DARESBURY LABORATORY

INFORMATION QUARTERLY for COMPUTER SIMULATION OF CONDENSED PHASES

LENDING CORY

An informal Newsletter associated with Collaborative Computational Project No.5 on Molecular Dynamics, Monte Carlo and Lattice Simulations of Condensed Phases. Number 11 JANUARY 1984

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Science & Engineering Research Council, Daresbury Laboratory, Daresbury, Warrington WA4 4AD, England.

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Editorial

Recipients of an unfamiliar newsletter entitled "Information Quarterly for the Computer Simulation of Condensed Phases" may be forgiven for thinking that newsletter distribution from Daresbury has finally lapsed into chaos. However, the puzzle is soon resolved. The new title for the CCP5 newsletter is intended to reflect the broadened scope of CCP5 under the terms of its renewal for the period 1983 to 1986. The scope of CCP5 now extends to the computer simulation of lattices in addition to the original subjects of MD and MC simulations, and the new title brings the newsletter in touch with this fact. We shall continue to publish articles on MD and MC as we have in the past, but will also include articles on the new subject area from now on. We hope our existing and new readers will find the newsletter a useful and stimulating reference.

Once again it is a pleasure to thank the contributors to the current issue. The CCP5 newsletter is a well-regarded periodical and this is obviously due to the efforts of our contributors. Long may they remain industrious on our behalf!

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General News

(a) CCP5 - POTENTIALS

The tenth CCP5 Meeting will be on the subject of 'Potentials' and will take place at University College London in September 1984. The principal organiser for this event will be Dr. C.R.A. Catlow who may be contacted at the Department of Chemistry, University College, 20 Gordon Street, London WClH OAJ.

(b) Solid State Meeting - THEORY OF LOCALISED ELECTRONIC STATES IN CONDESNED MATTER

A three day meeting on the "Theory of Localised Electronic States in Condensed Matter" is scheduled to be held in London on April 10th-12th 1984. The meeting is being organised by Dr. C.R.A. Catlow and Dr. W.C. Mackrodt. The cost of the meeting will be £25 per person. Further information is available from Dr. C.R.A Catlow at the address given above (item (a)).

(c) CCP5 Symposium - QUANTUM MECHANICAL COMPUTER SIMULATION A 12 day symposium on the treatment of quantum effects in (or by) computer simulation will be held in Oxford on March 12th to 13th. The purpose is mainly educational; to learn to implement current methods including:

- (i) Green's function Monte Carlo for systems at T=OK.
- (ii) Path integral methods for equilibrium properties (T≠OK).
- (iii) Semi-classical methods based on approximate path integral techniques

or the Wigner-Kirkwood h² expansion, or wave packet propagation. The number of participants will not exceed 20. Preference will be given to those already active in the field or about to become so. Applications for financial support (travel and subsistence) will be sympathetically considered by the CCP5 Excecutive Committee. Participants will include Dr. S.W. De Leeuw, Prof. J.G. Powles and Prof. K. Singer. Interested persons should write to Dr. S.W. De Leeuw, Department of Theoretical Physics, I Keble Road, Oxford, OXI 3NP, not later than February 5th. Please give reasons for wishing to attend.

(d) The CCP5 Steering Committee wish to remind participants in CCP5 that, within the limited resources of the Project it is willing to sponsor or assist financially the endeavours of computer simulation scientists in the U.K. Applications for financial assistance should be submitted to the CCP5 Secretary, Dr. W. Smith, SERC Daresbury Laboratory, Daresbury, Warrington, WA4 4AD in the first instance. All applications will be considered on merit by the CCP5 Executive Committee.

- (e) Readers will not be surprised to hear of the success of the recent CCP5 Meeting on 'Phase Transitions' which took place at Southampton. On behalf of the participants, it is a pleasure to thank Dr. Dominic Tildesley and Dr. David Adams for their organisation of the Meeting and Prof. G.R. Luckhurst for hosting the Meeting at Southampton. We hope to present a review of the Meeting in our March issue of the newsletter.
- (f) The news from Rutherford and Appleton Laboratory (RAL) is that, in October, they replaced their IBM 308D computer with a brand new IBM 308D. This they managed to do without incurring any cost to the SERC. Not surprisingly, they are very pleased with themselves. The present system has 24 M bytes of storage, which will rise to 32 M bytes in April 1984. April should also see the end of the installation of the M860 Mass Storage System for the central processors. The M860 is a tape cartridge store, which can load the tape cartridges into the read/write stations automatically. Each cartridge holds 170 M bytes and the entire M860, will hold 110 G bytes. The system will be used as a first level backup store for MVS users and will function as though it were additional disc space from which on-line datasets will be stored and recalled. Users in future will be encouraged to keep data on disc, from where it will migrate to the M860 store. This, it is thought, will be more efficient than storing data on magnetic tape.
- (g) The University of Manchester Regional Computer Centre (UMRCC) has recently seen the departure of its Director, Professor Gordon Black, who will continue links with UMRCC as a Consultant. His replacement as Director is Professor Frank H. Summer.

On the CYBER 205 Project, the hardware tests have been completed and the initial acceptance of the FORTRAN 77 compiler (FORTRAN 200) is scheduled for 31st January 1984. An experimental service is scheduled for 1st March 1984 and a full service for August 1984. As for the Amdahl V7A Project, the hardware tests have been completed and a full performance test wasscheduled for completion by 21st November 1983. A full service should start on 1st January 1984. At the time of writing, the testing of the Remote Host Facility software is still underway.

(h) The University of London Computer Centre is continuing with its intention to provide an archiving facility for the Amdahl V/8 computer. They have implemented the commercially available package called DMS/OS, which presently is operational in batch mode. The system resembles that in

existence at Daresbury but with some distinguishing features. Firstly, the datasets archived will have a limited life-time (3 years). Secondly, one hundred versions of a dataset may be archived with version numbers 0 to -99 (0 for the most recent version). Thirdly, users will be restricted in archive allocation, which, when exceeded, will prevent further archiving. The ubiquitous MASSTOR M860 storage system will provide the archive storage in the New Year. A new version of the Siemens FORTRAN 77 compiler (V10/L10) is available on

the Amdahl V/8. The features of this compiler are described in the ULCC November Newsletter. The December issue describes the Release 2.0 IBM FORTRAN 77 compiler (VS FORTRAN). Essential reading for Amdahl users The user service to the CDC 6600 and 7600 computers will cease on 1st February 1984.

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(i) Anyone wishing to make use of the CCP5 Program Library is invited to do so. Documents and programs are available, free of charge to academic centres, upon application to Dr. M. Leslie* at Daresbury Laboratory. Listings of programs are available if required, though use of magnetic tape (provided by the applicant) is recommended. (Note! Please do not send tapes using 'Jiffy' Bags as these invariably cause difficulties!) Readers interested in the lattice simulation programs available should also write to Dr. M. Leslie.

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Anyone wishing to donate programs to the CCP5 Program Library should contact Dr. M. Leslie, who will be overwhelmed by their generosity.

* Full address: SERC, TCS Division, Daresbury Laboratory, Warrington, WA4 4AD.

List of Programs in the CCP5 Program Library.

MDATOM by S. M. Thompson.

M.D. simulation of atomic fluids. Uses 12/6 Lennard - Jones potential function and fifth order Gear integration algorithm. Calculates system average configuration energy, kinetic energy, virial, mean square force and the associated R.M.S. deviations and also system pressure, temperature, constant volume specific heat, mean square displacement, quantum corrections and radial distribution function.

HMDIAT by S. M. Thompson.

M.D. simulation of diatomic molecule fluids. Uses 12/6 Lennard -Jones site - site potential functions and a fifth order Gear algorithm for centre - of - mass motion. Angular motion is calculated by fourth order Gear algorithm with quaternion orientation parameters. Calculates system average configuration energy, kinetic energy, virial, mean square force, mean square torque and the associated R.M.S. deviations and also system pressure, temperature, constant volume specific heat, mean square displacement and quantum corrections.

MDLIN by S. M. Thompson.

