6. Molecular Dynamics

Present your solutions to the following problems using latex, if you have figures make sure they are publication quality, include your code in the solutions. Print your pdf files and bring them to class.

1. Argon Gas

Implement the Verlet molecular dynamics method for a 2-d gas of argon atoms. Use the reduced units discussed in class. Use toroidal boundary conditions, a uniform initial configuration (with possible small random translations), and ensure that the centre of mass momentum is zero. Compute the following quantities

(i) the total energy vs. time

(ii) the CM velocity vs. time

(iii) temperature vs. time as estimated from the equipartition theorem

(iv) the distribution for v_x. Fit your distribution to T and compare to (iii).

(v) the pair correlation function $g(r)/r$ vs. r. Obtain an analytic expression for the peaks of the pair correlation function assuming a triangular lattice. Place markers on your plot indicating these peak locations.

(vi) the pair correlation function $g(r)$ vs. r at high temperature. Obtain an analytic expression for g in this case and place it on the same plot.

For (i-v) use N=100, R=10, dt = 0.005, 1000 time steps, $v_0 = 0$. The distributions in (iv-v) look better if you only collect data after an equilibration time (try 400 steps). For (vi) run with the same parameters but use $v_0 = 8$. Show your derivation of all analytic results. Describe how you did the fit in (iv).