CHM695A: Molecular Modeling
Project Work – 2

Project Submission and Presentation: 12.03.2018 (5:00 pm)

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1. Write a molecular dynamics code in Fortran or in C for a system of 864 Lennard–Jones particles, following the classic paper of A. Rahman, Physical Rev. **136**, A405 (1964). Use the inter atomic potential, density, temperature and other simulation parameters as per the work of Rahman.

2. By carrying out MD simulations of this system, reproduce the following figures of the aforementioned paper of Rahman: (a) pair–correlation function $g(r)$ (Figure 2 of the paper); (b) velocity auto correlation function (Figure 4 of the paper)

   Refs: A. Rahman, Physical Rev. **136**, A405 (1964), Molecular Modeling by A. R. Leach, Understanding Molecular Simulation by Frenkel & Smith.

   Note: take care of the special reduced units used in their work - this is discussed in the book of Frenkel & Smith.
   In summary:

Quantity	New Units	Relation
Energy	E^*	E/ϵ
Length	R^*	R/σ
Mass	m^*	mM^{-1}
Time	t^*	$t\sigma^{-1}\sqrt{\epsilon/M}$
Density	ρ^*	$N\sigma^3/V$
Temperature	T^*	$k_B T/\epsilon$
Force	F^*	$F\sigma\epsilon^{-1}$