Weekly Report: May 27 -May 31

-Vatsa Shah

Familiarized myself with palmetto and ran previous week's simulation's on palmetto.

Created box of water (tip4p) of dimension's 10x10x10 nm^3, 12x12x12 nm^3, and 14x14x14 nm^3 and inserted ice-seed (Type Ih / hexagonal ice) of radius 1.8 nm, 3 nm, and 4 nm in them respectively, keeping system at 300K temperature ,constant volume and constant number of molecules.

Performed simulation in order to fill gap between ice and water ->

gmx grompp -f em.mdp -c ice-water.gro -r ice-water.gro -p seed-water.top -o em.tpr
gmx mdrun -s em.tpr -v -deffnm em -ntmpi 4

Performed Annealing step to lower system's temperature.

For 1.8 nm ice seed in 10x10x10 nm^3 box of water, annealing was done from 300K to 220K,230K, and 240K.
For 3 nm ice seed in 12x12x12 nm^3 box of water, annealing was done from 300K to 240K,245K,250K and 255K.
For 4 nm ice seed in 14x14x14 nm^3 box of water, annealing was done from 300K to 255K and 260K.

eg. annealing for 1.8 nm ice seed in 10x10x10 nm^3 box of equilibrium water.

gmx grompp -f anneal-300-220.mdp -c em.gro -r ice-water.gro -p seed-water.top -o anneal_1.8_10x10x10_220.tpr

gmx mdrun -s anneal_1.8_10x10x10_220.tpr -v -deffnm anneal_1.8_10x10x10_220 -ntmpi 4

Performed Production Run.

gmx grompp -f nptprod-t220.mdp -c anneal_1.8_10x10x10_220.gro -p tip4p-ice.top -o prod_1.8_10x10x10_220.tpr -maxwarn 1

gmx mdrun -s prod_1.8_10x10x10_220.tpr -v -deffnm prod_1.8_10x10x10_220 -ntmpi 4

Visualized the output annealed gro file and production gro file.

vmd anneal_1.8_10x10x10_220.gro anneal_1.8_10x10x10_220.xtc
vmd prod_1.8_10x10x10_220.gro prod_1.8_10x10x10_220.xtc

Creation of Energy.xvg file ->

gmx energy -h (for help)
gmx energy -f prod_1.8_10x10x10_220.edr

Then select the y-axis options and all data will be stored in *energy.xvg* file

Plotted system's energy curve in each case.

Used gnuplot.

p "energy.xvg" u 1:2 w p/l (Potential energy Vs Time graph)
p "energy.xvg" u 1:3 w p/l (Kinetic Energy Vs Time graph)
p "energy.xvg" u 1:4 w p/l (Total Energy Vs Time graph)
p "energy.xvg" u 1:5 w p/l (Temperature Vs Time graph)
p "energy.xvg" u 1:6 w p/l (Pressure Vs Time graph)

Read following research paper's ->

1) Identification of Clathrate Hydrates, Hexagonal Ice, Cubic Ice, and Liquid Water in Simulations: the CHILL+ Algorithm. -Andrew H. Nguyen and Valeria Molinero.
2) Accurate determination of crystal structures based on averaged local bond order parameters. -Wolfgang Lechner, and Christoph Dellago
3) Preordering of water is not needed for ice recognition by hyperactive antifreeze proteins. -Arpa Hudaita , Daniel R. Mobergb , Yuqing Qiua , Nathan Odendahla , Francesco Paesanib and Valeria Molinero.
4) Combined molecular dynamics and neural network method for predicting protein antifreeze activity. -Daniel J. Kozucha , Frank H. Stillingerb , and Pablo G. Debenedetti.

Visualized *prod_xx_dxdxd_2X0.gro* files ->

1) Created Index file->

gmx make_ndx -f prod_1.8_10x10x10_220.tpr

2) Created xtc file taking time step as 500 ps ->

gmx trjconv -f prod_1.8_10x10x10_220.xtc -s prod _1.8_10x10x10_220.gro -dt 500
mv trajout.xtc prod_1.8_10x10x10_220-dt500.xtc (Renaming file)

3) Final output ->

/scratch2/tianmuy/MasterCode/analysis/q6-navg-march2019/g_q6-navg -f prod_1.8_10x10x10_220-dt500.xtc -s anneal_1.8_10x10x10_220-dt500.gro -n index.ndx -vis largest-cluste-dt500r.xvg

4) Visualizing through graph ->

In gnuplot.

p "q6navg.xvg" u 1:2 w l/p

We can see that number of molecules sticking to ice increases hence the ice seed grows.