Assignment #5
CH_ENG 8452, Spring 2017
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This (short!) project will be your last assignment for the semester in this course.

I have written a short (114-line) program in Fortran, available on Canvas, to calculate the radial distribution function for the hard sphere potential based on the Monte Carlo method (Metropolis–Hastings algorithm). I have also written an input file for the molecular dynamics program LAMMPS[1] that calculates the same radial distribution function for a Lennard-Jones fluid based on time-averaging at constant E, V, and N. The as-written settings assume a molecular density of $\rho^* = 0.75$ (using Lennard-Jones/hard sphere reduced units).

1. Download LAMMPS and/or connect to a computer that has it installed already. Follow the instructions to build it from source (you want the "serial" target—try `make serial` from the `src` directory), or download the pre-built binary version.[1]

2. Use the LAMMPS script available on Canvas to run the molecular dynamics simulation using the Lennard-Jones model. Plot the total energy, temperature, and pressure in the simulation (as output by LAMMPS) as a function of time for three different random number seeds (specify those seeds).[2] Discuss, given your knowledge of statistical mechanics, what you think the actual thermodynamic properties *should* be for this system; explain your reasoning.

3. Plot the radial distribution function (see the file created by LAMMPS via the `compute rdf` command) for the Lennard-Jones fluid for three different lengths of time integration (I recommend values like 1000 steps, 5000 steps, 10000 steps, 100000 steps, and 1000000 steps).

4. Compile the program encoded in `hard_spheres.f90`[3]; if using the GNU Fortran compiler, try

   ```
   gfortran -O2 hard_spheres.f90 -o hard_spheres
   ```

   If you have the Intel Fortran compiler, try

   ```
   ifort -O2 hard_spheres.f90 -o hard_spheres
   ```

   Any other compiler that supports Fortran 2003 will also work (if you only have an old one, try changing `ERROR_UNIT` to `0` and `OUTPUT_UNIT` to `*` and removing the "`use, intrinsic`" line at the top of the file).

5. Run the Monte Carlo program for increasing numbers of steps (e.g., 1000, 10000, 100000, and 1000000 steps), reporting the radial distribution function for each value.

[1] Andrea and Jiasen can help you do this if you are unsure where to start.

[2] No one should use the random number seed I gave you—please choose a different one! It can be any integer between 1 and 2 billion or so.

[3] You will need a Fortran compiler to do this; if you do not have access to a Fortran compiler or a UNIX-based machine (which will typically have such a compiler available), please see the instructor.

[1] Plimpton, S. "Fast Parallel Algorithms for Short-Range Molecular Dynamics." *Journal of Computational Physics* **117** (1): 1–19 (1995). `http://lammps.sandia.gov/`.

6. Comment on similarities and differences between the two sets of results, particularly with respect to whether you think the hard sphere model is a reasonable model of liquids at reasonable densities.[4]

7. If you make modifications to the code provided, please print them out with changes highlighted (or note the changes more succinctly in the written part) and hand them in so any errors/questions during grading can be answered and partial credit given

It is important to note that both the molecular dynamics *and* Monte Carlo examples here are *not* periodic—there will be some edge effects. The simulations could easily be made periodic if such was desired; this would give a radial distribution function more consistent with a bulk liquid.

[4]Please note: LAMMPS was written over the course of 22 years, whereas my Monte Carlo program was written in more like 22 hours. As such, please do *not* comment on the relative *speed* of the two programs, as I have done very little if any to optimize the Monte Carlo program! I also think I may have screwed up the normalization factor on the radial distribution function, so take that as qualitative-only for now. Sorry about that.