Projects

3.1) Estimate the volume of a 10-dimensional unit sphere using the midpoint method (given as a template) and the hit-and-miss MC method. Study the integration error. Plot, for both methods, the computational time as a function of the error. (The exact answer is $\pi^5/120$)

Projects continued

3.2 a) Implement the LJ potential and force (with $\sigma = 1$ and $\varepsilon=1$) in the template. A correct implementation should give good conservation of the total energy. Use a temperature of 1 and increase the time step until things go very wrong. Study the quality of the integration by monitoring the drift in the total energy for several different time steps just before things go wrong.

b) Run a LJ simulation with initial velocities at a temperature of 0.2. What happens with the kinetic and potential energy?

c) Implement an Andersen thermostat that thermalises all particles simultaneously at a fixed step interval and run simulations at T =1 and 0.2. What differences in collective behavior do you observe between 1 and 0.2 at long times? A physics question: can you explain what you see?

Projects continued

3.2 d) Use MD with the thermostat to calculate the average energy and heat capacity between T=0.2 and 1. Make sure the results are sufficiently converged (choose your own definition of sufficient). Can you explain the behavior of the heat capacity by looking at the sampled configurations of the particles?