

Weekly Report: July 1 - July 5

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Created Ice structure from scratch using Python code ->

1) `python /scratch2/tianmuy/Mastercode/analysis/gen-ice -h` (for help)

2) `python /scratch2/tianmuy/Mastercode/analysis/gen-ice -a 1 -b 1 -c 1 -i xyzs/oxygen_1h.xyz -o ice_1x1x1.gro`

a=nos. Of unit cells in x direction.

b=nos. Of unit cells in y direction.

c=nos. Of unit cells in z direction.

a, b, and c can only be positive integers.

1 unit cell length in x direction = 0.782 nm

1 unit cell length in y direction = 0.677 nm

1 unit cell length in z direction = 0.736 nm

3) Above nos. of units to length conversion help's us create specific dimension of hexagonal ice.

From command in 2 nd point we will get hexagonal ice of dimension 0.782 x 0.677 x 0.736 nm³
By changing nos. Of a,b and c we can create different dimensions of ice.

**Adjusted Protein file (.gro) such that protein molecule is completely inside the water system.
(Use the below commands only if the protein molecule protrudes out of the water box.)**

1) `gmx editconf -translate 0 0 5 -f original_protein.gro -o protein.gro`

Above command will translate the protein in water system in upward direction by 5 nm (+z direction).

You can shift the system in any direction by changing the x,y and z lengths in above command.

2) `gmx trjconv -f protein.gro -s protein.gro -pbc atom -o new_protein.gro`

Above command will fill up the pbc box by water molecules and resolve the problem of protein molecule protruding out of water box.

Adjusting Protein file (.gro) and ice file (.gro) such that they stack up on one another.

1) To change the dimension of pbc box size, go to the last line of protein.gro file and change the x,y and z co-ordinates such that ice structure can be placed beneath the protein-water system.

2) Then using combine.py code combine the protein and ice files (.gro) in order to get the protein on ice system.

`module load anaconda3/5.1.0`

`python combine_grofile.py -i1 protein.gro -i2 ice.gro -d 1 -o protein_on_ice.gro`

Make sure that protein file just fits above the ice file and have atmost 1 nm gap between them.