M.D. simulation of linear molecule fluids. Uses 12/6 Lennard -Jones site - site potential functions and a fifth order Gear algorithm for centre - of - mass motion. Angular motion is calculated by fourth order Gear algorithm with quaternion orientation parameters. List of calculated properties is the same as HMDIAT.

MDLINQ by S. M. Thompson.

M.D. simulation of linear molecule fluids. Uses 12/6 Lennard -Jones site - site potential functions plus a point electrostatic quadrupole. Uses a fifth order Gear algorithm for centre - of mass motion. Angular motion is calculated by fourth order Gear algorithm with quaternion orientation parameters. List of calculated properties is the same as HMDIAT.

MDTETRA by S. M. Thompson.

M.D. simulation of tetrahedral molecule fluids. Uses 12/6 Lennard -Jones site - site potential functions and a fifth order Gear algorithm for centre - of - mass motion. Angular motion is calculated by fourth order Gear algorithm with quaternion orientation parameters. List of calculated properties is the same as HMDIAT.

MDPOLY by S. M. Thompson.

M.D. simulation of polyatomic molecule fluids. Uses 12/6 Lennard -Jones site - site potential functions and a fifth order Gear algorithm for centre - of - mass motion. Angular motion is calculated by fourth order Gear algorithm with quaternion orientation parameters. List of calculated properties is the same as HMDIAT.

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and the second M.D. simulation of polyatomic molecule mixtures. Uses 12/6 Lennard - Jones site - site potential functions and a Verlet leapfrog algorithm for centre - of - mass motion. Angular motion is calculated by the Fincham leapfrog algorithm using quaternion orientation parameters. Calculates system average configuration energy, kinetic energy and virial and associated R.M.S. deviations and also pressure and temperature.

M.D. simulation of polyatomic molecule mixtures. Uses 12/6 Lennard - Jones site - site potential functions and point electrostatic multipoles (charge, dipole and quadrupole). Long range electrostatic effects are calculated using the Ewald summation method. Uses a Verlet leapfrog algorithm for centre - of - mass motion. Angular motion is calculated by the Fincham leapfrog algorithm using quaternion orientation parameters. Calculates system average configuration energy, kinetic energy and virial and associated R.M.S. deviations and also pressure and temperature.

MDMPOL by W. Smith & D. Fincham.

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M.D. simulation of polyatomic molecule mixtures. Uses 12/6 Lennard - Jones site - site potential functions and fractional charges to represent electrostatic multipoles. Long range electrostatic effects are calculated using the Ewald summation method. Uses a Verlet leaping algorithm for centre - of - mass motion. Angular motion is calculated by the Fincham leapfrog algorithm using quaternion orientation parameters. Calculates system average configuration energy, kinetic energy and virial and associated R.M.S. deviations and also pressure and temperature.

DENCOR by W. Smith.

A A REACT DECK PROPERTY Calculation of density correlation functions. Processes atomic M.D. data to produce the Fourier transform of the particle density, the intermediate scattering functions and the dynamic structure factors.

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CURDEN by W. Smith

Calculation of current density correlation functions. Processes atomic M.D. data to produce the Fourier transform of the current density, the current density correlation functions and their temporal Fourier transforms.

HLJ1 by D. M. Heyes.

M.D. simulation of atomic fluids. Uses 12/6 Lennard - Jones site site potential function and a Verlet leapfrog algorithm for centre - of - mass motion. Calculates system average configuration energy and kinetic energy and associated R.M.S. deviations and also pressure, temperature, mean square displacements and radial distribution function.

HLJ2 by D. M. Heyes.

M.D. simulation of atomic fluids. Uses 12/6 Lennard - Jones site site potential function and a Verlet leapfrog algorithm for centre - of - mass motion. Calculates system average configuration energy and kinetic energy and associated R.M.S. deviations and also pressure, temperature, mean square displacements, radial distribution function and velocity autocorrelation function.

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HLJ3 by D. M. Heyes.

M.D. simulation of atomic fluids. Uses 12/6 Lennard - Jones site site potential function and a Verlet leapfrog algorithm for centre - of - mass motion. The link - cell method is employed to enable large simulations. Calculates system average configuration energy and kinetic energy and associated R.M.S. deviations and also pressure, temperature, mean square displacements and radial distribution function.

HLJ4 by D. M. Heyes.

M.D. simulation of atomic fluids. Uses 12/6 Lennard - Jones site site potential function and a Verlet leapfrog algorithm for centre - of - mass motion. The algorithm allows either the temperature or the pressure to be constrained. Calculates system average configuration energy and kinetic energy and associated R.M.S. deviations and also pressure, temperature, mean square displacements and radial distribution function.

HLJ5 by D. M. Heyes.

M.D. simulation of atomic fluids. Uses 12/6 Lennard - Jones site site shifted potential function and a Verlet leapfrog algorithm for centre - of - mass motion. This method removes the discontinuities at the potential cutoff radius. Calculates system average configuration energy and kinetic energy and associated R.M.S. deviations and also pressure, temperature, mean square displacements and radial distribution function.

HLJ6 by D. M. Heyes.

M.D. simulation of atomic fluids. Uses 12/6 Lennard - Jones site site shifted potential function and the Toxvaerd algorithm for centre - of - mass motion. This algorithm is more accurate than the Verlet algorithm. Calculates system average configuration energy and kinetic energy and associated R.M.S. deviations and also pressure, temperature, mean square displacements and radial distribution function.

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MCRPM by D. M. Heyes.

M.C. simulation of electrolytes. Monte Carlo program using restricted primitive model of an electrolyte. The potential is regarded as infinite for r d and Coulombic for r d. The properties calculated are the average configuration energy and its R.M.S. deviation, the pair radial distribution function and the melting factor.

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HSTOCH by W. F. van Gunsteren & D. M. Heyes.

S.D. or M.D. simulation of molecules in vacuo or in a rectangular cell with solvent or lattice atoms (i.e. Langevin or Brownian dynamics of large molecules).

dynamics of large molecules). MDATOM by D. Fincham.

M.D. simulation of atomic fluids. Uses 12/6 Lennard - Jones potential function and Verlet leapfrog integration algorithm. Calculates system average configuration energy, kinetic energy, virial and the associated R.M.S. deviations and also system pressure, temperature, mean square displacement and radial distribution function.

MDDIAT by D. Fincham.

M.D. simulation of diatomic molecule fluids. Uses 12/6 Lennard -Jones site - site potential functions and the Verlet leapfrog algorithm for centre - of - mass motion. Angular motion is is calculated using the constraint algorithm. Calculates system average configuration energy, kinetic energy, virial and the associated R.M.S. deviations and also system pressure, temperature and mean square displacement.

MDDIATQ by D. Fincham.

M.D. simulation of diatomic fluids. Uses 12/6 Lennard - Jones site - site potential functions and a point quadrupole electrostatic term. Employs the Verlet leapfrog algorithm for centre - of - mass motion. Angular motion is calculated using the constraint algorithm. Calculates system average configuration energy, kinetic energy, virial and the associated R.M.S. deviations and also system pressure, temperature and mean square displacement.

MDIONS by D. Fincham & N. Anastasiou. A Second for the second states of the second sec

M.D. simulation of electrolytes. Uses exp/6/8 potential function and the Coulomb electrostatic potential. Long range interactions are calculated using the Ewald summation method. Uses the Verlet leapfrog algorithm for particle motion. Calculates system average configuration energy, kinetic energy, virial and the associated R.M.S. deviations and also system pressure, temperature, radial distribution functions, static structure factors and mean square displacements.

MDMANY by D. Fincham & W. Smith.

M.D. simulation of polyatomic molecules. Uses 12/6 Lennard - Jones site - site potential functions and fractional charges to represent electrostatic multipoles. Long range electrostatic effects are calculated using the Ewald summation method. Uses a Verlet leapfrog algorithm for centre - of - mass motion. Angular motion is calculated by the Fincham leapfrog algorithm using quaternion orientation parameters. Calculates system average configuration energy, kinetic energy and virial and associated R.M.S. deviations and also pressure and temperature. FORTRAN 77 standard program.

CARLOS by B. Jonsson & S. Romano.

