CZ3272 MC & MD, Tutorial 5 & 6
(*for week 12 & 14, Wed 1 & 15 Nov 06*)

1. Show that the Metropolis transition probability
$$W(X \to X') = T(X \to X') \min\left(1, P(X')/P(X)\right)$$
satisfies detailed balance as long as matrix *T(...)* is symmetric.

2. Consider the Ising model. One way to simulate the Ising model is to pick a site at random and flip the spin with probability min$[1, \exp(-\Delta E/(kT))]$. Show that the detailed balance is satisfied also for
   (a) (Glauber dynamics) Flip the spin with probability
$$\frac{1}{2}\left[1 - \sigma_i \tanh\left(\frac{J}{kT}\sum_{\langle i,j\rangle}\sigma_j\right)\right],$$
where site i is the center site whose spin is to be flipped; the summation is over the nearest neighbors of the center site.
   (b) (Heat-bath algorithm) Reset of the center spin as
$$\sigma_i = \mathrm{sign}\left(\xi - \frac{e^{-\Delta}}{1+e^{-\Delta}}\right), \quad \Delta = \frac{2J}{kT}\sum_{\langle i,j\rangle}\sigma_j$$
where ξ is a uniformly distributed random number between 0 and 1.

3.
   (a) Show that the symplectic algorithm C,
$$\hat{q} = q + \frac{h}{m}p + \frac{h^2}{2m}F(q),$$
$$\hat{p} = p + \frac{h}{2}\left[F(q) + F(\hat{q})\right],$$
is a second order algorithm – that is, the local truncation errors are of order O(h^3). Here p and q are current values of position and momentum at time t and hat(ed) version are new values at $t+h$. [Hint, compare Taylor expansion of exact result and the above formula]. (b) Show that the algorithm is exactly time-reversible. (c) Show that the algorithm viewed as a transformation preserves the phase space volume (assuming a 2D phase space).

4. Show that for the Nosé-Hoover dynamics
$$m\dot{\mathbf{v}}_i = \mathbf{F}_i - \zeta m\mathbf{v}_i, \quad \dot{\zeta} = \frac{1}{\tau^2}\left[\frac{K}{K_0} - 1\right], \quad K = \sum_{i=1}^{N}\frac{1}{2}m\mathbf{v}_i^2,$$
the quantity

$$C = K + V + K_0 \left(\tau\zeta\right)^2 + 2K_0 \int_0^t \zeta(t')dt'$$

is indeed a constant of the motion, namely dC/dt = 0.

5. Discuss on numerical methods to solve the one-dimensional Lengevin/Brownian dynamics equation

$$m\frac{d^2x}{dt^2} = -\gamma\frac{dx}{dt} + \xi(t),$$

where ξ is a stochastic variable with mean zero and delta-correlated:

$$\left\langle \xi(t)\xi(t')\right\rangle = kT\gamma\delta(t-t').$$

CZ3272 MC&MD, Lab 5 (*for week 11-13, 23 Oct – 10 Nov 2006*)

Due 10 Nov 2006

1. Consider a one-dimensional system of length L of N Lennard-Jones particles. The potential energy between pair of particles is

$$V(r) = 4\varepsilon\left[\left(\sigma/r\right)^{12} - \left(\sigma/r\right)^{6}\right],$$

r=$|x_i - x_j|$. Compute the equation of states, pressure P vs particle density ρ=N/L for a fixed temperature T=300 Kelvin using molecular dynamics and from the virial equation

$$P = NkT/L + \frac{1}{L}\left\langle \sum_{i<j}(x_i - x_j)F_{ij}\right\rangle,$$

where x_i is the one-dimensional coordinate of the particle and F_{ij} is the force between the two particles. The angular brackets mean average over molecular dynamics trajectories. Write the simulation program in reduced units. However, report your result (a plot of P vs ρ) in physical units with parameters ε= 1.67×10^{-21} J and σ = 3.40 Å suitable for the Ar gas. The mass of Ar is 40 a.m.u. The Boltzmann constant is k = 1.38×10^{-23} J/K.