MM553/837 - Computational Physics
Tutorial Exercise - Week 40

This tutorial concerns the **ideal gas law**. In order to understand the ideal gas law we have to talk about **temperature** (T) and **pressure** (P). For our purposes, temperature is defined as the average square velocity:

$$T = \langle v^2 \rangle,$$

where the average is taken over all the particles in the gas.
Pressure is defined as force per area. Calculate the force on the walls due to the particles by $F = \frac{\Delta p}{\Delta t}$ using the values from the constraint class which reflects the particles off the walls.
Consider a gas of N particles which do not interact but collide elastically inside a box L on a side.

- Take a look at the files `particle_box.cc`, `integrators.h`, `examples.h`, `constraints.h`, and `particle_box.py`. Change `particle_box.cc` to integrate the equations of motion for no central forces between the particles. You could do this by using the `CentralForce` class with its template parameter set to `NoForce`. For the constraints, use the `SquareBox` class. After compiling `particle_box.cc`, use `particle_box.py` to play an animation of the particles.

- Perform a simluation of $N = 40$ particles. Initialize the positions and velocities, then run for some time to let the system equilibriate. However, during this run monitor the total energy of the system to ensure it does not change very much. What happens if the stepsize ϵ gets too large?

- After the particles have come to equilibrium, calculate the pressure and temprature by averaging over all the particles for many steps.

- Repeat this for various inital velocities, to see if the ideal gas law holds:

$$PV = nRT,$$

  where n is the number of particles and R is some constant.

- Turn on some central forces and repeat the above procedure. Can you observe deviations from the ideal gas behavior?