M.C. simulation of a polyatomic solute molecule in an aqueous cluster. (i.e. a molecule surrounded by water molecules). The water - water potential is calculated using an analytical fit to an ab initio potential energy surface due to Matsuoka et al. The solute-solvent potential is optional. The program provides an energy and coordinate 'history' of the M.C. simulation. An analysis program CARLAN for processing the data produced by CARLOS is also available.

MCN by N. Corbin.

M.C. simulation of atomic fluids. Standard (Metropolis) Monte Carlo program for atomic fluids.

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SCN by N. Corbin. M.C. simulation of atomic fluids. Standard (Rossky, Friedman and Doll) Monte Carlo program for atomic fluids. SMF by N. Corbin.

M.C. simulation of atomic fluids. Standard (path integral method) Monte Carlo program for atomic fluids.

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ALGORITHMS FOR CONSTANT TEMPERATURE AND/OR CONSTANT PRESSURE ENSEMBLES. IN MOLECULAR DYNAMICS SIMULATIONS OF ATOMIC LIQUIDS

D., Brown, and J.H.R.; Clarke share a straight about the state of the

Conventionally molecular dynamics (MD) simulations of liquids at equilibrium are carried out using the constant energy ensemble. This is the usual microcanonical (N,V,E) ensemble of constant number of particles, N, constant volume, V_{c} and constant total energy, E, augmented by the fourth constraint of zero total linear momentum. Over the years several schemes have been proposed for performing MD calculations in alternative ensembles more comparable with the usual laboratory conditions of constant temperature and/or constant pressure. These include the (N,V,T) [1-4], the second (N, P, H) and (N, P, T) ensembles [3,5] and also the N, S, H ensemble [6], where S is the stress tensor. In most cases the relevant articles [1-11] have concentrated on the theoretical justification of the methods and the results obtained using them. In some cases results obtained from different ensembles have been compared [5,7-10] but in general little information is given of the specific algorithms used to integrate the different equations of motion. This can be disheartening for the potential user of these methods who finds that apparently rigorous mathematical expressions do not: lend themselves to easy numerical integration and is thus left to ponder how the originator circumvented the problems. Having spent many happy hours in trying to develop ways in which some of the methods can be implemented in a MD program it may be of some use to relate these ideas to those most likely to be interested through the pages of this newsletter. Most of the ideas applied in what follows will be familiar to anyone who has ever written a MD program but the context in which they are used may. not be. The 'new' algorithms presented for (N,V,T), (N,P,H) and (N,P,T) MD are by no means the last word and there is certainly room for improvement. They do work, however, and hopefully this article will spur others into revealing their better integration schemes.

Given below are the five algorithms which have been recently compared in a series of five MD simulations on the well worn LJ argon system close to the triple point. The results from these simulations will be presented and discussed in detail elsewhere [12].As has been found previously [7,9,10] all these methods produce essentially identical results for the thermody-

namic properties, the velocity auto-correlation function and the time dependence of the mean squared displacement. The first two algorithms contain nothing new but are included for completeness and for comparison with the three 'new' algorithms. The five MD algorithms are then:-

<u>ALG 1</u> Constant energy <u>ALG 2</u> Constant temperature, using 'ad hoc' rescaling [1] <u>ALG 3</u> Constant temperature, using the damped force method of Hoover [4] and Evans [11] <u>ALG 4</u> Constant pressure, Andersen's method [3] <u>ALG 5</u> Constant temperature and pressure, combination of damped force and Andersen's method.

and <mark>ALG 1, (N,V,E)</mark> and a back has each brack as a fill of the second state of the s

The equations of motion are integrated using the 'leapfrog' form of the Verlet algorithm [10]

 $\underline{\underline{v}_{i}}(t + \Delta t/2) = \underline{\underline{v}_{i}}(t - \Delta t/2) + \underline{\underline{P}_{i}}(t) \Delta t/m \qquad (1.1)$ $\underline{\underline{R}_{i}}(t + \Delta t) = \underline{\underline{R}_{i}}(t) + \underline{\underline{v}_{i}}(t + \Delta t/2) \Delta t \qquad (1.2)$ $\underline{\underline{v}_{i}}(t) = [\underline{\underline{v}_{i}}(t - \Delta t/2) + \underline{\underline{v}_{i}}(t + \Delta t/2)]/2 \qquad (1.3)$ where $\underline{\underline{v}_{i}}(t - \Delta t/2) = (\underline{\underline{R}_{i}}(t) - \underline{\underline{K}_{i}}(t - \Delta t))/\Delta t \qquad (1.4)$

The total internal energy U(t) is calculated from the total potential energy, $\Phi(t)$, and the temperature at time t, T(t).

ALG 2, (N,V,T) ('ad hoc' rescaling of velocities).

In this case the only modification is that velocities at the previous <u>half</u> time step are scaled, so that

$$\underline{V}_{i}(t + \Delta t/2) = \underline{V}_{i}(t - \Delta t/2)\beta + \underline{F}_{i}(t) \Delta t/m \qquad (2.1)$$
 where

$$\beta^{2} = (3(N - 1)kT_{r}/m) / \sum_{i=1}^{N} \frac{v^{2}(t - \Delta t/2)}{i}$$
(2.2)

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and T_r is the required temperature. The factor N-1 rather than N occurs in equation (2.2) as a result of the removal of three degrees of freedom by the constraint of zero total linear momentum.

ALG 3, (N,V,T) (damped force method)

This involves the integration of a modified set of Hamiltonian equations of motion [4]

$$\underline{\dot{p}}_{i} = \underline{F}_{i} - \alpha \underline{p}_{i} / \mathfrak{m} \text{ or } \underline{\dot{V}}_{i} = (\underline{F}_{i} - \alpha \underline{V}_{i}) / \mathfrak{m}$$

$$\underline{\dot{q}}_{i} = \underline{p}_{i} / \mathfrak{m} \text{ or } \underline{\dot{R}}_{i} = \underline{V}_{i} + \underline$$

(3:1):

where α is a constant. For constant temperature we require that dT/dt = 0.

Since
$$T = (m/3(N - 1)k) \sum_{i=1}^{N} \frac{v_i}{-i}$$
. $\frac{v_i}{-i}$ differentiation w.r.t. time gives

$$\hat{T} = (2\pi/3(N-1)k) \sum_{i=1}^{N} \frac{\hat{y}_i}{\hat{y}_i} \cdot \underline{y}_i$$
(3.3)

Substituting for
$$\underline{v}_i$$
 from eqn.(3.1) gives

$$\dot{\mathbf{T}} = (2\pi/3(N-1)k) \sum_{i=1}^{N} (\underline{\mathbf{F}}_{i} \cdot \underline{\mathbf{V}}_{i} - \underline{\mathbf{c}}\underline{\mathbf{V}}_{i} \cdot \underline{\mathbf{V}}_{i})/m \qquad (3.4)$$

and for $\mathbf{T} = 0$

$$\alpha = \sum_{i=1}^{N} \frac{F_{i}}{i} \cdot \frac{\nabla_{i}}{i} / \sum_{i=1}^{N} \frac{\nabla_{i}}{i} \cdot \frac{\nabla_{i}}{i}$$
(3.5)

Equation (1.1) now becomes

$$\underline{V}_{i}(t + \Delta t/2) = \underline{V}_{i}(t - \Delta t/2) + \underline{F}_{i}(t)\Delta t/m - \alpha \underline{V}_{i}(t)\Delta t/m \qquad (3.6)$$

The constant α can be found by the following procedure. Firstly, we implement the Verlet algorithm, eqn.(1.1), to obtain a projected velocity \underline{v}_i '(t) which is different from the constrained velocity \underline{v}_i (t)

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$$\underline{\mathbf{v}}_{\mathbf{i}}'(t) = \underline{\mathbf{v}}_{\mathbf{i}}(t - \Delta t/2) + \underline{\mathbf{F}}_{\mathbf{i}}(t) \Delta t/2m . \qquad (3.7)$$

Then

$$\underline{V}_{i}(t) = \underline{V}_{i}'(t) - \alpha \underline{V}_{i}(t) \Delta t / 2m = \underline{V}_{i}'(t)\beta \qquad (3.8)$$

where

$$\beta = (1 + \alpha \Delta t / 2m)^{-1} . \qquad (3.9)$$

The constant temperature condition requires $\sum_{i=1}^{N} \frac{\nabla_i^2}{i!} = 3(N-1)kT_r/m$ and since the constants α and β are ensemble properties

$$\beta^{2} = (3(N-1)kT_{r}/m) / \sum_{i=1}^{N} \frac{v_{i}}{2}(t)$$
 (3.10)

It is unnecessary to calculate α and $\underline{V}_i(t)$ explicitly since it is easily shown that eqn.(3.6) becomes

$$v_{i}(t + \Delta t/2) = \underline{v}_{i}(t - \Delta t/2) (2\beta - 1) + \beta \underline{F}_{i}(t) \Delta t/m$$
 (3.11)

Thus for the 'leapfrog' algorithm the damped force method reduces to simple scaling of the velocities and the forces at each integration step (for other algorithms this may not be the case). It does ensure that T(t) is constant at every time step whereas the method in ALG 2 only produces a mean constant temperature.

