1.2.1: Molecular Dynamics Simulation

The following simulation shows an adjustable number of gas molecules in a container. The molecules interact with a slight attraction which will cause them to stay connected with each other to form a a solid. But if they have enough kinetic energy they will begin to move around each other while still connected and the solid becomes a liquid. With even more kinetic energy they separate from each other and become a gas. Energy can be added or removed from the molecules with the 'cool' and 'heat' buttons to show changes of phase from solid to liquid to gas. The total energy (E), temperature and pressure (P) are given below the simulation.

The units used in the simulation are called 'natural units' where many constants (such as Boltzmann's constant, the mass of the molecules, the width of the molecules, etc.) are set equal to one. For the values to be in the usual units of joules for energy, pascal for pressure and kelvin for temperature they would have to be multiplied by scale factors which will depend on exactly what gas is being modeled. For our purposes here we can ignore these details and just talk about energy, pressure and temperature; see the references below the simulation for further details.

The initial simulation shows the system as a gas. The molecules are yellow if they have a lot of kinetic energy, red if they have a medium amount and blue if they have very little kinetic energy. There are several preset choices which can be selected from the pull down menu.

Credits

The Molecular Dynamics Exploration was developed by Wolfgang Christian at Davidson College using the Easy Java/JavaScript Simulation (EjsS) modeling and authoring tool created by Francisco Esquembre. This EjsS simulation is based on a pure JavaScript + HTML 5 simulation developed by Daniel V. Schroeder, Physics Department, Weber State University. Schroeder's simulation is described in Interactive Molecular Dynamics article (pdf), published in the American Journal of Physics **83** (3), 210-218 (2015), arXiv:1502.06169 [physics.ed-ph]. (Thanks to John Mallinckrodt for inspiring several of the presets.) Many of these presets use features that are only available in the original simulation by Dan Schroeder. We have imported the configuration file generated with Schroeder's simulation into the EjsS model.

Simulation Questions:

1. Start the simulation. What state is the system in when the simulation starts?
2. Do all the molecules have the same kinetic energy? (Does the simulation show them all with the same color?)
3. The average kinetic energy of the molecules in a substance is proportional to the temperature. Use the 'cool' button to decrease the temperature. What do you notice about the average kinetic energy as the temperature is lowered?
4. At about what temperature do the molecules begin to clump together and form a liquid? (Heat it up and cool it off several times to check your initial guess.)
5. Recall that pressure is force divided by area. In this case the force is supplied by the molecules hitting the sides of the container. What happens to the pressure as the temperature goes down? What if the temperature goes up?
6. Cool the system even more until it is a solid. At about what temperature do the molecules stop moving around each other to form a solid?
7. Stop the simulation and use the pull down menu to choose the bouncing ball preset. Run the simulation. What do you notice about the kinetic energy of the molecules (lighter color means higher kinetic energy) after the ball hits the ground?
8. For the bouncing ball, we know energy is conserved. But the ball does not return to its original height after it bounces so it doesn't end up with the same gravitational potential energy it started with. Based on your observations in the previous question, what happened to some of the gravitational potential energy of the ball after it hit the ground?
9. Reset the simulation and run the 'Hot and Cold' preset. The molecules in the upper solid have more kinetic energy than the molecules in the lower solid. What do you think will happen when the two solids touch? Run the simulation to see what happens. Were you correct?
10. Reset the simulation and run the 'Friction' preset. You will notice the molecules of the incline and the sliding object gain kinetic energy as the objects slides down the incline. Where does this energy come from?
11. Reset the simulation and run the 'Plucked String' preset. What part of the string has the most energy when it is plucked?

Chapter Two Summary

Forces cause accelerations, not velocities (objects will keep moving with constant velocity if the net force is zero). For every force there is always a second reaction force of the same amount but acting on a different object and in the opposite direction. Pressure is force distributed over an area. Bernoulli's principle is the result of air flow at different speeds and different pressures and causes baseballs to curve and the lips of a trumpet player to buzz. Energy comes in many forms and the total amount of energy is conserved (we can't create it or destroy it, only convert it from one type to another). When energy is converted from one form to another some of it has to end up in a less useful form (heat that generally isn't useful). Also, as you go through this book remember that: Science words have specific narrow definitions; Any number you see in science is a measurement of something, unlike in math class; and The laws of physics are always true with no exceptions.
