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INFORMATION QUARTERLY for COMPUTER SIMULATION OF CONDENSED PHASES

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

Number 24 March 1987

Contents

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Editorial.

It is probably part of the natural cycle of things that it occasionally becomes necessary to appeal for contributions for the CCP5 Newsletter. Such is the case now. This does not however indicate that there is a diminishing interest in the newsletter itself, as rarely a day goes by when we are not asked to add more names to our mailing list. It is therefore important to remind our readers that the newsletter is very dependent on their enthusiasm if it is to keep going.

The CCP5 newsletter is an interesting publication in a number of ways: it published regularly, articles appears quickly (within three months or less), it has an international readership and it is informal enough to allow the publication of novel or speculative ideas. Added to these is the fact that there are surprisingly few publications that discuss the computational details of simulation methods warts and all. For these reasons it should be well worth supporting.

So to encourage our readership we announce that we would be pleased to receive contributions from anyone active in the field of computer simulation of condensed phases, anywhere in the world! We would also be particularly pleased to publish material from postgraduate researchers, who often have some original ideas to contribute to the computational art. We await your contributions!

In view of this appeal it is a special pleasure to thank the contributors to this months issue. Long may they prosper!

Contributors:

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General News.

a) CCP5 is to organise a meeting entitled "Industrial Applications of Computer Simulation". The meeting will take place at the Royal Institution in London from 11th. to 13th. January 1988. The purpose of the meeting is to discuss the application of the simulation methods associated with CCP5 (i.e. molecular dynamics, Monte Carlo, energy minimisation etc.) to industrially significant problems. The organisers of the meeting will be Prof. C.R.A. Catlow and Dr. N. Quirke. Readers interested in taking part in this meeting should write to: Dr. N. Quirke, B.P. Research Centre, Chertsey Road, Sunbury-on-Thames, Middlesex TW16 7LN.

Further news of this meeting will be announced later.

b) CCP5 is also to organise a meeting on the subject of bio-organic applications of computer simulation, which provisionally, is scheduled for Easter 1988. More details of this will be revealed as the organisation develops.

c) At the last meeting of the CCP5 Steering Committee which took place on 9th. January the composition of the Executive Committee was changed in accordance with the usual procedure. Professor C.R.A. Catlow was elected as the new CCP5 Chairman to replace Dr. J.H.R. Clarke. In addition Drs. R. Lynden-Bell, S. Parker and M.P. Allen were elected to the Executive Committee. The outgoing members being Drs. N. Quirke and P.A. Madden. In addition to these changes; Dr. M. Leslie has taken the responsibility of Secretary to CCP5 and Dr. W. Smith will now handle the CCP5 Program Library. The composition of the Executive Committee is thus:

Professor C.R.A. Catlow (Keele University and Daresbury)-Chairman,
Dr. M.P. Allen (Bristol University)
Dr. D.M. Heyes (Royal Holloway and Bedford New College)
Dr. M. Leslie (Daresbury) - Secretary
Dr. R. Lynden-Bell (Cambridge University)
Dr. S. Parker (Bath University)
Dr. W. Smith (Daresbury) - Program Librarian

This would seem to be the place to thank the past members of the Executive Committee for their work on behalf of the CCP5 community. In particular it is appropriate to thank Julian Clarke, under whose chairmanship for the past three years CCP5 has been extremely successful.

d) The CCP5 Executive Committee wish to announce to all U.K. participants in CCP5 that it has set aside a part of the CCP5 budget for the purpose of assisting collaborative work in the U.K. simulation community. These funds are to assist with expenses for travel between collaborating centres. So far, CCP5 has agreed to assist the following collaborating groups:
J. Clarke and D. Tildesley (Transport Properties),
S. Parker and G. Price (Lattice Simulations),
M. Allen and G. Evans (Hard Ellipsoids),
K. Singer and W. Smith (Quantum Simulations).
Other groups who wish to be considered for this assistance should write to the CCP5 Chairman, Prof. C.R.A. Catlow, Department of Chemistry, University of Keele, Keele, Staffs. ST5 5BG.

e) The CCP5 Executive Committee also wishes to remind U.K. participants that it has an annual allocation of Cray time at each of the centres: London (Cray 1s) and Rutherford (Cray XMP-48), which is available for the development of simulation programs prior to a grant allocation. At present CCP5 is allocated 15 hours a year at London and 5 hours quarterly at Rutherford. Readers who wish to use some of this allocation should write to the CCP5 Secretary, Dr. M. Leslie, TCS Division, SERC Daresbury Laboratory, Daresbury, Warrington WA4 4AD.

f) The Rutherford and Appleton Computer Centre Cray XMP/48 is now up and running. It is currently accessible to a few privileged users, who are running jobs to test the machine in a working environment before it becomes available to the wider academic community in April.

In time it is expected that the CCP5 Program Library will be modified to run on the XMP and users who would like to see any specific programs converted immediately should contact the CCP5 Program Librarian, Dr. W. Smith.

g) The University of Manchester Regional Computing Centre has described the new VM/CMS service which they will be running soon on the Amdahl 5890/300. It was originally intended to run the three domains of the Multiple Domain Facility to deal with: (i) the service currently supplied by the Amdahl 470 V/8; (ii) a national VM/CMS service and (iii) a Manchester local service. However only two domains are possible with the current hardware and so the last two services will run initially on one domain. Some disruption of the existing service is expected 20-23 March to reconnect the peripherals of the 470 V/8 to the 5890/300, followed by acceptance tests. The experimental VM/CMS service is expected to be available in early May. A useful description of the VM/CMS service appears in the March UMRCC Newsletter. An important aspect of the operation of all the national computing centres (London, Manchester and Rutherford-Appleton) will be the new Peer Review system for the allocation of computing resources. Everyone involved in scientific computing in the UK should become familiar with this. The UMRCC newletter for March 1987 and the ULCC newsletter for February 1987 both carry details of the agreed procedure and are thus recommended reading.

h) The University of London Computing Centre has now upgraded its front end computer to an Amdahl 5890. The second phase of this upgrade will involve the introduction of new disc storage devices (Amdahl 6380 disc drives, which are 3380 compatible). During this phase both 3380 and 3350 discs will be used but eventually only 3380 discs will prevail. This change will have an impact on data storage at London and users are advised to reassess their data storage habits.

i) U.K. CCP5 participants are reminded that at Daresbury Laboratory the S.E.R.C. has available an FPS 164 attached processor, currently with 3 MAX (matrix accelerator) boards, which is available for grant supported computing within the Science Board Community. U.K. research groups are invited to apply informally to Dr. J.E. Inglesfield, at Daresbury, for time on the FPS for benchmarking purposes. If the FPS proves viable for a given project, a formal application may be made. Advice on using the FPS at Daresbury may be obtained from the User Interface Group (in the person of Dr. D. Taylor) or from the CCP5 representative Dr. W. Smith. A document entitled 'Using the FPS Attached Processor at the Daresbury Laboratory' by Dr. M.F. Guest is available from the User Interface Group.

j) Concurrent Computing Initiative at Daresbury.

A new advanced research computing group has been set up at Daresbury to develop large scale computational codes for a number of scientific applications in a highly parallel computer environment. Central to this project is the recently acquired FPS-T20 hypercube, 16 powerful processors interconnected as a 4 dimensional hypercube or tesseract (hence T for tesseract and $20_8=2^4$).

Each node of the T-machine comprises an Inmos transputer, 1Mb of memory and 3 Weitek floating point chips, giving a realisable 12 Mflop performance per node on highly vectorised code. Thus the total peak performance is 192 Mflop with 160 Mflop having already been demonstrated on a distributed matrix multiply. The machine is frontended by a Micro-Vax II running Micro-VMS 4.4 and initially the T-machine is only programmable in occam. However a software release scheduled for August will provide both Fortran and C, and also move to a Unix frontend operating system.

Plans for upgrades are already in place and it is anticipated that the system will evolve to be an extremely powerful Fortran engine for both scalar and vector code. It is only by exploting the inherent parallelism of most scientific applications that one can hope for the several orders of magnitude increase in computational power required by many applications. Current supercomputers with small numbers of expensive processors sharing memory cannot realise the 1000 fold increase in power offered by highly concurrent, distributed memory architectures.

R.J.Harrison and M.F.Guest.

SERC, Daresbury Laboratory, Warrington WA4 4AD.

k) The international conference entitled 'The Impact of Supercomputers on Chemistry' is due to take place in the University of London from 13 - 16 April 1987 The conference will cover all aspects of the use of supercomputers; applications and methodology. Some of the talks that are to be given include: "Supercomputer Simulation of Solids" by M.J. Gillan, "The Impact of Quantum Monte Carlo on Chemistry" by D.M. Ceperley, "Quantum Chemistry, Statistical Mechanics and Fluid Dynamics" by E. Clementi, "Chemistry as a Many-Particle Problem" by H.J.C. Berendsen and "Protein Structure, Computer Simulation and Graphics in the Design of Novel Molecules" by T.L. Blundell.

Enquiries regarding the conference should be addressed to Dr. J. Altmann, ISOC 87 Secretariat, Room 209, University of London Computer Centre, 20 Guildford Street, London WC1N 1DZ. (Telex 8953011).

l) Readers may also be interested in the Seventh Summer School on Computing Techniques in Physics, which takes place on 9th-18th. June 1987 at Bechyne Castle near Tabor, Czechoslovakia. This year's theme is 'Microcomputers in Physics'. The organiser is Dr. J. Nadrchal, address; Summer Schools on Computational Physics, Institute of Physics, Czechoslovak Academy of Sciences, Na Slovance 2, CS-180 40 Praha 8, Czechoslovakia.

m) The Institute of Physics is organising the 1987 Solid State Physics Conference for 16-18 December at the H.H. Wills Physics Laboratory, University of Bristol and it will contain a number of symposia that will undoubtedly be of interest to participants in CCP5. Among the intended symposia are: Statistical Mechanics of Disordered and Inhomogeneous Systems; Physics of Sputtering Processes; Polymers and Liquid Crystals; Scattering of Neutrons from Disordered Systems and The Physics of Solids at High Pressures. People interested in attending or contributing a paper should contact Dr. B.L. Gyorffy or Dr. R. Rvans at the H.H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8 1TL. We will provide more information in our next newsletter.

n) It has been suggested to the CCP5 Editors that it would be useful for CCP5 participants to have a list of the EARN and BITNET addresses of other members of the project. For this purpose we would be happy to receive from our readers their addresses, which we shall collect here at Daresbury for publication in the newsletter at a later date. So that we don't fall foul of the 'Data Protection Act', it should be understood by all participants that the contributed addresses will be available to everyone.

o) The CCP5 Program Library. Documents and programs are available free of charge to academic centres upon application to Dr. W. Smith, TCS Division, S.E.R.C. Daresbury Laboratory, Daresbury, Warrington WA4 4AD, U.K. Daresbury Laboratory. Listings of programs are available if required but it is recommended that magnetic tapes (to be supplied by the applicant) be used. It may also be possible to transfer a small number of programs over the JANET network to other computer centres in the U.K.. Please note that use of inappropriate packing for magnetic tapes (e.g. padded bags) may result in them being considered unusable by Daresbury Computing Division and returned without the required software. Please ensure that these forms of packaging are not used. A list of programs available is presented in the following pages.

We should also like to remind our readers that we would welcome contributions to the Program Library. The Library exists to provide support for the research efforts of everyone active in computer simulation and to this end we are always pleased to extend the range of software available. If any of our readers have any programs they would like to make available, please would they contact Dr. Smith.

THE CCP5 PROGRAM LIBRARY

MDATOM by S. M. Thompson. M.D. simulation of monatomic fluids.

HMDIAT by S. M. Thompson. M.D. simulation of homonuclear diatomic fluids.

MDLIN by S. M. Thompson. M.D. simulation of linear molecules.

MDLINQ by S. M. Thompson. M.D. simulation of linear molecules with quadrupole.

MDTETRA by S. M. Thompson. M.D. simulation of tetrahedral molecules.

MDPOLY by S. M. Thompson. M.D. simulation of polyatomic molecule fluids.

ADMIXT by W. Smith. M.D. simulation of monatomic molecule mixtures.

MDNACL by W. Smith. M.D. simulation of alkalai halide salts.

MDMIXT by W. Smith. M.D. simulation of polyatomic molecule mixtures.

MDMULP by W. Smith. M.D. simulation of polyatomic molecule mixtures.

MDMPOL by W. Smith & D. Fincham. M.D. simulation of polyatomic molecule mixtures.

MDZOID by W. Smith & K. Singer. M.D. simulation of ellipsoidal gaussian molecules.

DENCOR by W. Smith. Calculation of density correlation functions.

CURDEN by W. Smith. Calculation of current density correlation functions.

HLJ1 by D. M. Heyes. M.D. simulation of atomic fluids.

HLJ2 by D. M. Heyes. M.D. simulation of atomic fluids (with VACF).

HLJ3 by D. M. Heyes. M.D. simulation of atomic fluids (link-cells).

HLJ4 by D. M. Heyes. M.D. simulation of atomic fluids (constant T or P).

HLJ5 by D. M. Heyes. M.D. simulation of atomic fluids (shifted force).

HLJ6 by D. M. Heyes. M.D. simulation of atomic fluids (Toxvaerd algorithm).

MCRPM by D. M. Heyes. M.C. simulation of electrolytes (restricted primitive model).

SURF by D. M. Heyes. M.D. simulation of model alkalai halide lamina.

HSTOCH by W. F. van Gunsteren & D. M. Heyes. MD or SD simulation of molecules in vacuo or rectangular cell with solvent or lattice.

MDATOM by D. Fincham. M.D. simulation of atomic fluids.

MDDIAT by D. Fincham. M.D. simulation of diatomic molecule fluids.

MDDIATQ by D. Fincham. M.D. simulation of diatomic fluids.

MDIONS by D. Fincham & N. Anastasiou. M.D. simulation of electrolytes.

MDMANY by D. Fincham & W. Smith. Simulation of rigid polyatomic molecules with/without fractional charges.

CARLOS by B. Jonsson & S. Romano. M.C. simulation of a polyatomic solute molecule in an aqueous cluster.

MCN by N. Corbin. M.C. simulation of atomic fluids (Metropolis).

SCN by N. Corbin. M.C. simulation of atomic fluids (Rossky, Friedman and Doll).

STATIC SIMULATION CODES

CASCADE by M. Leslie and W. Smith. Calculates the structure and energy of a defect in an ionic crystal for a given potential model.

THBREL Determines the minimum energy configuration of a perfect lattice for a given potential.

THBFIT Empirically fits a potential to experimentally observed properties of a perfect lattice.

SYMLAT Determines the minimum energy configuration of a perfect lattice for a given potential.

THBPHON Calculates phonon dispersion curves for ionic crystals with three-body terms in the potential.

University of London

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ext. 3401

DEPARTMENT OF CHEMISTRY
The Bourne Laboratory

Dr. D.M. Heyes

10th March 1987

Dear Colleague,

At the 5th March 1987 CCP5 executive committee meeting it was decided to look into the possibility of holding a CCP5 sponsored workshop on " Transport Processes ".

I am writing to you to discover if you would be interested in attending such a meeting and if so the directions you would like it to take. An obvious area would be equilibrium and non-equilibrium MD routes to viscosity, self-diffusion and thermal conductivity of fluids. Transport in solids and algorithms for performing the molecular dynamics are other areas of interest. We would appreciate your opinions on this matter, and also on the months in this year most suitable to you.

Best wishes,

Yours sincerely,

David Heyes

MEETING ANNOUNCEMENT:

THERMODYNAMICS AND STATISTICAL MECHANICS OF SMALL SYSTEMS

A meeting is being organised by the Royal Society of Chemistry Statistical Mechanics and Thermodynamics Group at the University of York on September 24-25 1987.

The topics for discussion include small system behaviour in porous media and as crystallites, clusters and micelles. Both theoretical and experimental aspects will be discussed and contributions are invited.

The speakers include Dr. R.J. Evans (Bristol), Prof. D.H. Everett (Bristol) and Prof. J.S. Rowlinson (Oxford).

Please contact Dr. J.H.R. Clarke, Department of Chemistry, U.M.I.S.T., Sackville Street, Manchester M60 1QD as soon as possible for details.

P.G. Francis

REVIEW OF THE CCP5 MEETING ON 'NEW HORIZONS IN THE COMPUTER SIMULATION OF CONDENSED PHASES' HELD AT UMIST 8 - 9 JANUARY 1987.

W. Smith

As the title of the meeting suggests, the latest CCP5 meeting was a forward looking affair, which was intended to highlight areas of computer simulation which seem likely to open new avenues of enquiry. The meeting was organised by the departing CCP5 Chairman, Dr. J.H.R. Clarke, with the assistance of his colleagues at the Department of Chemistry and was attended by seventy simulation scientists from the United Kingdom, Europe and North America. As is always the case with CCP5 meetings, many interesting questions were raised and Dr. Clarke wisely allowed sufficient time for discussion. As a result it was generally held to be a stimulating and informative meeting.

