Physics 640
October 21, 2011

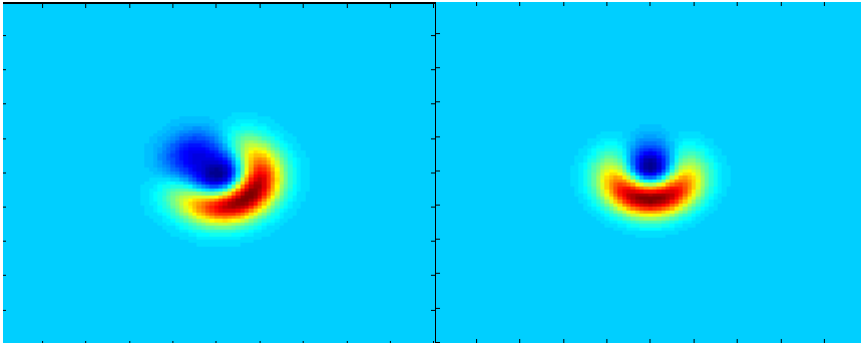Project 3 options (all with animations)

   1) Direct extension of FDTD 1D to 2D, surface waves, with ABC
How many time instants we will need to initialize? 2, 4, 6?
Please discuss this in your report

2D versus 1D: stability requires dt<= δ/c/sqrt(2) versus dt<= δ/c in 1D; this requires
initialization at k=2 at ibar+1/sqrt(2). This makes the ABC more involved than in 1D.

   2) FDTD1D for EM waves with ABC and implement a least two media, should see
      reflection and transmission (FDTD can handle any number of media we may
      have)

From higher index to lower index, artificial bump before the interface is due to the
different numerical speed in that medium
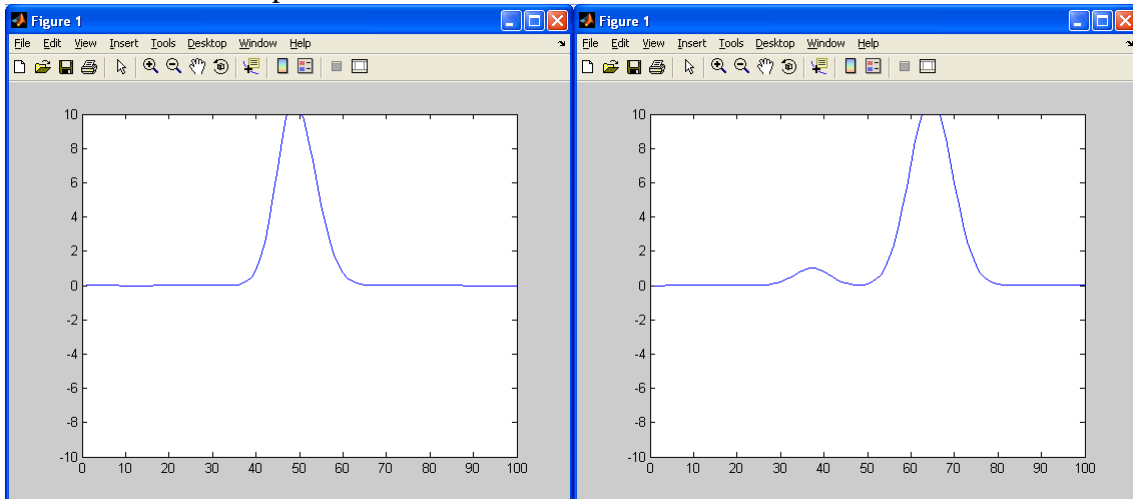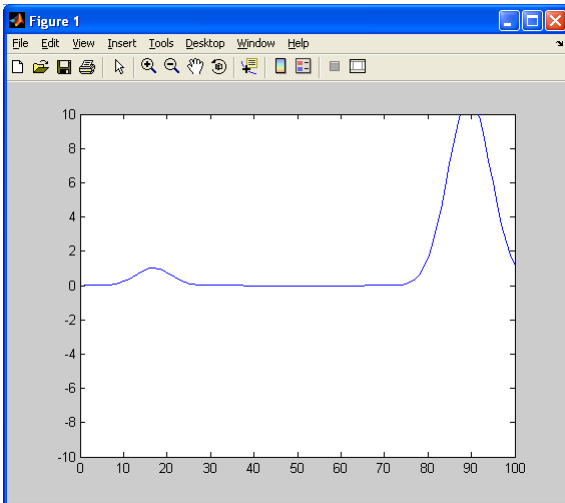
3) Use existing FDTD2D with Mur ABC but implement a correct mode for waveguide coupling. You can implement two parallel waveguides into the FDTD code, then feed in a correct mode
As expected.

