KATHOLIEKE UNIVERSITEIT LEUVEN

Exam Computational Physics 2007/2008

1 Integrals

Let us suppose that you have at your disposal a uniform random number generator (RNG) in the interval $[0, 1[$.

• Give a schematic description on how to use this RNG for a Monte Carlo evaluation of the following integral:

$$\int_{-\infty}^{+\infty} \frac{x^2}{1+x^4}\, e^{-x^4}\, dx$$

• Is it possible to devise a Metropolis algorithm to perform the same type of calculation? If so, give the transition probability $P(x \to x')$ of the associated Markov chain.

• Which of the two methods is expected to perform better for the calculation of the integral. Justify your answer!

2 Detailed balance

Consider a system with N states labeled by $n = 1, 2, \ldots N$. Each state has an energy $E_n = \varepsilon_0 n^2$ with $\varepsilon_0 > 0$. The system is at a temperature T.

Consider a discrete Markov chain where the following transition at a time step Δt are allowed $n \to n \pm 1$. We take as selection probabilities $g(n \to n \pm 1) = 1/2$ for $1 < n < N$.

• Give at least two different choices of acceptance ratios $A(n \to n \pm 1)$ such that the detailed balance condition is satisfied. Include in your discussion also the two states $n = 1$ and $n = N$.

• Which of the two or more choices is the best for setting up a Monte Carlo simulation scheme converging to thermal equilbrium? Justify your answer.

3 Non-local Kawasaki algorithm

Consider a two dimensional Ising model at temperature T with an Hamiltonian given by given by

$$H = -J \sum_{(ij)} s_i s_j \tag{1}$$

with $J > 0$ and $s_i = \{\pm 1\}$.

• Given the spin configurations μ and ν defined in Fig. 1 calculate the transition probabilities $P(\mu \to \nu)$ and $P(\nu \to \mu)$ for a non-local Kawasaki algorithm.

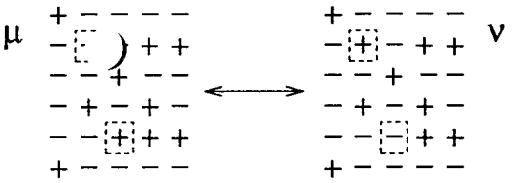

Figure 1: Spin exchange in the non-local Kawasaki algorithm.

4 Chemical Reactions

We consider the following system of coupled chemical reactions

$$A + B \xrightarrow{k_1} C \tag{2}$$

$$C \xrightarrow{k_2} 2A \tag{3}$$

$$C \xrightarrow{k_3} 2B \tag{4}$$

where k_1, k_2 and k_3 are the associated rates. We analyze the stochastic evolution of this system using the Gillespie algorithm.

Let us consider first for simplicity the case $k_1 = k_2 = k_3 = 10^6\ s^{-1}$.

• Given that at time $t = 0$ there are $N_A = N_B = 10$ and $N_C = 20$ particles, what is the average time one has to wait until the next reaction occurr?

• What are the relative probabilities (in %) that the next reaction is of type 1,2 or 3?

• Let us consider again the general case of different k_1, k_2 and k_3. Write down the deterministic differential equations describing the time evolution of the average number of particles. Are there stationary points?

5 Heat conduction through a rod

The differential equation describing the temperature T throughout a linear cooling element is given by

$$kA\frac{d^2T}{dx^2} - hP\,(T - T_{omg}) = 0 \tag{5}$$

k is the thermal conduction coefficient, A area of a section of the rod, h the convection coefficient and P the perimeter of the rod. We rewrite this equation in reduced quantities ($u = T - T_{omg}$; $\mu^2 = \frac{hP}{kA}$)

$$\frac{d^2u}{dx^2} - \mu^2\, u = 0 \tag{6}$$

Take as boundary conditions:

$$\frac{du(x)}{dx}(x = 0) = 0 \qquad \text{insulation, no heat loss} \tag{7}$$

$$u(x = L) = 1 \tag{8}$$