The first contributor to the meeting was Prof. W.L. Jorgensen (Purdue University), who spoke on the subject of computer simulations of organic reactions. The objective of this work was the determination of the rates of organic reactions from first principles. Prof. Jorgensen first considered the S_{N2} reaction beloved of organic chemists, in particular, the reaction between chloromethane CH_3Cl and chloride anion Cl^-. S_{N2} reactions are bimolecular and sterospecific, they do not have intermediates and have an activation energy that increases with the polarity of the solvent. Prof. Jorgensen's approach involved the calculation of the gas phase potential reaction surface followed by its modification to include solute-solvent effects and finally a simulation of the reaction along a suitable reaction coordinate. The first step was achieved through ab initio methods; calculating the energy of the transition state (i.e. the $[Cl.....CH_3.....Cl]^-$ complex) over the reaction coordinate. The solute-solvent interactions were determined by the ab initio calculation of clusters of solvent molecules with the reactive species. The purpose of the simulation (by Monte Carlo method) was to determine the density function $g(r_c)$ giving the probability of the reacting species being at a separation r_c on the reaction coordinate. From this the 'reaction force' $w(r_c)=-kT\ ln(g(r_c))$ could be obtained. The simulation involved the reacting system plus 250 'TIP4P' water molecules within a periodic system. The MC procedure required the simulation to be done for several overlapping 'windows' of the reaction coordinate, using a biasing technique to sample each window adequately. The final set of overlapping windows gave the full $g(r_c)$ function. The NTP ensemble required 1-2M equilibration steps and 2-6M steps averaging for each window. In the simulation the potential functions used were Lennard-Jones 12-6 functions with fractional charges to represent the Coulombic forces. However the parameters were described as functions of the reaction coordinate, fitted to the ab inito calculations.

The results for the example reaction showed that the relatively complicated energy barrier of the gas phase reaction was replaced by a single, higher peak in aqueous solution. These results tally with experimental observations, which show the gas reaction to be much faster, and that the solvated reaction has no intermediates. Interestingly, in the less polar solvent DMF, the energy barrier showed more structure, particularly the occurrence of minima suggestive of intermediates. (This latter suggestion has some experimental NMR evidence in its favour.) Calculations of the energy and number distributions showed that the number of solvating water molecules about the reacting species is constant throughout the reaction, contrary to expectations. The relative reduction of the solvation energy of the transition state (a factor contributing to the energy barrier increase) is due to a weakening of the solute-solvent bonding, not to the expected reduction in solvent coordination numbers. Further calculations using thermodynamic perturbation theory indicate that the structure of the transition state in gas and solvent is very similar.

Prof. Jorgensen concluded with a study of the S_N1 reaction of t-butyl chloride with Cl^- and showed that the formation of a contact ion pair $[t\text{-}Bu]^+.Cl^-$ was clearly apparent, but the evidence for a solvent separated ion pair was much less clear. Throughout his talk Prof. Jorgensen presented excellent graphics revealing the stereochemical aspects of the reactions being described.

Dr. S. Toxvaerd (Panum Institute) described his studies in the implementation of the Generalised Langevin Equation (GLE). He was was concerned to show how the GLE could be used to simulate the system of a polymer in solution for the fraction of the cost of a full molecular dynamics simulation but with comparable accuracy. The system he considered was a nonomer consisting of Lennard-Jones atoms bound by harmonic forces and suspended in a solution with 509 Lennard-Jones atoms. Following the work of Bossis, Quentrec and Boon, the GLE for this system is is written as:

$$m d\underline{v}_i(t)/dt = -m\int dt' M_i(t-t')\underline{v}_i(t') + \underline{r}_i + \underline{e}_i(t)$$

where $\underline{v}_i$ is the velocity of the i'th. bead, $\underline{r}_i$ the stochastic force, $\underline{e}_i$ the bead-bead forces on bead i, and $M_i(t)$ the memory function. The division of the forces into stochastic and bead-bead contributions is only valid if the correlation function $\langle \underline{v}_i . \underline{r}_i \rangle$ is zero throughout. Dr. Toxvaerd has checked this using simulation and has established that it is true except at short times, where small deviations occur.

Once the memory functions M_i are known, the GLE can be solved numerically and Dr. Toxvaerd described his procedure for obtaining them. The memory function for the whole system is replaced by a Mori expansion. These terms cannot in general be resolved into intramolecular and solvent contributions, with the exception of the first term K_1. Nevertheless the higher terms can be calculated by molecular dynamics via the time derivatives of the velocities. Explicit consideration of the first two terms of the Mori expansion; comparison of the values for the pure solvent with values obtained for the polymer solution allows physically reasonable approximations to the memory functions M_i to be made. The memory functions are then written as:

$$M_i(t) = K_{1,i}(s,t)\exp(-K_2 t^2/2)$$

In which $K_{1,i}(s,t)$ is the instantaneous value of the solvent dependent part of K_1 (which is dependent on the bead number i) and K_2 is the second Mori coefficient for the pure solvent. This approximation has been implemented in a simulation program using the Fourier method of Wang and Uhlenbeck and the results have been compared with molecular dynamics and a simpler Langevin Equation (LE) simulation.

The results show that small differences arise between the MD and the GLE and LE simulations of the bead-bead bondlength distribution, but the bead velocity autocorrelation functions are well reproduced. The approximate GLE method was shown to give essentially exact results for the centre of mass diffusion. Studies of the end-to-end distance R^2 and the radius of gyration S^2 and the corresponding correlation functions showed that very long runs are necessary for good statistics (prohibitively for the MD simulations) and about 10^6 timesteps are required for the molecule to establish the mean shape. Within the limitations on the studies occasioned by these difficulties, the MD and stochastic dynamics results were good. A study of the effects of the solvent on the molecular conformation was undertaken, by means of a comparison with a 'free molecule' simulation of the nonomer. For the state points studied, the molecule was rather globular, and no great effects of the solvent were seen. It was concluded that the GLE method described was a very useful method for studying polymers in solution.

Dr. D. Rapaport (Bar-Ilan University) spoke on the new subject of microscale hydrodynamics, by means of which he has successfully simulated some of the macroscopic features of fluid flow. He began by describing the kinds of phenomena seen in real flow experiments, such as fluid flow past a stationary object. At low flow rates (low Reynolds number) the flow is laminar (Stokes flow). As the flow inreases stationary eddies form. At yet higher rates the eddies become unstable and move away from the object (vortex shedding) and give rise to a wake pattern known as the vortex or von Karman street. At very high flow rates turbulence results.

Dr. Rapaport described how he had simulated many of these features in a molecular dynamics simulation on the parallel assembly of FPS attached processors at IBM, Kingston, New York. The simulation was of two-dimensional flow past a fixed cylinder of 25 nm diameter. The fluid consisted of 170,000 'soft sphere' molecules in a 150 nm wide system with periodic boundaries. A fluid density of 0.83 and a flow speed of 330 m/s was used. A force field of 10^{11}g was employed to drive the flow and rethermalisation of the molecules at the down-field boundary was used to maintain the periodic conditions. The entire simulation cell was partitioned into 'slabs' to permit efficient parallelisation of the system and reduce data communication between processors to a minimum. The resulting flow pattern was presented graphically. The simulation cell was partitioned into a 60x60 grid and a short time average of the particle velocities in each sub-cell was calculated at intervals of 5 timesteps. The average velocity vector for each sub-cell was then plotted as a field of flow. Approximately 100 hours of CPU time were required on a system of four FPS 264 processors in parallel.

The results showed clearly the development of the different regimes of flow behaviour described above i.e. laminar flow, eddy formation, incipient instability of the eddies and vortex shedding and finally the von Karman street. The method clearly has great potential in elucidating the microscopic features that underlie the continuum behaviour of fluids in flow. Dr. Rapaport concluded by discussing the limitations of the method (short times, small spatial scales and subsonic velocities) and possible extensions of the method to three dimensional simulations.

Dr. M.P. Allen (University of Bristol) described his work done in a collaboration with D. Frenkel (Utrecht) on the molecular dynamics simulation of the isotropic to nematic phase transition in a system of hard ellipsiods. (The phase diagram for this system had been obtained previously by Frenkel and Mulder.) Dr Allen described the technique by which the hard ellipsoid system was simulated. (A detailed description of this appears in CCP5 Info. Quart. No. 23 p.28.) In practice the system simulated consisted of 144 ellipsoids and generated 10^6 collisions per hour on a CYBER 205 computer. The ellipsoids studied had axial ratios (a/b) of 2 and 3. The objective was to calculate single and collective time-dependent orientational correlation functions in the region of the isotropic-nematic phase transition and deduce the values of parameters important in the DeGennes and Keyes/Kivelson theories.

The single particle correlation functions were defined as:

$$c_L^s(t) = < P_L(\underline{e}_i(0)\cdot\underline{e}_i(t) >$$

and the collective correlations functions as:

$$c_L^c(t) = \Sigma_j < P_L(\underline{e}_i(0)\cdot\underline{e}_j(t)) > / \Sigma_j < P_L(\underline{e}_i(0)\cdot\underline{e}_j(0)) >$$

in which P_L is a Legendre polynomial of order L and $\underline{e}_i$ is a unit vector aligned along the major axis of the ellipsoid. These functions were calculated for L=1 and 2 at various densities. The functions showed exponential decay at long times in the expected manner. The characteristic decay times τ for the collective correlation functions were significantly longer than the decay times for the single particle correlations, particularly near nematic-isotropic phase transition. The behaviour of the ratio $\tau_2{}^s/\tau_2{}^c$ was shown in a plot against density and revealed a critical slowing down effect at the transition for the axial ratio 3. This slowing down was interpreted using the Kivelson expression:

$$\tau_2{}^s/\tau_2{}^c = (1+j_2)/(1+g_2)$$

where g_2 is the static second-rank Kirkwood factor and j_2 is a dynamical quantity that is describable in terms of the orientational memory functions. Calculations of the factor $(1+g_2)^{-1}$ for different densities allowed the above equation to be used to calculate j_2, which was found to be insensitive to the density. The calculated mean values were given as $1+j_2=0.74+/-0.16$ (a/b=2) and $1+j_2=0.92+/-0.05$ (a/b=3). These results find experimental evidence in their favour from the work of Flygare et al. on p - methoxy - benzylidene - n - butylaniline (MBBA), which provided an estimate of $1+j_2$ of the order 0.7 and also supported the mean field predictions of DeGennes that g_2 diverges at the critcal density. Further systematic investigations of these and related systems are planned.

Dr. D. Tildesley (University of Southampton) described the method he has devised with his collaborators M.R. Stapleton (Southampton) and N. Quirke (BP Sunbury-on-Thames) for simulating variable polydispersed liquids which he defined as systems in which the dispersed particles (micelles) change size when the density of the system changes. The systems examined were the hard-sphere system and a modified Lennard-Jones system, in both of which every particle possessed a different effective diameter (i.e. $\sigma_{eff} = (\sigma_i+\sigma_j)/2$). The simulation method was a modified Monte Carlo algorithm in which the sizes of the particles as well as their locations were changed as the simulation proceeded. The sampling of the particle sizes at each MC move was taken from an appropriate particle size distribution function, which in this case was the Shultz function:

$$f_z(\sigma) = z!^{-1}((z+1)/\sigma)^{z+1}\,\sigma^z\,\exp(-((z+1)/\sigma)\sigma) \text{ if } [a<\sigma<b]$$

$$= 0 \text{ otherwise}$$

Where z is a parameter controlling the form of the function. (The distribution function changes with density and temperature for the LJ fluid.) A move was accepted or rejected according to the change in the inter-micellar interaction energy resulting from the move. Special care was needed for the long range corrections. Applications of this method to hard spheres showed that as the number density of the particles increases, they tend to become smaller, while for Lennard-Jones particles there is an initial average increase in the particle diameters followed by a decrease at higher densities. The initial increase was thought to be due to the attractive component of the LJ potential, which encourgaged particles to approach, but this effect was outweighed by repulsive component when the density of the particles was high.

For fluids in which the distribution function is symmetric an adequate description is possible using a monodispersed fluid with the appropriate packing fraction, which is a function of the density and the third moment of the equilibrium distribution of diameters; M_3. A mean field theory for M_3 has been developed in collaboration with Dr. T. Sluckin (Southampton). The chemical potential distributions of the hard sphere polydispersed fluids were calculated by means of Widom's particle insertion method with lattices of different particle sizes. The scaled particle theory of Salacuse and Stell gave good agreement with the simulated chemical potential obtained with both low density distribution functions.

The second day began with a talk by Dr. D. Price on the computer simulation of minerals important in the understanding of geological processes. The minerals of greatest significance being silicates. It is extremely important that the properties of these materials be fully understood before realistic models of geological processes such as plate techtonics can be developed. The problem however is that these materials most commonly exist in regions of high pressure and temperature in the earth's core and is is not practicable to perform suitable experiments in the laboratory. (Perovskite, a high pressure phase of magnesium silicate, for example is thought to constitute 40 percent of the earth by volume, but it is still very little understood). Computer simulation is therefore an essential tool for investigating such materials. The simulations need to provide information on several properties of the minerals to assist the geologist; the equation of state, (P vs. T) phase diagram, bulk and shear moduli, rheological properties and diffusion processes among them.

A number of methods are available for modelling these systems: (i) the ab initio Hartree-Fock method employing periodic boundaries (accurate but limited to small systems); (ii) ab initio calculations on SiO clusters to obtain the potential energy surfaces (good for some properties, though there is a loss in accuracy resulting from harmonic fitting of the surfaces); (iii) modified electron gas potentials with fitting of the potential surface using empirical (e.g. Buckingam) potentials (poor estimates of the elastic constants result) and (iv) The ionic model using fitted empirical potentials, plus coulombic interactions and the shell model (massless charged shell coupled to ion core by harmonic spring) to account for polarisability. The whole periodic crystal structure is modelled. To offset the effects of covalency non integer charges and bond bending forces are sometimes used.

Of the four methods described only the last is presently useful for providing geological data. The method is employed in the large lattice simulation programs CASCADE, THBREL and THBPHON and give excellent crystal structure data and elasticity constants (e.g. the predicted structures of olivine, spinel and ilmenite are very good).

Phonon data are also available and allow the calculation of heat capacity, Gruneisen parameters, thermal expansion, entropy and defect entropies. Also the phonon spectrum has been found to be in close agreement with infra red and Raman frequencies. The eigenvectors provide details of the vibrational motions of the ions which is not easily available from experiments. The calculations of the entropies and heat capacities have been found to be very accurate. Thermal expansion coefficients and the phase diagrams of minerals have been obtained by this method and compare fairly well with experimental data. Lastly, defect energy calculations, using the CASCADE program, have allowed reasonable estimates of the diffusion rates of ions.

In the future Dr. Price expects to see the ionic model being used successfully to determine unknown phases and the incorporation of better three-body forces such as the Axilrod-Teller type. It is also expected that ab initio and modified electron gas potentials will be sufficiently advanced to assist with this type of work.

Dr. R. Lynden-Bell (University of Cambridge) delivered a talk on the subject of phase transitions and the fluctuations in orientationally disordered crystals. Dr. Lynden-Bell has used molecular dynamics to study these phenomena in a variety of systems; CH_4, CBr_4, CCl_4, $Na^+.CN^-$, tBuBr and SF_6. The value of the molecular dynamics approach is that it complements existing experimental and theoretical methods and naturally introduces the effects of temperature and entropy. The theory of ordering studied by Dr. Lynden-Bell is the Landau theory, in which the free energy of a system is given by the expression:

$$G = G_o + a(T-T_c)Y^2 + cY^4$$

In which Y is the 'order parameter'. This function has a single minimum for temperatures $T>T_c$ (indicating a stable, orderered phase) a very broad minimum when $T=T_c$ (indicating incipent instability) and a double minimum when $T<T_c$ (indicating a new preferential ordering). The order parameter Y is itself a function of the orientation of the molecules and is an irreducible representation of the space group of the crystal. Its spatial Fourier transform is represented by:

$$Y(\underline{k}) = \Sigma_i^{mol}\exp(i\underline{k}.\underline{r}_i^{eq})\ K_{\Gamma M}^{L}(\Omega_i)$$

In which the function $K_{\Gamma M}^{L}(\Omega_i$ is a combination of spherical harmonics (e.g. Kubic harmonics) appropriate to the crystal symmetry. The index L indicates the type of ordering; thus

L=1 implies dipolar ordering, L=2 quadrupolar ordering and L=3 octupolar ordering. Fluctuations in the order parameter Y (i.e $\langle Y^2 \rangle$) are largest when a change in phase is incipient and plots of $\langle Y^2 \rangle$ vs. k vector provide information on the crystallographic features of the transition e.g. a peak at k=0 (Γ point) indicates no change in the number of molecules in the unit cell, at k=zone boundary implies a doubling (or similar) in the unit cell and at intermediate k values, an incommensurate phase is expected.

Dr. Lynden-Bell illustrated these principles with examples of the orientational properties of sodium nitrite and nitrogen on graphite. The concluding example was an investigation of tertiary butyl bromide (tBuBr) to determine whether the ordering was dipolar (L=1) or octupolar (L=3); the former indicating the dominance of the molecular dipole in the crystal structure and the latter the dominance of the tetrahedral geometry of the molecule. A comparison of the $\langle Y^2 \rangle$ vs. k plots of these two alternatives with the corresponding plots of CBr_4, showed the closer resemblance to the octupolar case.

Prof. C.R.A. Catlow (University of Keele / Daresbury) described the investigation of the structure and conductivity of β alumina. Two forms of β alumina exist; the stoichiometric form $Na_2O.11Al_2O_3$ and the non-stoichiometric form $(Na_2O)._{1.3}11Al_2O_3$. The believed structures are complex spinel blocks in which the sodium atoms occur in layers at alternate hexagonal sites (the so-called Beevers-Ross (BR) sites). The sodium ions are mobile in these layers and give rise to conductivity. The non-stoichiometric sodium ions reside in bridging locations between oxygen ions. The structures were investigated both by static lattice methods (which used a shell model for the ions) and by molecular dynamics (which used a rigid ion model and the Ewald sum to handle the long range forces). The objectives were to determine the role of non-stoichiometry in conduction, the migration mechanism, the structure of the conduction plane and the temperature dependence of the conduction.

