NATIONAL UNIVERSITY OF SINGAPORE

SEMESTER EXAMINATION FOR THE DEGREE OF B. SC.

COMPUTATIONAL SCIENCE III

(Computational Physics Option)

CZ372 Computational Techniques in Theoretical Physics

April/May 1996 — Time: 2 hours

INSTRUCTIONS TO CANDIDATES

1. This examination paper contains FIVE (5) questions and comprises FOUR (4) printed pages.
2. Answer any **FOUR (4)** questions. All questions carry equal weight.

1. Site Percolation

For the purpose of testing a computer simulation program, it is desirable to know the exact expressions for cluster numbers n_s. For this we work on a very small 2×2 square lattice.

(a) Define the average cluster number n_s.

(b) Give expressions of n_s as functions of occupation probability p, for $s = 1$, 2, 3, and 4, on the 2×2 square lattice.

(c) What should be the sum $\sum_{s=1}^{4} s n_s$? You need not compute it explicitly, but it gives you a consistent check.

2. Monte Carlo Method, Markov Chain

Consider a situation where we have only one Ising spin with two possible states, $+$ and $-$. The spin is in a magnetic field so that the energy is $-\mu B$ in the $+$ state and μB in the $-$ state [i.e., $H(\sigma) = -\mu B \sigma$]. The spin is in thermal contact with a heat bath at a temperature T.

(a) Applying the Metropolis algorithm to the above system, write down the transition probability matrix elements $W(+ \to +)$, $W(- \to +)$, $W(+ \to -)$, and $W(- \to -)$.

(b) What is the equation relating the transition matrix W to the invariant (equilibrium) probability distribution P_+ and P_-? Solve the equation for (P_+, P_-).

(c) State the detailed balance condition, and show that detailed balance is satisfied for the single spin system.

3. Monte Carlo Method, Ising Model

Consider a one-dimensional Ising model with the Hamiltonian (energy function)

$$H(\{\sigma\}) = -J \sum_{i=1}^{N} \sigma_i \sigma_{i+1} - K \sum_{i=1}^{N} \sigma_i \sigma_{i+2} - B \sum_{i=1}^{N} \sigma_i,$$

with the periodic boundary condition $\sigma_{N+i} = \sigma_i$. According to statistical mechanics, the probability for a particular configuration $\{\sigma\}$ is proportional to the Boltzmann weight $\exp\bigl(-H(\{\sigma\})/k_B T\bigr)$. This probability distribution can be realized by the *Metropolis* Monte Carlo method.

(a) Write the central part of the (pseudo) code which performs one spin updating.

(b) How do you compute the total magnetization, $M = \langle \sum_{i=1}^{N} \sigma_i \rangle$, and the heat capacity, $C = dU/dT$, where $U = \langle H \rangle$, directly from the simulation?

4. Symplectic Algorithm

The second-order time-reversible symplectic algorithm (for unit mass $m = 1$) is given by

$$\begin{aligned} p_{\frac{1}{2}} &= p + \frac{h}{2} F(q), \\ \hat{q} &= q + h\, p_{\frac{1}{2}}, \\ \hat{p} &= p_{\frac{1}{2}} + \frac{h}{2} F(\hat{q}), \end{aligned}$$

where F is the force, p and q are the momentum and position at time t, and $\hat{p}$ and $\hat{q}$ are the values at $t + h$.

(a) Apply this general difference scheme to the coupled oscillator system:

$$H(p_x, p_y, x, y) = \frac{1}{2}\left(p_x^2 + p_y^2 + x^2 + y^2\right) + xy^2.$$

That is, give the transformation from phase space point (p_x, p_y, x, y) at time t to $(\hat{p}_x, \hat{p}_y, \hat{x}, \hat{y})$ at time $t + h$.

(b) On the basis of the properties of symplectic algorithms, what is the value of the Jacobian,

$$\frac{\partial(\hat{p}_x, \hat{p}_y, \hat{x}, \hat{y})}{\partial(p_x, p_y, x, y)},$$

of the transformation? What is the significance of this result?

(c) Give the inverse transformation.