ALG 4, (N,P,H) (Andersen's method)

In the constant pressure method of Andersen [3] the Hamiltonian for the system in terms of the scaled variables

$$\underline{\mathbf{r}}_{i} = \underline{\mathbf{R}}_{i} / \mathbf{V}^{1/3} \tag{4.1}$$

$$\dot{\underline{r}}_{i} = \underline{p}_{i} / \mathfrak{m} V^{1/3} \tag{4.2}$$

can be written as [7]

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and

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$$H(\{\underline{r}\},\{\underline{\dot{r}}\},V,V) = \frac{V^{2/3}}{2} \sum_{i=1}^{N} m \, \underline{\dot{r}}_{i} \cdot \underline{\dot{r}}_{i} + \sum_{i=1}^{N} \sum_{j \ge i} \phi(r_{ij}V^{1/3}) + (1/2)MV^{2} + P_{E}V$$
(4.3)

where V is the volume of the system, M is a constant and P_E is the external pressure. The first two terms are exactly equivalent to the internal energy, U, of the particles of the system whereas terms three and four are the kinetic and potential energy associated with the change in volume. The conserved quantity is the total energy H associated with the Hamiltonian given in eqn.(4.3). The ensemble average $\langle H(t) \rangle$ differs from the enthalpy of the N-particle system by 1/2kT which is the average kinetic energy associated with the volume functions i.e. $\langle 1/2 \text{ MV}^2(t) \rangle$.

The coupled Newtonian equations of motion for this system have been given previously [7].

$$\underline{\underline{r}}_{i} = \underline{\underline{F}}_{i} / m v^{1/3} - (2/3) \underline{\underline{r}}_{i} \, \underline{\underline{V}} / v$$
(4.4)

$$\mathbf{v} = (\mathbf{P} - \mathbf{P}_{\mathbf{E}})/\mathbf{M}$$
(4.5)

P is the calculated pressure in the system and is given by

$$P = (1/3V) \left(\sum_{i=1}^{N} m(\underline{p}_{i}/m) \cdot (\underline{p}_{i}/m) + \sum_{i=1}^{N} \sum_{j>i} \underline{R}_{ij} \cdot \underline{F}_{ij} \right) \quad (4.6)$$

Where $\underline{R}_{ij} = \underline{R}_{i} - \underline{R}_{j}$ and \underline{F}_{ij} is the force on molecule i due to molecule j.

The direct application of the 'leapfrog' algorithm to integrate eqn. (4.4) is not possible because of the term involving $\underline{\dot{r}}$. However, this difficulty can be overcome by transforming the equation back into cartesian space [14]. Differentiating eqn.(4.1) w.r.t. time gives

$$\underline{\dot{r}}_{i} = (1/v^{1/2}) (\underline{\dot{R}}_{i} - \underline{R}_{i} \dot{v}/3v)$$
 (4.7)

which defines the relationship between the momentum and the velocity, since $\underline{\dot{r}}_i \nabla^{1/3} = \underline{p}_i / m$, as

$$\underline{\mathbf{p}}_{\mathbf{i}}/\mathbf{m} = \frac{\dot{\mathbf{R}}_{\mathbf{i}}}{\mathbf{R}_{\mathbf{i}}} - \underline{\mathbf{R}}_{\mathbf{i}} \dot{\mathbf{V}}/3\mathbf{V} . \tag{4.8}$$

Differentiating eqn.(4.7) w.r.t. time and substituting for \underline{r}_i and \underline{r}_i in eqn.(4.4) gives

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$$\frac{R_{i}}{R_{i}} = \frac{F_{i}}{m} + (\frac{R_{i}}{3V}) [V - (2/3) (\dot{V}/V)^{2}]$$
(4.9)

which can be integrated as we do know \underline{R}_i and \underline{R}_i at the time t.

A similar problem exists in the integration of eqn.(4.5) as strictly speaking the momenta at time t are needed to evaluate the pressure from eqn.(4.6) but these are generally calculated after eqn.(4.9) has been integrated. The procedure adopted is to evaluate the kinetic contribution to the pressure, NkT/V, using an approximation to the momenta calculated from the previous two time steps, $\underline{p}_i(t) = 2\underline{p}_i(t - \Delta t) - \underline{p}_i(t - 2\Delta t)$, and to combine this with the potential part evaluated at the present time step to obtain a pressure, P(t). The approximation used is simply the result of applying Verlet's algorithm to momenta rather than positions and ignoring the terms in Δt^2 . A test of the stability of the numerical integration of eqns.(4.5) and (4.9) using the method outlined is the constancy of the total energy, H, of the system given by the Hamiltonian, eqn.(4.3).

Prior to integrating the equations of motion of the particles the Verlet algorithm is used to obtain $V(t + \Delta t)$ and $\tilde{V}(t)$ as follows

$$V(t + \Delta t) = 2V_i(t) - V(t - \Delta t) + (P(t) - P_E)\Delta t^2/M$$
 (4.10)

$$\hat{\mathbf{v}}_{i}(t) = (\mathbf{v}(t + \Delta t) - \mathbf{v}(t - \Delta t))/2\Delta t \qquad (4.11)$$

The leapfrog algorithm for updating the velocities in ALG 4 becomes $\underline{v}_{i}(t + \Delta t/2) = \underline{v}_{i}(t - \Delta t/2) + \left[\underline{F}_{i}(t)/m + (R_{i}(t)/3V(t))(V(t) - \frac{2}{3}(\frac{\dot{V}(t)}{V(t)})^{2}\right] \Delta t \qquad (4.12)$

The remaining steps in the algorithm are as in ALG 1.

ALG 5, (N,P,T)

In ALG 5 the methods used in ALG 3 and ALG 4 are combined. Projected velocities at time t are calculated using

$$\frac{\Psi_{i}'(t) = \Psi_{i}(t - \Delta t/2)$$

$$+ \left[\frac{F_{i}(t)}{m} + (R_{i}(t)/3V(t)) [V(t) - 2\Psi^{2}(t)/3V^{2}(t)] \right] \Delta t/2$$
(5.1)

Eqn.(4.8) is then used to calculate the projected momenta at time t

$$\underline{p}_{i}'(t)/m = \underline{V}_{i}'(t) - \underline{R}_{i}(t)\dot{V}(t)/3V(t)$$
 (5.2)

and thus the scaling factor, β , from

$$\beta^{2} = (3(N - 1)kT_{r}/m) / \sum_{i=1}^{N} (\underline{p}_{i}'(t)/m)^{2}$$
(5.3)

It is then straightforward to show that the leapfrog algorithm for updating the velocities becomes

$$\underline{v}_{i}(t + \Delta t/2) = \underline{v}_{i}(t - \Delta t/2) (2\beta - 1) + [2\underline{R}_{i}(t)\dot{v}(t)/3V(t)] (1 - \beta)$$
(5.4)

+
$$\beta(\underline{F_i}(t)/m + (R_i(t)/3V(t))[V(t) - 2V^2(t)/3V^2(t)])\Delta t$$
.

