Report

The students who have chosen option 2 are expected to write an individual report covering issues addressed in Tasks II (Molecular dynamics of Lennard-Jones liquid) and VI (Monte-Carlo simulation of Lennard-Jones liquid).

In particular, this report should contain:

- Task II

  1. A plot and discussion of the radial pair correlation function $g(r)$ and the comparison with the results from [1].
  2. A plot and discussion of the structure factor $S(k)$ computed as (a) a Fourrier transform of $g(r)$ and (b) via direct sampling.
  3. Values of the diffusion coefficient D computed (a) using Einstein's relation and (b) by integrating the velocity correlation function. Error estimates for both values should be provided.

- Task VI

  1. A plot and discussion of $g(r)$ and $S(k)$ computed in the NVT ensemble at 94K. The results should be compared to the ones obtained in Task II and in [1].
  2. A plot and discussion of the evolution of the block-averaged errors on the energy as the block size increases.

All the numbers are expected to be in physical and not L.J. units, errors and a discussion of the results are expected to be provided whenever possible. All quantities that are plotted and/or discussed in the report should be defined.

References

[1] A. Rahman, *Correlations in the Motion of Atoms in Liquid Argon*. Phys. Rev **136** A405 (1964)