Projects: Monte Carlo

3.1) Use the Metropolis method to calculate:

$$\langle x \rangle = \frac{\int_0^\infty x\, e^{-x}\, dx}{\int_0^\infty e^{-x}\, dx}$$

Here $P(x) = e^{-x}$. Use probability $P(x) = 0$ for $x < 0$. Try different values of the parameter delta in the range between 0.01 and 10. Study $\sigma/\sqrt{N}$ and compare with the actual difference to the exact answer. (note: N_0 is not critical when $x_0 = 0$)

Projects: Molecular Dynamics

3.2 a) Implement the LJ potential and force (with $\sigma = 1$ and $\epsilon = 1$) 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.

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

3.2 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?

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 from the behavior of the system that you observe in the animations?

Projects: Molecular Dynamics (continued)

3.2 e) Now we will look at the pressure. Can you explain the differences in pressure between the different temperatures? Also run with a 4 times as large unit cell by doubling L. What happens to the pressure at different T? How does the pressure compare with that of an ideal gas?