Ideal Gas simulation

The simulation program is composed of four panes. In the upper left is a visualization of the simulation. The particles behave as a 2-D ideal gas and do not interact with each other. All momentum exchanges made by the particles take place either at the walls of the simulation box or with the piston. The piston applies pressure to the system, which is represented by the mass drawn on top of it. The color of each particle describes the particle’s kinetic energy: blue particles have a low energy, while red particles have a higher energy. Likewise, the color of the piston reflects the temperature of the system. To the right of the Visualization are graphs of the systems temperature, volume and pressure, as well as a PV diagram. Note that the units for time are given in simulation times steps, simulation volume is measured in pixels, and that temperature and pressure are subsequently based upon these units. The bottom two panes control the parameters of the simulation.

1) Open the simulation and allow the system to equilibrate for a while. The simulation starts with a fixed pressure and an adjustable temperature. You will notice that the system oscillates in pressure and volume for a while, but will eventually approach an equilibrium state: why does this happen?

2) If you double the temperature (move the slider to the far right) how are the volume and pressure affected? What happens if you halve the temperature?

3) If you drop the temperature to zero, you will notice that just as the piston bottoms out there is a small increase in the temperature, even though it is being controlled by the thermostat: why does this happen?

4) Reset the temperature to somewhere near its starting value and let the system equilibrate again. Select the “Constant temperature adjustable pressure” ensemble. If you double the pressure, how are the volume and temperature affected? What happens if you halve the pressure?

5) Select the “constant energy adjustable pressure” ensemble. In this ensemble, the walls of the simulation act as perfect insulators, so for a given temperature and pressure the total energy of the system remains constant. Notice that temperature, pressure and volume all oscillate and do not reach an equilibrium state: why is this? How are the oscillations of temperature, pressure, and volume related to one another?

6) Observe the PV diagram in each ensemble. In each case, adjust the free variable to see how it changes the behavior of the PV plot. What are the differences between the PV diagrams for each ensemble? What causes these differences?