

Physics 640
October 25, 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.

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

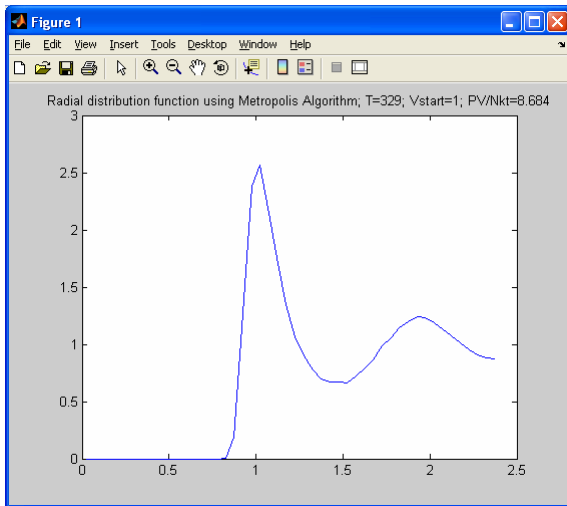
```
TEMPERATURE = 329.0 VSTAR = 1.00
```

```
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.