The static lattice calculations were performed with the CASCADE program and showed that the interstitial sodium ions occupied the 'anti- Beevers-Ross' sites and that the conduction path for the sodium ions was different in the non-stoichiometric and stoichiometric cases. The molecular dynamics were performed with the program FUNGUS, which was adapted for the parallel assembly of FPS processors at Kingston N.Y.. The simulations used 500 ions per MD cell; the stoichiometric case possessing 24 Na^+ ions. The non-stoichiometric cases had 4 and 8 more Na^+ ions (plus compensating O^{2-} ions) respectively.

The stoichiometric cases showed the sodium ions to be at the BR sites but NO diffusion (i.e. conductivity) was evident in the temperature region 600K to 900K, though the Na^+ ions showed large thermal parameters. The non-stoichiometric ($+4Na^+$) case showed signs of diffusion at 600K and definite diffusion at 900K. The interstitial sodium ions occupied anti-BR sites with some displacement due to strong interaction with the excess O^{2-} ions. There was some evidence of conduction paths. Surprisingly, the non-stoichiometric ($+8Na^+$) case showed significantly less diffusion and extensive interactions between the excess sodium and oxygen ions. The excess sodium ions were displaced towards the mid O-O bridge.

The conclusions of this work were that the stoichiometric β alumina is not a sodium ion conductor, while in the highly non-stoichiometric form conduction is surpressed. In the low non-stoichiometric form the excess sodium ions occupy anti-BR sites, but are displaced towards the oxygens at higher non-stoichiometry. Conduction by the sodium ions appears to involve distinct pathways.

The session on the quantum mechanical methods of simulation began with a talk by Dr. M. Gillan (Harwell) on the Path Integral Monte Carlo (PIMC) method, which is a method for simulating quantum systems at nonzero temperatures and has its origins in the path integral formulation of quantum mechanics due to Feynmann. Beginning with the one dimensional, single particle case, Dr. Gillan explained the derivation of the method. At the core of the method is the mathematical function known as the density matrix, in terms of which the partition function of a system and the mean value of any static (equilibrium) observable quantity may be calculated. The form of the density matrix is:

$$\rho(x,x';\beta) = \Sigma_n \; \varphi^*_n(x) \; \exp(-\beta E_n) \; \varphi_n(x')$$

which closely resembles the Green's function or propagator used in the path integral formulation of Feynman. This means that a substitution of the time variable by $i\beta h/2\pi$ permits the formal use of the path integral method to calculate the partition function for the system of interest. In reality the density function has only been derived for two cases; the free particle and the harmonic potential, and no analytical solution is known for complex potentials or many-body systems. However Feynman's formalism allows the partitioning of a given path integral into shorter paths over the span of which the harmonic potential may be used as a good approximation. (This is the so-called short-time approximation.) If this strategy is adopted, it emerges that the resultant expression for the partition function is formally equivalent to that of a classical model ring polymer in which the atoms are coupled by harmonic springs with a force constant of $2mP(\pi)^2/(h\beta)^2$ and each atom is in a potential field of strength V/P, where P is the number of atoms in the ring and V is the potential in the original Hamiltonian.

The physical significance of the polymer is that collectively it represents the delocalisation of the parent particle in agreement with the Uncertainty Principle. The effective reduction of the potential energy by the factor 1/P is what enables the parent particle to tunnel into classically forbidden regions. The spring constant is largest when the temperature or the mass of the parent particle is large. This means that the ring polymer reduces in extent (i.e. reduced delocalisation) under these circumstances, which comply with the classical limit. Generalisation of the method to many dimensions and many particles is easily accomplished (but may be computationally expensive).

Simulations using this method require only that some realistic way of generating the configurations of the isomorphic polymer be available. Either molecular dynamics, Monte Carlo or stochastic dynamics methods may be employed. (No significance should be attached to the time dependent aspects of MD and SD.) Dr. Gillan prefers the stochastic method over MD since it avoids the problems of ergodicity encountered in MD when the spring constants are large. Dr. Gillan gave a number of examples of the application of the method and concluded with his own work on the dissolution of hydrogen in metals in which he has been able to reproduce many of the observed features of these remarkable systems.

Dr. B.H. Wells (University of Oxford) continued the quantum mechanical theme in a talk on the new developments that have taken place in the Green's Function Monte Carlo method. Dr. Wells began by describing the two basic methods currently in use; the Variational Monte Carlo and Diffusion Monte Carlo methods. Both are methods for dealing with the electronic wavefunctions of molecular systems. The Variational method is used to calculate the energy of a system from a known wavefunction. In the method an inital set of electron positions are moved using a gaussian propagator and the moves accepted according to a probability based on the square of the wavefunction. The so-called local energy $E_L(\underline{r}')$ is calculated and accumulated at each step, following an equilibration period. In Diffusion Monte Carlo the wavefunction itself is calculated, starting from an initial trial wavefunction. In this method the gaussian propagation is augmented by an exponential branching term, for which a trial state energy is required and is updated as the simulation proceeds. Excited states can be calculated provided the initial wavefunction possesses the correct symmetry. The standard method uses the 'fixed node' approximation, which requires the nodes of the wavefunction to be accurately known. This knowledge prevents negative configuration densities arising in the sampling procedure . Configurations which cross a node boundary in the course of the calculation are deleted. but provided the trial energy is close to the actual state energy, the population of configurations will be maintained. The method has been successfully applied calculations of the correlation energy in small molecules.

Among the advances in the methods that have been taking place recently are the removal of the short-time approximation in the Green's function propagator, the removal of the 'fixed-node' constraint and the development of the differential Monte Carlo method to enable calculations of physical quantities, such as the molecular dipole, which depend on small energy differences. (The essential feature of the latter method is the calculation of two distinct systems, one the minor perturbation of the other, using the same random walk to reduce the variances of the calculated property.) Example applications of the methods described by Dr. Wells included the $e_2^+e^-$ bound system, e^-H^+ systems at a dielectric surface (for both of which good binding energies were obtained) and the calculations of H_3^+ and H_5^+ systems with and without the Born-Oppenheimer approximation.

The final speaker of the meeting was Dr. D. Fincham (University of York) who provided an overview of the current developments in parallel computing. He began by defining the concept of a parallel computer, which is a computer possessing more than one processing unit, all or some of which could be active simultaneously under the direction of the user's program. Parallel computers may be SIMD (Single Instruction Multiple Datastream) or MIMD (Multiple Instruction Multiple Datastream) machines.

There are currently three main architectures for parallel computers. The first of these is the mainframe which has a small number of processors with shared memory (e.g. Cray XMP/48). The second is the switching network, in which there are separate processors and interconnected memories (e.g. ULTRA). In the third architecture, the processors are connected but have their own memory boards. An important feature of all parallel computers is the topology of the connections between processing units, Dr. Fincham gave four examples; the square array (e.g. ICL DAP), the hypercube (e.g. INTEL hypercube), the pyramid (devised by the University of Erlangen) and the Waterloop Ring. Each of these topologies has its own features and advantages e.g. the hypercube, which possesses 2^n nodes with n connections to each, has other connectivities as subsets of this, and these can be exploited in specific applications such as the periodic boundary.

A recent significant development in the parallel computing concept has been the introduction of the TRANSPUTER, which is a high performance microprocessor which has been specifically designed to be linked to other TRANSPUTERS so creating a parallel processor. Each processor is itself a complete computer, which will soon acquire a hardware floating point unit (currently floating point arithmetic is handled by software). By way of an example application Dr. Fincham described a molecular dynamics application of the TRANSPUTER, that was suitable for simulating biological molecules. Other recent significant developments are: the INTEL iPSC and iPSC/VX computers which have the hypercube topology and up to 128 processors; the FPS T series, which has hypercube topology and vector processors at each node; the ICL Mini-DAP, a SIMD machine, and the Reconfigurable Processor Array (RPA) at Southampton, in which the processing elements can be dynamically configured to suit the application.

Dr. Fincham concluded with a few comments on the (unlikely) transportability of parallel codes and the commercial pressures likely to encourage the development of larger machines with fewer processors instead of smaller multi-processor machines.

Throughout the meeting a number of poster displays were on view. These included:

"Dynamical Simulation of a Model Reverse Micelle", by D. Brown and J.H.R. Clarke.
"Simulated Annealing of Atomic Clusters", by L.T. Wille.
"Computer Simulation of Plasticity in Minerals", by M. Heggie, R. Jones and Y. Zhang.
"Simulation Studies on Adsorption of Methanol over Silicalite", by R. Vetrivel, C.R.A. Catlow and E.A. Colbourn.

"Computer Simulation of Zeolite Stability and Structure", by R.A. Jackson.
"Generalised Hydrodynamics and Eigenmodes for a Lennard-Jones Fluid", by C. Bruin.
"Computer Simulation of a Classical Fluid with Internal Quantum States", by J. Talbot, P. Ballone, Ph. de Smedt and J.L. Lebowitz.

Acknowledgements

I am grateful to Dr Julian Clarke, Professor Konrad Singer and to several of the speakers for their assistance in preparing this review. Any errors that are present are entirely of my own making.

Computer Simulation Studies of Zeolite Structure and Stability

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Introduction

Atomistic computer simulation techniques have been applied to a range of zeolites, with a view to predicting the structures and relative stabilities of these materials.

Details of the Method

The atomistic computer simulation technique that has been used in this work is lattice energy minimisation. This technique enables lattice energies to be calculated and the associated minimum energy structures to be obtained. It relies on the availability of interatomic potentials to describe the interactions of atoms in the crystal; the potential model used for zeolites has been applied to a wide range of ionic and semi-ionic solids, and the parameters have been used in a successful simulation of the structures of α- quartz and its polymorphs(1). An important feature of this model is the inclusion of a 3 body term to account for covalent effects in silicon-oxygen bonding.

A second derivative minimisation method has been used in all calculations; it should be noted that in the case of silicalite, the CRAY X-MP/48 was required for the calculations.

DARESBURY LABORATORY

INFORMATION QUARTERLY for COMPUTER SIMULATION OF CONDENSED PHASES

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

Number 24 March 1987

Contents

Editor: Dr. William Smith
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Editorial.

It is probably part of the natural cycle of things that it occasionally becomes necessary to appeal for contributions for the CCP5 Newsletter. Such is the case now. This does not however indicate that there is a diminishing interest in the newsletter itself, as rarely a day goes by when we are not asked to add more names to our mailing list. It is therefore important to remind our readers that the newsletter is very dependent on their enthusiasm if it is to keep going.

The CCP5 newsletter is an interesting publication in a number of ways: it published regularly, articles appears quickly (within three months or less), it has an international readership and it is informal enough to allow the publication of novel or speculative ideas. Added to these is the fact that there are surprisingly few publications that discuss the computational details of simulation methods warts and all. For these reasons it should be well worth supporting.

So to encourage our readership we announce that we would be pleased to receive contributions from anyone active in the field of computer simulation of condensed phases, anywhere in the world! We would also be particularly pleased to publish material from postgraduate researchers, who often have some original ideas to contribute to the computational art. We await your contributions!

In view of this appeal it is a special pleasure to thank the contributors to this months issue. Long may they prosper!

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General News.

a) CCP5 is to organise a meeting entitled "Industrial Applications of Computer Simulation". The meeting will take place at the Royal Institution in London from 11th. to 13th. January 1988. The purpose of the meeting is to discuss the application of the simulation methods associated with CCP5 (i.e. molecular dynamics, Monte Carlo, energy minimisation etc.) to industrially significant problems. The organisers of the meeting will be Prof. C.R.A. Catlow and Dr. N. Quirke. Readers interested in taking part in this meeting should write to: Dr. N. Quirke, B.P. Research Centre, Chertsey Road, Sunbury-on-Thames, Middlesex TW16 7LN.

Further news of this meeting will be announced later.

b) CCP5 is also to organise a meeting on the subject of bio-organic applications of computer simulation, which provisionally, is scheduled for Easter 1988. More details of this will be revealed as the organisation develops.

c) At the last meeting of the CCP5 Steering Committee which took place on 9th. January the composition of the Executive Committee was changed in accordance with the usual procedure. Professor C.R.A. Catlow was elected as the new CCP5 Chairman to replace Dr. J.H.R. Clarke. In addition Drs. R. Lynden-Bell, S. Parker and M.P. Allen were elected to the Executive Committee. The outgoing members being Drs. N. Quirke and P.A. Madden. In addition to these changes; Dr. M. Leslie has taken the responsibility of Secretary to CCP5 and Dr. W. Smith will now handle the CCP5 Program Library. The composition of the Executive Committee is thus:

Professor C.R.A. Catlow (Keele University and Daresbury)-Chairman,
Dr. M.P. Allen (Bristol University)
Dr. D.M. Heyes (Royal Holloway and Bedford New College)
Dr. M. Leslie (Daresbury) - Secretary
Dr. R. Lynden-Bell (Cambridge University)
Dr. S. Parker (Bath University)
Dr. W. Smith (Daresbury) - Program Librarian

This would seem to be the place to thank the past members of the Executive Committee for their work on behalf of the CCP5 community. In particular it is appropriate to thank Julian Clarke, under whose chairmanship for the past three years CCP5 has been extremely successful.

d) The CCP5 Executive Committee wish to announce to all U.K. participants in CCP5 that it has set aside a part of the CCP5 budget for the purpose of assisting collaborative work in the U.K. simulation community. These funds are to assist with expenses for travel between collaborating centres. So far, CCP5 has agreed to assist the following collaborating groups:
J. Clarke and D. Tildesley (Transport Properties),
S. Parker and G. Price (Lattice Simulations),
M. Allen and G. Evans (Hard Ellipsoids),
K. Singer and W. Smith (Quantum Simulations).
Other groups who wish to be considered for this assistance should write to the CCP5 Chairman, Prof. C.R.A. Catlow, Department of Chemistry, University of Keele, Keele, Staffs. ST5 5BG.

e) The CCP5 Executive Committee also wishes to remind U.K. participants that it has an annual allocation of Cray time at each of the centres: London (Cray 1s) and Rutherford (Cray XMP-48), which is available for the development of simulation programs prior to a grant allocation. At present CCP5 is allocated 15 hours a year at London and 5 hours quarterly at Rutherford. Readers who wish to use some of this allocation should write to the CCP5 Secretary, Dr. M. Leslie, TCS Division, SERC Daresbury Laboratory, Daresbury, Warrington WA4 4AD.

f) The Rutherford and Appleton Computer Centre Cray XMP/48 is now up and running. It is currently accessible to a few privileged users, who are running jobs to test the machine in a working environment before it becomes available to the wider academic community in April.

In time it is expected that the CCP5 Program Library will be modified to run on the XMP and users who would like to see any specific programs converted immediately should contact the CCP5 Program Librarian, Dr. W. Smith.

g) The University of Manchester Regional Computing Centre has described the new VM/CMS service which they will be running soon on the Amdahl 5890/300. It was originally intended to run the three domains of the Multiple Domain Facility to deal with: (i) the service currently supplied by the Amdahl 470 V/8; (ii) a national VM/CMS service and (iii) a Manchester local service. However only two domains are possible with the current hardware and so the last two services will run initially on one domain. Some disruption of the existing service is expected 20-23 March to reconnect the peripherals of the 470 V/8 to the 5890/300, followed by acceptance tests. The experimental VM/CMS service is expected to be available in early May. A useful description of the VM/CMS service appears in the March UMRCC Newsletter.

An important aspect of the operation of all the national computing centres (London, Manchester and Rutherford-Appleton) will be the new Peer Review system for the allocation of computing resources. Everyone involved in scientific computing in the UK should become familiar with this. The UMRCC newletter for March 1987 and the ULCC newsletter for February 1987 both carry details of the agreed procedure and are thus recommended reading.

h) The University of London Computing Centre has now upgraded its front end computer to an Amdahl 5890. The second phase of this upgrade will involve the introduction of new disc storage devices (Amdahl 6380 disc drives, which are 3380 compatible). During this phase both 3380 and 3350 discs will be used but eventually only 3380 discs will prevail. This change will have an impact on data storage at London and users are advised to reassess their data storage habits.

i) U.K. CCP5 participants are reminded that at Daresbury Laboratory the S.E.R.C. has available an FPS 164 attached processor, currently with 3 MAX (matrix accelerator) boards, which is available for grant supported computing within the Science Board Community. U.K. research groups are invited to apply informally to Dr. J.E. Inglesfield, at Daresbury, for time on the FPS for benchmarking purposes. If the FPS proves viable for a given project, a formal application may be made. Advice on using the FPS at Daresbury may be obtained from the User Interface Group (in the person of Dr. D. Taylor) or from the CCP5 representative Dr. W. Smith. A document entitled 'Using the FPS Attached Processor at the Daresbury Laboratory' by Dr. M.F. Guest is available from the User Interface Group.

j) Concurrent Computing Initiative at Daresbury.

A new advanced research computing group has been set up at Daresbury to develop large scale computational codes for a number of scientific applications in a highly parallel computer environment. Central to this project is the recently acquired FPS-T20 hypercube, 16 powerful processors interconnected as a 4 dimensional hypercube or tesseract (hence T for tesseract and $20_8=2^4$).

Each node of the T-machine comprises an Inmos transputer, 1Mb of memory and 3 Weitek floating point chips, giving a realisable 12 Mflop performance per node on highly vectorised code. Thus the total peak performance is 192 Mflop with 160 Mflop having already been demonstrated on a distributed matrix multiply. The machine is frontended by a Micro-Vax II running Micro-VMS 4.4 and initially the T-machine is only programmable in occam. However a software release scheduled for August will provide both Fortran and C, and also move to a Unix frontend operating system.

Plans for upgrades are already in place and it is anticipated that the system will evolve to be an extremely powerful Fortran engine for both scalar and vector code. It is only by exploting the inherent parallelism of most scientific applications that one can hope for the several orders of magnitude increase in computational power required by many applications. Current supercomputers with small numbers of expensive processors sharing memory cannot realise the 1000 fold increase in power offered by highly concurrent, distributed memory architectures.

