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BE21B004

BT4110 – Computational Biology Lab

Practical 2

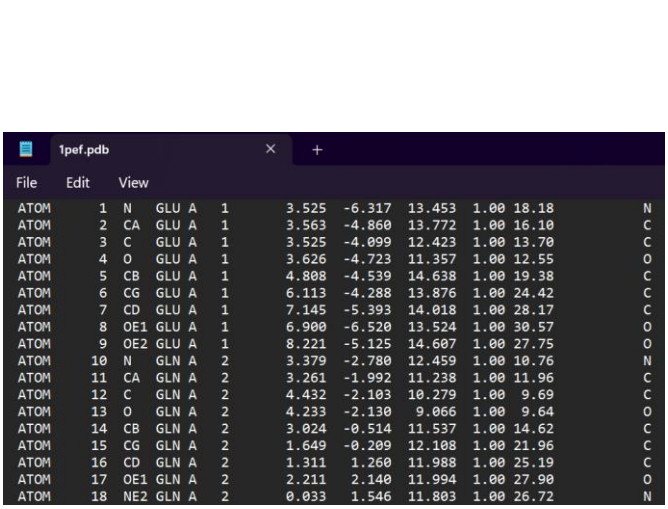
Task 1

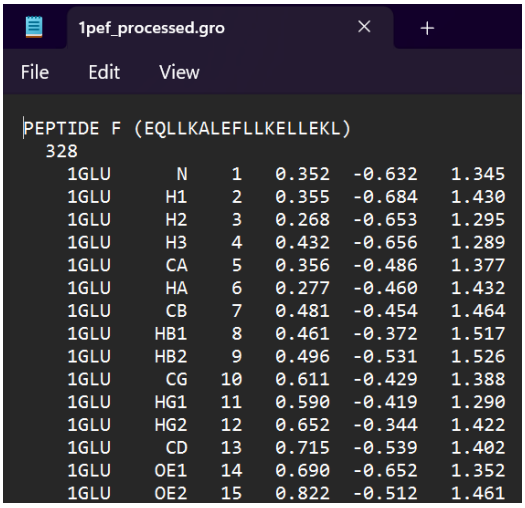
Steps followed

- The .pdb file for 1PEF was downloaded from the Protein Data Bank.
- Water molecules were removed from the .pdb file using a `grep` command.
- A .gro file was created using `pdb2gmx`. CHARMM27 was used as the force field and TIP3P was chosen as the water model.

Question 1a

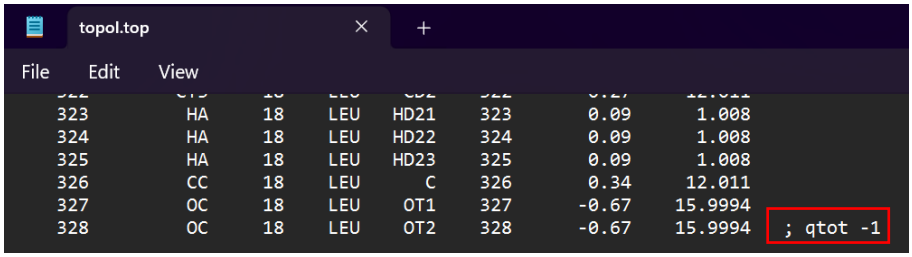
- The .gro file produced by `pdb2gmx` is much more compact than the input .pdb file.
- All the remarks given in the .pdb file are erased and only the atomic coordinates are retained.
- The .pdb file may or may not have hydrogen coordinates but the .gro file includes hydrogen coordinates.
- The .gro file complies with a user-defined force field.
- The coordinates in .pdb are in angstrom units while those in the .gro file are in nanometre units.





Question 1b

According to the topol.top file, the protein currently has a net charge of −1.

