Exploring a given Molecular Trajectory Farhad Ramezanghorbani

Final Project Time-line

Till December 18th (one week):

- Being familiar with Radial Distribution Function Algorithm by reading articles about that, then see what does Gromacs do for calculating RDF
- How RDF works in Gromacs for a single snapshot of a simulation trajectory, then try to get some results for my system which I am working on. This system contains 512 molecules.

Till December 27th (one week):

- Being familiar with MDAnalysis library of Python
- Defining some criteria for interaction between molecules in this system.
- Then obtain an interaction matrix. It will show that if two molecules interact based on our criteria, the related element of matrix is 1 and if they do not interact it should be 0.

Till January 13th (tow weeks):

- I will use the interaction matrix to find an aggregate distribution and I will show that distribution like a graph for a single frame.
- Using MDAnalysis to find out about aggregates distribution
- Using Network X library or other method to create aggregate distribution
- being familiar with TCL scripting that I am going to use for separating aggregate visually