It is important to note that in the constant pressure methods that the velocity of a particle is dependent upon its position since from eqn.(4.8)

$$\underline{\dot{R}}_{i} = \underline{p}_{i}/\pi + \underline{R}_{i}\dot{V}/3V .$$

So if at a particular time t the sidelength of the MD cell is L then the velocities of its images are, for the x-direction,

$$\dot{R}_{x}' = p_{x}/m + (R_{x} \pm L)\dot{V}/3V$$

 $\dot{R}_{x}' = R_{x} \pm L\dot{V}/3V$

so that

Therefore, both the position and velocity of a particle have to be altered if a boundary is crossed. It is also worth noting that the time dependence of the particle mean squared displacements, $\langle R^2 \rangle(t)$, was evaluated as

$$\langle \mathbb{R}^2 \rangle$$
(t) = $\langle \mathbb{N}^{-1} \sum_{i=1}^{\infty} \left(\int_0^t \underline{p}_i(t) / \mathfrak{m} dt \right)^2 \rangle$

so as not to include any displacements due to volume fluctuations in the constant pressure simulations, and similarly the auto-correlation function for the 'velocity' was calculated from

$$C_V(t) = M^{-2} \langle \underline{p}_i(o) \cdot \underline{p}_i(t) \rangle$$

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GRAND ENSEMBLE MONTE CARLO

David Nicholson

For some years now we have made extensive use of grand ensemble (μ , V, T,) simulations in the study of adsorbate phases.¹ This choice seems a natural one for such systems since experimental data are very often collected as isotherms οĒ surface excess versus pressure as an independent, variable. The very low pressures frequently employed in adsorption work, are of course readily calculated from . The use of this technique although by now fairly familiar, raises some questions which may be of interest to other practitioners.

The algorithm for carrying out GEMC work can be constructed in slightly different ways. Our initial method (when we also believed that we were the first to apply the technique to non-lattice systems) used a mixture of real and ghost particles with a fixed total number, in which creation or destruction steps could transfer particles from one category to the other. Subsequently we adopted the method proposed by Norman and Filinov which is more economical in the use of computer time. The decision for a creation/destruction attempt is determined by the conditions:

 $\exp(-\Delta E/kT) \ge RN$ (move)

 $\left[1 + \frac{Zy}{N} \exp(\Delta E/kT)\right]^{-1} > RN$ (destroy)

 $\left[1 + \frac{N+1}{ZV} \exp(\Delta E/kT)\right]^{-1} \ge RN$ (create)

where ΔE is the change in energy for the proposed step in the chain, Z is the activity, N the number of particles, V the volume of the box and RN a random number in the interval (0,1). The activity can be expressed in terms of the chemical potential μ

The realisation of the Markoff chain is straightforward. Each step is an attempt to MOVE, CREATE and DESTROY molecules. Under the constraint imposed by detailed balancing equal numbers of creation and destruction steps should be attempted. This leaves the programmer free to choose the fraction of trials devoted to moves out of the total numbers as well as the maximum step length as is usual for canonical ensemble simulations.

One problem which particularly vexed early work is that of applying long range corrections. Although perhaps obvious with hindsight, it did not seem apparent initially that (a chosen variable) would require any correction of this kind. However such a correction is in fact essential because density fluctuates during a run, and when incorporated, accounts for the discrepency between grand ensemble and the more tedious canonical ensemble calculations of the transition from the liquid phase in argon.^{1,3,4} Adsorbates are vapour of course ĽΟ non~ uniform so that long-range correction becomes somewhat more problematic for these, but suitable methods can be found, at least for non-polar species 5.

To highlight the use of the GEMC method it is interesting to examine some MD simulations on 2D adsorbed Ar.⁶ These of course were carried out with fixed N and snapshots for

runs clearly showed solid-like and gas-like (and less sòne clearly liquid-like) areas of co-existence. One might ask what would become of such a system if GE creation/destruction trials were switched into the system ? Clearly there would be a tendency less dense regions to fill or the more dense to empty for the until a (statistically) uniform density was achieved. The fixed number chosen in this example must in fact correspond to physically unstable state. But in that case what significance can attached to the local structure in the dense and rarefied regions ? Is the system large enough to claim that these correspond to co-existing stable states, and if so how might one go about analysing properties such as distribution functions. Clearly one recourse for getting away from manifestly unstable states in MD or canonical MC is to choose a new value for N. But it is by no means always clear, especially in dealing with systems possessing density gradients, whether a given (N,V,T) or (N, V, E) corresponds to an unstable, stable or metastable state. Indeed we have found that metastable states can continue quite happily for several million configurations in a converged, or at least apparently converged, simulation run 7.

The last observation in fact also underlines another advantage of using GEMC in that, at the expense of calculating the pressure virial, it is possible to compare free energies for two such apparently converged simulations in order to determine which is the more stable. It may be of course that the free energy minimum can only be easily reached from an initial configuration which the simulator never even dreamt of, and which

is hidden behind ergodic barriers from all those which he/she has tried.

It may be argued then that the reasons for applying the grand ensemble method to this type of investigation are very compelling. But are there disadvantages, apart from the trivial (!) one of extra programming ? One difficulty is the choice of the parameters, maximum step length, and $\alpha_{\rm CD}$, the fraction of creation or destruction trials. Criteria for these seem to be somewhat arbitrary at the best, so that the extra freedom of choice is not altogether welcome, but in many cases the freedom is less real that might appear.

It is easy to show that if α^1 is the fraction of trials accepted and α^1_M , α^1_CD that of the move and creation/destruction trials respectively, then

 $\alpha^{1} = (\alpha_{M}^{1} - \alpha_{M}^{1}) \alpha_{CD}^{1} + \alpha_{M}^{1}$ where α_{CD}^{1} is the fraction of trials which are either creation or destruction out of the total. It is possible of course to regulate α_{M}^{1} by changing the maximum step length, but α_{CD}^{1} cannot be easily regulated in a similar way. It turns out that this quantity can be quite a small fraction (.001) when there is a sharp boundary between the dense and rarefied parts of the system (e.g. for a monolayer near to completion), but higher by perhaps an order of magnitude, for multilayer simulations. For practical purposes therefore the overall acceptance fraction is :

 $\alpha^{1} \cong \alpha^{1}_{M} (1-\alpha_{CD}) \cong \alpha^{1}_{M} \alpha_{M}$

Obviously most of the creation or destruction occurs in the less dense regions, but because of the non-uniformity of the system, the variations in density gradient so caused will influence

ossible moves in the more dense regions of the adsorbate. How, can the optimum values for α^1 and α^1 be decided? Clearly systematic investigation would be very time consuming. Our own experience suggests that vastly increasing $\alpha_{\rm exp}$ does not CD significantly affect thermodyamic quantities and intuitively it would seem that a low value for $\alpha_{\rm CD}$ is preferable, since, there should be several passes for each creation/destruction in order that relaxation can occur. The extra time involved in attempting creation hore, destruction is, also a disadvantage of the the method. However this is not quite as demanding as might at first appear. the first place the rejection of a creation attempt usually Ιn occurs, because, the new particle overlaps, too, much with its neighbors - a situation which can be trapped immediately at the beginning of the CREATE subroutine.Secondly both the CREATE and DESTROY subroutines involve far fewer programming steps than the MOVE subroutine. For these reasons the computing time per configuration is substantially lower than in a canonical ensemble simulation.

Another problem, the need to reorder the indices referring to a large number of molecules after a successful destruction step, can also be circumvented. This is done by updating a vector, LOC(I) whose elements are associated with those molecules which are currently in existence. The array elements (IS say) of these molecules are obtained by running through the index I = 1,NMOL with IS = LOC (I). Detroyed molecules are placed in the section of the LOC vector not accessed in the DO loops.

