MASSACHUSETTS INSTITUTE OF TECHNOLOGY
DEPARTMENT OF MECHANICAL ENGINEERING
2.370/2.37 Fundamentals of Nanoengineering
Spring 2018
PROJECT DESCRIPTION

The project report is due on Thursday, May 17, at 5:00pm.

Below we propose a representative project on molecular dynamics simulation for which a Matlab code template is provided. Students should feel free to define an alternative project that better matches their interests. The alternative project description can be formulated in consultation with the TA and the instructor-in-charge. The final version of the project description **needs to be approved by the instructor-in-charge by March 23.**

General project description: Molecular Dynamics simulation
Develop a molecular dynamics simulation program for a Lennard-Jones potential. The temperature in the simulation can be calculated from average thermal energy of N particles using

$$T = \frac{2}{3Nk_B} \sum_{i}^{N} \frac{1}{2} m_i \left(\vec{c}_i - \vec{u}\right)^2 \tag{1}$$

where $\vec{c}_i$ is the velocity of particle i and $\vec{u}$ is the average flow velocity.

The *configurational part* of the pressure is the average of the diagonal terms of the stress tensor whose $i-j$ term is given by

$$\mathcal{P}_{ij} = \frac{1}{V} \sum_{k}^{N} \sum_{l>k}^{N} (r_{kl})_i (F_{kl})_j \tag{2}$$

Thus the pressure is given by

$$PV = Nk_BT + \frac{V}{3}(\mathcal{P}_{xx} + \mathcal{P}_{yy} + \mathcal{P}_{zz}) \tag{3}$$

Note that the pressure calculated using (3) will not exactly match reference results when the cutoff radius is small. For this, a long range correction needs to be applied. Also note that some time needs to be allowed for the material to reach equilibrium; averaging needs to start after *sufficient* time has elapsed.

Deliverables:
Validate your code by calculating equilibrium properties of Argon and comparing your answers to the ones used to validate the Monte Carlo code in homework. Also calculate the energy, pressure and coefficient of diffusion of liquid Argon at 158K and a number density $n = 8 \times 10^{27}/\mathrm{m}^3$.

In your report clearly describe your algorithm and the basic features of your numerical implementation. Discuss any important approximations you have introduced and their potential effect on your results. Also discuss any discrepancies you observe between your simulation results and reference results.