Physics 640
October 21, 2008

Project 4
Week 7 & 8:
-Introduction to Molecular Dynamics/Metropolis Algorithm/Monte Carlo

Molecular Dynamics:
Numerical algorithm to solve Newton's equations:

$$-\frac{d\Phi}{dt} = f = m\ddot{x} = m\frac{d^2x}{dt^2}$$

where Φ is the interaction potential between molecules. Typical interaction potential between molecules are:

-Hard spheres
-Hooke's Law
-Lennard-Jones

The Lennard-Jones interaction between two molecules located at x_1 and x_2 is (no external forces are considered!):

$$\Phi(x_1, x_2) = \frac{1}{|x_1 - x_2|^{12}} - \frac{2}{|x_1 - x_2|^6}$$

This potential is repulsive at short distances and no interacting at large distances between molecules, being the point of minimum potential at mid range.

Assuming equal masses molecules, for a system of 4 molecules, we need to solve the following equations:

$$1)\ m\frac{d^2x_1}{dt^2} = -\frac{d\Phi}{dx_1} = 12\sum_{j=2}^{4}\left[\frac{1}{(x_1 - x_j)^{13}} - \frac{1}{(x_1 - x_j)^7}\right]$$

$$2)\ m\frac{d^2x_2}{dt^2} = -\frac{d\Phi}{dx_2} = 12\sum_{j=1,3,4}\left[\frac{1}{(x_2 - x_j)^{13}} - \frac{1}{(x_2 - x_j)^7}\right]$$

3)...
4)...

-Use finite-difference to approximate the derivatives
-The differential equations of 2nd order require two initial conditions for each molecule: position and velocity

Example in this input file "md.in" for "molec_dyn.f"

```
4  0.001  0.10  60.0
 0.50  0.00  0.00
-1.00  0.00 -0.00
-0.50  0.00  0.00
 1.00  0.00 -0.00
 0.00 -1.00  0.00
 0.00  0.00  1.00
 0.00  1.00  0.00
```

```
 0.00  0.00 -1.00
* NATOM –Number of atoms (IN) is 4
* H - Time step. (IN) is 0.001
* HP - Time interval between printing.   (IN) is 0.10
* TEND - Time at end of computation: TEND = H*NSTEP.  (IN) is 60
* The next 8 lines specify the initial positions (cartesian
coordinates) and velocities of the atoms
```

Example output file "md.out"

```
     4
      600
      0.000000     0 -4.078430E+00  2.000000E+00 -2.078430E+00
      0.000000     1  5.000000E-01  0.000000E+00  0.000000E+00
      0.000000     1 -1.000000E+00  0.000000E+00  0.000000E+00
      0.000000     2 -5.000000E-01  0.000000E+00  0.000000E+00
      0.000000     2  1.000000E+00  0.000000E+00  0.000000E+00
      0.000000     3  0.000000E+00 -1.000000E+00  0.000000E+00
      0.000000     3  0.000000E+00  0.000000E+00  1.000000E+00
      0.000000     4  0.000000E+00  1.000000E+00  0.000000E+00
      0.000000     4  0.000000E+00  0.000000E+00 -1.000000E+00
      0.000000     0 -3.617130E+00  1.538704E+00 -2.078426E+00
      0.100000     1  4.475015E-01  0.000000E+00  0.000000E+00
      0.100000     1  5.895949E-01  0.000000E+00  0.000000E+00
      0.100000     2 -4.475015E-01  0.000000E+00  0.000000E+00
      0.100000     2 -5.895949E-01  0.000000E+00  0.000000E+00
      0.100000     3  0.000000E+00 -9.753933E-01  9.917767E-02
      0.100000     3  0.000000E+00  4.894474E-01  9.754606E-01
      0.100000     4  0.000000E+00  9.753933E-01 -9.917767E-02
      0.100000     4  0.000000E+00 -4.894474E-01 -9.754606E-01
       .........
```

```
WRITE(3,99)INT(1000.*K*H),0,PE,KE,PE+KE
DO I = 1,NATOM
     WRITE(3,99)K*H,I,X(I),Y(I),Z(I)
     WRITE(3,99)K*H,I,U(I),V(I),W(I)
END DO
```

(where k is from the time looping)

*NATOM is 4

*NSTEP is 600

*Then for each time iteration line "0" contains information on PE, KE, and PE+KE for all atoms

Outcomes for Project 4 part a), to be included in the report:

1) Animation of the position of a chosen number of molecules (4 or higher) over time given at least two different initial conditions. You should be able to confirm a result from your intuition in these animations based on the initial conditions. Explain in report.
2) Animate the motion of one of the molecules in phase space (x and v_x)