Most of our work with the grand ensemble technique has been

directed towards the investigation of the rare gas/graphite adsorption system, where we have found repeatedly that apparently converged runs can be obtained on either of the branches of a transition. It is particularly frustrating to see a run phase reach apparent stability over perhaps a million or so configurations and then suddenly begin to eject particles rapidly before achieving a new plateau, and it would indeed be valuable to have new or additional techniques which could speed up the stabilization process. Force bias applied to the external field part of the potential is a promising candidate. However the very existence of this type of phenomenon lends support to the conviction that a method of this type is essential if one is to assured that simulation data for stable phases is being be The $extsf{acquired}$. The end of the end of the second problem is the second state of the second state

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MOLECULAR GRAPHICS USING THE DAP

Rod Hubbard and David Fincham

We have recently been exploring the use of the DAP in drawing realistic pictures of molecules. By 'realistic' we mean the type of picture often known as 'shaded space-filling'. An example appears in figure 1, though it is unlikely that the reproduction does full justice to the original which is a colour transparency. These pictures have the following features. The individual atoms are represented by spheres of the appropriate van der Waal's radius; and are coloured according to atom type or some other relevant criterion. The spheres are shaded as if illuminated by a point source, to give an impression of shape; full removal of hidden surfaces is carried out.

Such computer-generated pictures are replacing laborious model building as a way to display the structures obtained by crystallographic techniques. This is more than just an exercise in producing pretty pictures as, particularly for the large molecules of biochemical interest, the chemical behaviour of the molecule is very much dependent on its shape and its surface topography. The space-filling picture then becomes an important research tool in studying biochemical activity.

At present these pictures can be produced by raster-graphics terminals which are usually driven by mini-computers. However, this is a slow process. For example the insulin dimer shown in figure lewould take several minutes to draw because of the several minutes to draw because of th extensive computations involved. There are two aspects to the computations; the removal of the hidden surfaces, including the calculations of the correct intersections between the parts of the atoms that are visible, and the shading to get the effect of a illumination, involving the specification of an intensity value for each point in the picture. Typically raster pictures consist of a 512x512 array of pixels (picture elements) so there are over a quarter of a million values to be specified. The reader will begin to appreciate why the most powerful Cray computer has been sold to a Hollywood movie company! However, this is a mis-use of such a machine. For most purposes computer-generated raster pictures need no more than 8 bit data values for each pixel, allowing 256 distinct shades, and the use of a 64 bit floating-point processor to calculate them is a real case of. overkill.

The potential and suitability of the DAP in tackling this problem should be obvious to all regular readers of this Newsletter. First, it consists of a square 64 by 64 array of processing elements working in parallel, so it is possible to process 4096 pixels simultaneously. Second, the processing elements can perform arithmetic at any required precision, and the lower the precision the faster the machine goes. Our approach is the following. The complete picture of 512 by 512 pixels is divided into blocks of 64 by 64. For each block two DAP matrices are stored, an INTEGER*1 matrix of colour levels (i.e 8 bits) and an INTEGER*2 matrix of z-values, the z direction being perpendicular to the plane of the picture.

For each distinct type of atom in the picture to be displayed we pre-compute a correctly shaded sphere within a similar 64 by 64 block, but outside the main picture store. The DAP Fortran routine to do this is shown in figure 2. Each pixel is given an x and y index (with the origin at the centre of the block) and the z value of each pixel, $SQRT(R^2 - (x^2 + y^2))$, is calculated. Also for each pixel an intensity level between 0 and 15 is defined; for a sphere illuminated from the front the intensity is simply proportional to z.

To draw the picture we loop over atoms one by one. A simplified version of the code which adds an atom into the picture is shown in figure 3. A copy of the previously computed sphere of appropriate radius is simply shifted, using built-in DAP Fortran shift functions, so that it occupies the correct position ready for copying into the appropriate picture block. (Extra code is needed to handle the case where the atom overlaps boundaries between picture blocks). Both the intensities and the z values are shifted, the colour bits are added into the intensities, and the z value of the atom centre is added to the sphere values. Where the resulting z values of the atom are greater than those already existing in the picture (i.e. a part of the new atom lies in front of the picture that has been created so far), the appropriate picture intensity and z values are updated with the atom values. This simple technique determines the correct intersections between the spheres without any geometrical calculations being required.

We have indeed found that the DAP is extremely effective in producing molecular pictures. The picture of insulin shown, which has about 900 atoms, took only half a second to calculate, and this is before any attempts to optimise the program. Smaller molecules are correspondingly quicker to compute. This opens up two exciting possibilities.

First, it should be possible to produce motion pictures to study dynamical processes. Members of CCPS are mostly interested in systems of many simple molecules, and here the application would be to study collective dynamical effects of a complicated nature which it is difficult to characterise in terms of simple response functions. Another group of people who could make use of such moves are the protein chemists. It is being increasingly realised that dynamical properties are crucial to many aspects of biological function, and the production of a movie is an unparalleled aid to understanding the behaviour of a simulated model system. Very few such movies have been made to date because of the slowness of production of individual frames on conventional systems. Now that we have demonstrated the ability of the DAP to perform these calculations we are trying to obtain funding to attach a high speed graphical output and recording system to facilitate movie-making.





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Second, it is well known that ICL have plans to develop a smaller

DAP in an interactive workstation environment. This work has

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demonstrated that it should be possible to produce real-time molecular modelling systems involving both graphical display of space-filling pictures with the necessary computational back-up such as energy minimisation calculations. 28

SUBROUTINE SPHEREGEN(IRAD, SPHEREZ, SPHEREI) INTEGER*1 IRAD, SPHEREZ(,), SPHEREI(,) this subroutine generates a 64*64 pixel shaded sphere of radius IRAD REAL*3 Z(,) INTEGER*2 SQUARES(,),INDEXVEC2(),IRADSQ INTEGER INDEXVEC() LOGICAL SPHERE(,) ХVЕР°Э) C IRADSO=LENGTH(IRAD,2)**2 CALL X05SHORTINDEX(INDEXVEC,-31) INDEXVEC2=INDEXVEC**2 SQUARES=MATC(INDEXVEC2)+MATR(INDEXVEC2) SPHERE=SQUARES.LT.IRADSQ Z=0.0 Z(SPHERE)=SQRT(FLOAT(LENGTH(IRADSQ-SQUARES,3))) SPHEREI=0 SPHEREI(SPHERE)=(16.0*Z/IRAD)-0.5 SPHEREZ=Z+0.5 TRACE S(SPHEREI) RETURN END Figure 2 SUBROUTINE ADDATOM(IB, JB, MOVEX, MOVEY, ICOL, ZCENTRE , SPHEREZ, SPHEREI , PICTUREZ, PICTUREI) 1 Ź INTEGER IB, JB, MOVEX, MOVEY INTEGER*1 ICOL INTEGER*2 ZCENTRE INTEGER*1 SPHEREZ(,), SPHEREI(,) INTEGER*2 PICTUREZ(,,8,8) INTEGER*1 PICTUREI(,,8,8) 00000000 This subroutine adds at atom into the picture. Its centre is in the block (IB,JB). The previously generated sphere needs to be shifted by (MOVEX,MOVEY) pixels. This simplified version does not handle atoms going over block boundaries, nor does it handle negative shifts. INTEGER*2 TEMPZ(;)
INTEGER*1 TEMPI(;)
LOGICAL SPHERE(;);MASK(;) C SPHERE=SPHEREI.NE.0 С TEMPI=SHSC(SHEC(SPHEREI,MOVEX),MOVEY)+ICOL TEMPZ=SHSC(SHEC(SPHEREZ,MOVEX),MOVEY)+ZCENTRE C MASK=TEMPZ.GT.PICTUREZ(,,IB,JB) PICTUREZ(MASK,IB,JB)=TEMPZ PICTUREI(MASK,IB,JB)=TEMPI C RETURN END

Figure 3

THE SHEAR STRESS AUTOCORRELATION FUNCTION

ne al la seconda de la companya de la **by D.M. Heyes** de la _{la} consultar activitation de la conseconda de la cons Seconda a sugli a seconda a de la consecutión de la conseconda de la consecutaria de la seconda de la consecuta

Perhaps the most helpful way of analysing liquid state collective motion is via time correlation functions, which are used to represent the relationship between a system property with another (or the same) property at a later time. As a liquid has no long-time permanence of structure, then functions which measure system quantities at one time relative to another are therefore usually the most meaningful means of characterisation. We concentrate here on the specific example of the shear stress autocorrelation function (or SACF), [1], although the treatment is very similar for most other correlation functions. The SACF is defined by,

