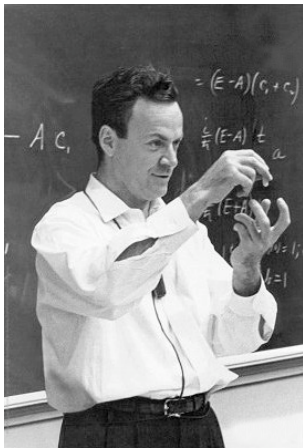


Molecular Dynamics for All Ages

Dan Schroeder, Weber State University



Richard Feynman

"If, in some cataclysm, all of scientific knowledge were to be destroyed, and only one sentence passed on to the next generation of creatures, what statement would contain the most information in the fewest words? I believe it is the *atomic hypothesis* (or the *atomic fact*, or whatever you wish to call it) that ***all things are made of atoms—little particles that move around in perpetual motion, attracting each other when they are a little distance apart, but repelling upon being squeezed into one another.*** In that one sentence, you will see, there is an *enormous* amount of information about the world, if just a little imagination and thinking are applied."

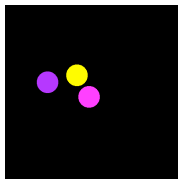
Every child should have a visual, interactive molecular dynamics simulation to play with.

Every physics major should write one.

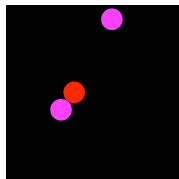


Physics major Rhett Zollinger with daughter Missy, age 3

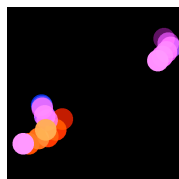
Visualizing Matter



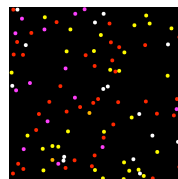
Attracting...



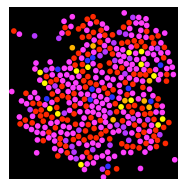
Repelling...



