PHYS 114 Contemporary Physics II - Rec 2

January 23, 2008

Breaking the Law!

Feel free to use old code you have written before, as long as it belongs to you.

- Create N=25 ideal (non-interacting) gas particles (mass=1kg) in a box. Let the box have dimensions of 1,1,1. Initially, place all the particles in the center of the box. Please draw in the sides of the box visually (look on the Visual Python webpage for help if needed).
- Give each particle an initial velocity of 1, pointed in a random direction (I will check this!).
- Let the particles evolve by simply moving them, there is no force acting on them and they do not interact with anything but the walls of the container. When they reach the ends of the box, let them bounce off elasticly. This time however, I would like you to update the particles motion using Velocity Verlet (see wikipedia's article on Velocity Verlet for an excellent primer). Notice that with constant force, Velocity Verlet and the old way of integration are the same.
- Let the code run for 10 seconds. Now take every particle and reverse its velocity. Run it for another 10 seconds. If you've done everything right, the particles are right back where they started!
- Now put the particles in a gravitational field (i.e. $\vec{F} = -g\hat{z}$). Repeat the same procedure and you will get the same results.
- Remember that the 2nd law of thermodynamics says: In a closed external system not in thermal eq. we have,

  $$\frac{dS}{dt} >= 0 \tag{1}$$

  Explain what is going on here! Note that this is the most integral part of the assignment, so even if you do not finish the simulation you must still explain this unexpected consequence.

For extra credit, build a simulation where the particles interact under the so-called Lennard-Jones potential:

$$V(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] \tag{2}$$

Feel free to chose ϵ and σ and new starting positions if you try this.