Molecular dynamics for the Lennard Jones system

Goal: The goal of this exercise is to explore the behaviour of a Lennard Jones fluid using Molecular Dynamics simulations.

1. Start by converting one of your Monte Carlo codes to a Molecular dynamics code in the NVE ensemble. Assume that the interactions between the particles is the Lennard Jones interaction. It can be useful for part 5 to use the so-called "Velocity Verlet" algorithm.
2. Now, include a thermostat converting your NVE MD simulation to a NVT MD simulation (Easiest is the Andersen).
3. Compare the NVE and NVT methods by examining the behaviour of both applied to a Lennard Jones fluid.
4. Confirm that the average energy at a specific state point (low density and high temperature, i.e. gas) is the same for your MD as it was for a NVT Monte Carlo simulation.
5. Read the set of notes on diffusion. Then, study the diffusive properties of the Lennard Jones fluid by
    - Calculating the velocity-velocity autocorrelation function in the NVT ensemble for a i) low density fluid, and ii) high density fluid.
    - Use the Green-Kubo relation to determine the diffusion coefficient for your system.

To be handed in: Your results should be handed in as a small document. The goal of the document is to demonstrate what you have done in this exercise, and to demonstrate both that your simulation works and that you understand the results that it produces. It should be seperated into two sections, a **Methods** section and a **Results** section. In particular, you should ensure that you include the following:

- A description of the integration scheme you used for the MD.
- A short description of the way you included the thermostat into your code (which thermostat did you use and how exactly did you implement it).
- A small description of the properties of the Lennard Jones system you studied. Make sure to include the system size, temperature, density, etc. of the state points you examined.
- A short analysis of the behaviour of the Lennard Jones system that you determined via the exercise, including figures and discussion of the velocity-velocity autocorrelation function and diffusion coefficients you measured.