 $C_{XZ}(t) = \langle P_{XZ}(t) \rangle \langle P_{XZ}(t) \rangle \langle P_{XZ}(t) \rangle \langle P_{XZ}(0) \rangle 2 \rangle, \qquad (1)$

where $\langle \dots \rangle$ denotes a statistical average over time origins and where $P_{XZ}(t)$ is the xz off-diagonal component of the pressure tensor (or shear stress), which is defined at the microscopic level by,

$$P_{xz} = V^{-1} \left[\sum_{i=1}^{N} m_{i} v_{xi}v_{zi} + \sum_{i=1}^{N} x_{ij}z_{ij}F_{ij}/r_{ij} \right], (2)$$

where V is the molecular dynamics (MD) cell's volume; N is the number of molecules in the MD cell; m_i is the mass of molecule i; v_{xi} and v_{zi} are the x and z components of the velocity of molecule i; r_{ij} is the separation between molecules i and j; x_{ij} and z_{ij} are the x and z components of r_{ij} ;

$$F_{ij} = (d/dr) \phi(r_{ij}), (3)$$

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 $O(r) = 4 E ((\sigma/r) 12 - (\sigma/r) 6), (4)$

and \bigoplus (r) is the Lennard-Jones (LJ) pair potential which is used here. Any off-diagonal component of the pressure tensor (e.g., xy or yz) could be considered but here the xz component is arbitrarily chosen. In practice all three components would be considered to improve the statistical accuracy with little extra work. Here the $P_{XZ}(t)$ is evaluated at times separated by the same time interval Δt (which is written as DT in FORTRAN). Hence the times are, t =(i-1) Δt , where i ranges from 1 to NTIM, which is the number of time steps in the correlation function. The shear stress needs to be stored for up to the previous (NTIM-1) time steps in array CXZO(NTIM). I favour calculating the SACF during the MD run and not as a post-simulation calculation from catalogued $P_{XZ}(t)$ (mainly because any unnecessary dataset manipulation is frequently very time consuming in terms of human effort!). The practical details of the recommended scheme are outlined in Table 1. In this application a time origin is started every time step. The necessary programming falls into three quite distinct regions.

(a) Read in parameters and array CXZ (containing the digitised discrete unnormalised SACF) if the calculation is to be continued from a previous run. Initialise the SACF integer accumulators.

(b) Each time step multiply the current shear stress components by their previous values taken from a maximum of (NTIM-1) time steps in the immediate past.

(c) At the end of the run obtain the SACF = $C_{XZ}(T)$, where T=(I-1)*DT and DT is the time step duration, by dividing CXZ(I) by NTO (the number of time origins accumulated so far). Here I ranges from 1 to NTIM. Note that it is necessary for NR (the number of time steps performed in the present run) to be an integer multiple of NTIM - rarely a serious restriction. This avoids problems associated with normalisation. This is performed in the program by the assignment of an arbitrarily large negative integer (-5000 in the example shown

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in Table 1) into NST(IOR) for any time origins started within (NTIM-1) time steps nearest to the end of the run.

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Evaluation of the Shear Stress Autocorrelation Function (SACF):

The FORTRAN Code Appropriate to the Lennard-Jones system.

Ċ NOTE THAT ONLY THE ESSENTIAL FORTRAN CODE IS GIVEN. N IS THE NUMBER OF LJ ATOMS. С С DT IS THE TIME STEP DURATION IN LJ UNITS. RHO IS THE DENSITY IN LJ UNITS. С SG IS THE LUNISIGNA'S IN MD BOX UNITS. **C** : C CU IS THE INTERACTION TRUNCATION DISTANCE IN UNITS OF SIGMA SQUARED. С RX(I), RY(I), RZ(I) ARE THE LJ COORDINATES IN UNITS OF С THE MD CELL SIDELENGTH. С DX(I), DY(I), DZ(I) ARE THE POSITION INCREMENTS IN VERLET'S ALGORITHM. C NTIM IS THE NUMBER OF TIME STEPS IN THE ACF. C NOR INDICATES HOW MANY TIME STEPS BACK THE ACF Ç ACCUMULATORS ARE ACCESSED AT STAGES IN THE RUN. C IOR IS THE ARGUMENT OF NST(...). Ç NST(IOR) HOLDS THE TIME STEP INDICATOR IT C FOR TIME ORIGIN IOR. C NR IS THE NUMBER OF TIME STEPS THIS RUN. С THE UNNORMALISED SACF IS ACCUMULATED IN ARRAY CXZ (MTIM). Ċ PXZO (NTIM) CONTAINS THE TIME STEP SHEAR STRESS UP TO (NTIM-1) C TIME STEPS BACK IN THE PAST. С NTOT IS THE TOTAL NUMBER OF TIME STEPS FROM ALL RUNS UNTIL C THE END OF THIS RUN. C NT IS THE NUMBER OF TIME STEPS READ IN FROM THE PREVIOUS RUN. С C C SG=(RHO/FLOAT(N)) ** (1.0/3.0) SG2=SG*SG SG2I=1.0/SG2SG3≍SG2*SG CFV=1.0/(SG*DT)С THE INTERACTION TRUNCATION DISTANCE IS HALF THE MD CUBE SIDELENGTH CU=1.0/(2.0*SG)CU2=CU*CU C IF IP EQUALS 0 ZERO SACF ACCUMULATORS IF (IP.NE.0) GOTO 99 NT=0 DO 100 I=1,NTIM CXZ(I)=0.0100 CONTINUE NTO=099 CONTINUE IOR=0 II-1 NOR=0 NTOT=NI+NR С С MAIN PROGRAM STARTS HERE С 6 CONTINUE С ZERO FORCE COMPONENT ARRAYS DO 110 I=1,N FX(I) = 0.0

--4--
	FY(I)=0.0
110	FZ(I)=0.0
C	EVALUATE FORCES AND THE STRUCTURAL PART OF THE SHEAR STRESS
	$\frac{1}{120} \frac{1}{1} $
	X = PX(T) = PY(T)
	$\mathbf{z} = \mathbf{R}\mathbf{Z} (\mathbf{I}) - \mathbf{R}\mathbf{Z} (\mathbf{J})$
С	APPLY PERIODIC BOUNDARY CONDITIONS
	X=X-INT(2.0*X)
	Y=Y-INT(2.0*Y)
_	Z=Z-INT(2.0*Z)
С	EVALUATE THE SEPARATION SQUARED IN UNITS OF SIGMA SQUARED
	$RR = (X \times X + Y \times Y + Z \times Z) \times SG2$
	$\frac{1}{10} (RR. GT. GJZ) GJIO 140$
	PGT=PRT*PRT*PRT
	RI2I=R6T*R6T
	FF=(R121+R121-R61)*RR1
· .	PXZS=PXZS+X*Z*FF
	FX (I) =FX (I) +X*FF
	FY(I) = FY(I) + Y + FF
	FZ(I) = FZ(I) + 2*FF
	FX (J) = FY (J) - Y*FY F7 (J) = F7 (J) - 7*FY
140	
130	CONTINUE
120	CONTINUE
	PXZK=0.0
	DO 150 I=1,N
	FX(I) = FX(I) * 24.0 * DT * DT
	FY (1)=FY (1)*24.0*DT*DT F7 (1)=F7 (1)*24.0*DT*DT
	₽ፚ\1/~₽ፚ\1/~24•0~D1~D1 VFT.X=DX(T)+0.5*FX(T)
	VELY=DY(T)+0.5*FY(T)
	VELZ=DZ(I)+0.5*FZ(I)
	PXZK=PXZK+VELX*VELZ*CFV*CFV
С	UPDATE POSITION INCREMENTS
	DX(I) = DX(I) + FX(I)
	DY(I) = DY(I) + FY(I)
Ċ	$\frac{D^2(1) = D^2(1) + t^2(1)}{D^2(1) + t^2(1)}$
C	PX(T) = PX(T) = TMP((PX(T) = 0.5) * 2.0)
	RY(I) = RY(I) - INT((RY(I) - 0.5) * 2.0)
	RZ(I) = RZ(I) - INT((RZ(I) - 0.5) * 2.0)
150	CONTINUE
С	CALCULATE THE SHEAR STRESS IN LJ UNITS
	PXZ=SG3*SG2I*PXZS*24.0+SG3*PXZK
C	CALCULATE THE SHEAR STRESS AUTOCORRELATION FUNCTION
	LE (NOR+GE-NTER) NOR=NTER TOR=TOR+1
	IF (IOR. GT. NTTM) TOR=1
	PXZO (IOR) = PXZ
	NST(IOR)=IT
	IF (IT.GT. (NR-NTIM+1)) $NST(IOR) = -5000$

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.

