Physics 640
October 23, 2008

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

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
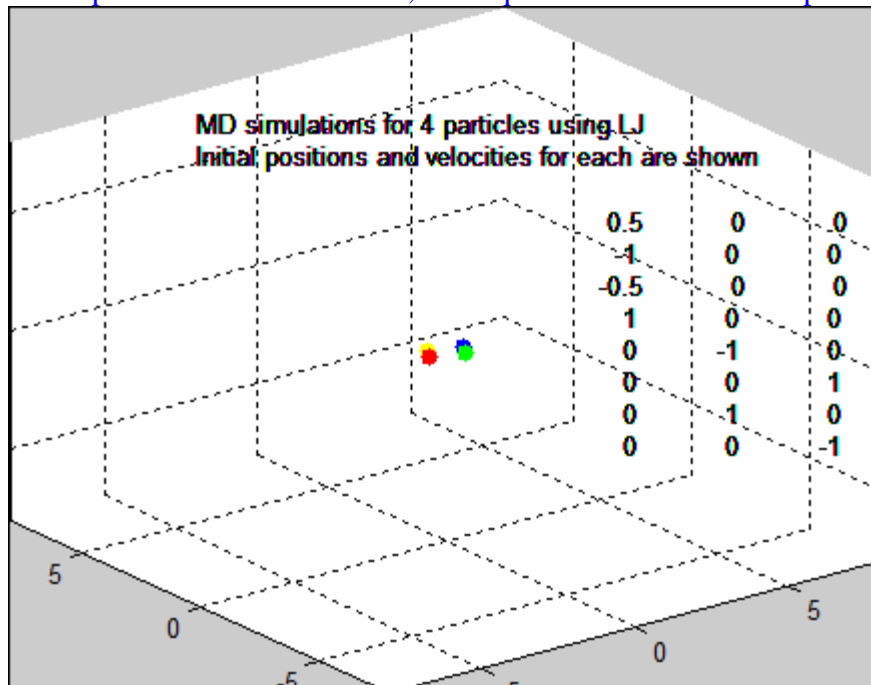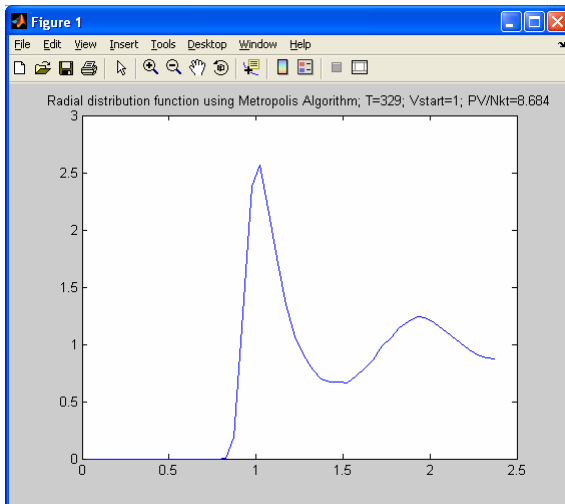

b) Execute an example program based on the <u>Metropolis algorithm</u>, varying on or
    two parameters, present results using Matlab

```
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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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.

    b) Execute an example program based on the <u>Metropolis algorithm,</u> varying one or
two parameters, present results using Matlab

"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.**

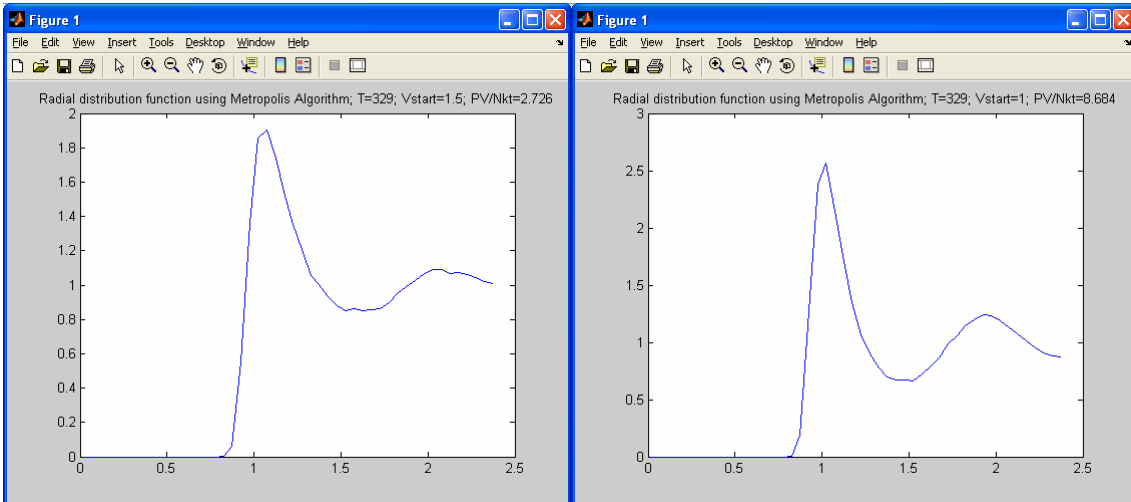The following portion describes how the code produces its outputs:

```
    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))
```
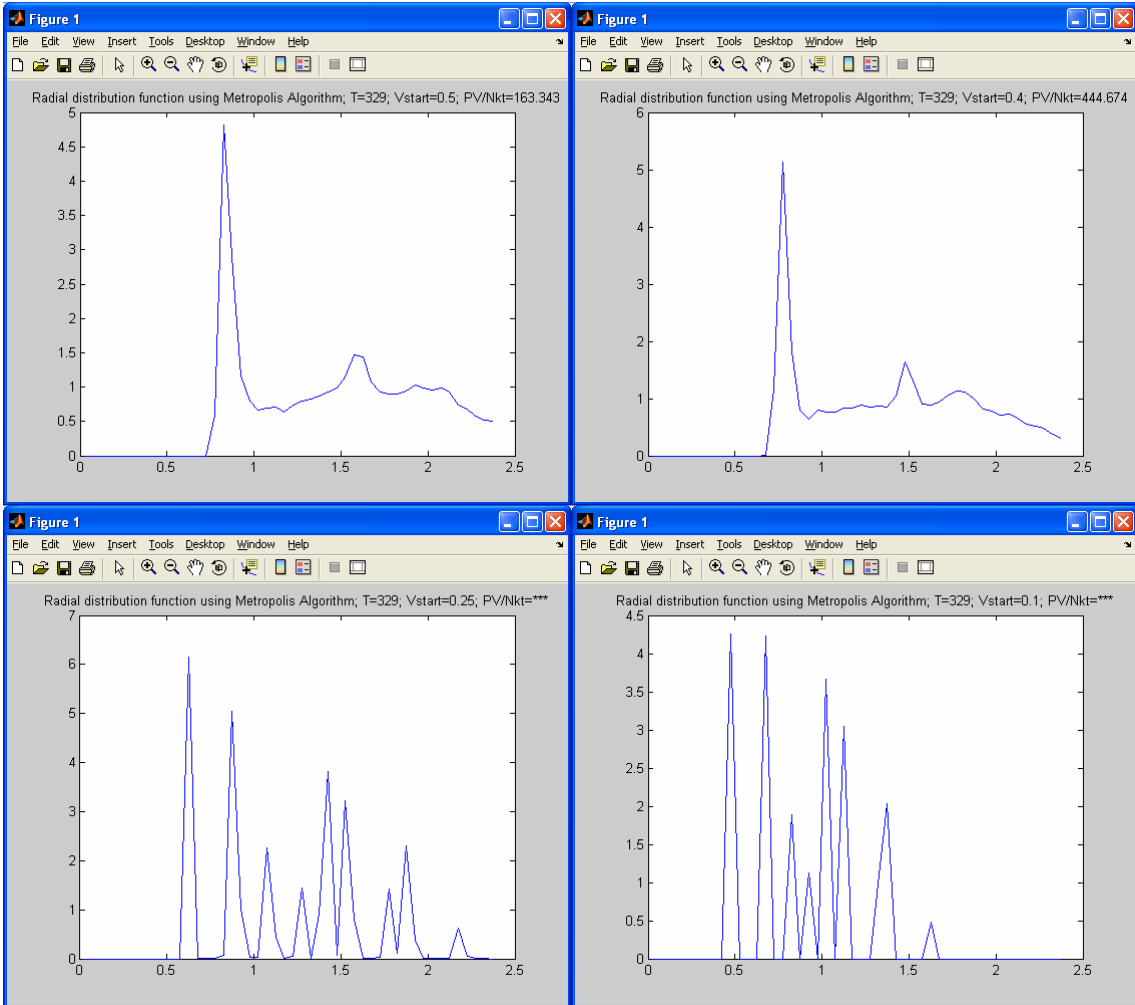
```
TEMPERATURE =  329.0 VSTAR =     1.00

 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
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     2.325     0.881240     2.375     0.872938
```


Radial distribution function using Metropolis Algorithm; T=329; Vstart=1.5; PV/Nkt=2.726

Radial distribution function using Metropolis Algorithm; T=329; Vstart=1; PV/Nkt=8.684

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. See example below:

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