R.J.Harrison and M.F.Guest.

SERC, Daresbury Laboratory, Warrington WA4 4AD.

k) The international conference entitled 'The Impact of Supercomputers on Chemistry' is due to take place in the University of London from 13 - 16 April 1987 The conference will cover all aspects of the use of supercomputers; applications and methodology. Some of the talks that are to be given include: "Supercomputer Simulation of Solids" by M.J. Gillan, "The Impact of Quantum Monte Carlo on Chemistry" by D.M. Ceperley, "Quantum Chemistry, Statistical Mechanics and Fluid Dynamics" by E. Clementi, "Chemistry as a Many-Particle Problem" by H.J.C. Berendsen and "Protein Structure, Computer Simulation and Graphics in the Design of Novel Molecules" by T.L. Blundell.

Enquiries regarding the conference should be addressed to Dr. J. Altmann, ISOC 87 Secretariat, Room 209, University of London Computer Centre, 20 Guildford Street, London WC1N 1DZ. (Telex 8953011).

l) Readers may also be interested in the Seventh Summer School on Computing Techniques in Physics, which takes place on 9th-18th. June 1987 at Bechyne Castle near Tabor, Czechoslovakia. This year's theme is 'Microcomputers in Physics'. The organiser is Dr. J. Nadrchal, address; Summer Schools on Computational Physics, Institute of Physics, Czechoslovak Academy of Sciences, Na Slovance 2, CS-180 40 Praha 8, Czechoslovakia.

m) The Institute of Physics is organising the 1987 Solid State Physics Conference for 16-18 December at the H.H. Wills Physics Laboratory, University of Bristol and it will contain a number of symposia that will undoubtedly be of interest to participants in CCP5. Among the intended symposia are: Statistical Mechanics of Disordered and Inhomogeneous Systems; Physics of Sputtering Processes, Polymers and Liquid Crystals; Scattering of Neutrons from Disordered Systems and The Physics of Solids at High Pressures. People interested in attending or contributing a paper should contact Dr. B.L. Gyorffy or Dr. R. Rvans at the H.H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8 1TL. We will provide more information in our next newsletter.

n) It has been suggested to the CCP5 Editors that it would be useful for CCP5 participants to have a list of the EARN and BITNET addresses of other members of the project. For this purpose we would be happy to receive from our readers their addresses, which we shall collect here at Daresbury for publication in the newsletter at a later date. So that we don't fall foul of the 'Data Protection Act', it should be understood by all participants that the contributed addresses will be available to everyone.

o) The CCP5 Program Library. Documents and programs are available free of charge to academic centres upon application to Dr. W. Smith, TCS Division, S.E.R.C. Daresbury Laboratory, Daresbury, Warrington WA4 4AD, U.K. Daresbury Laboratory. Listings of programs are available if required but it is recommended that magnetic tapes (to be supplied by the applicant) be used. It may also be possible to transfer a small number of programs over the JANET network to other computer centres in the U.K.. Please note that use of inappropriate packing for magnetic tapes (e.g. padded bags) may result in them being considered unusable by Daresbury Computing Division and returned without the required software. Please ensure that these forms of packaging are not used. A list of programs available is presented in the following pages.

We should also like to remind our readers that we would welcome contributions to the Program Library. The Library exists to provide support for the research efforts of everyone active in computer simulation and to this end we are always pleased to extend the range of software available. If any of our readers have any programs they would like to make available, please would they contact Dr. Smith.

THE CCP5 PROGRAM LIBRARY

MDATOM by S. M. Thompson. M.D. simulation of monatomic fluids.

HMDIAT by S. M. Thompson. M.D. simulation of homonuclear diatomic fluids.

MDLIN by S. M. Thompson. M.D. simulation of linear molecules.

MDLINQ by S. M. Thompson. M.D. simulation of linear molecules with quadrupole.

MDTETRA by S. M. Thompson. M.D. simulation of tetrahedral molecules.

MDPOLY by S. M. Thompson. M.D. simulation of polyatomic molecule fluids.

ADMIXT by W. Smith. M.D. simulation of monatomic molecule mixtures.

MDNACL by W. Smith. M.D. simulation of alkalai halide salts.

MDMIXT by W. Smith. M.D. simulation of polyatomic molecule mixtures.

MDMULP by W. Smith. M.D. simulation of polyatomic molecule mixtures.

MDMPOL by W. Smith & D. Fincham. M.D. simulation of polyatomic molecule mixtures.

MDZOID by W. Smith & K. Singer. M.D. simulation of ellipsoidal gaussian molecules.

DENCOR by W. Smith. Calculation of density correlation functions.

CURDEN by W. Smith. Calculation of current density correlation functions.

HLJ1 by D. M. Heyes. M.D. simulation of atomic fluids.

HLJ2 by D. M. Heyes. M.D. simulation of atomic fluids (with VACF).

HLJ3 by D. M. Heyes. M.D. simulation of atomic fluids (link-cells).

HLJ4 by D. M. Heyes. M.D. simulation of atomic fluids (constant T or P).

HLJ5 by D. M. Heyes. M.D. simulation of atomic fluids (shifted force).

HLJ6 by D. M. Heyes. M.D. simulation of atomic fluids (Toxvaerd algorithm).

MCRPM by D. M. Heyes. M.C. simulation of electrolytes (restricted primitive model).

SURF by D. M. Heyes. M.D. simulation of model alkalai halide lamina.

HSTOCH by W. F. van Gunsteren & D. M. Heyes. MD or SD simulation of molecules in vacuo or rectangular cell with solvent or lattice.

MDATOM by D. Fincham. M.D. simulation of atomic fluids.

MDDIAT by D. Fincham. M.D. simulation of diatomic molecule fluids.

MDDIATQ by D. Fincham. M.D. simulation of diatomic fluids.

MDIONS by D. Fincham & N. Anastasiou. M.D. simulation of electrolytes.

MDMANY by D. Fincham & W. Smith. Simulation of rigid polyatomic molecules with/without fractional charges.

CARLOS by B. Jonsson & S. Romano. M.C. simulation of a polyatomic solute molecule in an aqueous cluster.

MCN by N. Corbin. M.C. simulation of atomic fluids (Metropolis).

SCN by N. Corbin. M.C. simulation of atomic fluids (Rossky, Friedman and Doll).

STATIC SIMULATION CODES

CASCADE by M. Leslie and W. Smith. Calculates the structure and energy of a defect in an ionic crystal for a given potential model.

THBREL Determines the minimum energy configuration of a perfect lattice for a given potential.

THBFIT Empirically fits a potential to experimentally observed properties of a perfect lattice.

SYMLAT Determines the minimum energy configuration of a perfect lattice for a given potential.

THBPHON Calculates phonon dispersion curves for ionic crystals with three-body terms in the potential.

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DEPARTMENT OF CHEMISTRY
The Bourne Laboratory

Dr. D.M. Heyes

10th March 1987

Dear Colleague,

At the 5th March 1987 CCP5 executive committee meeting it was decided to look into the possibility of holding a CCP5 sponsored workshop on " Transport Processes ".

I am writing to you to discover if you would be interested in attending such a meeting and if so the directions you would like it to take. An obvious area would be equilibrium and non-equilibrium MD routes to viscosity, self-diffusion and thermal conductivity of fluids. Transport in solids and algorithms for performing the molecular dynamics are other areas of interest. We would appreciate your opinions on this matter, and also on the months in this year most suitable to you.

Best wishes,

Yours sincerely,

David Heyes

MEETING ANNOUNCEMENT:

THERMODYNAMICS AND STATISTICAL MECHANICS OF SMALL SYSTEMS

A meeting is being organised by the Royal Society of Chemistry Statistical Mechanics and Thermodynamics Group at the University of York on September 24-25 1987.

The topics for discussion include small system behaviour in porous media and as crystallites, clusters and micelles. Both theoretical and experimental aspects will be discussed and contributions are invited.

The speakers include Dr. R.J. Evans (Bristol), Prof. D.H. Everett (Bristol) and Prof. J.S. Rowlinson (Oxford).

Please contact Dr. J.H.R. Clarke, Department of Chemistry, U.M.I.S.T., Sackville Street, Manchester M60 1QD as soon as possible for details.

P.G. Francis

REVIEW OF THE CCP5 MEETING ON 'NEW HORIZONS IN THE COMPUTER SIMULATION OF CONDENSED PHASES' HELD AT UMIST 8 - 9 JANUARY 1987.

W. Smith

As the title of the meeting suggests, the latest CCP5 meeting was a forward looking affair, which was intended to highlight areas of computer simulation which seem likely to open new avenues of enquiry. The meeting was organised by the departing CCP5 Chairman, Dr. J.H.R. Clarke, with the assistance of his colleagues at the Department of Chemistry and was attended by seventy simulation scientists from the United Kingdom, Europe and North America. As is always the case with CCP5 meetings, many interesting questions were raised and Dr. Clarke wisely allowed sufficient time for discussion. As a result it was generally held to be a stimulating and informative meeting.

The first contributor to the meeting was Prof. W.L. Jorgensen (Purdue University), who spoke on the subject of computer simulations of organic reactions. The objective of this work was the determination of the rates of organic reactions from first principles. Prof. Jorgensen first considered the S_{N2} reaction beloved of organic chemists, in particular, the reaction between chloromethane CH_3Cl and chloride anion Cl^-. S_{N2} reactions are bimolecular and sterospecific, they do not have intermediates and have an activation energy that increases with the polarity of the solvent. Prof. Jorgensen's approach involved the calculation of the gas phase potential reaction surface followed by its modification to include solute-solvent effects and finally a simulation of the reaction along a suitable reaction coordinate. The first step was achieved through ab initio methods; calculating the energy of the transition state (i.e. the $[Cl.....CH_3.....Cl]^-$ complex) over the reaction coordinate. The solute-solvent interactions were determined by the ab initio calculation of clusters of solvent molecules with the reactive species. The purpose of the simulation (by Monte Carlo method) was to determine the density function $g(r_c)$ giving the probability of the reacting species being at a separation r_c on the reaction coordinate. From this the 'reaction force' $w(r_c)=-kT\ ln(g(r_c))$ could be obtained. The simulation involved the reacting system plus 250 'TIP4P' water molecules within a periodic system. The MC procedure required the simulation to be done for several overlapping 'windows' of the reaction coordinate, using a biasing technique to sample each window adequately. The final set of overlapping windows gave the full $g(r_c)$ function. The NTP ensemble required 1-2M equilibration steps and 2-6M steps averaging for each window. In the simulation the potential functions used were Lennard-Jones 12-6 functions with fractional charges to represent the Coulombic forces. However the parameters were described as functions of the reaction coordinate, fitted to the ab inito calculations.

The results for the example reaction showed that the relatively complicated energy barrier of the gas phase reaction was replaced by a single, higher peak in aqueous solution. These results tally with experimental observations, which show the gas reaction to be much faster, and that the solvated reaction has no intermediates. Interestingly, in the less polar solvent DMF, the energy barrier showed more structure, particularly the occurrence of minima suggestive of intermediates. (This latter suggestion has some experimental NMR evidence in its favour.) Calculations of the energy and number distributions showed that the number of solvating water molecules about the reacting species is constant throughout the reaction, contrary to expectations. The relative reduction of the solvation energy of the transition state (a factor contributing to the energy barrier increase) is due to a weakening of the solute-solvent bonding, not to the expected reduction in solvent coordination numbers. Further calculations using thermodynamic perturbation theory indicate that the structure of the transition state in gas and solvent is very similar.

Prof. Jorgensen concluded with a study of the S_{N1} reaction of t-butyl chloride with Cl^- and showed that the formation of a contact ion pair $[t\text{-}Bu]^+.Cl^-$ was clearly apparent, but the evidence for a solvent separated ion pair was much less clear. Throughout his talk Prof. Jorgensen presented excellent graphics revealing the stereochemical aspects of the reactions being described.

Dr. S. Toxvaerd (Panum Institute) described his studies in the implementation of the Generalised Langevin Equation (GLE). He was was concerned to show how the GLE could be used to simulate the system of a polymer in solution for the fraction of the cost of a full molecular dynamics simulation but with comparable accuracy. The system he considered was a nonomer consisting of Lennard-Jones atoms bound by harmonic forces and suspended in a solution with 509 Lennard-Jones atoms. Following the work of Bossis, Quentrec and Boon, the GLE for this system is is written as:

$$m d\underline{v}_i(t)/dt = -m\int dt' M_i(t-t')\underline{v}_i(t') + \underline{r}_i + \underline{e}_i(t)$$

where $\underline{v}_i$ is the velocity of the i'th. bead, $\underline{r}_i$ the stochastic force, $\underline{e}_i$ the bead-bead forces on bead i, and $M_i(t)$ the memory function. The division of the forces into stochastic and bead-bead contributions is only valid if the correlation function $\langle \underline{v}_i . \underline{r}_i \rangle$ is zero throughout. Dr. Toxvaerd has checked this using simulation and has established that it is true except at short times, where small deviations occur.

Once the memory functions M_i are known, the GLE can be solved numerically and Dr. Toxvaerd described his procedure for obtaining them. The memory function for the whole system is replaced by a Mori expansion. These terms cannot in general be resolved into intramolecular and solvent contributions, with the exception of the first term K_1. Nevertheless the higher terms can be calculated by molecular dynamics via the time derivatives of the velocities. Explicit consideration of the first two terms of the Mori expansion; comparison of the values for the pure solvent with values obtained for the polymer solution allows physically reasonable approximations to the memory functions M_i to be made. The memory functions are then written as:

$$M_i(t) = K_{1,i}(s,t)\exp(-K_2t^2/2)$$

In which $K_{1,i}(s,t)$ is the instantaneous value of the solvent dependent part of K_1 (which is dependent on the bead number i) and K_2 is the second Mori coefficient for the pure solvent. This approximation has been implemented in a simulation program using the Fourier method of Wang and Uhlenbeck and the results have been compared with molecular dynamics and a simpler Langevin Equation (LE) simulation.

The results show that small differences arise between the MD and the GLE and LE simulations of the bead-bead bondlength distribution, but the bead velocity autocorrelation functions are well reproduced. The approximate GLE method was shown to give essentially exact results for the centre of mass diffusion. Studies of the end-to-end distance R^2 and the radius of gyration S^2 and the corresponding correlation functions showed that very long runs are necessary for good statistics (prohibitively for the MD simulations) and about 10^6 timesteps are required for the molecule to establish the mean shape. Within the limitations on the studies occasioned by these difficulties, the MD and stochastic dynamics results were good. A study of the effects of the solvent on the molecular conformation was undertaken, by means of a comparison with a 'free molecule' simulation of the nonomer. For the state points studied, the molecule was rather globular, and no great effects of the solvent were seen. It was concluded that the GLE method described was a very useful method for studying polymers in solution.

Dr. D. Rapaport (Bar-Ilan University) spoke on the new subject of microscale hydrodynamics, by means of which he has successfully simulated some of the macroscopic features of fluid flow. He began by describing the kinds of phenomena seen in real flow experiments, such as fluid flow past a stationary object. At low flow rates (low Reynolds number) the flow is laminar (Stokes flow). As the flow inreases stationary eddies form. At yet higher rates the eddies become unstable and move away from the object (vortex shedding) and give rise to a wake pattern known as the vortex or von Karman street. At very high flow rates turbulence results.

Dr. Rapaport described how he had simulated many of these features in a molecular dynamics simulation on the parallel assembly of FPS attached processors at IBM, Kingston, New York. The simulation was of two-dimensional flow past a fixed cylinder of 25 nm diameter. The fluid consisted of 170,000 'soft sphere' molecules in a 150 nm wide system with periodic boundaries. A fluid density of 0.83 and a flow speed of 330 m/s was used. A force field of 10^{11}g was employed to drive the flow and rethermalisation of the molecules at the down-field boundary was used to maintain the periodic conditions. The entire simulation cell was partitioned into 'slabs' to permit efficient parallelisation of the system and reduce data communication between processors to a minimum. The resulting flow pattern was presented graphically. The simulation cell was partitioned into a 60x60 grid and a short time average of the particle velocities in each sub-cell was calculated at intervals of 5 timesteps. The average velocity vector for each sub-cell was then plotted as a field of flow. Approximately 100 hours of CPU time were required on a system of four FPS 264 processors in parallel.

The results showed clearly the development of the different regimes of flow behaviour described above i.e. laminar flow, eddy formation, incipient instability of the eddies and vortex shedding and finally the von Karman street. The method clearly has great potential in elucidating the microscopic features that underlie the continuum behaviour of fluids in flow. Dr. Rapaport concluded by discussing the limitations of the method (short times, small spatial scales and subsonic velocities) and possible extensions of the method to three dimensional simulations.

Dr. M.P. Allen (University of Bristol) described his work done in a collaboration with D. Frenkel (Utrecht) on the molecular dynamics simulation of the isotropic to nematic phase transition in a system of hard ellipsiods. (The phase diagram for this system had been obtained previously by Frenkel and Mulder.) Dr Allen described the technique by which the hard ellipsoid system was simulated. (A detailed description of this appears in CCP5 Info. Quart. No. 23 p.28.) In practice the system simulated consisted of 144 ellipsoids and generated 10^6 collisions per hour on a CYBER 205 computer. The ellipsoids studied had axial ratios (a/b) of 2 and 3. The objective was to calculate single and collective time-dependent orientational correlation functions in the region of the isotropic-nematic phase transition and deduce the values of parameters important in the DeGennes and Keyes/Kivelson theories.

