Homework H3 Solution

1. Turn in Go to the MD simulation …Select "Presets" "Two atoms."
a. Does a diatomic molecule form or not? What type of motion does this molecule undergo?
b. Now make sure that "Mouse/touch" is set to drag, and use the mouse to drag one of the atoms just a little. Now what motions does the molecule undergo (name all three types)?
c. Keep things running, and increase the box size to 15. (You may have to click/drag that slider a few times! It will look like the molecule shrinks and slows down; that's just because it plots the bigger box in the same black space). Now hit "Faster" several time carefully. What happens to the amplitude of the vibration? As you keep hitting "Faster," the molecule will eventually dissociate. What happens to the frequency of the vibration just before it dissociates (slower or faster than before)?

Solution:

a) Yes a diatomic molecule forms: the atoms move back and forth and cannot separate from one another. The back-and-forth is vibrational motion.
b) The molecule now undergoes translational (moves about in the box), vibrational, and rotational (spins around) motion.
c) The amplitude of the vibration increases. Just before the molecule dissociates, the frequency is slower than before. This may seem a bit counterintuitive because you are putting energy into the molecule to dissociate it. The reason is that the Lennard-Jones potential flattens out at large interatomic distance r, so the restoring force becomes weak when the bond is stretched very long. Thus the atoms are accelerated towards one another very slowly. The technical term for this is "anharmonicity." A harmonic oscillator will not do this, no matter how much energy you add into it.

2. Now run Preset "Hot and Cold." … What happens to the temperature of the two drops after they merge? Look carefully: does the back end of the blue droplet instantly turn more red?

Solution:
The temperature of the two droplets equilibrates after they merge. The back end of the blue droplet does not instantly turn red, it takes time (albeit a short time in the simulation) for thermal motion to be propagated through the blue droplet in response to the red droplet.

3. Now run "Friction:" A large molecule will slide down an inclined plane. What happens to the temperature of the molecule as it slides down? Eventually, the molecule comes to a rest at the bottom. So first, potential energy was converted into kinetic energy when the particle slid down. After it's all over, where did the energy go? (Energy is conserved.)

Solution:
The temperature of the molecule increases as a result of friction. In the case of the simulation, some of the potential energy of the molecule first converts to kinetic energy (it slides down). The kinetic energy leads to collisions of the molecule's atoms with the atoms in the ramp. This converts the kinetic energy of motion into thermal energy. As proof of this principle, notice that after the simulation is over atoms which started off as blue are now red and yellow and vibrating.