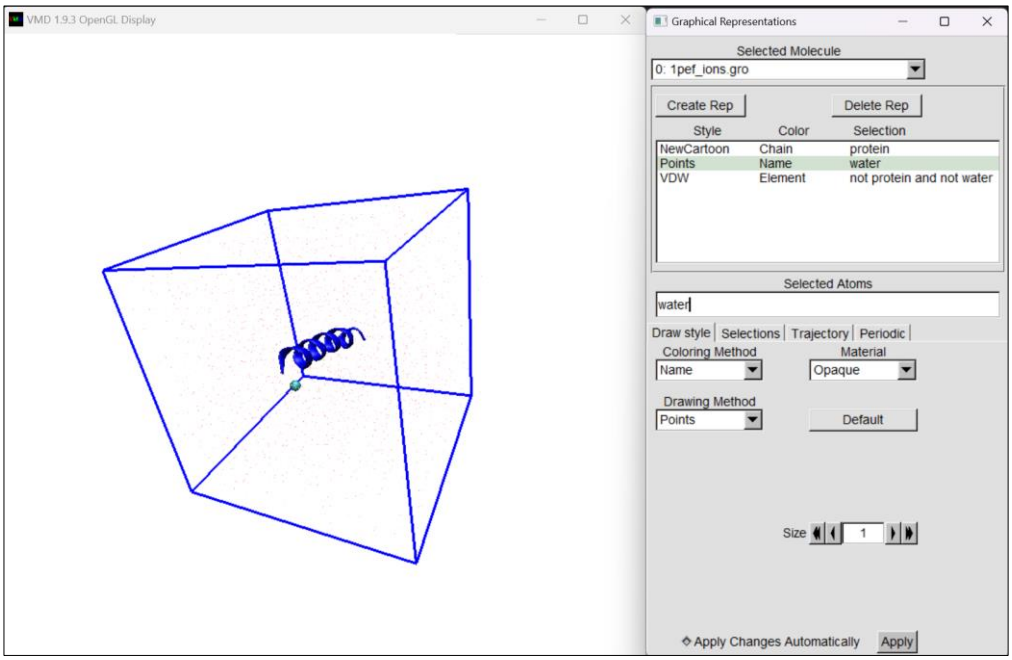


Task 2

Steps followed

- A cubic box was created using `editconf` with the protein at the centre and a padding distance of 1 nm.
- The box was solvated using `solvate`.
- Ions were added using `grompp` and `genion`. 1 Na^+ ion was added since the net charge was −1

Question 2a



We can visualise the solvated box with the protein in VMD. To do so, we have to first load the solvated and neutralized .gro file in VMD. We can represent the protein with NewCartoon, the solvent with Points, and the ion with VDW as the Drawing Method. Then, in the Tk Console , we can run the command

```
draw pbcbox
```

Question 2b

The volume of the cubic box is 131.692 nm^3.

4175 water molecules were added during solvation.

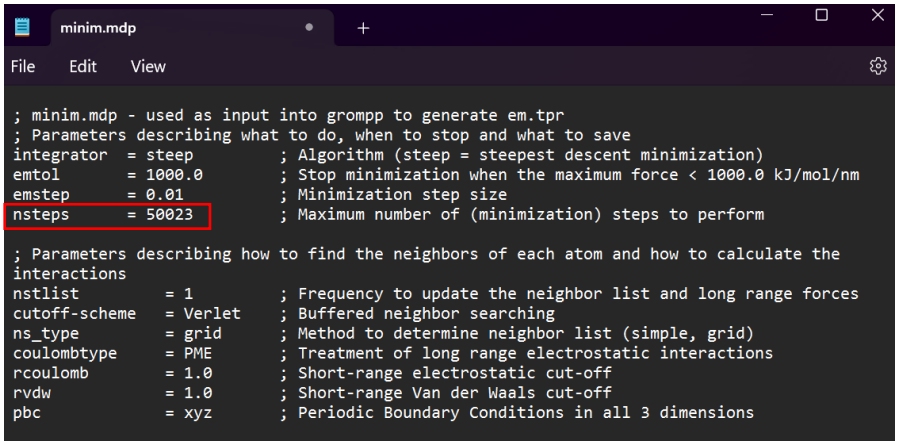
```
Output configuration contains 12853 atoms in 4193 residues
Volume                 :     131.692 (nm^3)
Density                :     977.915 (g/l)
Number of solvent molecules:   4175
```

