Scientific Programming in Python
Project
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The Physics of Colliding Balls: Part 3

Now we can use the physics of collisions to simulate an ideal gas. We will assume that the gas particles are just solid balls that can collide with the walls of a containing box, as well as with one another. One additional element that we will consider here is the temperature of the gas.

Temperature

The temperature of an ideal gas is related to the average kinetic energy of the atoms in the gas.

$$T = \frac{2}{3} k_B^{-1} \overline{E_K}, \tag{1}$$

where T is the temperature, $\overline{E_K}$ is the average kinetic energy of all the atoms, and

$$k_B \approx 1.380650 \times 10^{-23} \text{ J/K} \tag{2}$$

is the Boltzmann constant. We can measure the temperature of the gas at any time by computing (1) and this value should stay constant if there is no external temperature influence. Remember that the kinetic energy is defined as

$$E_K = \frac{1}{2} m v^2 \tag{3}$$

where m is the mass of the moving object and v is the speed.

If we *do* want to model an external heat bath, we can assign temperatures to each of the walls of the box containing the gas. Whenever an atom collides with a wall, we change the temperature (i.e. the kinetic energy) of that atom to match the temperature of the wall. The image below shows what happens when we have one cold wall (on the left) and one warm wall (on the right). A temperature gradient is created, as well as a density gradient. Note that the atoms on the left are more closely packed (denser) and more blue (colder) than the atoms on the right.