Physics 332, Spring 2022
Problem Set 1

Due Wednesday April 6th - either bring to class or e-mail to Prof. Driscoll by 1:00 pm.

For problems which ask you to explore things using simulations, please include snapshots of the simulations (screen shots, or even a picture taken with your phone) that support your conclusions in your answers. The simulations run in any web browser, and can be accessed at compadre.org/stpbook. The simulations for this homework set are under the link 'Thermal Physics'.

1. **Nature of temperature**
   (a) Summarize what you know about temperature. What reasons do you have for thinking it has something to do with energy?
   (b) Discuss what happens to the temperature of a hot cup of coffee. What happens, if anything, to the temperature of its surroundings?
   (c) If you add energy to a pot of *boiling* water, does its temperature change?

2. **Identification of the temperature.** Use the program *ThermalContact* to simulate two systems, A and B, of particles that interact through the Lennard-Jones potential, $u(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$. Both systems are in a square box of size $L = 12$; periodic boundary conditions are not used. The simulation begins with the particles surrounded by fixed walls (made of particles of infinite mass), and the inner wall can be removed, allowing the two systems to come into contact with each other.
   (a) Initialize the simulation with 81 red particles and 64 green particles, using the default time step of $\Delta t = 0.01$. Run the simulation and monitor the kinetic and potential energy until the system appears to reach equilibrium. How long does it take for the system to come into equilibrium? What is the average potential and kinetic energy of each system (not per particle as reported)? Is the total energy of each system constant (to within numerical error)?
   (b) Let the two systems interact with each other: remove the barrier by stopping the simulation and clicking 'Contact', then restarting the simulation. What quantity is exchanged between the two systems?
   (c) After you decide the system is again in equilibrium, compare the average kinetic and potential energies of each system (not per particle) to their values before you allowed the systems to come into contact.
   (d) What quantity is the same in both systems after equilibrium has been established? Does it make more sense to compare the average total kinetic and potential energies, or the average kinetic and potential energies per particle? What can conclude about the possible identification of temperature in this system?

3. **Irreversibility** Read section 1.7 and use the program *Chaos* to explore sensitivity to initial conditions. Program *Chaos* simulates a system of $N = 11$ particles with a special initial condition: they are all placed in a line and are given the same initial velocity.
   (a) Run the program until time = 60. What do you observe?
   (b) Now, perturb the velocity of particle 6 by clicking on 'Perturb'; note the strength of the perturbation is only one part in 10^5. What do you observe? How long does it take for the system to exhibit new behavior?
   (c) Reinitialize the simulation and click 'Perturb', but now stop the simulation at a time t after the perturbation. Click on 'Reverse' to reverse the particle velocities. Confirm that if t is sufficiently short, the particles will return approximately to their initial state (e.g. in a line). What is the maximum value of t that allows the particles to return approximately to their initial positions?