

Physics 640  
October 28, 2011

#### Project 4

#### Week 7 & 8:

-Introduction to Molecular Dynamics/Metropolis Algorithm/Monte Carlo

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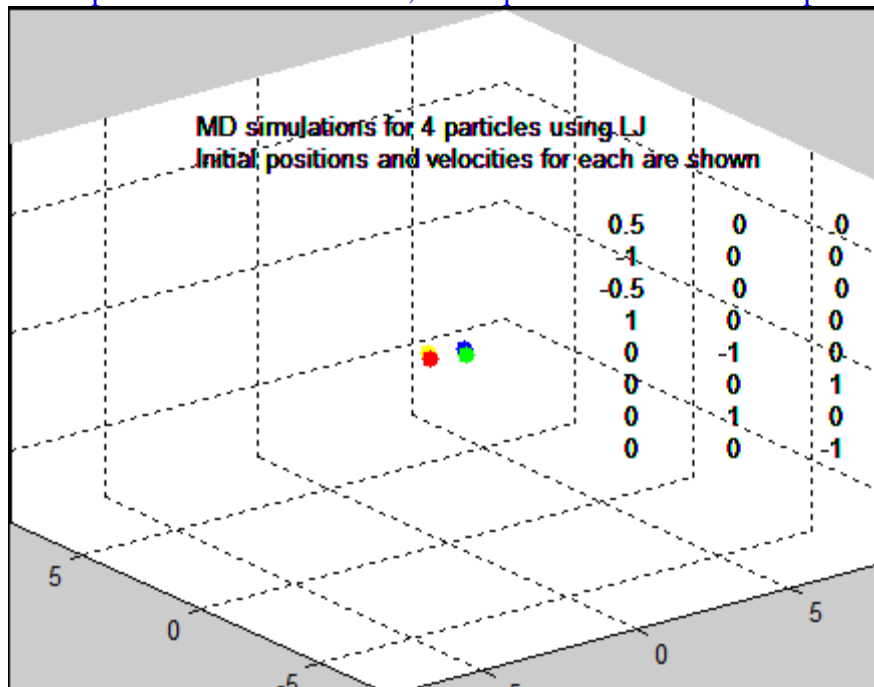
- a) Molecular interactions, execute the Example Program MolDyn for several particles with different initial conditions, is there low or high sensitivity on these conditions? Use output files to visualize animations of particle motions using Matlab.

What is this about?

You mainly need to run the existing code in Fortran 77, will need to modify the input file to set different initial conditions for the particles (position and velocity), the code will produce dynamics of these molecules in time. Major part involves writing a Matlab code to read in the output files of MolDyn and visualize the particles adequately.

The output file contains information on position and velocity, you can visualize in position space using position only or in phase space using position versus velocity. You may want to eliminate the first two data (or comment out the corresponding write statement in the F77 code) to use load in Matlab. To plot a second graph on top of the first one (the second dot while holding the first dot) you can use “hold on” after the first “plot” statement, then do the next “plot” statement.

The input file is called “md.in”, the required information is explained within the code



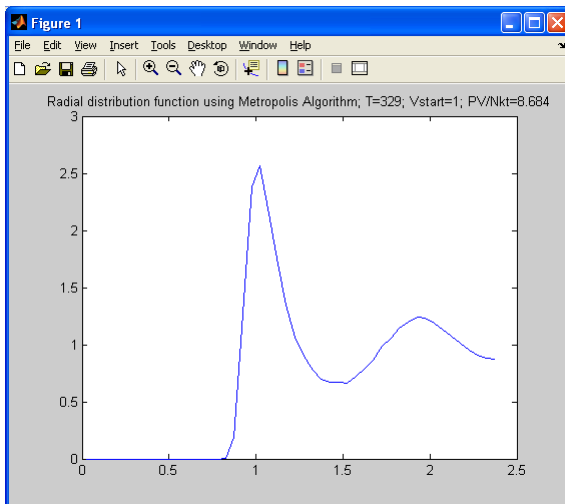
- b) Execute an example program based on the Metropolis algorithm, varying on or two parameters, present results using Matlab