The single particle correlation functions were defined as:

$$c_L^{s}(t) = < P_L(\underline{e}_i(0).\underline{e}_i(t) >$$

and the collective correlations functions as:

$$c_L^{c}(t) = \Sigma_j < P_L(\underline{e}_i(0).\underline{e}_j(t)) > / \Sigma_j < P_L(\underline{e}_i(0).\underline{e}_j(0)) >$$

in which P_L is a Legendre polynomial of order L and $\underline{e}_i$ is a unit vector aligned along the major axis of the ellipsoid. These functions were calculated for L=1 and 2 at various densities. The functions showed exponential decay at long times in the expected manner. The characteristic decay times τ for the collective correlation functions were significantly longer than the decay times for the single particle correlations, particularly near nematic-isotropic phase transition. The behaviour of the ratio τ_2^{s}/τ_2^{c} was shown in a plot against density and revealed a critical slowing down effect at the transition for the axial ratio 3. This slowing down was interpreted using the Kivelson expression:

$$\tau_2^{s}/\tau_2^{c} = (1+j_2)/(1+g_2)$$

where g_2 is the static second-rank Kirkwood factor and j_2 is a dynamical quantity that is describable in terms of the orientational memory functions. Calculations of the factor $(1+g_2)^{-1}$ for different densities allowed the above equation to be used to calculate j_2, which was found to be insensitive to the density. The calculated mean values were given as $1+j_2=0.74+/-0.16$ (a/b=2) and $1+j_2=0.92+/-0.05$ (a/b=3). These results find experimental evidence in their favour from the work of Flygare et al. on p - methoxy - benzylidene - n - butylaniline (MBBA), which provided an estimate of $1+j_2$ of the order 0.7 and also supported the mean field predictions of DeGennes that g_2 diverges at the critcal density. Further systematic investigations of these and related systems are planned.

Dr. D. Tildesley (University of Southampton) described the method he has devised with his collaborators M.R. Stapleton (Southampton) and N. Quirke (BP Sunbury- on-Thames) for simulating variable polydispersed liquids which he defined as systems in which the dispersed particles (micelles) change size when the density of the system changes. The systems examined were the hard-sphere system and a modified Lennard-Jones system, in both of which every particle possessed a different effective diameter (i.e. $\sigma_{eff} = (\sigma_i+\sigma_j)/2$). The simulation method was a modified Monte Carlo algorithm in which the sizes of the particles as well as their locations were changed as the simulation proceeded. The sampling of the particle sizes at each MC move was taken from an appropriate particle size distribution function, which in this case was the Shultz function:

$$f_z(\sigma) = z!^{-1}((z+1)/\sigma)^{z+1} \sigma^z \exp(-((z+1)/\sigma)\sigma) \text{ if } \{a<\sigma<b\}$$

$$= 0 \text{ otherwise}$$

Where z is a parameter controlling the form of the function. (The distribution function changes with density and temperature for the LJ fluid.) A move was accepted or rejected according to the change in the inter-micellar interaction energy resulting from the move. Special care was needed for the long range corrections. Applications of this method to hard spheres showed that as the number density of the particles increases, they tend to become smaller, while for Lennard-Jones particles there is an initial average increase in the particle diameters followed by a decrease at higher densities. The initial increase was thought to be due to the attractive component of the LJ potential, which encourgaged particles to approach, but this effect was outweighed by repulsive component when the density of the particles was high.

For fluids in which the distribution function is symmetric an adequate description is possible using a monodispersed fluid with the appropriate packing fraction, which is a function of the density and the third moment of the equilibrium distribution of diameters; M_3. A mean field theory for M_3 has been developed in collaboration with Dr. T. Sluckin (Southampton). The chemical potential distributions of the hard sphere polydispersed fluids were calculated by means of Widom's particle insertion method with lattices of different particle sizes. The scaled particle theory of Salacuse and Stell gave good agreement with the simulated chemical potential obtained with both low density distribution functions.

The second day began with a talk by Dr. D. Price on the computer simulation of minerals important in the understanding of geological processes. The minerals of greatest significance being silicates. It is extremely important that the properties of these materials be fully understood before realistic models of geological processes such as plate techtonics can be developed. The problem however is that these materials most commonly exist in regions of high pressure and temperature in the earth's core and is is not practicable to perform suitable experiments in the laboratory. (Perovskite, a high pressure phase of magnesium silicate, for example is thought to constitute 40 percent of the earth by volume, but it is still very little understood). Computer simulation is therefore an essential tool for investigating such materials. The simulations need to provide information on several properties of the minerals to assist the geologist; the equation of state, (P vs. T) phase diagram, bulk and shear moduli, rheological properties and diffusion processes among them.

A number of methods are available for modelling these systems: (i) the ab initio Hartree-Fock method employing periodic boundaries (accurate but limited to small systems); (ii) ab initio calculations on SiO clusters to obtain the potential energy surfaces (good for some properties, though there is a loss in accuracy resulting from harmonic fitting of the surfaces); (iii) modified electron gas potentials with fitting of the potential surface using empirical (e.g. Buckingam) potentials (poor estimates of the elastic constants result) and (iv) The ionic model using fitted empirical potentials, plus coulombic interactions and the shell model (massless charged shell coupled to ion core by harmonic spring) to account for polarisability. The whole periodic crystal structure is modelled. To offset the effects of covalency non integer charges and bond bending forces are sometimes used.

Of the four methods described only the last is presently useful for providing geological data. The method is employed in the large lattice simulation programs CASCADE, THBREL and THBPHON and give excellent crystal structure data and elasticity constants (e.g. the predicted structures of olivine, spinel and ilmenite are very good).

Phonon data are also available and allow the calculation of heat capacity, Gruneisen parameters, thermal expansion, entropy and defect entropies. Also the phonon spectrum has been found to be in close agreement with infra red and Raman frequencies. The eigenvectors provide details of the vibrational motions of the ions which is not easily available from experiments. The calculations of the entropies and heat capacities have been found to be very accurate. Thermal expansion coefficients and the phase diagrams of minerals have been obtained by this method and compare fairly well with experimental data. Lastly, defect energy calculations, using the CASCADE program, have allowed reasonable estimates of the diffusion rates of ions.

In the future Dr. Price expects to see the ionic model being used successfully to determine unknown phases and the incorporation of better three-body forces such as the Axilrod-Teller type. It is also expected that ab initio and modified electron gas potentials will be sufficiently advanced to assist with this type of work.

Dr. R. Lynden-Bell (University of Cambridge) delivered a talk on the subject of phase transitions and the fluctuations in orientationally disordered crystals. Dr. Lynden-Bell has used molecular dynamics to study these phenomena in a variety of systems; CH_4, CBr_4, CCl_4, $Na^+.CN^-$, tBuBr and SF_6. The value of the molecular dynamics approach is that it complements existing experimental and theoretical methods and naturally introduces the effects of temperature and entropy. The theory of ordering studied by Dr. Lynden-Bell is the Landau theory, in which the free energy of a system is given by the expression:

$$G = G_o + a(T-T_c)Y^2 + cY^4$$

In which Y is the 'order parameter'. This function has a single minimum for temperatures $T>T_c$ (indicating a stable, orderered phase) a very broad minimum when $T=T_c$ (indicating incipent instability) and a double minimum when $T<T_c$ (indicating a new preferential ordering). The order parameter Y is itself a function of the orientation of the molecules and is an irreducible representation of the space group of the crystal. Its spatial Fourier transform is represented by:

$$Y(\underline{k}) = \Sigma_i^{mol} \exp(i\underline{k}.\underline{r}_i^{eq})\ K_{\Gamma M}^{L}(\Omega_i)$$

In which the function $K_{\Gamma M}^{L}(\Omega_i$ is a combination of spherical harmonics (e.g. Kubic harmonics) appropriate to the crystal symmetry. The index L indicates the type of ordering; thus

L=1 implies dipolar ordering, L=2 quadrupolar ordering and L=3 octupolar ordering. Fluctuations in the order parameter Y (i.e $\langle Y^2 \rangle$) are largest when a change in phase is incipient and plots of $\langle Y^2 \rangle$ vs. k vector provide information on the crystallographic features of the transition e.g. a peak at k=0 (Γ point) indicates no change in the number of molecules in the unit cell, at k=zone boundary implies a doubling (or similar) in the unit cell and at intermediate k values, an incommensurate phase is expected.

Dr. Lynden-Bell illustrated these principles with examples of the orientational properties of sodium nitrite and nitrogen on graphite. The concluding example was an investigation of tertiary butyl bromide (tBuBr) to determine whether the ordering was dipolar (L=1) or octupolar (L=3); the former indicating the dominance of the molecular dipole in the crystal structure and the latter the dominance of the tetrahedral geometry of the molecule. A comparison of the $\langle Y^2 \rangle$ vs. k plots of these two alternatives with the corresponding plots of CBr_4, showed the closer resemblance to the octupolar case.

Prof. C.R.A. Catlow (University of Keele / Daresbury) described the investigation of the structure and conductivity of β alumina. Two forms of β alumina exist; the stoichiometric form $Na_2O.11Al_2O_3$ and the non-stoichiometric form $(Na_2O)._{1.3}11Al_2O_3$. The believed structures are complex spinel blocks in which the sodium atoms occur in layers at alternate hexagonal sites (the so-called Beevers-Ross (BR) sites). The sodium ions are mobile in these layers and give rise to conductivity. The non-stoichiometric sodium ions reside in bridging locations between oxygen ions. The structures were investigated both by static lattice methods (which used a shell model for the ions) and by molecular dynamics (which used a rigid ion model and the Ewald sum to handle the long range forces). The objectives were to determine the role of non-stoichiometry in conduction, the migration mechanism, the structure of the conduction plane and the temperature dependence of the conduction.

The static lattice calculations were performed with the CASCADE program and showed that the interstitial sodium ions occupied the 'anti- Beevers-Ross' sites and that the conduction path for the sodium ions was different in the non-stoichiometric and stoichiometric cases. The molecular dynamics were performed with the program FUNGUS, which was adapted for the parallel assembly of FPS processors at Kingston N.Y.. The simulations used 500 ions per MD cell; the stoichiometric case possessing 24 Na^+ ions. The non-stoichiometric cases had 4 and 8 more Na^+ ions (plus compensating O^{2-} ions) respectively.

The stoichiometric cases showed the sodium ions to be at the BR sites but NO diffusion (i.e. conductivity) was evident in the temperature region 600K to 900K, though the Na^+ ions showed large thermal parameters. The non-stoichiometric ($+4Na^+$) case showed signs of diffusion at 600K and definite diffusion at 900K. The interstitial sodium ions occupied anti-BR sites with some displacement due to strong interaction with the excess O^{2-} ions. There was some evidence of conduction paths. Surprisingly, the non-stoichiometric ($+8Na^+$) case showed significantly less diffusion and extensive interactions between the excess sodium and oxygen ions. The excess sodium ions were displaced towards the mid O-O bridge.

The conclusions of this work were that the stoichiometric β alumina is not a sodium ion conductor, while in the highly non-stoichiometric form conduction is surpressed. In the low non-stoichiometric form the excess sodium ions occupy anti-BR sites, but are displaced towards the oxygens at higher non-stoichiometry. Conduction by the sodium ions appears to involve distinct pathways.

The session on the quantum mechanical methods of simulation began with a talk by Dr. M. Gillan (Harwell) on the Path Integral Monte Carlo (PIMC) method, which is a method for simulating quantum systems at nonzero temperatures and has its origins in the path integral formulation of quantum mechanics due to Feynmann. Beginning with the one dimensional, single particle case, Dr. Gillan explained the derivation of the method. At the core of the method is the mathematical function known as the density matrix, in terms of which the partition function of a system and the mean value of any static (equilibrium) observable quantity may be calculated. The form of the density matrix is:

$$\rho(x,x';\beta) = \Sigma_n \varphi^*_n(x) \exp(-\beta E_n) \varphi_n(x')$$

which closely resembles the Green's function or propagator used in the path integral formulation of Feynman. This means that a substitution of the time variable by $i\beta h/2\pi$ permits the formal use of the path integral method to calculate the partition function for the system of interest. In reality the density function has only been derived for two cases; the free particle and the harmonic potential, and no analytical solution is known for complex potentials or many-body systems. However Feynman's formalism allows the partitioning of a given path integral into shorter paths over the span of which the harmonic potential may be used as a good approximation. (This is the so-called short-time approximation.) If this strategy is adopted, it emerges that the resultant expression for the partition function is formally equivalent to that of a classical model ring polymer in which the atoms are coupled by harmonic springs with a force constant of $2mP(\pi)^2/(h\beta)^2$ and each atom is in a potential field of strength V/P, where P is the number of atoms in the ring and V is the potential in the original Hamiltonian.

The physical significance of the polymer is that collectively it represents the delocalisation of the parent particle in agreement with the Uncertainty Principle. The effective reduction of the potential energy by the factor 1/P is what enables the parent particle to tunnel into classically forbidden regions. The spring constant is largest when the temperature or the mass of the parent particle is large. This means that the ring polymer reduces in extent (i.e. reduced delocalisation) under these circumstances, which comply with the classical limit. Generalisation of the method to many dimensions and many particles is easily accomplished (but may be computationally expensive).

Simulations using this method require only that some realistic way of generating the configurations of the isomorphic polymer be available. Either molecular dynamics, Monte Carlo or stochastic dynamics methods may be employed. (No significance should be attached to the time dependent aspects of MD and SD.) Dr. Gillan prefers the stochastic method over MD since it avoids the problems of ergodicity encountered in MD when the spring constants are large. Dr. Gillan gave a number of examples of the application of the method and concluded with his own work on the dissolution of hydrogen in metals in which he has been able to reproduce many of the observed features of these remarkable systems.

Dr. B.H. Wells (University of Oxford) continued the quantum mechanical theme in a talk on the new developments that have taken place in the Green's Function Monte Carlo method. Dr. Wells began by describing the two basic methods currently in use; the Variational Monte Carlo and Diffusion Monte Carlo methods. Both are methods for dealing with the electronic wavefunctions of molecular systems. The Variational method is used to calculate the energy of a system from a known wavefunction. In the method an inital set of electron positions are moved using a gaussian propagator and the moves accepted according to a probability based on the square of the wavefunction. The so-called local energy $E_L(\underset{\sim}{r}')$ is calculated and accumulated at each step, following an equilibration period. In Diffusion Monte Carlo the wavefunction itself is calculated, starting from an initial trial wavefunction. In this method the gaussian propagation is augmented by an exponential branching term, for which a trial state energy is required and is updated as the simulation proceeds. Excited states can be calculated provided the initial wavefunction possesses the correct symmetry. The standard method uses the 'fixed node' approximation, which requires the nodes of the wavefunction to be accurately known. This knowledge prevents negative configuration densities arising in the sampling procedure. Configurations which cross a node boundary in the course of the calculation are deleted, but provided the trial energy is close to the actual state energy, the population of configurations will be maintained. The method has been successfully applied calculations of the correlation energy in small molecules.

Among the advances in the methods that have been taking place recently are the removal of the short-time approximation in the Green's function propagator, the removal of the 'fixed-node' constraint and the development of the differential Monte Carlo method to enable calculations of physical quantities, such as the molecular dipole, which depend on small energy differences. (The essential feature of the latter method is the calculation of two distinct systems, one the minor perturbation of the other, using the same random walk to reduce the variances of the calculated property.) Example applications of the methods described by Dr. Wells included the $e_2^+e^-$ bound system, e^-H^+ systems at a dielectric surface (for both of which good binding energies were obtained) and the calculations of H_3^+ and H_5^+ systems with and without the Born-Oppenheimer approximation.

The final speaker of the meeting was Dr. D. Fincham (University of York) who provided an overview of the current developments in parallel computing. He began by defining the concept of a parallel computer, which is a computer possessing more than one processing unit, all or some of which could be active simultaneously under the direction of the user's program. Parallel computers may be SIMD (Single Instruction Multiple Datastream) or MIMD (Multiple Instruction Multiple Datastream) machines.

There are currently three main architectures for parallel computers. The first of these is the mainframe which has a small number of processors with shared memory (e.g. Cray XMP/48). The second is the switching network, in which there are separate processors and interconnected memories (e.g. ULTRA). In the third architecture, the processors are connected but have their own memory boards. An important feature of all parallel computers is the topology of the connections between processing units, Dr. Fincham gave four examples; the square array (e.g. ICL DAP), the hypercube (e.g. INTEL hypercube), the pyramid (devised by the University of Erlangen) and the Waterloop Ring. Each of these topologies has its own features and advantages e.g. the hypercube, which possesses 2^n nodes with n connections to each, has other connectivities as subsets of this, and these can be exploited in specific applications such as the periodic boundary.

A recent significant development in the parallel computing concept has been the introduction of the TRANSPUTER, which is a high performance microprocessor which has been specifically designed to be linked to other TRANSPUTERS so creating a parallel processor. Each processor is itself a complete computer, which will soon acquire a hardware floating point unit (currently floating point arithmetic is handled by software). By way of an example application Dr. Fincham described a molecular dynamics application of the TRANSPUTER, that was suitable for simulating biological molecules. Other recent significant developments are: the INTEL iPSC and iPSC/VX computers which have the hypercube topology and up to 128 processors; the FPS T series, which has hypercube topology and vector processors at each node; the ICL Mini-DAP, a SIMD machine, and the Reconfigurable Processor Array (RPA) at Southampton, in which the processing elements can be dynamically configured to suit the application.

Dr. Fincham concluded with a few comments on the (unlikely) transportability of parallel codes and the commercial pressures likely to encourage the development of larger machines with fewer processors instead of smaller multi-processor machines.

