

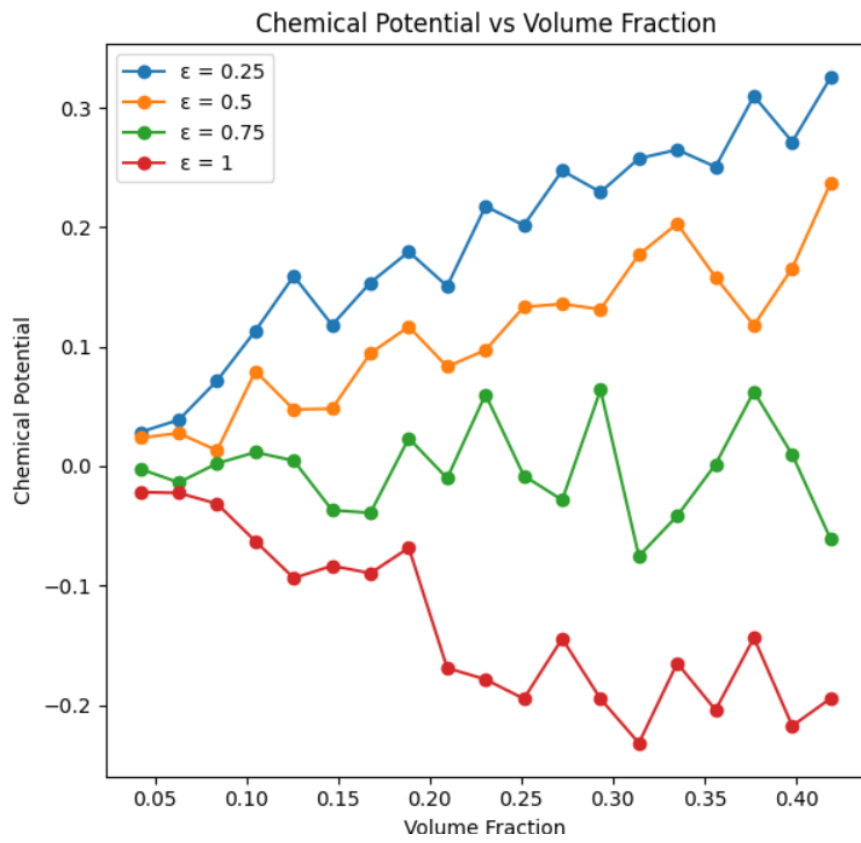
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Report Date:	August 25, 2024
Assignment:	2 (3D Lennard Jones Fluid)

Introduction

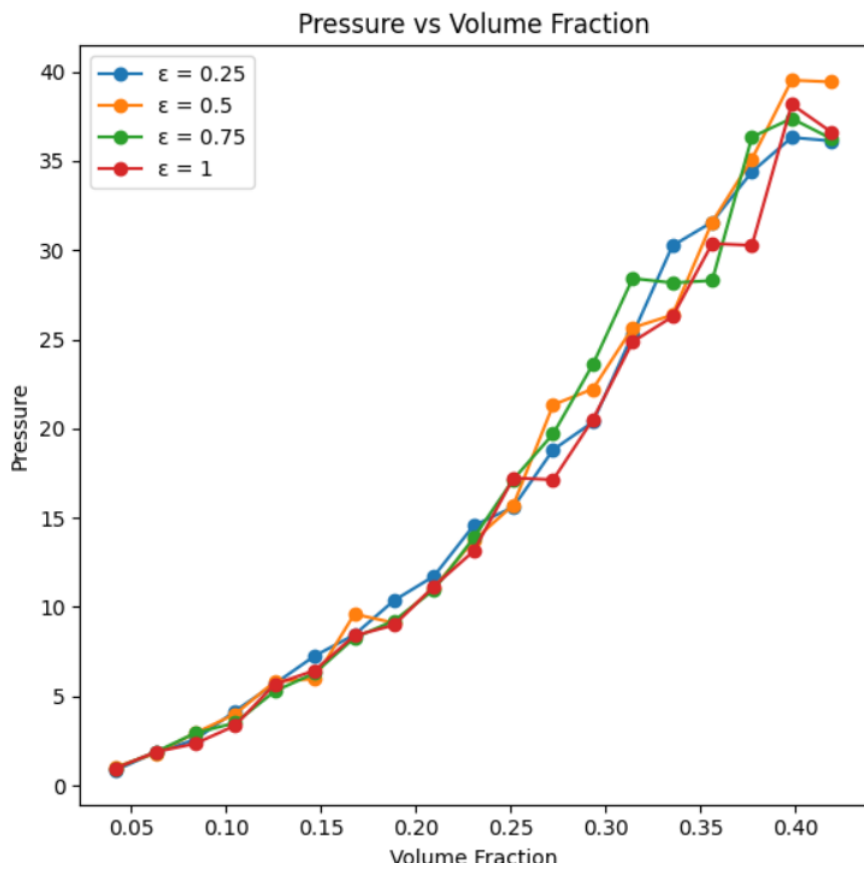
This Assignment required a Monte Carlo simulation of a 3D Lennard Jones simulation. A 3D cubic box with a large number of particles as points in 3D was simulated. Lennard-Jones (continuous) Interparticle interactions were added to the simulation. 'Metropolis Algorithm' was used to converge to Boltzmann distribution. After convergence, The chemical potential and pair correlation function were computed. The pressure was computed using the pair correlation function. The complete simulation was repeated for varying values of epsilon of Lennard-Jones potential.

