Assignment 3 – Due Nov. 12th by electronic submission to azp@princeton.edu

On the book's website you can find a Molecular Dynamics (MD) program for the cut-and-shifted Lennard-Jones potential in the NVE ensemble (under "Exercise 10"). Unfortunately, the program does not conserve energy, because it contains three errors.

1. Find the three errors in the code. Hint: there are two errors in *integrate.f* and one in *force.f* . List the lines containing errors and their corrected versions. You will need to use a Unix system to run the book code – see this link for an introduction to Unix at Princeton.

2. Test the energy drift of the numerical integration algorithm as a function of the total run time, time step used, temperature and density for N=100. You need to make minor changes to the code so that the energy drift is reported in a separate file; plot the results in appropriate coordinates.

3. Compute the diffusivity of this system for T = 2 and densities ρ = 0.7, 0.8 and 1.0 from the Einstein relationship for the mean-square displacement as a function of time. You may modify the code of Exercise 10, or use the code of Case Study 5.

4. Use the Andersen thermostat (Case Study 10) or Nosé-Hoover thermostat (Case Study 11) and compare the mean energy, pressure and mean-square displacement for for T = 2 and ρ = 0.7.

5. Lennard-Jones parameters for Ar are reported[1] as σ = 3.405 Å, ε/k = 118.2 K. The self-diffusion coefficient for liquid Ar at T=84.3 K, ρ=1413 kg/m^3 has been measured[2] as D=2.07 × 10^{-5} cm^2/s. How well is this property predicted from the LJ potential?

Please submit your solution (graphs, comments, code changed you made) as a single PDF file similar to that provided as solution to assignment 1. I will assign 20% of the grade to "aesthetics" of your solution: how easy it is to follow, quality and proper labeling of graphs, information density etc.

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[1] A. D. White, *J. Chem. Phys.*, **111**: 9352 (1999).

[2] J. W. Corbett and J. H. Wang, *J. Chem. Phys.*, **25**: 422 (1956).