Queen Mary & Westfield College
UNIVERSITY OF LONDON
MSci EXAMINATION

PHYS- 970 Computational Physics

Time Allowed : two hours.

Date: 10th May 1999 Time: 14.30

Answer TWO questions only. All questions carry equal marks.

1 (a) Explain briefly what is meant by a *molecular dynamics* computer simulation. Discuss examples of the types of useful physical outputs you would expect from such simulations. [4]

(b) Describe briefly the Verlet algorithm for integrating the equations of motion explaining the advantages and disadvantages. [4]

(c) Explain briefly what is meant by the *radial distribution function*, $g(r)$. What are the values of $g(r)$ at the origin and at infinity for a Lennard-Jones fluid? Briefly describe how it can be measured and how other quantities are related to it. [4]

(d) The radial distribution function is simply related to the pair distribution function defined by

$$\frac{V}{N^2}\sum_{i\neq j} < \delta(\mathbf{r}_i - \mathbf{r}_j - \mathbf{r}) >$$

Give a brief outline of the steps needed to compute this quantity within a molecular dynamics simulation. [4]

(e) Explain briefly how you would characterise the *temperature* in a MD simulation. Describe the procedure you would use to equilibrate a system of particles appropriate to a canonical ensemble at the temperature T. [4]

2 (a) Discuss the usefulness of Monte Carlo methods in computer simulations. Illustrate your discussion with a couple of examples. [4]

(b) Describe how you would use the Monte Carlo method to do a multidimensional integral and explain why it becomes more efficient than a straight forward extension of Simpson's rule as the dimensionality is increased. [4]

(c) The Hamiltonian of the Ising model is given by

$$H = -J\sum_{<ij>} s_i s_j - B\sum_i s_i.$$

Give a physical interpretation of the Ising model and explain what is meant by the various quantities in H. Discuss its usefulness in computer simulations and the types of problems for which it is most suited. [4]

(d) Explain briefly the terms *microstate* and *macrostate* and gives examples of them for a 2x2 Ising model. [3]

(e) Explain the term *importance sampling*. Outline the *Metropolis algorithm* and explain how importance sampling is achieved within it. [5]

© University of London 1999

3 (a) Describe briefly what is meant by algebraic computing and discuss the type of problems which can be tackled with such techniques. [6]

(b) Explain briefly what is meant by *microparallelism* and *macroparallelism* in parallel computing and the types of computer architecture to which they relate. [4]

(c) Describe briefly what is meant by Variational Monte Carlo (VMC) simulation for quantum systems and explain how one can obtain useful information about the ground state by choosing suitable variational parameters. [3]

(d) In a particular VMC calculation the trial wave function is taken to be a Slater determinant wave function corresponding to an electron gas. Explain why calculation of the total energy requires "updates" of the determinant. [3]

(e) Consider a matrix M; denote its determinant and the inverse of its transpose by Δ and $\overline{M}$ respectively. If M' denotes the matrix M with its j^{th} column replaced then it can be shown that the corresponding determinant Δ' is given by

$$\frac{\Delta'}{\Delta} = Q = \sum_p \overline{M}_{pj} M'_{pj}.$$

Furthermore the columns of $\overline{M'}$ are expressible in terms of the corresponding ones in $\overline{M}$ and the replaced j_{th} column. Explain how this result may be used in a parallel algorithm to update determinants in a Variational Monte Carlo calculation. [4]

END OF PAPER