Week 7 & 8:
-Introduction to Molecular Dynamics/Metropolis Algorithm/Monte Carlo
Project 4: this project consists of two parts
a) Molecular interactions, execute the Example Program MolDyn for several particles with different initial conditions, is there low or high sensitivity on these conditions? Use output files to visualize animations of particle motions using Matlab. Include some conclusion on final outcome based on initial conditions.

What is an example of the visualization for this code?
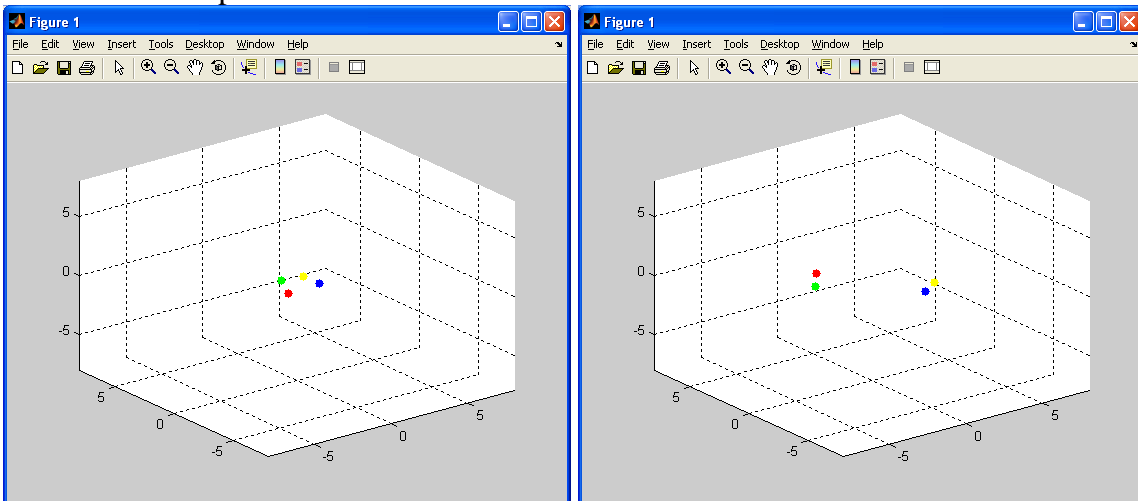
b) Execute an example program based on the Metropolis algorithm, varying one or two parameters, present results using Matlab

Bibliography:

Error! Bookmark not defined.-F. Ercolessi, A Molecular Dynamics Primer, http://www.fisica.uniud.it/~ercolessi/

Error! Bookmark not defined.-M. Field, A Practical Introduction to the Simulation of Molecular Systems

Error! Bookmark not defined.-N. Metropolis, A.W. Rosenbluth, M.N. Rosenbluth, A.H. Teller and E. Teller, (1953) *J. Chem. Phys.* **21**, 1087-1092.

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Error! Bookmark not defined.-Rasmussen, J. L. (1984). A Fortran program for statistical evaluation of pseudorandom number generators. Behavior Research Methods and Instrumentation, 16, 63-64.

Error! Bookmark not defined.-The Basics of Monte Carlo Simulations: http://www.cs.cornell.edu/jwoller/samples/montecarlo/default.html

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)