Throughout the meeting a number of poster displays were on view. These included:

"Dynamical Simulation of a Model Reverse Micelle", by D. Brown and J.H.R. Clarke.
"Simulated Annealing of Atomic Clusters", by L.T. Wille.
"Computer Simulation of Plasticity in Minerals", by M. Heggie, R. Jones and Y. Zhang.
"Simulation Studies on Adsorption of Methanol over Silicalite", by R. Vetrivel, C.R.A. Catlow and E.A. Colbourn.

"Computer Simulation of Zeolite Stability and Structure", by R.A. Jackson.
"Generalised Hydrodynamics and Eigenmodes for a Lennard-Jones Fluid", by C. Bruin.
"Computer Simulation of a Classical Fluid with Internal Quantum States", by J. Talbot, P. Ballone, Ph. de Smedt and J.L. Lebowitz.

Acknowledgements

I am grateful to Dr Julian Clarke, Professor Konrad Singer and to several of the speakers for their assistance in preparing this review. Any errors that are present are entirely of my own making.

Computer Simulation Studies of Zeolite Structure and Stability

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Introduction

Atomistic computer simulation techniques have been applied to a range of zeolites, with a view to predicting the structures and relative stabilities of these materials.

Details of the Method

The atomistic computer simulation technique that has been used in this work is lattice energy minimisation. This technique enables lattice energies to be calculated and the associated minimum energy structures to be obtained. It relies on the availability of interatomic potentials to describe the interactions of atoms in the crystal; the potential model used for zeolites has been applied to a wide range of ionic and semi-ionic solids, and the parameters have been used in a successful simulation of the structures of α- quartz and its polymorphs(1). An important feature of this model is the inclusion of a 3 body term to account for covalent effects in silicon-oxygen bonding.

A second derivative minimisation method has been used in all calculations; it should be noted that in the case of silicalite, the CRAY X-MP/48 was required for the calculations.

Results and Discussion

The work carried out falls into two sections. First, Na^+ Zeolite A has been studied extensively, since reliable experimental data exist for this zeolite which enable the computer simulation methods to be tested. Secondly, the relative stabilities of a range of zeolites have been calculated.

In the case of Na^+ zeolite A, a number of potential models have been used, ranging from a rigid ion description of all ions to the use of the shell model to describe oxygen ion polarisability. In the simulations it is most important that the positions of the framework ions be accurately reproduced; the non-framework cations (in this case Na^+) are not so accurately located experimentally. This has been achieved in general, but some oxygen ion displacements are too large. Some refitting of the potential model (originally fitted to α-quartz) may be necessary.

In the case of calculations of relative stabilities, these have been obtained for the siliceous forms of zeolite A, faujasite and silicalite. Results are given in table 1. The corresponding value for α-quartz is given for comparison. It should be noted that these simulations were carried out to constant pressure, i.e. all strains, both internal and external, were removed.

An important extension of this work is the calculation of minimum Gibbs energies for these zeolites, as relative stability over a range of temperatures is important. This work is in progress.

Table 1

Lattice energies per SiO_2 unit after relaxation to constant pressure

	lattice energy/eV
Zeolite A	-123.66
Faujasite	-123.48
Silicalite	-123.89
quartz	-123.90

Acknowledgements

We are grateful to Shell Research BV for funding this work.

References

1. Sanders, M.J., Leslie, M. and Catlow, C.R.A., J.Chem.Soc.Chem.Commun. 1984, p1273.

SOME "AD HOC" NOTES ON ISOKINETIC AND (N,V,T) DYNAMICS

Les Woodcock

All equilibrium particle simulations comprise at least two stages; an equilibration period and a sample period. The relative computational requirements can vary enormously depending on the size of the system. For very large systems, > ~ 10000 particles the sample period for equilibrium properties may be instantaneous (one configuration). For very small systems eg. 2, any low energy configuration can be regarded as being in equilibrium. The computational overheads for equilibration of large systems with long relaxation time could be considerable; it is practical considerations such as these which will determine the choice of dynamical equations for the practitioner. The same applies to steady-state NEMD simulations.

When the non-equilibrium behaviour is of no interest the particles and momenta are set as close as possible to equilibrium. This usually involves placing the particles in a low-energy initial configuration and allocating a normal distribution of velocities. Irrespective of the mean and half-width of this initial velocity distribution $(\underline{v}_1 \ldots \underline{v}_N)$ the requisite initial kinetic energy corresponding to an instantaneous temperature T_o, defined by

$$3N^{\ddagger}k\ T_o = \Big(\sum_{i=1}^{N} \underline{p}_i^2/m\Big)_{t=0} = \Big\langle \sum_{i=1}^{N} \underline{p}_i^2/m \Big\rangle \qquad (1)$$

is <u>exactly</u> obtained by the scaling

$$(\underline{p}_1\ \ldots\ \underline{p}_N)_{T_o} = f_o\ m(\underline{v}_1\ \ldots\ v_N)_{\text{initial}} \qquad (2)$$

The scaling factor f_o is defined by

$$f_o^2 = \frac{3N^{\ddagger}k\ T_o}{\sum_{i=1}^{N} \underline{p}_i^2/m} \qquad (3)$$

The simplest method of isothermal constraint dynamics is to incorporate this momentum renormalisation procedure continuously into the equations of motion. The objective is to generate isothermal (constant kinetic energy) dynamics with the minimum disturbance to the particle trajectories and momenta [1]. In the original continuous renormalisation method [2] a scaling factor f(t) defined as above was incorporated directly into the second-order central difference algorithm of Verlet [3]. The finite difference equations (1) and (2) together with equation (7) of reference [2] are equivalent to the constraint equations of motion

$$d\underline{r}_i = \underline{p}_i \; dt \tag{4}$$

$$d\underline{p}_i = \underline{F}_i \; dt + (f(t) - 1)\underline{p}_i \tag{5}$$

$$f^2(t) = \frac{3N^{\ddagger} k \; T_o m}{\sum\limits_{i=1}^{N} \left(\underline{p}_i + \underline{F}_i \; dt\right)^2} \tag{6}$$

In equations (4) to (6) the force $\underline{F}_i$ is $\nabla\phi(\underline{r}_i)$ where ϕ_i is the potential at $\underline{r}_i$.

If we substitute into equation (5) for f and square the bracket we obtain the continuous renormalisation equation for the acceleration

$$d\underline{p}_i = \underline{F}_i \; dt + \left(\left(\frac{3N^{\ddagger} k \; T_o m}{\sum\limits_{i=1}^{N} \underline{p}_i^2 + \sum\limits_{i=1}^{N} 2\underline{p}_i \; \underline{F}_i \; dt + \sum\limits_{i=1}^{N} \left(\underline{F}_i \; dt\right)^2}\right)^{1/2} - 1\right) \underline{p}_i \tag{7}$$

substituting for T_o from equation (1), expanding the inner bracket, and taking the limit dt → 0 gives

$$d\underline{p}_i = \underline{F}_i \; dt - \frac{\sum\limits_{i=1}^{N} \underline{p}_i \cdot \underline{F}_i}{\sum\limits_{i=1}^{N} \underline{p}_i^2/m} \; \underline{p}_i \; dt \tag{8}$$

Equation (8) is the isokinetic constraint equation of motion used by

Hoover et al.(4) and derived by Evans et al (5) from Gauss's principle minimum constraint using a Lagrange undetermined multiplier. The derivati and some applications are reviewed by Evans and Morriss [1] where it is referred to as the method of Gaussian isokinetic dynamics.

Equations (1) to (8) show that the methods of continuous renormalisation [2] and Gaussian isokinetic dynamics are essentially the same. That the equations of motion (4-6) lead to isokinetic dynamics can be shown by deriving f from the constraint, additional to equation (1) for the average T_o, that the time-derivative of the "instantaneous temperature" be zero, i.e.

$$\frac{dT(t)}{dt} = \frac{d}{dt}\,\frac{\sum_{i=1}^{N} \underline{p}_i^2/m}{3N^{\ddagger}k} = \frac{2\sum_{i=1}^{N} \underline{p}_i\cdot\underline{F}_i}{3N^{\ddagger}km} = 0 \qquad (9)$$

substituting in equation (9) for $\underline{F}_i(t)$ from equation (5) gives the exact expression for f consistent with the constraint equation (9)

$$\frac{2}{3N^{\ddagger}k}\sum_{i=1}^{N}\left(\frac{d\underline{p}_i + (f-1)\underline{p}_i}{dt}\right)\underline{p}_i = 0 \qquad (10)$$

$$\therefore \sum_{i=1}^{N} \underline{F}_i\cdot\underline{p}_i = -\sum_{i=1}^{N}\frac{(f-1)\underline{p}_i^2/m}{dt} \qquad (11)$$

$$\therefore f = 1 + \frac{\sum_{i=1}^{N} \underline{F}_i\cdot\underline{p}_i}{\sum_{i=1}^{N} \underline{p}_i^2/m}\,dt \qquad (12)$$

[Interpretation of f : time derivative of (f-1) is a moderating factor which slows or speeds all the particles uniformly in momentum space].

The formal proof that this method generates truly isokinetic dynamics and, simultaneously reproduces the distribution in coordinate space of a canonical ensemble of statistical thermodynamics has been given recently by Nose [6].

Equation (6) is preferred to equation (12) for f in the implementation of these equations into a finite difference integration scheme because the continuous renormalisation has the advantages that:

(i) the reference temperature T_o enters the equations-of-motion
(ii) it is self-starting
(iii) it is more efficient for the equilibration period
and (iv) it is self-stabilising up to much larger values of the finite time difference Δt.

That the continuous renormalisation method is practicable for the various finite difference algorithms normally employed for Newtonian MD has been demonstrated by many comparisons with N,V,E microcanonical calculations on similar systems. Actually it is generally found to stabilise the algorithms to larger values of the finite difference Δt. The net effect, however, of the temptation to use a larger Δt, is to unwittingly introduce some "Brownian motion" and this effect upon the time-dependent properties of the trajectories may be undesirable.

Several other schemes very closely related to the continuous renormalisation method have also appeared in the literature recently [7-10].

Brown and Clarke [7] have compared MD schemes, including a method which they refer to the "ad hoc" method of momentum scaling. Brown and Clarke's "ad hoc" method differs from the continuous renormalisation method in that the particles are slightly less constrained due to the absence of the $\underline{F}dt$ term in their scaling factor (equation (6)). The net effect of this is to introduce some fluctuations in T of the order $N^{-1/2}$, and linear in Δt; this was evidenced by the comparisons of Brown and Clark with their Gaussian isokinetic calculations at the same mean T. It would appear that any "ad hoc" variation from equations (4-6) would to some degree loosen the constraint of constant kinetic energy, as also would too large a finite time increment.

Haille and Gupta [8] have introduced an alternative method of momentum scaling; they propose the equations of motion

$$d\underline{p}_i = \underline{F}_i \, dt \qquad (13)$$

$$d\underline{r}_i = (\underline{p}_{i/m}) f_{HG} \, dt \qquad (14)$$

where f_{HG}, the momentum scaling factor, is defined as f_o in equation (3). As with the "ad hoc" method of Brown and Clarke, the Haille-Gupta momentum scaling equations lead to deviations linear or first order, in dt, but they derive the equations from a generalised driving potential and indicate that the canonical coordinate distributions is generated. Nose [6], however, suggested that these H-G equations yield a modified canonical coordinate distribution with differences of the order $N^{-1/2}$.

Broughton et al.[9] have examined the effect of discontinuous renormalisation or periodic scaling.

Heyes et al [10] have added two further "ad hoc" methods to the growing list of variations of renormalisation techniques.

Any number of "ad hoc" methods can be derived but only where the algorithm reduces to equations (4-6) as $\Delta t \to 0$ does it correspond to the continuous renormalisation method of reference [2].

Berendsen et al [11] have derived a set of constraint equations of motion for isothermal (but not <u>isokinetic</u>) behaviour. They begin with the Langevin equation for macromolecule behaviour but remove the stocastic element. The Berendsen equations are isothermal, deterministic but not time reversible, and in the present notation take the form

$$\underline{dp}_i = \underline{F}_i \, dt + \gamma \left(\frac{3N^{\ddagger} k \; T_o}{\sum\limits_{i=1}^{N} \underline{p}^2{}_i/m} - 1 \right) \underline{p}_i \, dt \qquad (15)$$

The constant γ is a coupling constant to an imaginary heat bath. When $\gamma dt = 0$ the system is effectively decoupled and Newtonian dynamics are recovered. When $\gamma dt = 1$ we obtain a constraint equation very closely related to the momentum scaling procedure

$$d\underline{p}_i = \underline{F}_i\, dt + (f_o^2(t) - 1)\, \underline{p}_i \tag{16}$$

All the previous constraint equations were derived without recourse to the total Hamiltonian equations of motion for both the system and heat bath. By fixing the constraint of constant T equation (9) a truly canonical distribution of both coordinates and momenta cannot be achieved since in a truly canonical (N,V,T) ensemble the total kinetic energy is distributed according to the Boltzmann probability

$$\frac{d \sum_{i=1}^{N} \underline{p}_i^2/m}{dn} \;\alpha\; \exp\left(\frac{\sum_{i=1}^{N} \underline{p}_i^2/m}{2k\, T_o}\right) \tag{17}$$

where n is the probability density.

This problem of simulating canonical kinetic energy fluctuations with reversible deterministic equations of motion has been solved by Nosé [6,13]. By writing down the extended system (i.e. system + heat exchanger) Hamiltonian and introducing a new scaling variable in time, Nosé was able to derive the deterministic constraint equations of motion that are both time-reversible and generate the canonical ensemble up to factors of the order D/6N where D is the number of degrees-of-freedom. The whole system may accelerate or decelerate to permit fluctuations in T without disturbing the coordinate distribution.

The Nosé ES (extended system) Hamiltonian for the system plus heat exchanger is

$$H_N = \Phi(\underline{r}_i \ldots \underline{r}_N) + \sum_i \frac{\underline{p}_i^2/2m}{s^2} + (N^{\ddagger} + 1)\, kT \log_e s + \frac{p_s^2}{2Q} \tag{18}$$

s is an arbitrary dimensionless time-scaling variable, p_s its conjugate momentum. Q (effective "mass") has units of energy time^2, p_s units of energy time.

The equations of motion derived by Nosé which correspond to his extended system Hamiltonian are

$$d\underline{r}_i = \frac{\underline{p}_i}{ms^2}\, dt \tag{19}$$

$$d\underline{p}_i = \underline{F}_i\, dt \tag{20}$$

$$d_s = \frac{p_s}{Q}\, dt \quad \sum_{i=1}^{N} \frac{\underline{p}_i^2\, (\underline{p}_i + \underline{F}_i\, dt)^2}{ms^3} - (N^{\ddagger} + 1)kT/s \quad dt \tag{21}$$

the additional degree of freedom $(N^{\ddagger} + 1)$ is due to the conjugate momentum of the heat exchanger.

Hoover [12] has observed that Nosé's equations can be written in a much more ammenable form by the simple expedient of reducing the global time-scale by the factor s, putting dt = sdt'

$$d\underline{r}_i = \frac{\underline{p}_i\, dt'}{ms} \tag{22}$$

$$d\underline{p}_i = \underline{F}_i\, sdt' \tag{23}$$

$$ds = \frac{sp_s\, dt'}{Q} \tag{24}$$

$$dp_s = \left(\sum_{i=1}^{N} \frac{p_i^2}{ms^2} - (N^{\ddagger} + 1)kT \right) dt' \tag{25}$$

re-writing the evolution equations (differentiate equation(22) with respect to time again and substitute from (23) and (24) for $d\underline{p}_i$ and ds.

The variable s is then eliminated by re-writing the second-order equation

$$\frac{d^2\underline{r}_i}{dt'^2} = \frac{1}{s}\, \frac{d\underline{p}_i/m}{dt'} - \frac{\underline{p}_i}{m_s}\, \frac{1}{s}\, \frac{ds}{dt'} \tag{26}$$

substitute from equation (24) for ds/s

$$= \frac{\underline{F}_i}{m} - \frac{d\underline{r}_i}{dt'}\,\frac{p_s}{Q} \tag{27}$$

The Nosé-Hoover canonical equations of motion are then (redefining dt)

$$d\underline{r}_i = \underline{p}_i/m \; dt \tag{28}$$

$$d\underline{p}_i = \frac{\underline{F}_i}{m}\,dt - \frac{p_s}{Q}\,\underline{p}_i \; dt \tag{29}$$

$$dp_s = \left(\frac{\sum_{i=1}^{N} \underline{p}_i^2/m - NkT}{Q} \right) dt \tag{30}$$

Any choice of the constant Q will yield the canonical equations so for practical purposes it is convenient to eliminate Q also by setting

$$Q = 3NkT(\Delta t)^2 \tag{31}$$

In this case the more specific equations of motion can then be simplified into a more recognisable form

$$\underline{dp}_i = \underline{F}_i \; dt - \left(\frac{p_s}{3NkTdt}\right) \underline{p}_i \tag{32}$$

denoting the dimensionless conjugate heat exchanger momentum as π_s then

$$d\pi_s = (f_o^2 - 1) \tag{33}$$

is <u>independent</u> of the time increment in the integration of the equations of motion.

