Brownian dynamics simulations

Goal: The goal of this exercise is to explore the behaviour of attractive and repulsive particles using both Brownian dynamics simulations and Molecular dynamics simulations.

1. Start by converting your Molecular Dynamics code into a Brownian Dynamics code for Weeks Chandler Anderson particles (WCA). Note that the WCA interaction is the same as the Lennard Jones potential, but cut off at the minimum of the potential and shifted back to zero at that point. As a result, it is purely repulsive.

    - Using your Brownian dynamics code, calcualte the mean square displacement for a low density fluid, and use this to determine the diffusion coefficient. Compare to what you observe with your MD simulation for the same state point. Also compare with what you predict from velocity-velocity correlations in your MD.
    - Do the same for a high density fluid.
    - Repeat for a face-centered-cubic crystal.
    - Finally, repeat this exercise for a low density and high density Lennard Jones fluid.

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 short description of the way you implemented the Brownian dynamics simulations.
- A small description of the mean square displacements you measured, including both an explanation of what you observe and figures that show this.