TEMPERATURE = 329.0 VSTAR = 1.00

THE FACTOR PV/NkT = 8.684

RADIAL DENSITY FUNCTION ON AN ABOLUTE SCALE

0.025	0.000000	0.075	0.000000
0.125	0.000000	0.175	0.000000
0.225	0.000000	0.275	0.000000
0.325	0.000000	0.375	0.000000
0.425	0.000000	0.475	0.000000
0.525	0.000000	0.575	0.000000
0.625	0.000000	0.675	0.000000
0.725	0.000000	0.775	0.000000
0.825	0.003650	0.875	0.191842
0.925	1.263791	0.975	2.385576
1.025	2.566855	1.075	2.148101
1.125	1.705648	1.175	1.347593
1.225	1.069640	1.275	0.899462
1.325	0.772841	1.375	0.701379
1.425	0.668434	1.475	0.669831
1.525	0.666207	1.575	0.723743
1.625	0.797710	1.675	0.867987
1.725	0.984701	1.775	1.060678
1.825	1.148412	1.875	1.201534
1.925	1.239367	1.975	1.228720
2.025	1.186895	2.075	1.126671
2.125	1.075798	2.175	1.014802
2.225	0.956140	2.275	0.906592
2.325	0.881240	2.375	0.872938



$EL=5.0 * SIG * VSTAR ** (1.0/3.0)$

Outcome: to include the analysis of final results with respect to Vstar: make a 3D plot (surface or mesh) where the x and y axes are the radius r (from the output file) and the Vstar, respectively, and the z axis is the radial distribution itself.

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“THIS IS A CELL-STRUCTURE MONTE CARLO PROGRAM IN WHICH THE CELL CONTAINS 125 MOLECULES. THE MOLECULES ARE FIRST PLACED ON A 5 X 5 X 5 REGULAR GRID AND THEN DISPLACED RANDOMLY BY UP TO  $D/20$  IN EACH PRINCIPAL DIRECTION WHERE D IS THE INITIAL SEPARATION. THE ALGORITHM IS BASED ON THAT IN N. Metropolis, A.W.Rosenbluth, DATA FOR THE LENNARD-JONES FORCE. SIG IS IN nm AND EPS AS EPS/k WHERE k IS BOLTZMANN'S CONSTANT. THE FIGURES ARE FOR ARGON. THE RANGE OF THE FORCE, DLIM, IS SET AT 2.4 X SIG CORRESPONDING TO WHERE THE FORCE FALLS TO 1% OF ITS MAXIMUM VALUE. THE SIDE OF THE CUBICAL CELL IS 5 X SIG FOR  $V^* = 1$ . THE VALUE OF  $V^*$  IS READ IN WHICH GIVES THE CELL EDGE, EL”

**In part b) you should modify the Fortran code to output different radial distributions for different VSTAR (different sizes for each of the 125 cells in the simulation, or different initial separations for the 125 argon molecules. Then plot the radial distributions against r and VSTAR in a 3D plot. Temperature will be fixed at 329 K.**

The following portion describes how the code produces its outputs:

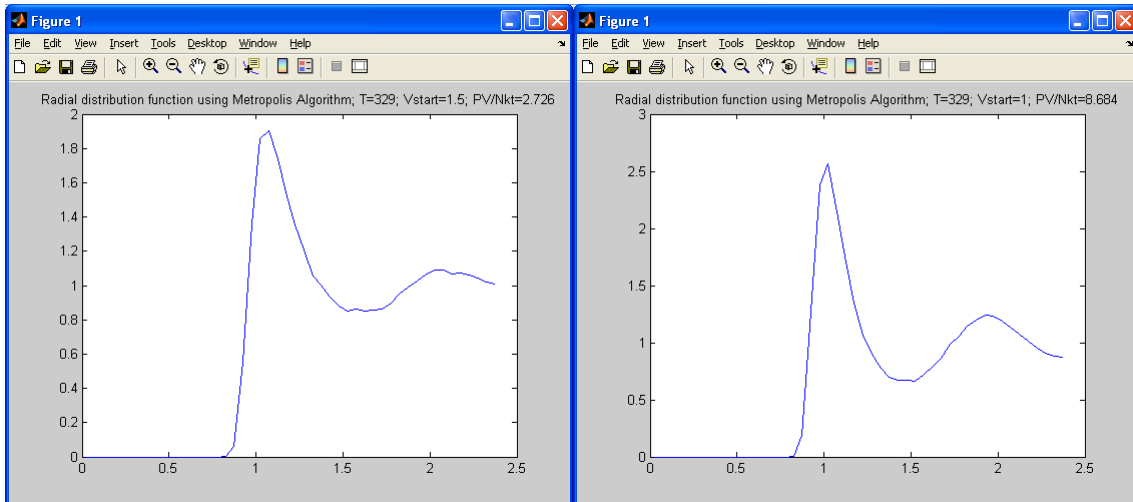
```
OPEN(UNIT=9,FILE='metropol.out')
C OUTPUT TEMPERATURE AND VSTAR
WRITE(9,350)T,VSTAR
350 FORMAT(15H TEMPERATURE = ,F6.1,9H VSTAR = ,F7.2)
WRITE(9,(' '))
C OUTPUT FACTOR
WRITE(9,200)FACTOR
200 FORMAT(21H THE FACTOR PV/NkT = ,F7.3)
C OUTPUT THE RADIAL DENSITY DISTRIBUTION  $4*\pi*R**2*RO(R)$  ON AN
C ABSOLUTE SCALE RELATIVE TO THE AVERAGE DENSITY.
DO 90 I=0,47
TAB(I)=6.161E-3*VSTAR*TAB(I)/((I+1.0)**3-I**3)
DD(I)=0.05*(I+0.5)
90 CONTINUE
WRITE(9,(' '))
WRITE(9,(' RADIAL DENSITY FUNCTION ON AN ABOLUTE SCALE '))
WRITE(9,300)(DD(I),TAB(I),I=0,47)
300 FORMAT(2(F10.3,F12.6))
```