Thus the Nosé-Hoover equation in a form suitable for conversion to a finite difference algorithm is

$$d\underline{p}_i = \underline{F}_i(t)\,dt - \int_0^t (f_o^2 - 1)\,\frac{dt}{t}\,\underline{p}_i \,. \tag{34}$$

Alternatively, for most practical applications imaginable, we have a practicable simple generalisation of the equations of motion

$$dp_i = \underline{F}_i\,dt + (f^n - 1)\,\underline{p}_i \tag{35}$$

n = 0 Newtonian
n = 1 Continuous renormalisation isokinetic
n = 2 Isothermal

Example: Verlet algorithm

$$\left.\begin{aligned} m\Delta\underline{r}_i &= \underline{p}_i(t^-)\Delta t + \underline{F}_i(t)\Delta t^2 - (\pi_s + f_o^2 - 1)\underline{p}_i(t^-)\Delta t \\ \Delta\underline{p}_i &= \underline{F}_i(t)\Delta t - (\pi_s + f_o^2 - 1)\underline{p}_i(t^-) \\ \Delta\pi_s &= (f_o^2 - 1) \end{aligned}\right\}\text{Nosé-Hoover} \tag{36}$$

or for the simple generalised form

$$m\Delta\underline{r}_i = \underline{p}_i(t^-)\Delta t + \underline{F}_i(t)\Delta t^2 - (f^n - 1)\underline{p}_i(t^-)\Delta t \tag{37}$$

If anyone were to find any differences between the results obtained from amongst the above methods which significantly affect applications, e.g. comparisons with experiment or theory, the topic would be of more interest. Differences between the ensembles become negligible anyhow for a system of sufficient size.

References

[1] D.J. Evans and G.P. Morriss, Comp. Phys. Report 1, 297 (1984)

[2] L.V. Woodcock, Chem. Phys. Lett. 10, 257 (1971)

[3] L. Verlet, Phys. Rev. 159, 98 (1967)

[4] W.G. Hoover, A.J.C. Ladd and B. Moran, Phys. Rev. Lett. 48, 1818 (1982) see also D.J. Evans, J. Chem. Phys. 78, 3297 (1983)

[5] D.J. Evans, W.G. Hoover, B.J. Failor, B. Moran and A.J.C. Ladd, Phys. Rev. A28, 1016 (1983)

[6] S. Nosé, Mol. Phys. 52, 255 (1984); J. Chem. Phys. 81, 511 (1984)

[7] D. Brown and J.H.R. Clarke, Mol. Phys. 51, 1243 (1984)

[8] J.M. Haille and S. Gupta, J. Chem. Phys. 17,3067 (1983)

[9] J.Q. Broughton, G.N. Gilmer, J.D. Weeks, J. Chem. Phys. 75, 5128 (1984)

[10] D.M. Heyes, Chem. Phys. 82, 285 (1983); see also D.M. Heyes et al CCP5 Newsletter No.17 page 25 June (1985)

[11] H.J.C. Berendsen, J.P.M. Patma, W.F. van Gunsteren, A. di Nola and J.R. Haak, J. Chem. Phys. 81, 3684 (1984)

[12] W.G. Hoover, Phys. Rev. A31, 1695 (1985)

[13] D.J. Evans and W.G. Hoover, Ann. Rev. Fluid Mech. 18, 243 (1986)

VECTORISING YOUR MD PROGRAM FOR THE CYBER 205
THE BRODE AND AHLRICHS WAY

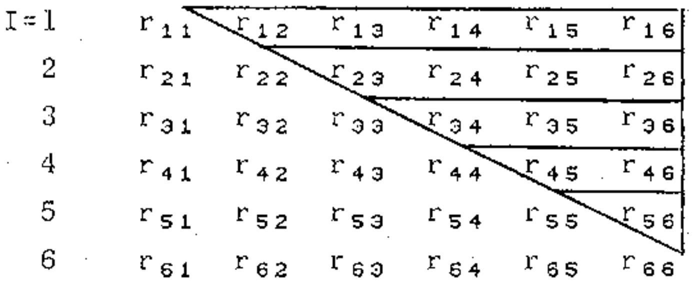
by David Brown, Chemistry Department, UMIST.

As a regular reader of this illustrious, World renowned informal newsletter I have been surprised that little, if anything, has appeared in its pages concerning the adaptation of MD programs to take advantage of the "vector" capability of the CYBER 205. In Britain access to the CYBER 205 at the University of Manchester Regional Computing Centre (UMRCC) has now been possible for over two years and despite some early teething problems, with compiler bugs and fragile links with the front-end, is now providing a fairly robust service. It seems reasonable to assume then that many people have already managed to vectorise their programs but have not taken up the unique opportunity that this newsletter provides of communicating their experience directly to those most likely to be interested. I have, therefore, taken it upon myself, at least partially, and *under absolutely no duress at all from the Editor-in-chief (Bill Smith)*, to redress this balance. Hopefully others will find faults with what I'm about to relate and will be spurred on to point these out in an article of their own.

As mentioned in the title, the method I have used has been lifted wholesale from a paper by Brode and Ahlrichs [Computer Physics Communications, 42, 51, (1986)] who report that significant savings (93%) in CPU time can be achieved using it. There are, however, some slight technical differences between my own implementation and that originally described to which I will allude in due course. Only a brief resumé of the method will be given here. For a fuller description the reader is directed towards the original article.

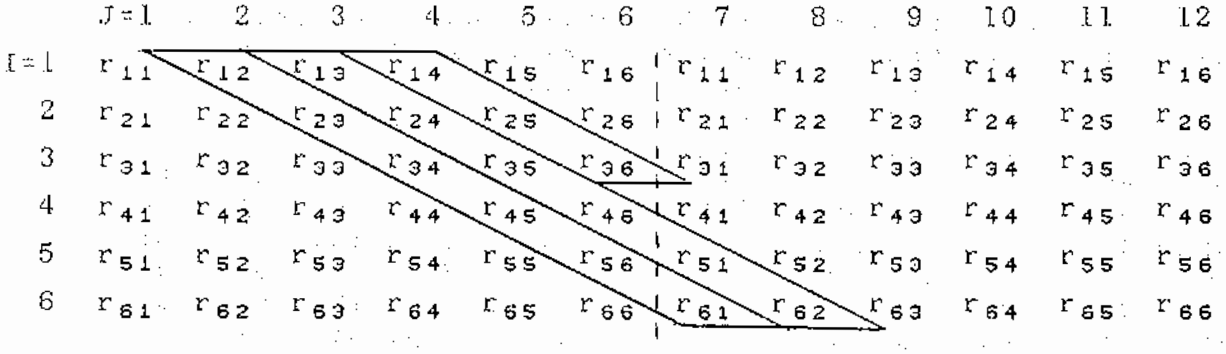
METHOD

In a conventional MD simulation the vast majority of the time is spent evaluating the forces between all possible interacting pairs. Schematically the conventional order of evaluating pair separations ($r_{ij}=r_i-r_j$), and hence forces, is shown below for a system of just N=6 particles.



$$\begin{array}{c|cccccc}
 & J=1 & 2 & 3 & 4 & 5 & 6 \\
I=1 & r_{11} & r_{12} & r_{13} & r_{14} & r_{15} & r_{16} \\
2 & r_{21} & r_{22} & r_{23} & r_{24} & r_{25} & r_{26} \\
3 & r_{31} & r_{32} & r_{33} & r_{34} & r_{35} & r_{36} \\
4 & r_{41} & r_{42} & r_{43} & r_{44} & r_{45} & r_{46} \\
5 & r_{51} & r_{52} & r_{53} & r_{54} & r_{55} & r_{56} \\
6 & r_{61} & r_{62} & r_{63} & r_{64} & r_{65} & r_{66}
\end{array}$$

This is achieved in Fortran quite simply within a double loop in which the first index, I, runs from 1 to N-1 and the second, J, runs from I+1 to N. On a scalar processor this represents an easy and efficient way of calculating the matrix for a reasonable number of particles, i.e. N of order 10^2. On the CYBER 205 though there are distinct disadvantages with this approach. Firstly, the vector lengths are short, at most N-1 and, secondly, they become shorter as I→N. The CYBER 205, however, only starts to approach its asymptotic speed when vector lengths are of order 10^3, due to penalties incurred in starting up an operation. Now consider the following scheme where the interaction matrix and an identical copy have been juxtaposed



$$\begin{array}{c|cccccc|cccccc}
 & J=1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 \\
I=1 & r_{11} & r_{12} & r_{13} & r_{14} & r_{15} & r_{16} & r_{11} & r_{12} & r_{13} & r_{14} & r_{15} & r_{16} \\
2 & r_{21} & r_{22} & r_{23} & r_{24} & r_{25} & r_{26} & r_{21} & r_{22} & r_{23} & r_{24} & r_{25} & r_{26} \\
3 & r_{31} & r_{32} & r_{33} & r_{34} & r_{35} & r_{36} & r_{31} & r_{32} & r_{33} & r_{34} & r_{35} & r_{36} \\
4 & r_{41} & r_{42} & r_{43} & r_{44} & r_{45} & r_{46} & r_{41} & r_{42} & r_{43} & r_{44} & r_{45} & r_{46} \\
5 & r_{51} & r_{52} & r_{53} & r_{54} & r_{55} & r_{56} & r_{51} & r_{52} & r_{53} & r_{54} & r_{55} & r_{56} \\
6 & r_{61} & r_{62} & r_{63} & r_{64} & r_{65} & r_{66} & r_{61} & r_{62} & r_{63} & r_{64} & r_{65} & r_{66}
\end{array}$$

This time all possible interactions have been taken, as $r_{ij}=-r_{ji}$, but the vector length has been kept to N except, in this case, for the last one which equals N/2. Of course, there are always (N-1)/2 blocks of N interactions, so for an *odd* number of particles there would be an integer number of blocks. This kind of procedure can be realised on the computer by doubling the length of the position arrays, such that $r_{i+N}=r_i$, and also the force arrays. A double loop could then be performed in which the outer loop controller takes values of the difference in the *indices of the arrays* J-I=1,2,3...etc. whilst the inner one runs from 1 to N *or until all possible interactions have been taken.* Then the total force will be given by f_i+f_{i+N}. In practice several blocks of N interactions are processed at the same time using additional vectors of length ~5000 so as to improve efficiency.

FORTRAN 200 CODE

To demonstrate the simplicity of this method selected sections of a "typical" MD code for an equilibrium simulation of a single component atomic system, interacting through a Lennard-Jones 12-6 potential, will be given.

The positions of the N particles reside in the arrays X, Y and Z of dimension N2=2*N and are contained in a periodic cube such that all coordinates lie within the range -FAC and +FAC. The forces will be accumulated in the vectors FX, FY and FZ again of length N2. All the other vectors used V1, V2, V3, V4, R2, XIJ, YIJ, ZIJ including the BIT VECTOR BV are of length NVECL where NVECL is usually, though not necessarily, a multiple of N in the region of 5000. Use of FORTRAN 200 shorthand has been used throughout so statements such as

```
      A(1;N)=B(1+N;N)**2
```

are short for

```
      DO 10 I=1,N
      A(I)=B(I+N)**2
   10 CONTINUE
```

Another way this can be written makes use of array DESCRIPTORs which also have to be declared. These are all suffixed with a "D" so as to avoid confusion with scalars. A descriptor contains a starting address and a length both set by an ASSIGN statement. The example above would then look like

```
      ASSIGN AD,A(1;N)
      ASSIGN BD,B(1+N;N)
      AD=BD**2
```

WARNING!! As the code given below has been lifted and adapted from more complicated programs it will not in itself have been tested on the computer. There remains, therefore, the possibility, although very slight, that it contains one or two small buggettes.

```
:
:
C     Declare arrays, descriptors and bit vectors etc.
C
      REAL X(N2),Y(N2),Z(N2),FX(N2),FY(N2),FZ(N2)
      REAL XIJ(NVECL),YIJ(NVECL),ZIJ(NVECL),R2(NVECL),
     +V1(NVECL),V2(NVECL),V3(NVECL),V4(NVECL)
      BIT BV(NVECL),BVD
      DESCRIPTOR BVD,XIJD,YIJD,ZIJD,R2D,V1D,V2D,V3D,V4D
C
:
:
C
C     Calculate from the number of interactions, NITCC,
C     the maximum number of blocks of N that can be processed
C     at any one time, NMAXCC, and the number of batches
C     required to account for all interactions, NTIMCC.
C
      NITCC=NINT(0.5*N*(N-1))
      NMAXCC=NVECL/N
      MAXCC=NMAXCC*N
      NTIMCC=NITCC/MAXCC
      MTIMCC=NTIMCC*MAXCC
      IF(MTIMCC.NE.NITCC)NTIMCC=NTIMCC+1
C
:
:
C
C     Zero potential energy and force accumulators.
C
      TCCPEN=0.0
      FX(1;N2)=0.0
      FY(1;N2)=0.0
      FZ(1;N2)=0.0
C
```

```
C     Normalize coordinates using RFAC=1.0/FAC so that they
C     lie between -1 and +1.
C
      X(1;N)=X(1;N)*RFAC
      Y(1;N)=Y(1;N)*RFAC
      Z(1;N)=Z(1;N)*RFAC
C
C     Copy coordinates onto the 1+N to N2 elements.
C
      X(1+N;N)=X(1;N)
      Y(1+N;N)=Y(1;N)
      Z(1+N;N)=Z(1;N)
C
C     Zero counters and start loop over the number of batches.
C
      L=0
      DO 2000 K=1,NTIMCC
      LL=0
C
C     Calculate the present value of the difference in
C     indices, JI=J-I.
C
      JI=(K-1)*NMAXCC
C
C     Loop over the number of blocks of N interactions in one
C     batch
C
      DO 2010 M=1,NMAXCC
C
C     Increment index difference counter
C
      JI=JI+1
C
C     Calculate the number of interactions in this set, JMAX,
C     allowing for the possibility that JMAX=N/2 or 0.
C
      JMAX=NITCC-L
      JMAX=MIN0(N,JMAX)
      IF(JMAX.EQ.0) GOTO 2030
C
C     Store separation vectors in elements offset by LL
C
      XIJ(LL+1;JMAX)=X(1;JMAX)-X(JI+1;JMAX)
      YIJ(LL+1;JMAX)=Y(1;JMAX)-Y(JI+1;JMAX)
      ZIJ(LL+1;JMAX)=Z(1;JMAX)-Z(JI+1;JMAX)
C
C     Update offsets
C
      L=L+JMAX
      LL=LL+JMAX
 2010 CONTINUE
 2030 CONTINUE
C
C     Processing the LL interactions stored
C
      ASSIGN BVD,BV(1;LL)
      ASSIGN R2D,R2(1;LL)
      ASSIGN XIJD,XIJ(1;LL)
      ASSIGN YIJD,YIJ(1;LL)
```

```
      ASSIGN ZIJD,ZIJ(1;LL)
      ASSIGN V4D,V4(1;LL)
C
C     Apply periodic boundaries making use of vector function
C     VAINT which returns into the target vector, in this
C     case V4D, the integer part of the subject vector as a
C     real.
C
      XIJD=XIJD-2.0*VAINT(XIJD;V4D)
      YIJD=YIJD-2.0*VAINT(YIJD;V4D)
      ZIJD=ZIJD-2.0*VAINT(ZIJD;V4D)
C
C     Calculate the square of the separation
C
      R2D=XIJD**2+YIJD**2+ZIJD**2
C
C     Set the elements of the bit vector to 1 if r² is
C     less than the square of the potential cutoff, CUTSQ.
C
      BVD=R2D.LT.CUTSQ
C
C     Count the number of interactions within cutoff using
C     special Q8 routine, Q8SCNT.
C
      NN=Q8SCNT(BVD)
C
C     Check for no contributing interactions
C
      IF(NN.EQ.0) GOTO 2000
C
C     Assign some descriptors to new length NN
C
      ASSIGN V1D,V1(1;NN)
      ASSIGN V2D,V2(1;NN)
      ASSIGN V3D,V3(1;NN)
      ASSIGN V4D,V4(1;NN)
C
C     Use the Q8VCMPRS instruction to compress the list of
C     square separations down to just those that contribute.
C
      V2D=Q8VCMPRS(R2D,BVD;V2D)
C
C     Re-assign array descriptor.
C
      ASSIGN R2D,R2(1;NN)
C
C     Calculate terms in potential and force using
C     CON1=σ²/FAC**2  and  CON2=48*FAC*ϵ/σ²
C
      R2D=CON1/V2D
      V2D=R2D**3
      V1D=V2D**2
      V3D=V1D-V2D
      V4D=CON2*R2D*(V1D-0.5*V2D)
C
C     Accumulate total potential energy (/4ϵ) using the Q8SSUM
C     instruction.
C
      TCCPEN=TCCPEN+Q8SSUM(V3D)
```

```
C
C     Compress down the components of the separation vector
C
      V1D=Q8VCMPRS(XIJD,BVD;V1D)
      V2D=Q8VCMPRS(YIJD,BVD;V2D)
      V3D=Q8VCMPRS(ZIJD,BVD;V3D)
C
C     Re-assign separation descriptors
C
      ASSIGN XIJD,XIJ(1;NN)
      ASSIGN YIJD,YIJ(1;NN)
      ASSIGN ZIJD,ZIJ(1;NN)
C
C     Calculate components of the force
C
      XIJD=V1D*V4D
      YIJD=V2D*V4D
      ZIJD=V3D*V4D
C
C     Accumulate the potential contribution to the pressure
C     tensor using the Q8SDOT instruction which returns the
C     sum of the dot product of two vectors.
C
      A11=A11+Q8SDOT(V1D,XIJD)
      A12=A12+Q8SDOT(V1D,YIJD)
      A13=A13+Q8SDOT(V1D,ZIJD)
      A22=A22+Q8SDOT(V2D,YIJD)
      A23=A23+Q8SDOT(V2D,ZIJD)
      A33=A33+Q8SDOT(V3D,ZIJD)
C
C     Re-assign descriptors for expansion.
C
      ASSIGN V1D,V1(1;LL)
      ASSIGN V2D,V2(1;LL)
      ASSIGN V3D,V3(1;LL)
C
C     Using the Q8VXPND instruction the force arrays are
C     expanded up to their original length using the control
C     bit vector BV to insert zeroes into non-contributing
C     interactions.
C
      V1D=Q8VXPND(XIJD,BVD;V1D)
      V2D=Q8VXPND(YIJD,BVD;V2D)
      V3D=Q8VXPND(ZIJD,BVD;V3D)
C
C     Calculate number of interactions already processed.
C
      LOLD=L-LL
C
C     Assign forces to particles using the reverse procedure
C     as that used above to assign separations and Newton's
C     law fij=-fji.
C
      LL=0
      JI=(K-1)*NMAXCC
      DO 2120 M=1,NMAXCC
      JI=JI+1
      JMAX=NITCC-LOLD
      JMAX=MIN0(N,JMAX)
```

```
      IF(JMAX.EQ.0) GOTO 2130
      FX(1;JMAX)=FX(1;JMAX)+V1(LL+1;JMAX)
      FY(1;JMAX)=FY(1;JMAX)+V2(LL+1;JMAX)
      FZ(1;JMAX)=FZ(1;JMAX)+V3(LL+1;JMAX)
      FX(JI+1;JMAX)=FX(JI+1;JMAX)-V1(LL+1;JMAX)
      FY(JI+1;JMAX)=FY(JI+1;JMAX)-V2(LL+1;JMAX)
      FZ(JI+1;JMAX)=FZ(JI+1;JMAX)-V3(LL+1;JMAX)
      LOLD=LOLD+JMAX
      LL=LL+JMAX
 2120 CONTINUE
 2130 CONTINUE
 2000 CONTINUE
C
C     End of force calculation.
C
C     Add forces in array elements I and I+N to obtain
C     total force on particle I.
C
      FX(1;N)=FX(1;N)+FX(1+N;N)
      FY(1;N)=FY(1;N)+FY(1+N;N)
      FZ(1;N)=FZ(1;N)+FZ(1+N;N)
C
:
:
```

It should be noted that with the vectorisation of the forces loop the rest of the integration algorithm can start to account for a sizeable percentage of the overall CPU time used. It is, therefore, essential that all these other parts of the code are also vectorised. This is generally straightforward as they usually consist of just N-particle loops.

