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Molecular Dynamics Simulations in GROMACS

(with visualization in VMD)

Molecular dynamics is based on classical Newtonian mechanics, where it is possible to simulate systems with millions of atoms and calculate intermolecular interactions. In this tutorial, I plan on walking through how to use GROMACS to simulate a water box with octane and visualize the system on VMD.

Installing GROMACS and VMD

GROMAC (GROningen MAchine for Chemical Simulations) and VMD (Visual Molecular Dynamics) can be downloaded from their respective websites.

Downloading CHARMM36 forcefield

The reason I am using CHARMM36 as a forcefield is because it is an improved force field for folded and intrinsically disordered proteins - which I am working with currently. However, you can use OPLS/AA force field too.

Water Box

The coordinate file and topology file of the water molecule are already in the forcefields, so we don't need to download water separately. The water model that we will be working with is TIP3P. The first step is to make a water box. So, open up your terminal window and use this command:

```
gmx solvate –box 5 5 5 –o waterbox.gro
```

This creates a 5x5x5 box of water molecules - my box gave me 4055 residues of water - with the file name waterbox.gro.

Next, generate the topology file of the waterbox.gro file:

```
gmx pdb2gmx –f waterbox.gro –p waterbox.top
```

Octane

The next step is to download the octane.pdb file, where the atom description matches the forcefield's description of the atom. I have included the correct pdb file for octane. Get the topology of octane:

```
gmx pdb2gmx –f octane.pdb –p octane.top
```

(This didn't have problems for me, but you can manually remove all the lines after dihedrals in the topology file.)

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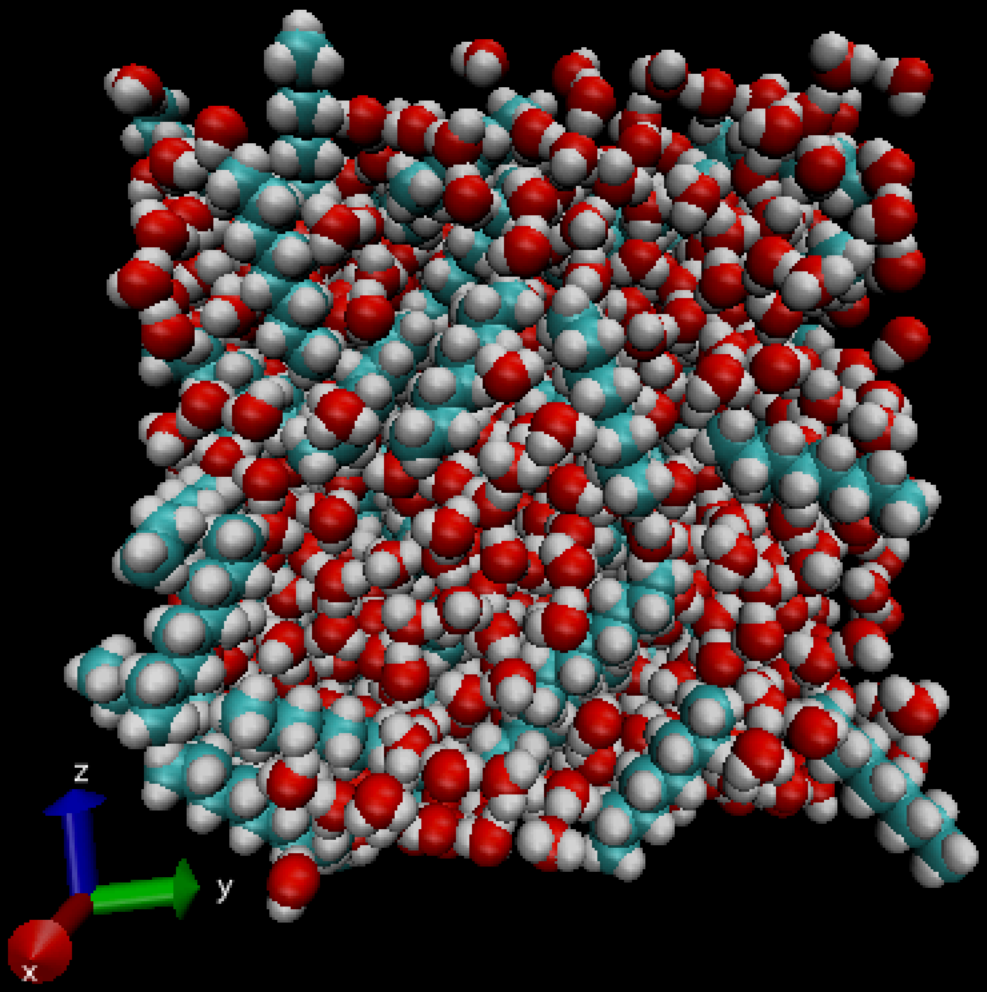
Octane in the water box

Run the following command to insert 100 olecules of octane into the water box:

```
gmx insert-molecules -nmol 100 -ci octane.gro -f waterbox.gro -o
octwater.gro -try 100000 -replace SOL
```

In the output line, it'll say how many residues of SOL molecules it has replaced, so manually remove that from the topology file (waterbox.top)



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Energy Minimization

The reason to do energy minimization is so that there are no steric clashes or unwanted geometry in the system. So run the following command:

```
gmx grompp –f minim.mdp –c octwater.gro –o em.tpr –p waterbox.top
```

This creates the em.tpr file, which you can use to run mdrun:

```
gmx mdrun –s em.tpr
```

This will output a confout.gro file and a traj.trr file, which you can load on VMD and see the relaxed state.

NVT and NPT equilibration

This is to make the temperature and pressure constant, so run the following commands. We are running the system in continuation, so make sure you don't re-run a system in the middle and overwrite the files.

NVT:

```
gmx grompp –p waterbox.top –c confout.gro –f nvt.mdp –o nvt.tpr
gmx mdrun –s nvt.tpr
```

NPT:

```
gmx grompp –p waterbox.top –c confout.gro –f npt.mdp –o npt.tpr
gmx mdrun –s nvp.tpr
```

Production MD

The last step is to run production MD to get the final state:

gmx grompp 0f md.mdp -c confout.gro -t state.cpt -p waterbox.top -o md_0_1.tpr
gmx mdrun -s md_0_1.tpr

Citations

GROMACS: https://github.com/ElsevierSoftwareX/SOFTX-D-15-00003

GROMACS Tutorials. Mdtutorials.com. http://www.mdtutorials.com/gmx/. Published 2018. Accessed August 18, 2020.