Physics 640
October 30, 2007

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

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.

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

The following portion describes how the code produces its outputs:

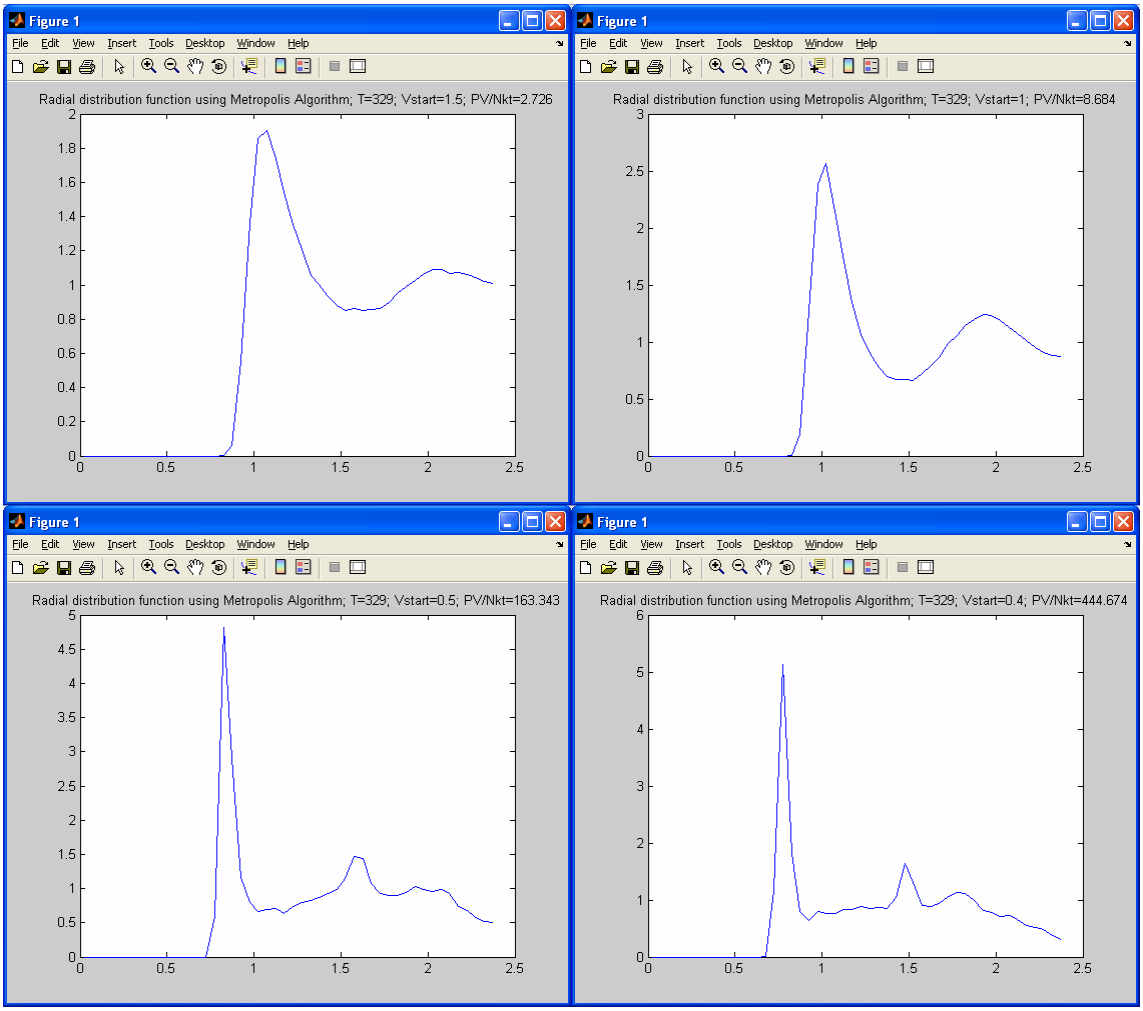
```
    OPEN(UNIT=9,FILE='metropol.out')
C  OUTPUT TEMPERATURE AND VSTAR
    WRITE(9,350)T,VSTAR
 350 FORMAT(15H TEMPERATURE = ,F6.1,9H VSTAR = ,F7.2)
    WRITE(9,(" "))
C  OUTPUT FACTOR
    WRITE(9,200)FACTOR
 200 FORMAT(21H THE FACTOR PV/NkT = ,F7.3)
C  OUTPUT THE RADIAL DENSITY DISTRIBUTION 4*PI*R**2*RO(R) 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))
```

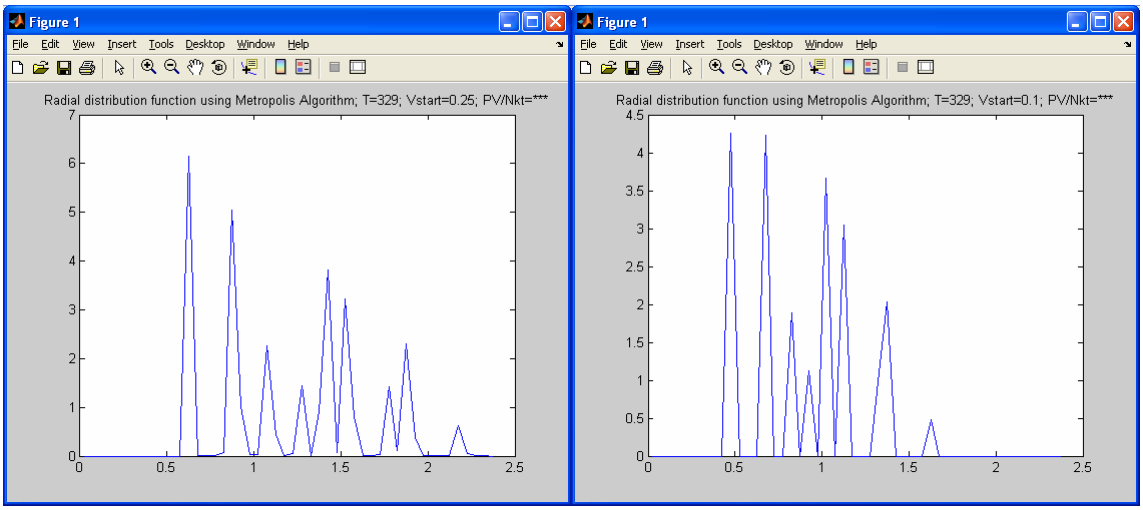
```
TEMPERATURE =  329.0 VSTAR =    1.00

 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
     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.