# CZ3272 MC & MD, Tutorial 4 (*for week 10, Wed 18 Oct 06*)

1. Suppose we want to generate random 3D points ($x$,$y$,$z$) uniformly distributed on a unit sphere, e.g., $x^2 + y^2 + z^2 = 1$. Give a method (or two) to do this.

2. Design a "good" simple sampling Monte Carlo method to compute the integral
$$\int_0^\infty \cos(x) e^{-x} dx .$$
Write down not only the estimator but also Monte Carlo error.

3. (a) Let assume that the transition matrix $W_i$ has invariant distribution $P$ for all $i$, i.e., $P = P\ W_i$, $i$=1,2,..,$N$. show that both the weighted sum $W_s = \Sigma_i \lambda_i W_i$ and product $W_p = \Pi_i W_i$ have invariant distribution $P$, where $\Sigma_i \lambda_i = 1$. How to implement $W_s$ and $W_p$ on computer?
(b) If $W_i$ satisfies detailed balance with respect to $P$, is $W_s$ and/or $W_p$ satisfy detailed balance?

4. Write down the transition matrix $W$ for a one-dimensional 3-spin Ising system with periodic boundary condition using Metropolis flip rate, where a spin is picked at random, and flip is accepted with probability $\min[1, \exp(-\Delta E/(kT))]$. What is $W$ if site is scanned sequentially? The energy function of a 1D Ising model is
$$E(\sigma) = -J \sum_{i=0}^{N-1} \sigma_i \sigma_{(i+1) \bmod N}, \quad \sigma_i = \pm 1.$$
Note that $N$=3 system has $2^3$ possible states.

## CZ3272 MC & MD, Lab 4 (*for week 9 & 10, 9-20 October 2006*)

Due Friday, 20 October 2006

**1.** Write a Monte Carlo simulation program for the two-dimensional nearest neighbor Ising model, using the Metropolis algorithm. Feel free to make reference or use whatever code you happen to see (on the web). But you must understand and be able to modify the code. Compute energy per site $e$ and heat capacity per spin $c$ as a function of temperature $T$ (taking the Boltzmann constant $k_B$=1 and coupling constant $J$ = 1), for system size of 16 by 16 spins. You need about $10^5$ Monte Carlo steps to get good looking data for each $T$. Verify that random selection of a spin and sequential scan to flip spins give the same results (within statistical error). Make plots of $e$ and $c$ vs $T$.