Building the final structure ARA-MEM & PVA-MEM

Lefteris Mainas – Michalis Lazaratos – Zoe Cournia

1. Firstly, we have the structure of the membrane (membrane.gro), that has been simulated in NPT ensemble for 100ns. The dimensions of the box are: 19.39170 – 19.43890 – 28.91430
2. We wish to cut the box so that we can reduce the number of total atoms of the system. Because the structure that we have, comes from a simulation that the usual periodic boundary conditions apply, atoms on the boundaries of the box are not whole. For this purpose we use the following command so that all the molecules are placed inside the box:

   gmx trjconv –f membrane.gro –s membrane.tpr –o new_structure.gro –pbc mol

3. Now we are in position to cut the box without facing any problems with atom topology. Load new_structure.gro in VMD. Go to “Graphics” in VMD Main Window and choose “Graphical Representation”. In the “Selected Atoms” area, write the following line:

   (same residue as z>20) and (same residue as z<260)

   In this way we choose only the atoms that have z-coordinate greater that 2 nanometers and less than 26 nanometers. The rest of the molecules are neglected. The next step is to save the cropped structure. Go to “File” option in VMD Main and choose “Save coordinates”. In the

window (Save Trajectory) that pops up select "(same residue as z>20) and (same residue as z<260)" and in the file type option choose "pdb". Finally, save the structure and name it cropped.pdb

4. Convert the pdb file into gro:

   gmx editconf –f cropped.pdb –o cropped.gro

5. Construct the new box:

   gmx editconf –f cropped.gro –o newbox.gro –c –d 0.0

6. You can see the dimensions of the new box by writing the following line in terminal:

   tail -1 newbox.gro

7. The dimensions are 19.39200 - 19.43900 - 24.28700. We cut the box in the z-direction only. Next, we want to place the magnetite inside the membrane system. For this reason we will firstly create a box, with the same dimensions as the membrane-system, around the magnetite and then we will center the molecule. Go to the magnetite structure file (e.g. mag-ara.gro or mag-pva.gro) and write in the last line of the file the following: 19.39200 19.43900 24.28700

8. Place the magnetite molecule in the center of the box:

   gmx editconf –f mag_ara.gro (or mag_pva.gro) –o mag_centered.gro –c

9. In the case we want to translate the magnetite molecule simply type:

gmx editconf –f mag_centered.gro –o mag_translated.gro –translate 0 0 2

This command translates the molecule 2 nanometers in the +z direction.

10. Merge the two structures:

    cat mag_translated.gro newbox.gro > all.gro

11. Correct the number of atoms in the second line of the file and remove the unnecessary lines between the end of the magnetite lines and the beginning of the membrane structure.

12. Load the all.gro structure in VMD and as in step three go to "Graphical Representation" and type:

    all and not (all and (same residue as (within 2 of resname MAG)) and not resname MAG)

    Save the new structure and convert it in gro format. In this way we removed the molecules (water molecules and ions) that overlap with the magnetite. Name the new structure overlap.gro so that you can keep track of the different .gro files.

13. Renumber the atoms from 1 so that there is compatibility between the topology of the system and the structure:

    gmx editconf –f overlap.gro –o renumber.gro –resnr 1

14. Update the topology. Count the number of atoms in the overlap.gro file.

15. After cutting the structure, it is possible that the total charge of the system is not zero. For this reason we may need to add some ions using the following two commands:

    gmx grompp –f ions.mdp –c overlap.gro –p topol.top –o ions.tpr

    if we want to add for example 5 chlorine atoms we type:

    gmx genion –s ions.tpr –o neutral.gro –p topol.top –pname SOD –nname CLA –nn 5

16. The system is now ready to proceed to energy minimization.