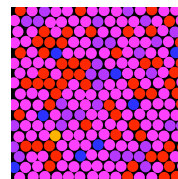
Perpetual motion



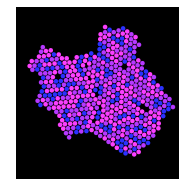
Gas



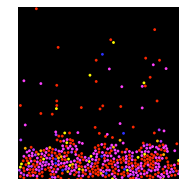
Liquid



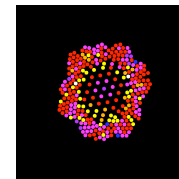
Solid



Dislocations

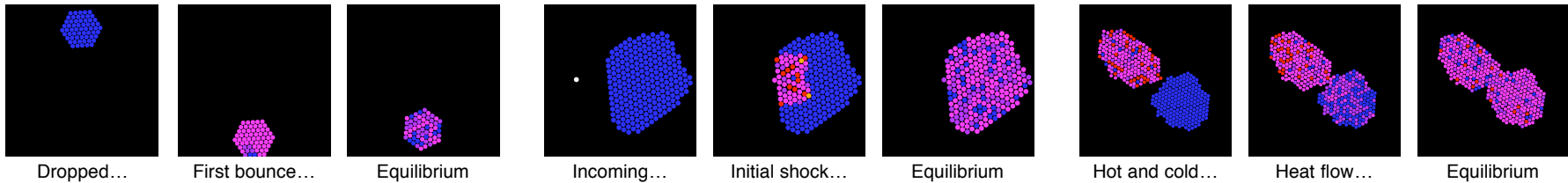


Evaporation

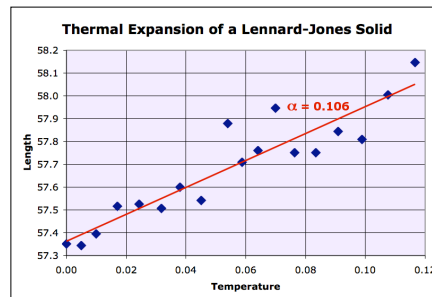
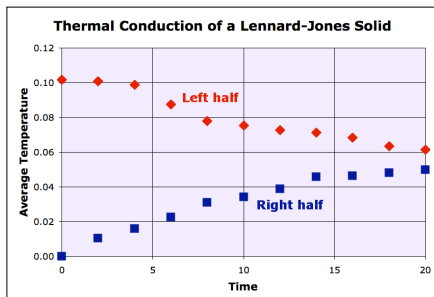
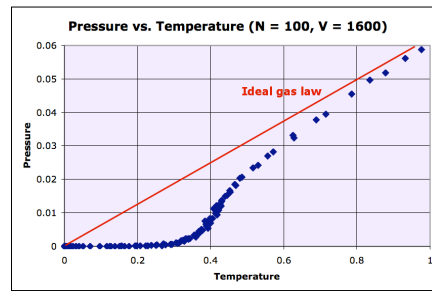
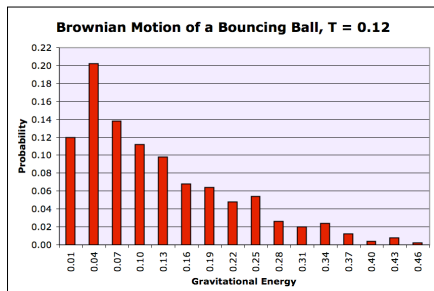
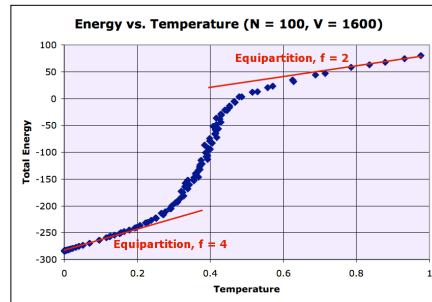
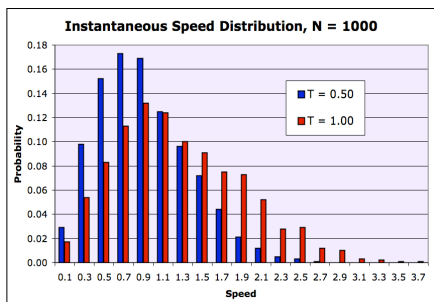


Explosion!

The Arrow of Time (Inspired by John Mallinckrodt)



Data Cornucopia

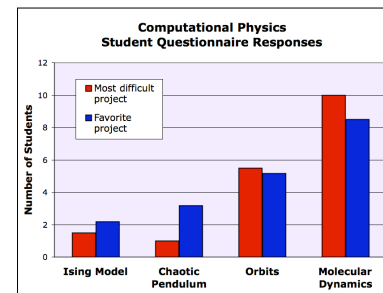


Coding (for Grownups)

In go Newton's laws...

```
// Lennard-Jones interactions (adapted from Gould and Tobochnik)
for (i = 0; i < N; i++) { // loop over all pairs of molecules
    for (j = 0; j < i; j++) {
        dx = x[i] - x[j];
        dy = y[i] - y[j];
        rSquared = dx*dx + dy*dy;
        attract = 1 / (rSquared * rSquared); // 1/r^6
        repel = attract * attract; // 1/r^12
        potentialE += 4 * (repel - attract);
        fOverR = 24 * ((2 * repel) - attract) / rSquared;
        fx = fOverR * dx;
        fy = fOverR * dy;
        ax[i] += fx; // add force to i's acceleration (m = 1)
        ay[i] += fy;
        ax[j] -= fx; // Newton's 3rd law
        ay[j] -= fy;
    }
}
```

...out comes thermodynamics.



Challenging...
but worth it.

Quit reading this flier and go run the applet:
<http://physics.weber.edu/schroeder/software>
(or just google "molecular dynamics applet")
Then write your own version, or improve mine!