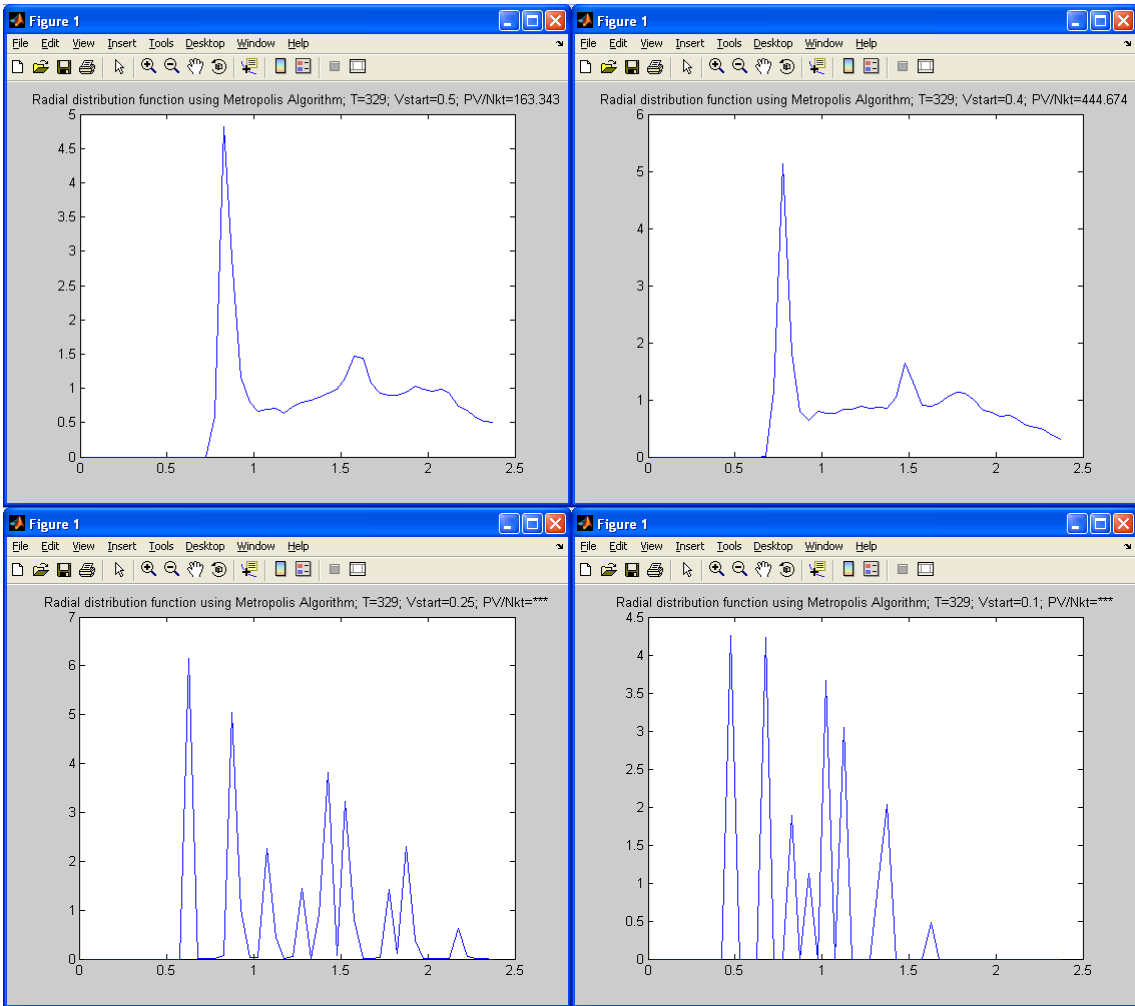
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Simulations of 125 Argon molecules using Metropolis Algorithm; T=329