IF (IT.LE. (NR-NTIM+1)) MIO=NIO+1 DO 160 IS=1,NOR JOR=TT+1-NST(IS) IF (JOR.GT.NTIM) GOTO 170 CXZ (JOR) =CXZ (JOR) +PXZO (IS) *PXZ 170 CONTINUE 160 CONTINUE . ÷ . . IT=II+1 NT=NT+1 IF (NT.LT.NIOT) GOTO 6 • • . . . AT THE END OF THE RUN: С CXZS=CXZ(1)/FLOAT(NIO) DO 180 I=1,NTIM CX21=CXZ(1)/CXZ(1)T=FLOAT(I-1)*DT WRITE(6,190)1,T,CX21 FORMAT(17,2F12.8) 190 1.80 CONTINUE STOP END

6.

RESEARCH INTERESTS OF THE MD GROUP AT ROYAL HOLLOWAY COLLEGE LINBAR AND NON-LINEAR RESPOnses OF DENSE LIQUIDS

In the modern world it is increasingly necessary to make things in the shortest possible time. This often involves applying extreme conditions to a material which, for example, could be used as an interface between other materials [1-3] or be moulded into a desired shape. To achieve the best results it is useful to understand the mechanism by which these materials respond to rapidly changing conditions. For example, the rheological properties of fluids are of particular importance to chemical and lubrication engineers who frequently encounter non-newtonian flow phenomena such as shear thinning (a decrease in shear viscosity with increasing shear rate), shear thickening (an increase in shear viscosity with increasing shear rate) and the behaviour of other non-newtonian materials, such as exhibited by the class of compounds known as Bingham plastics.

It would be interesting to discover what factors are needed in the characteristics of a molecule to produce the observed behaviour in these fields.

It has been shown [4-6] that there is a remarkable similarity between the response of many complex materials, such as glasses, lubricants at high pressure, polymer solutions and melts and those of simple model liquids to sudden changes in applied conditions. It has been revealed that even the Lennard-Jones (LJ) liquid exhibits many features in common with the above more complex materials and it is currently being used in MD to provide a mechanistic framework on which to base analytical representations of polymer, glass and pressurised-lubricant non-linear viscoelastic behaviour. Provided appropriate normalisation with respect to internally derived characteristic timescales is made, these disparate systems manifest very similar reductions in relative shear

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viscosity when shear rate increases. The effect of shear straining implemented during MD, or in an integral equation formulation, has already gone part way towards establishing the theoretical ground-rules which bring about these common features [1-6]. In particular, a coupling of shear and 'bulk' structural distortions from the equilibrium structure seems essential to account for certain fascinating viscoelastic properties.

It is hoped that such simulation and theoretical treatments will be useful in interpreting a wide variety of technologically important roles for liquids both in the linear [7-8] and non-linear regimes [1-6].

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المان معالمه في معالمة المان معالمة من كالمان الترويون المان المام الأربية المان والسعور. المان معالمة أن المان الملاقة المعالمة من معالل من المراجع ومن المان المام من المان المان المعالم والسعور. المان معالمة معالمة معالمة المان المعالمة المعالمة من المان معالمة من المان المان المان المعالمة المعالمة المعا المان معالمة معالمة المان المعالمة معالمة المعالمة من المعالمة من المان المان المان المعالمة المعالمة المعالمة

-3-38 Singer on the Root

Jack Powles

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The specialised fast square root recipe proposed by Konrad Singer (CCP5 Inf. Quart. March 1983, p.47) has, it appears, been very popular and rightly so. It is based on the least squares polynomial fit for, say four terms to square root of x from x=0.1 to 1.0,

root x = a0+x*(a1+x*(a2+x*a3)).

However the values of the ai given by Singer are wrong! The correct values are, I hope (Singer's in brackets),

a0=0.188030699 (0.1882532) a1=1.48359853 (1.428264) a2=-1.0979059 (-1.097209) a3=0.430357353 (0.430526)

The fit to root x, x=0.1,0.05,1.0, now has a rms devn. of 0.0028 (0.0333).

If users have not noticed this DO NOT PANIC.

Singer's iterations soon give the right answer to any desired accuracy, even on the CDC which gave the wrong values for the ai! However with the correct parameters at least one fewer iteration is needed, depending on your machine. Since the whole object is to make it fast this is surely worth having, so change your BLOCK DATA.

This routine is so fast it is difficult to time. It is no good, for instance using a DO loop i=1,10000, say, because the looping overheads swamp it. In fact I do not know how to do it. Maybe our kind Editor will add the answer to the end of this Note - if they still have a computer in Daresbury?

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Yes we do indeed still have a computer at Daresbury, though not alas, the Cray-1. Presently we 'make do' with the NAS AS 7000 which has replaced our departed IBM 370/165.

The problem posed by Professor Powles is not a trivial one. It is surprisingly difficult to extract accurate values for the execution times for a given routine from amongst the many operations that occur in even the simplest of jobs. Such an evaluation must inevitably be system dependent and I confess I know of no general way of obtaining an accurate one. However, in the usual hand-waving way that computational (as opposed to computer) scientists work, a rough estimate is possible.

To prevent the swamping of the square-root timing by the DO-loop overheads I have evaluated 256 double precision square-roots in the same 1000 step loop. I have also averaged the results over 10 runs, to obtain a figure less susceptible to system vagaries. The time for the execution of the corresponding 'empty loop' was similarly obtained and subtracted. The system SQRT routine averaged 4.705 seconds for 256,000 square roots. The Singer/Powles algorithm (which I call SPSQRT) averaged 5.173 seconds for the same number (assuming two cycles of the Newton-Raphson procedure).

This result is not too encouraging until one realises that it is not necessary to use the SPSQRT routine as an external function (as is the system SQRT). Inserting the relevant code in-line, at the point where the squre root is required, removes the overheads associated with an external function call. Using SPSQRT in this manner gave a result of 2.004 seconds for our 256,000 square roots. Such a substantial improvement over the system SQRT routine is not to be ignored!

On the subject of accuracy, I have compared the Singer and Powles algorithms (each assuming two cycles of the Newton-Raphson interation) with the system SQRT routine. Assuming the SQRT routine to be 100% accurate, the Singer algorithm gave an average error of -.4E-6 with a RMS deviation about this error of -.4E-6. The averages being obtained from a determination of 10,000 square roots in the range 0.1 to 1.0. The Powles algorithm was noticably better, with an average error of -.2E-9 and a RMS deviation about this error of .2E-8.

Lastly, assuming that the Powles formulation of the Singer algorithm with two here. Newton-Raphson iterations is acceptably accurate, the algorithm can be made yet more efficient if the two Newton-Raphson steps are with as an explicit formula thus:-

Y=((.430357353*X-1.0979059)*X+1.48359853)*X+.188030699

Z=.25*(Y-X/Y) + X/(Y+X/Y)where $Z = \sqrt{X}$ $Z= \sqrt{X}$ $Z= \sqrt{X}$

This algorithm then requires 1.543 seconds to evaluate our 256000 square roots.

W. Smith provide the state of t

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CCP5 Literature Survey

F. Gibb and W. Smith

The literature survey produced in this month's newsletter follows on from that printed in the March 1983 newsletter and covers the period between September 1982 and August 1983 approximately. The search was conducted on the current INSPEC file on Lockheed Dialog's Information Retrieval System at Palo Alto, California.

While retaining the original categories of published material, we have attempted to broaden the search to include more theoretical and experimental papers (as opposed to computer simulation alone). We hoped thereby to 'capture' some material mysteriously missing from our first survey. The success of this is best judged by our readers, from whom we would be delighted to receive comments. We would also gladly publish missing references in an "Addendum", to appear in the following issue of the newsletter.

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CCP5 LITERATURE SURVEY

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