1 Abstract

After further discussion on the project, the purpose of this project is adjusted to "Modeling a bulk of water with comparison of different potentials to calculate the surface tension force using LAMMPS". It would break down into several steps as it comes along:

- Create a bulk of H_2O with associated potentials (SPC, SPC/E,TIP3P, TIP4P, TIP4P-Ew). It is known that different water models are developed to fit well with some specific parameters (i.e., the radial distribution function, the density anomaly or other critical parameters) [1], thus it requires some tests on which model provides a better fit for surface tension forces. A preliminary test has been run with a flexible SPC/E model developed by Zhang et al. [2], and the $g(r)$ after running for 60,000 steps with step size 0.5fs is shown in Fig. 1. The reference LAMMPS input file comes from [3] with 6400 atoms with a setting to melt ice and equilibrate at 298K.

- Based on the preliminary results, tests can be run with PBC, and I'm currently in the progress of finding an indicator to confirm the relaxation of the system, then compare if `nvt` or `npt` works better for the system. I noticed in the previous lab that we could have equilibration stage and production stage written in the input file, but still need to understand which condition (`nvt`/`npt`) might be proper for which stage and why.

- After being comfortable with the single phase water model, a vacuum phase needs to be added with a small volume to allow atoms close to surface some space to relieve their energy. At this point, the main challenge would be how to remove the PBC while still being able to stabilize the system (need to start with some examples on liquid/vacuum interface or liquid/vapor interface and look at how boundary conditions are treated).

- When the water model is constructed with proper boundary conditions to stabilized the system, surface tension force will be obtained from pressure following the equations in [4], then compared with their results.

- Subsequently, different water models (SPC, SPC/E, TIP3P, TIP4P, TIP4P-Ew) will be tested to explore their advantages, mostly as a verification of what has been proposed in the literatures, but would be helpful in getting more insight for the physical concept behind different models, rather than simply taking the parameters themselves.

As an interesting side note, when learning about LAMMPS, I found that LAMMPS includes a SPH USER package, where they create an `atom_style` called `meso` to represent SPH particles, and they used the same paper as the one I am working on for my research project. Getting some insight into their source code could be a "bonus" to this project.

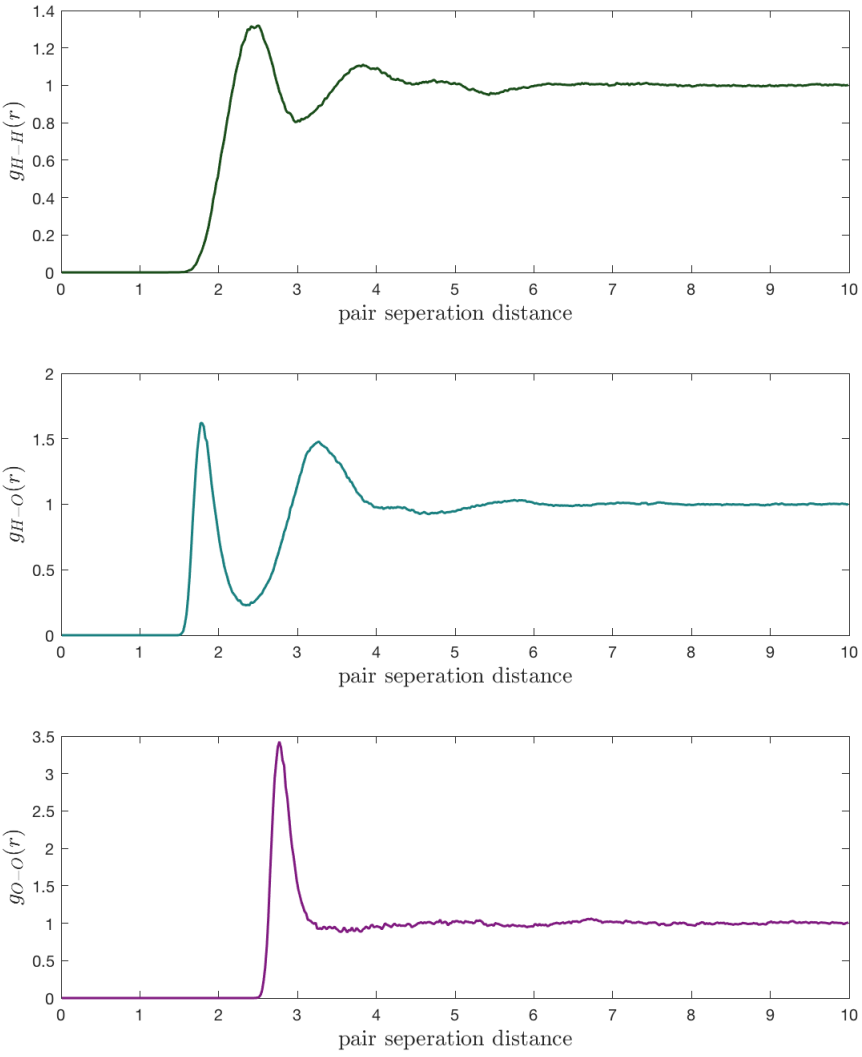

Figure 1: Radial distribution function g(r) with flexible SPC/E model developed by Zhang et al. [2] after running for 60,000 steps with step size 0.5fs at 298K

References

[1] http://www1.lsbu.ac.uk/water/water_models.html.

[2] Xin Bo Zhang, Qing Lin Liu, and Ai Mei Zhu. An improved fully flexible fixed-point charges model for water from ambient to supercritical condition. *Fluid Phase Equilibria*, 262(1-2):210–216, 2007.

[3] https://sites.google.com/a/ncsu.edu/cjobrien/tutorials-and-guides/working-with-water-in-lammps.

[4] Ahmed E Ismail, Gary S Grest, and Mark J Stevens. Capillary waves at the liquid-vapor interface and the surface tension of water. *The Journal of chemical physics*, 125(1):014702, 2006.