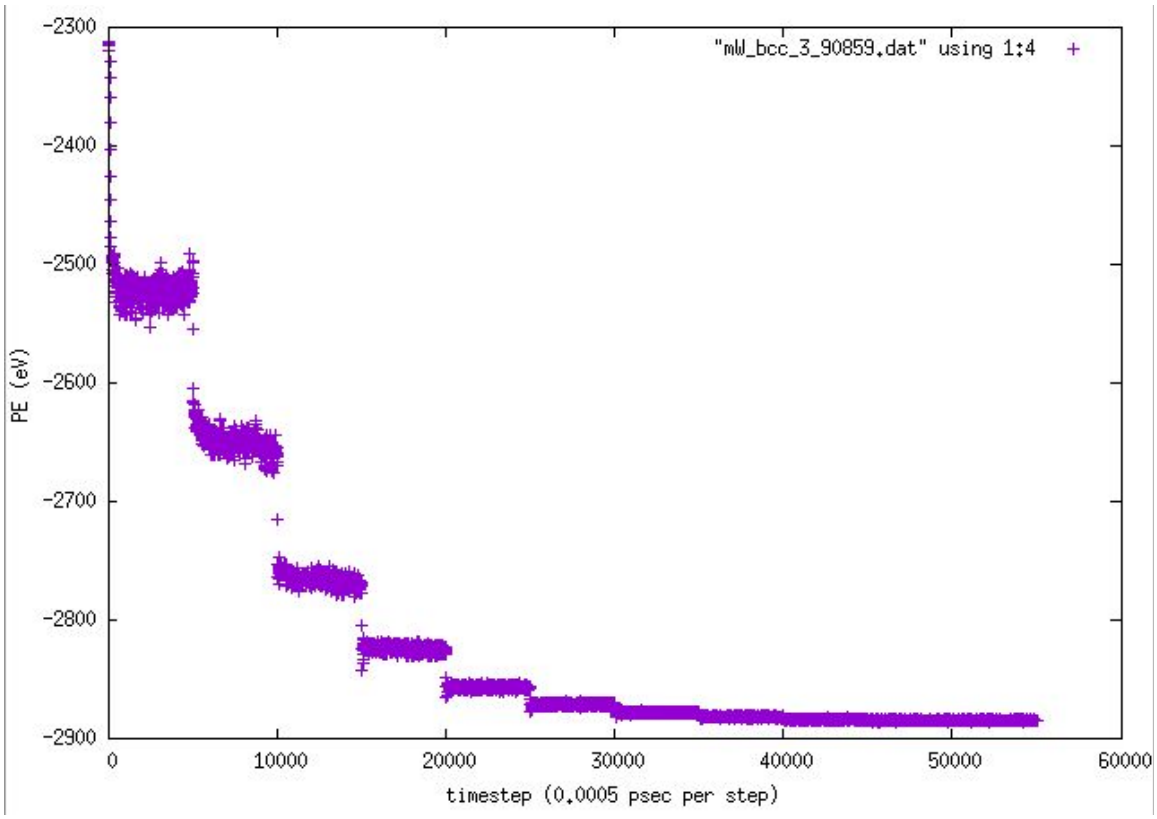
I could do some sort of parameter sweep (maybe over initial lattice densities?) until I see liquid behavior

Check what expected self-diffusion rate is for liquid water, will it be an obvious upward trend in the time scale of my simulation?

Check what expected pressure fluctuations should be, is my system having too large fluctations? Why?

Extra:


"mW_bcc_3_90859.dat" using 1:2
Temperature (K)
timestep (0.0005 psec per step)
0
1000
2000
3000
4000
5000
6000
7000
8000
0
10000
20000
30000
40000
50000
60000


"mW_bcc_3_90859.dat" using 1:4
PE (eV)
timestep (0.0005 psec per step)
-2300
-2400
-2500
-2600
-2700
-2800
-2900
0
10000
20000
30000
40000
50000
60000