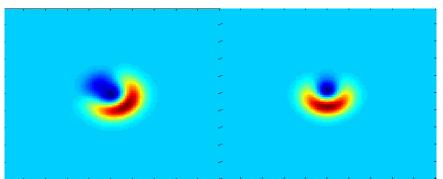
Physics 640 October 18, 2007

Project 3 options (all with animations)

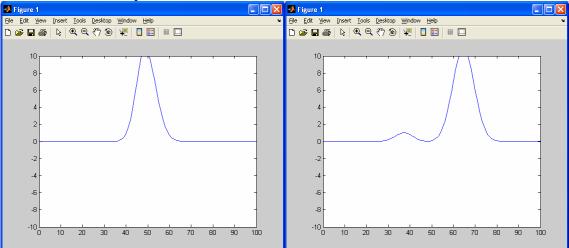
1) Direct extension of FDTD 1D to 2D, surface waves, with ABC (Team 1) How many time instants we will need to initialize? 2, 4, 6? Please discuss this in your report

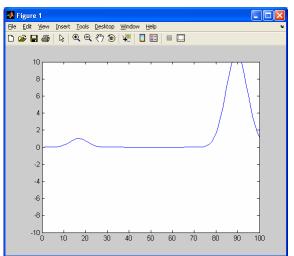


2D versus 1D: stability requires  $dt \le \delta/c/sqrt(2)$  versus  $dt \le \delta/c$  in 1D; this requires initialization at k=2 at ibar+1/sqrt(2). This makes the ABC more involved than in 1D.

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) (Team 3)

From higher index to lower index, artificial bump before the interface is due to the different numerical speed in that medium





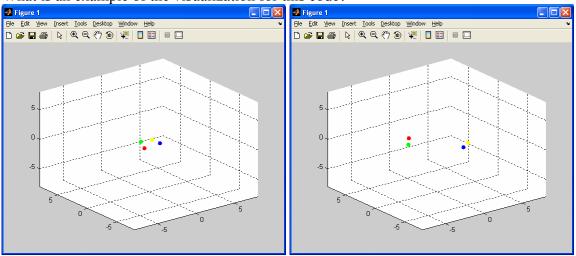
 Use existing FDTD2D with Mur ABC but implement a correct mode for waveguide coupling. You can implement two parallel waveguides into the FDTD code, then feed in a correct mode (Team 2). As expected.

## 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 <u>MolDyn</u> 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 <u>Metropolis algorithm</u>, varying one or two parameters, present results using Matlab

Bibliography:

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

**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.

Error! Bookmark not defined..-Z.Q. Li and H.A. Scheraga, (1987) Proc. Natl. Acad. Sci. USA 84, 6611-6615.

**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