5. Molecular Dynamics

Consider N point particles moving in a one-dimensional box of length L. The particles interact pairwise through a potential $V(r)$, where r is the distance between two particles. The mass of each particle is m. A microcanonical molecular dynamics simulation is made so that we know the positions x_i and momenta p_i ($i = 1, 2, \cdots, N$) at time t.

(a) How does one compute the temperature T of the system?

(b) How does one estimate the error in T?

(c) How does one compute the average force (analog of pressure in three-dimensional system) exerted by the particles on one of the walls of the box?

— End of the Paper —

Computational Techniques in Theoretical Physics, Answers

1: (a) n_s is the average number of clusters of size s per lattice site.

(b) By enumerating all the states (16 of them), we get $n_1 = p(1-p)^2$, $n_2 = p^2(1-p)^2$, $n_3 = p^3(1-p)$, $n_4 = \frac{1}{4}p^4$.

(c) $\sum_s s n_s = p$.

2: (a) $W(+ \to +) = 1 - \lambda$, $W(+ \to -) = \lambda$, $W(- \to +) = 1$, $W(- \to -) = 0$, where $\lambda = \exp(-2\mu B/k_B T)$.

(b) The equation is

$$\begin{pmatrix} 1-\lambda & 1 \\ \lambda & 0 \end{pmatrix} \begin{pmatrix} P_+ \\ P_- \end{pmatrix} = \begin{pmatrix} P_+ \\ P_- \end{pmatrix}.$$

The solution $P_+ = 1/(1+\lambda)$, $P_- = \lambda/(1+\lambda)$,

(c) Detailed balance for this problem $P_+ W(+ \to -) = P_- W(- \to +)$, or $1 \cdot \lambda = \lambda \cdot 1$ is satisfied.

3: (a) The important result looking for is that $\delta H = 2J\sigma_0(\sigma_{-1} + \sigma_1) + 2K\sigma_0(\sigma_{-2} + \sigma_2) + 2B\sigma_0$. Code omitted.

(b) $M = 1/n \sum_i^n M_i$, $C = (\langle H^2 \rangle - \langle H \rangle^2)/(k_B T^2 N)$.

4: (a) The symplectic algorithm applies to the coupling oscillator is

$$\begin{aligned}
u_{1/2} &= u + \frac{h}{2}(-x - y^2), \\
v_{1/2} &= v + \frac{h}{2}(-y - 2xy), \\
x' &= x + h u_{1/2}, \\
y' &= y + h v_{1/2}, \\
u' &= u_{1/2} + \frac{h}{2}(-x' - y'^2), \\
v' &= v_{1/2} + \frac{h}{2}(-y' - 2x'y'),
\end{aligned}$$

where $(p_1(t), p_2(t), x(t), y(t)) = (u, v, x, y)$ and $(p_1(t+h), p_2(t+h), x(t+h), y(t+h)) = (u', v', x', y')$.

(b) Symplecticity implies

$$\frac{\partial(u', v', x', y')}{\partial(u, v, x, y)} = 1.$$

The map preserves the phase space volume.

(c) Inverse is simply (a) with h replaced by $-h$.

5: (a) By equipartition theorem, $\langle \frac{1}{2} m v^2 \rangle = \frac{1}{2} k_B T$, we get $T = \langle \sum_i^N m v_i^2 \rangle / (k_B N)$, where the average is over a period of time.

(b) Error in T can be estimated by $\delta T = \sigma/\sqrt{n}$, where σ is variance of T and n is number of samples taken.

(c) One can repeat the process of derivation of virial theorem to get the force. A quick way is to use the virial theorem directly. Note that in three dimensions, $PV = N k_B T + \frac{1}{6} \langle \sum_{i,j}^N \mathbf{F}_{ij} \cdot (\mathbf{r}_i - \mathbf{r}_j) \rangle$. Applying this in one dimension, $PV = (F/A)(AL) = FL$, we get

$$F = N k_B T / L + \frac{1}{2L} \langle \sum_{i,j}^{N} F_{ij} (x_i - x_j) \rangle.$$