Task 3

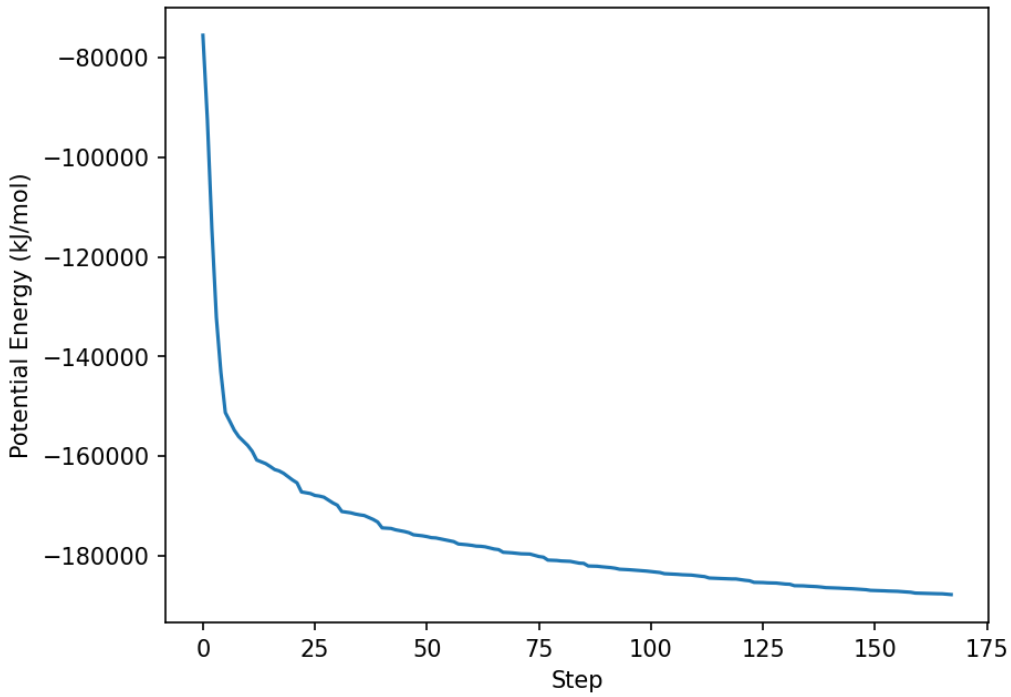
Steps followed

- The minim.mdp file was modified as required.
- Energy minimisation was performed using `grompp` and `mdrun`.
- The potential energy as a function of time was obtained using `energy`.

Question 3a



Question 3b



This was plotted using the following Python code:

```
import numpy as np
import matplotlib.pyplot as plt


x,y=np.loadtxt("potential.xvg",comments=["#","@"],unpack=True)
plt.figure(dpi=150)
plt.plot(x,y)
plt.xlabel("Step")
plt.ylabel("Potential Energy (kJ/mol)")
plt.show()
```

The system converged to its minimum energy state in 168 steps.

```
Steepest Descents converged to Fmax < 1000 in 168 steps
Potential Energy  = -1.8783233e+05
Maximum force     =  9.8512854e+02 on atom 28
Norm of force     =  5.2512326e+01
```

Task 4

Steps followed

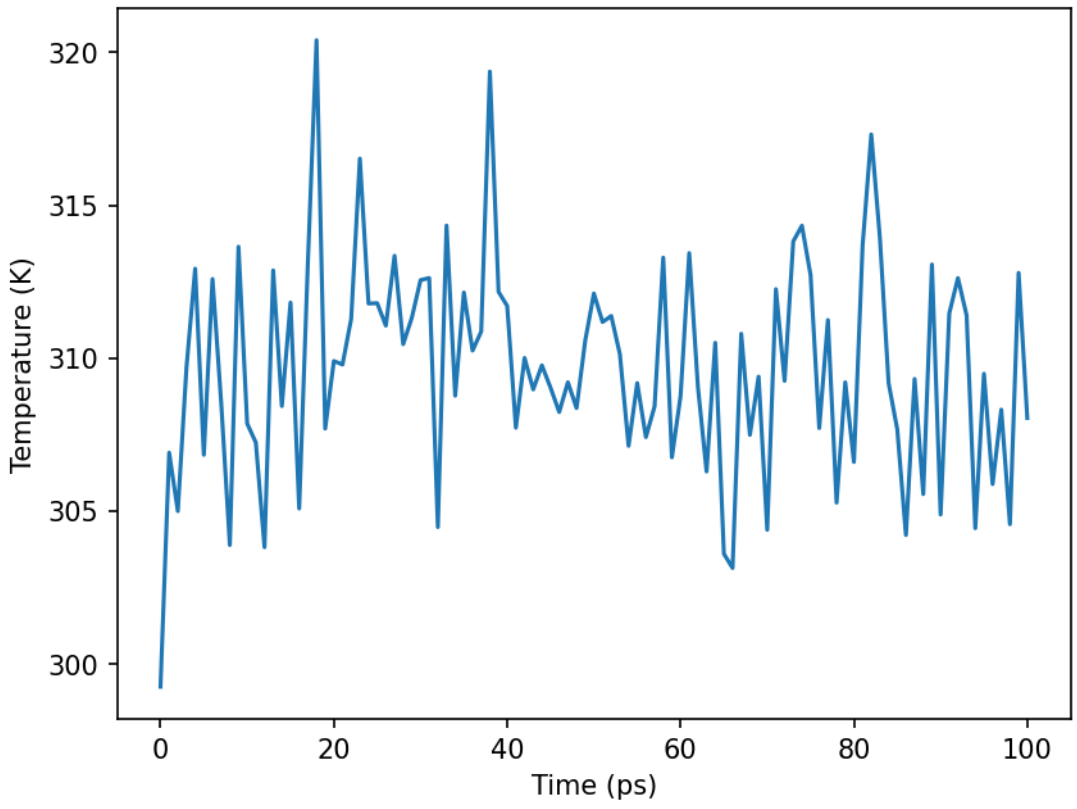
- The nvt.mdp file was modified to perform equilibration at 310 K.
- NVT equilibration was performed using `grompp` and `mdrun`.
- The temperature as a function of time was obtained using `energy`.

