Fys4460 – 2017 – Project 4

Final Project

Through this project we will develop one of the subjects of the course further in an individual project. The project should take up to 2 days of full time work to complete and your presentation of the project will be a part of the final, oral exam in the course. The following are ideas that may form the basis of your final project. You are expected to be able to expand the project to fill the suggested time span, and you should relate the project results with other parts of the course contents where this is reasonable. You may collaborate on the projects, but project presentations are individual. If you collaborate, you should provide details of who you collaborated with during the exam.

Extended studies of Lennard-Jones systems

(a) Use Green-Kubo relations to measure thermodynamic properties. Compare with other measurement approaches and discuss advantages and disadvantages.

(b) Introduce the Noose-Hover thermostat and measure rms-displacement using various thermostats. Discuss advantages and disadvantages of the various thermostats for various thermodynamic measures.

(c) Characterize the equation of state for a liquid and gas and compare with van der Waals theory. Characterize the system at phase equilibria, if possible, and visualize and discuss the results.

Studies of parallellization approaches

(d) Develop a parallel version of the molecular dynamics code. Characterize its scaling performance and discuss advantages and disadvantages of various parallellization and optimization techniques.

Nanoporous systems – extended modeling

(e) Extend your studies of the nanoporous system by studying either significantly longer times or larger systems. Discuss challenges.

(f) (Challenging) Generate a very large MD system. Measure porosity over a length $d \ll L$. Measure the permeability in smaller parts of the system (of size d), and use these values in a flow solver on a L/d sized grid to find the permeability of the whole system.

(g) Measure diffusion in a large nanoporous system and compare with results from random walks on a percolation cluster. Coarse-grain your nanoporous system for a direct comparison with a discretized percolation system.

(h) (Challenging) Implement the Weber-Stillinger potential for Si and make a nanoporous Si system. Characterize the elastic behavior of the system as a function of porosity.

(i) (Challenging) Implement the SiO_2 potential from Vashishta et al. and characterize the resulting system, for example by studying SiO_2 liquid at $T = 4000$K.

The system may be characterized by addressing $T(t)$ and $g(r)$. Compare with a Lennard-Jones liquid and comment.

Percolation

(j) Measure $n(s, p_c, L)$ and find a finite size scaling theory and demonstrate the theory by a finite size scaling data collapse.

(k) Study percolation in correlated systems: Generate an initial matrix using correlated noise (of your choice) and study percolation in this system using methods you have aquired.

(l) Characterize a nanoporous system using aspects of percolation theory: Coarse-grain the atomic system and study flow or diffusion processes on the coarse-grained system.

(m) Characterize the behavior of a self-avoiding random walker on the spanning cluster.

(n) Characterize the geometry of a diffusion front using percolation theory.

(o) Develop a model for invasion-percolation in three-dimensions. Characterize the size distribution of invasion events – the distribution of the number of sites invaded when the pressure is increased.

End of Project 4