Project II
Chemistry 5021/8021, Spring, 2005
Assigned: February 23, 2005. Due: March 23, 2005

This project is to help to learn the "control" of energy calculations, options for integrating dynamics equations, and analyses of MD trajectories.

1. Carry out a molecular dynamics simulation for liquid water in (1) the canonical ensemble (NVT) if you take CHEM5021, or (2) the isothermal-isobaric (NPT) ensemble if you take CHEM8021, both of which at 25 ^{o}C and at (or correspond to) 1 atm for a system containing 216 water molecules. Use the TIP3P model for water along with periodic boundary conditions. It is the aim of this project for you to experience and decide a reasonable choice for the cutoff distances in energy calculations, starting and equilibrating the system for productive MD simulations, criteria for evaluating "convergence" or "being equilibrated" of the system, and specific integration schemes. Then, perform and save the trajectory for 50 ps, to be used in the next problem.

2. Use the trajectory, saved along the 50 ps trajectory on every 10 fs, to determine the mean-square displacement and, then, the diffusion coefficient of water.