Question 4a

The average temperature at the end of the NVT run was 309.788 K.

```
Energy                      Average   Err.Est.       RMSD  Tot-Drift
-------------------------------------------------------------------------------
Temperature                 309.788       0.32    3.56599   0.540081  (K)
```

Question 4b



This was plotted using the following Python code:

```
import numpy as np
import matplotlib.pyplot as plt
x,y=np.loadtxt("temperature.xvg",comments=["#","@"],unpack=True)
plt.figure(dpi=150)
plt.plot(x,y)
plt.xlabel("Time (ps)")
plt.ylabel("Temperature (K)")
plt.show()
```

Task 5

Steps followed

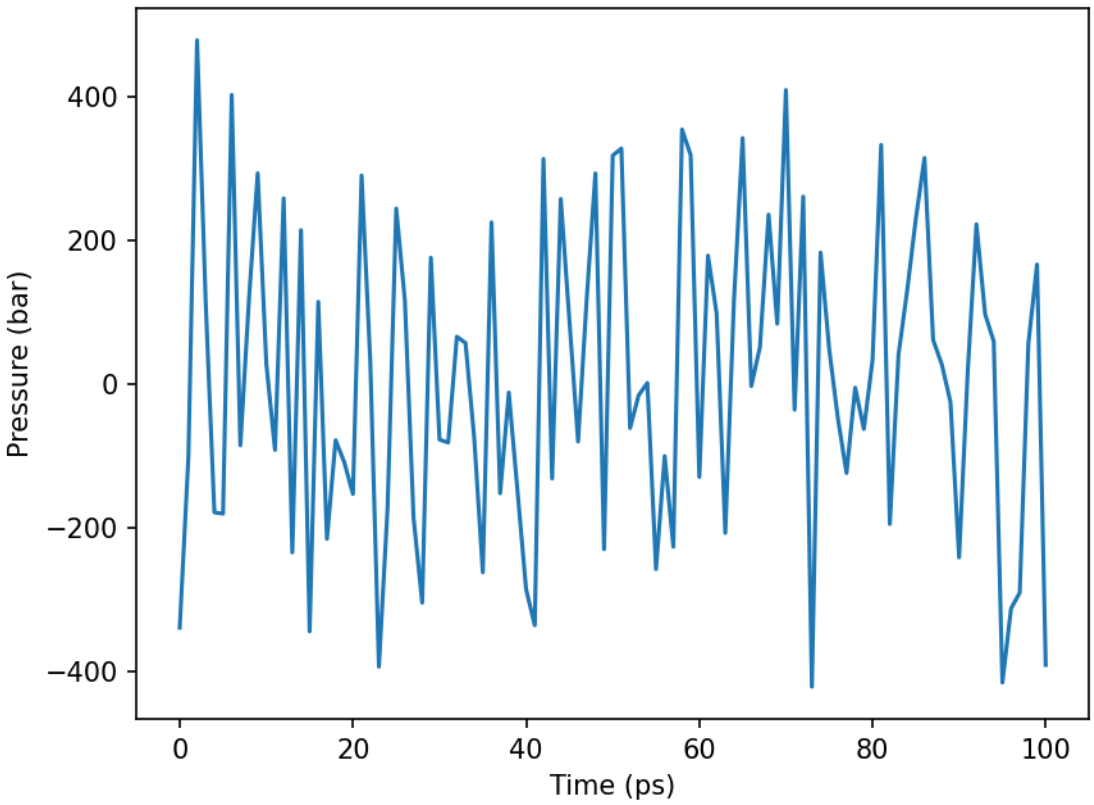
- The npt.mdp file was modified to perform equilibration at 310 K and 1 bar.
- NPT equilibration was performed using `grompp` and `mdrun`.
- The pressure as a function of time was obtained using `energy`.

Question 5a

The average temperature at the end of the NPT run was 0.0602295 bar.

```
Energy                      Average   Err.Est.       RMSD  Tot-Drift
-------------------------------------------------------------------------------
Pressure                 0.0602295          3    220.301    -14.007  (bar)
```

Question 5b



This was plotted using the following Python code:

```
import numpy as np
import matplotlib.pyplot as plt
x,y=np.loadtxt("pressure.xvg",comments=["#","@"],unpack=True)
plt.figure(dpi=150)
plt.plot(x,y)
plt.xlabel("Time (ps)")
plt.ylabel("Pressure (bar)")
plt.show()
```

After this, the md.mdp file was modified to perform a 500,000 step (1 ns) simulation at 310 K and 1 bar, and a production MD run was carried out using `grompp` and `mdrun`.