ChemE I5800 **Molecular Simulation** **Spring 2019**

Problem Set 10 – due May 9

The problem is to compute the molecular diffusivity of the Lennard-Jones liquid by two methods.

1. Use the mean-square displacement calculation built into the basic lj.f program. Plot $\langle \Delta \mathbf{r}^2 \rangle$ as a function of time and find D from the slope. Also plot the early-time behavior and determine the transition time for going from ballistic to diffusive behavior.

2. Measure the velocity autocorrelation function and find D from its time integral. Pay particular attention to the dependence on the integration limit.

If you're feeling adventurous, you could instead determine the shear viscosity. In this case you would measure and integrate the shear stress autocorrelation function and compare the result to either the value obtained from the curvature of the Poiseuille flow profile from Problem Set 8 or (better) impose Lees-Edwards boundary conditions and compute the average shear stress.