Problem Set 9 – due Nov. 20

Do **either** of the following two problems.

1. Add a Langevin thermostat to the MD code *lj_vv.f.* In this case the old constant kinetic energy thermostat should be used during equlibration (the first 1000 steps, say) to fix the temperature precisely, and afterwards the new thermostat should be called instead for the remaining 1000. The relaxation time parameter γ should be chosen by trial and error to produce a stable temperature.

2. Compute the surface tension of the Lennard Jones liquid at temperature 1.0 and density 0.8, using the method discussed in class. Also, compute the density profile in z.