Simulation parameters

- Box dimension, $L = 3$
- particle radius, $\sigma = 0.3$
- Boltzmann constant time temperature, $k_b T = 2$
- potential cut-off at 2.5σ
- LJ epsilon = 0.25, 0.5, 0.75, 1
- Number of Equilibration steps = 2000



(a) Chemical potential vs volume fraction



(b) Pressure vs volume fraction

Remarks about plots

the chemical potential seems to be linearly related to volume fraction. It increases with volume fraction for high values of Lennard Jones epsilon and decrease with volume fraction for low values of Lennard Jones epsilon.

The pressure increases with volume fraction as expected since number of particles is increasing but due to the Lennard Jones potential, the pressure increase is not as the ideal gas case.

Conclusion

The chemical potential and pressure increase nearly linearly as a function of volume fraction in a Lennard-Jones fluid due to the following reasons:

- **Increased Particle Interactions:** **Chemical Potential:** The chemical potential represents the change in the free energy of the system when an additional particle is added. As the volume fraction (the ratio of the volume occupied by the particles to the total volume) increases, the number of particles in a given volume increases. This leads to more interactions between particles, primarily due to the attractive part of the Lennard-Jones potential at short distances. As these interactions increase, the energy cost of adding an additional particle also increases, resulting in a higher chemical potential. **Pressure:** Pressure in the system is related to the force that particles exert on the walls of the container. With more particles in the same volume (higher volume fraction), there are more collisions and interactions, leading to a higher force exerted per unit area, which increases the pressure.
- **2. Volume Fraction and Density Relationship:** **Density:** The volume fraction is directly related to the number density of the system (number of particles per unit volume). As the volume fraction increases, the density increases as well. **Linear Response:** For moderate volume fractions, the system is not highly compressed, and the interactions between particles are not extreme enough to deviate significantly from ideal behavior. In this regime, both the chemical potential and pressure can respond linearly to changes in density, and by extension, to changes in volume fraction.
- **3. Energy Landscape:** **Potential Energy:** The Lennard-Jones potential has a short-range repulsive part and a longer-range attractive part. As volume fraction increases, particles are slightly pushed closer together, increasing the repulsive interactions, which increases the overall energy linearly within this moderate regime before any significant nonlinear effects (such as crowding or phase transitions) take place. In summary, the nearly linear increase of chemical potential and pressure with volume fraction is due to the moderate increase in particle interactions, the direct relationship between volume fraction and density, and the fact that the system is still in a regime where the properties can be approximated by a linear response to changes in volume fraction. As the system becomes denser, the interactions between particles increase in a nearly predictable manner, contributing to a linear rise in both chemical potential and pressure.