Problem Set 11 – due Dec. 11

Use the Green-Kubo formulas

$$D = \frac{1}{3}\int_0^\infty dt\, \langle \mathbf{v}(t) \cdot \mathbf{v}(0) \rangle$$

and

$$\mu = \frac{1}{3k_B TV} \sum_\alpha \int_0^\infty dt\ \langle \sigma_\alpha(t) \sigma_\alpha(0) \rangle$$

to calculate the diffusion coefficient and the shear viscosity of the Lennard-Jones fluid at density 0.8 and (reduced) temperature 1.0. Check the diffusivity against the direct calculation of the mean-square displacement built into the code, and the viscosity against the result of the previous problem set.