The Molecular Dynamics Method I: Oscillator

One of the most powerful computational methods is called "Molecular Dynamics" (MD). It is used in solid state physics to understand the stucture and vibrations of solids, in astrophysics to figure out how galaxies formed, in chemistry and biology to describe the properties of molecules (eg how proteins "fold"), in engineering to model aircraft wing vibrations, etc etc.

The idea of MD is very simple: If an object is currently at a position x and has a velocity v then if you let a small time dt pass, the new position is $x + v * dt$. As an example, a car which is at the $x = 205$ mile marker on the freeway, moving at 60 miles/hour, will, after $dt = 0.05$ hours have passed, be located at $x = 205 + 60 * 0.05 = 208$ miles.

In the description above, I used the phrase "small time" to label dt. The reason dt must be small is that the formula $x + v * dt$ assumes the velocity v is constant. If you consider our example again and let $dt = 4$ hours instead of $dt = 0.05$ hours, you would predict that the car would move to $205 + 60 * 4 = 445$ miles. But in fact it is very likely instead that the car would have encountered a traffic jam, stopped for gas, or had something which changed v from $v = 60$ in the course of four long hours!

But this restriction that dt be small does not mean MD cannot predict the value of the position a large time in the future. It just means we need to allow for the possibility that the velocity might change and build up large time intervals from many short ones. In other words, we need a formula for getting a new v analogous to the formula $x = x + v * dt$ for the new position. Here is where physics enters the problem. I will just tell you the rule and let your physics teacher go into the detailed reasoning. Forces (pushes and pulls on an object) are the things that cause the velocity to change. More precisely, if there is a force F acting on an object of mass m for a time interval dt, then the velocity changes my $F/m * dt$. Notice that the appearance of the mass m in the denominator is reasonable: It is harder to change the velocity of an object which has a big mass.

In summary, if we know enough physics that we possess a formula for the force F on the object, then the rule for getting the new velocity is $v = v + F/m * dt$ where m is the mass of the object.

So MD works this way: You figure out the formula for the force F and then stick the two equations

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x=x+v*dt
v=v+F/m*dt
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into a loop and let it fly. The loop generates a whole sequence of positions and velocities. Because we are allowing v to change in the correct way, this loop can correctly precict the trajectory a long time (many, many steps dt) into the future.

A first example problem to test MD: Mass on a Spring

The formula for the force F for a spring is called "Hooke's law": $F = -k * x$ where k is the "spring constant". A spring with a big k is very hard to stretch. A small k spring is easy to stretch. Hooke's law tells you that the more you stretch the spring (the larger x is) the larger the force F which tries to pull you back becomes. In fact, F grows linearly with x. (Can you explain the minus sign in the formula? Think about the direction of the force compared to the direction in which the spring is deformed.)

Using Hooke's law, write a MD program for a mass on a spring. You will need to input k, m, dt and also the total number of steps you want taken. Also you need to tell the program the starting position and velocity. The core of your program will be a loop containing:

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x=x+v*dt
v=v-k*x/m*dt
t=t+dt
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The last line computes the time by adding the little increment of time dt which passes each time the loop is executed.

You might start with the values $k = 5, m = 4, dt = 0.01$ and do $N = 5000$ steps (so the final time is $5000 * 0.01 = 50$). Start the mass off at $x = 3$ with no initial velocity. Then try some other values and see if you can figure out what the effects of each parameter are. What happens if m doubles? How about doubling k? what does making v nonzero at the beginning do?

Print out the time t and the position x and velocity v. Make a plot of x vs t. What does it look like? A good check on your code is that the "period" (the time it takes for your mass to return to its original location) should be $2\pi\sqrt{m/k}$.

This MD problem can be solved without pretty easily. The answer is

$$x(t) = x(0)\cos\sqrt{\frac{k}{m}}\,t + v(0)\,\sqrt{\frac{m}{k}}\,\sin\sqrt{\frac{k}{m}}\,t$$

Here $x(0)$ is the initial position and $v(0)$ is the initial velocity. Can you plot both your MD data and this exact solution on the same graph to see that MD is agreeing?

If friction is present, the formula for the force now has an additional term, $F = -k*x - A*v$. The constant "A" is big if there is a lot of friction. Change your MD code to input A and plot $x(t)$ again. What has changed? Is the change reasonable, ie is the effect what you might suppose friction would have been likely to do?

The friction problem can also be solved without a computer, but here's one that cannot: When a spring is stretched too much it becomes *anharmonic* and the force law changes to $f = -kx - bx^3$. It would be super easy for you to change your MD program to include the anharmonic term (try it!), yet to do that problem with pencil and paper is **not** possible! This observation illustrates the power of MD in solving problems that otherwise would be impossible.