DISCUSSION

The scheme described differs slightly from that of the originators in three main respects :-

1) The separation vectors are compressed before multiplying by V4 to obtain the resultant forces instead of expanding V4 and then multiplying by XIJ etc.

Although more compressions and expansions are required this process represents a significant saving in CPU time, particularly if the pressure tensor is being calculated.

2) Exact force and potential calculations are carried out rather than using tabulated forces and potentials.

For inverse even power potentials there is little saving using tables by the time all the gathering and interpolating has been done. If constant temperature algorithms are being used in conjunction with constant shear rate or stress methods a high degree of accuracy is required in the force calculation to prevent a drift in the constrained properties.

3) Calculation of g(r) is omitted from the main loop.

Accumulating the radial distribution function presents quite a problem as it is inherently non-vectorisable due to the random access of array elements. If needs be a separate loop could be constructed containing the necessary Fortran and accessed periodically instead of the above loop. As configurations tend to be well correlated for many steps there is little point accumulating g(r) too often. For my own part I prefer to store coordinates etc. on magnetic tape for processing later and calculate g(r) if and when necessary.

Another point to note is that correlation functions have also been calculated from data stored on magnetic tape using the Fourier transform method described by Smith [see CCP5 Newsletters 5 and 7]. This is a very efficient way of calculating correlation functions as the fast Fourier transform (FFT) library of routines on the CYBER 205 is also vectorized.

In all, the method described results in increases of speed by a factor of about 15 compared to a scalar optimized program run on either the CDC 7600 or CYBER 176 machines also at UMRCC (though, sadly, soon to depart for that big computer centre in the sky). Although this comparison does not include the extra time needed to calculate g(r). Even so the increase in speed is at least an order of magnitude, which is not to be sneezed at. It is also possible that the above scheme may improve performance figures on CRAY machines as well. This may have already been tried by someone, in which case I would like to hear from them.

MINIDAP AT DAPSU

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DAPSU (DAP Support Unit) took delivery of a prototype Mini-DAP as part of a collaboratve grant between SERC and ICL during April of last year. Since then the mini-DAP has been in daily use, producing demonstrations for a variety of projects including hydrodynamics, molecular graphics, finite element work and for general development.

DAPs (Distributed Array Processors) are already well known in the molecular simulation field and various articles describing their use have appeared in this newsletter and other publications (see for example references at end). Essentially a DAP is a collection of individual processors all of which are simultaneously able to execute the same instruction. Each processor has its own memory but also has links with its four nearest neighbours and 'highways' are present for broadcasting data simultaneously to all processors. In addition each processor has its own on/off switch, which is used, for example, to map directly onto conditional clauses in user programs, thus implementing them very efficiently.

Mini-DAP

Mini-DAP grew out of a previous version of the DAP, one of which was installed at QMC in 1980 and has been used by the scientific community worldwide, though mainly in this country, since then. The term mini-DAP is deserved for two reasons;

1) The original DAP at QMC was built in MSI (medium scale integration) technology and occupied several double filing cabinet size boxes, whereas the mini-DAP is built in LSI (large scale integration) and fits under a table.

2) MSI DAPs have 4096 processors, mini-DAP has 1024.

The new production version of DAP is primarily intended for use in a single user workstation environment with the DAP as an attached processor to either a SUN or a microVAX. The prototype at QMC is currently attached to a PERQ II.

Although the DAP was originally manufactured by ICL, since November 1986 the DAP has been placed in the control of a new company called 'Active Memory Technology' (AMT) who are exploiting the DAP comercially. AMT has close links with DAPSU (several ex DAPSU members have become founder members of AMT) and many of the current mini-DAP demonstrations to be seen at computer exhibitions were written by DAPSU staff.

Mini-DAP Software Environment

Mini-DAP has a very similar software environment to the MSI DAP, although there are four significant changes,

1) The array size is 1024 instead of 4096

2) The data area in DAP and HOST are no longer shared

3) A fast I/O channel (FIO) operating at rates up to 40 Mbytes/sec is available

4) Asynchronous working of DAP and HOST is possible.

1) This change is fundamental and will require many of the existing DAP programs which make specific reference to either the total number of processors (4096) or edge size (64) of the MSI DAP, to be altered. The syntax of the DAP FORTRAN declarations for vector and matrix working, e.g.

```
REAL*3 R( ), S( )
```

remains the same, but the value of the constrained dimensions is 32 for the mini-DAP.

2) Whereas the MSI DAP used common store for DAP and HOST sections of the program, mini-DAP requires data to be sent to, or received from the DAP. This transfer is actually performed by the HOST program and two routines DAPSEN and DAPREC are provided for this purpose. Conversion of data to DAP storage mode must still be carried out as on the MSI DAP.

3) The fast I/O provides new ways of accessing the results of a DAP run, or of inputting data quickly. For example, a video board has been designed to sit on the FIO enabling the DAP store to be used in the same way as a conventional frame store, but at a much higher rate. The DAP FIO is asynchronous with the working of the DAP, so that data can be fed in or read out whilst DAP processing continues.

4) The ability to use DAP and HOST machines asynchronously creates several programming possibilities. Some of the current demonstrations which use external graphics processors to display their results have the DAP calculating the next picture, while the HOST is displaying the current one. Semaphore systems have been devised to allow either machine to poll the other to find if it has finished the next step in the calculations.

At DAPSU the prototype mini-DAP has a full set of system software allowing programs to be compiled, ran and interactively 'debugged'. In addition DAPSU staff have been converting routines from the MSI DAP subroutine library for use on the mini-DAP and ~100 routines will be available in the first release.

ICL, who have rights to mini-DAP for defence contracts in this country are supplying software for use with the video board and Intercept Systems, a software house are supplying software for a variety of DAP related problems. Further graphics work will continue at DAPSU.

Performance

It is generally reckoned that the MSI DAP was approximately one third the power of the CRAY 1S for computationally intensive calculations. Our own estimate in DAPSU show the prototype mini-DAP to be one third the power of the MSI DAP and based on discussions with AMT we believe the production machines will be one half the power of the MSI DAP, 1/6th of the CRAY 1S. Memory sizes on production machines will range from 4-128 Mbyte.

Support for mini-DAP

At present there is no front line support for mini-DAPs. However anyone wishing to use the mini-DAP in a 'pump-priming' fashion should write to Carol Hirst at DAPSU explaining what they would like to do, so that, where possible, time and resources can be made available.

The possibility of installing a large (32 Mbyte) mini-DAP at QMC and using it to provide a national service, replacing the current ICL 2980/DAP service, is being explored. At this point in time the choice of HOST is unclear as is a start date for such a service. However it is envisaged that the two machines would run in parallel for a number of months before the 2980/DAP is removed, allowing users time to move from one DAP to the other.

In addition to this service a number of research groups are applying to various grant awarding bodies for the provision of their own mini-DAP.

References

See for example

Gauge Theory and Condensed Matter Calculations on an Edinburgh DAP : MG/11849 R.A.Cowley, G.S.Pawley, D.J.Wallace & J.G.Burns Final Report 10/9/85

Parallel Programming for Lattice Problems on the DAP : D.Fincham and N.Quirke CCP5 Newsletter No.11 (Dec. 83)

Quasicritical Behaviour and First-Order Transition in the *d = 3* Random-Field Ising Model : A.P.Young & M.Nauenberg Phys. Rev. Letters 54-22 June 1985

Order of the phase Transition of a Two Dimensional Rotor System: A. Hurler Zeischrift fur Physik B, 61-5

CCP5 LITERATURE SURVEY 1986.

We present in the following pages the CCP5 literaure survey for the year 1986. The survey was conducted with the help of the INSPEC service at the University of London Computing Centre and we thank Dr. J. Altmann of U.L.C.C. for her essential contribution. Thanks are also due to Mrs. Anne Ireland of the Daresbury Reprographics Division for typing and sorting the entries appearing here and to Mrs. C.M. Smith for helping with the proof reading.

We invite readers who have knowledge of other relevant papers, articles or books to send us the details, which we shall pleased to publish in an Addendum in our next newsletter.

W. Smith

Abraham, F.F. and Broughton, J.Q.
Pulsed melting of silicon (111) and (100) surfaces simulated by molecular dynamics
Phys. Rev. Lett. 56 (1986) 734-7.

Abramo, M.C., Pizzimenti, G. and Carini, G.
Molecular dynamics of a silver borate glass
J. Non-Cryst. Solids, 85 (1986) 233-8.

Adamczyk, Z. and Nowotny, J.
Effect of segregation on near-surface and bulk transport phenomena in ionic crystals
J. Phys. and Chem. Solids 47 (1986) 11-27.

Aguilera-Navarro, V.C., Baker, G.A,., Jr., and De Llano, M.
Ground-state energy of jellium
Phys. Rev. B 32 (1985) 4502-6.

Ahlrichs, R., Bohm, H.-J., Hertz, H.G., et al
The hydration of F$^-$: an explicit demonstration of a basic discrepancy between NMR results and those obtained from various computations and neutron diffraction experiments
Z. Phys. Chem. Neue Folge 142 (1984) 67-80.

Ala-Nissila, T., Amar, J. and Gunton, J.D.
Wetting in the two-dimensional ANNNI model
J. Phys. A 19 (1986) L41-7.

Ala-Nissila, T., Gunton, J.D. and Kaski, K.
Kinetics of the order-disorder transition of the two-dimensional anisotropic next-nearest-neighbour ising model with Kawasaki dynamics
Phys. Rev. B 33 (1986) 7583-93.

Allen, M.P. and Marechal, G.
Non-equilibrium molecular dynamics simulation of a molecular fluid subjected to an oscillatory shear perturbation
Mol. Phys. 57 (1986) 7-19.

Allison, S.A., Northrup, S.H. and McCammon, J.A.
Extended brownian dynamics of diffusion controlled reactions
J. Chem. Phys. 83 (1985) 2894-9.

Amarendra, G. and Ananthakrishna, G.
Monte Carlo study of percolation of random discs in two dimensions: variable range interaction
Solid State Commun. 58 (1986) 873-5.

Amitrano, C., Bunde, A. and Stanley, H.E.
Diffusion of interacting particles on fractal aggregates
J. Phys. A 18 (1985) L923-9.

Anayev, Yu.A.
On the application of the Monte Carlo method to calculations of laser pumps
Opt. and Spektrosk. 58 (1985) 188-9.

Anderson, J., Ullo, J.J. and Yip, S.
Inelastic neutron scattering by benzene: direct spectral analysis using molecular dynamics simulation
Physica B and C 136 (1986) 172-6.

Angles D'Auriac, J.C. and Rammal, A.
Critical behaviour of the kinetic ising model on a fractal lattice
J. Phys. A 19 (1986) L655-61.

Aoki, N. Hasegawa, H. and Yasui, I.
X-ray diffraction studies and molecular dynamics calculations of the structure of alkali disilicate glasses
Yogyo-Kyokai-Shi (Japan), 94 (1986) 539-44.

Aoki, N., Yambe, S., Inoue, H., et al
An x-ray diffraction study of the structure of Na_2O, Al_2O_3, $2SiO_2$ glass
Phys. and Chem. Glasses, 27 (1986) 124-7.

Aquilanti, V. and Cavalli, S.
Coordinates for molecular dynamics; othogonal local systems
J. Chem. Phys. 85 (1986) 1355-61.

Aqvist, J.
A simple way to calculate the axis of an alpha-helix
Comput. and Chem. 10 (1986) 97-9.

Asanovich, V.Ya., Katysheva, L.V. and Ukhov, V.F.
On calculating the electronic structure of iron melts
Izv. Akad. Nauk. SSR Met. 4 (1984) 56-8.

Athienitis, A.K., Chandrashekar, M. and Sullivan, H.F.
Modelling and analysis of thermal networks through subnetworks for multizone passive solar buildings
Appl. Math. Modelling 9 (1985) 109-16.

Attard, G.S. and Williams, G.
Molecular dynamics of a smectic liquid-crystalline side-chain polymer in itw unaligned and aligned states as studied by dielectric relaxation spectroscopy
Liq. Cryst. 1 (1986) 253-69.

Aucouturier, M.
Grain boundary segregtion. Grain boundary diffusion
Polycrystalline Semiconductors: Physical Properties andApplications. Proc. Int. School of Materials.

Axe, J.D. and Yamada, Y.
Scaling relations for grain autocorrelation functions during nucleation and growth
Phys. Rev. B 34 (1986) 1599-606.

Baalss, D. and Hess, S.
Nonequilibrium molecular-dynamics studies on the anisotropic viscosity of perfectly aligned nematic liquid crystals
Phys. Rev. Lett. 57 (1986) 86-9.

Badke, R., Rittenberg, V. and Ruegg, H.
A test of conformal invariance: correlation functions on a disc
J. Phys. A 18 (1985) L867-71.

Bagmet, A.D. and Tsykalo, A.L.
Computer simulation study of the Frederics transition dynamics
Ukr. Fiz. Zh. 31 (1986) 387-93.

Balcelis, M., Giro, A. and Padro, J.A.
Correlations in the Ar-Kr liquid mixture
Physica A, 135A (1986) 414-25.

Ball, R.D.
Strong anharmonicity in ionic crystals: self-consistent phonons and shell models
J. Phys. C 19 (1986) 1293-309.

Baltar, V.L.V. and Pol, M.E.
On the Z(4) spin model
J. Phys. A 19 (1986) 743-9.

Bansil, R., Herrmann, H.J. and Stauffer, D.
Kinetic percolation with mobile monomers and solvents as a model for gelation
J. Polym. Sci. Polym. Symp. 73 (1985) 175-80.

Baranyai, A., Ruff, I. and McGreevy, R.L.
Monte Carlo simulation of the complete set of molten alkali halides
J. Phys. C 19 (1986) 453-65.

Barker, J.A.
Many-body interactions in rare gases: krypton and xenon
Phys. Rev. Lett. 57 (1986) 230-3.

Barnett, R.N., Cleveland, C.L. and Landman, U.
Structure and dynamics of a metallic glass: molecular-dynamics simulations
Phys. Rev. Lett. 55 (1985) 2035-8.

Barocchi, F., Spinelli, G. and Magli, R.
Molecular dynamics calculation of the density dependence of S(K) of krypton
J. Phys. Colloq. 46 (1985) 23-6.

Bartelt, N.C. and Einstein, T.L.
Finite-size effects on the critical structure factor of the two-dimensional ising model
J. Phys. A 19 (1986) 1429-38.

Bator, G., Jakubas, R., and Malarski, Z.
Molecular dynamics in the alpha-alpha-dicyclohexyl-cyclohexane-methanol single crystal $(C_6H_{11})_3COH)$
J. Phys. C 19 (1986) 2799-809.

Baumgartner, A.
Diffusion and Brownian motion of polymeric liquids
J. Polym. Sci. Polym. Symp. 73 (1985) 181-6.

Baumgartner, A.
Phase transitions of semiflexible lattice polymers
J. Chem. Phys. 84 (1986) 1905-8.

Baumgartner, A. and Muthukumar, M.
Disentangling of two intertwined chains
J. Chem. Phys. 84 (1986) 440-3.

Bedanov, V.M., Gadiyak, G.V. and Lozovik, Yu.E.
Melting of two-dimensional crystals
Zh.Eksp. and Teor. Fiz. 88 (1985) 1622-33.

Bedanov, V.M., Gadiyak, G.V., Lozovik, Yu.E.
Modified Lindemann criterion for two-dimensional melting
Fiz. Tverd. Tela 27 (1985) 2207-9.

Beenakker, C.W.J. and Ross, J.
Monte Carlo study of a model of diffusion-controlled reactions
J. Chem. Phys. 84 (1986) 3857-64.

Belashchenko, D.K.
Modelling of the structure of amorphous iron
Fiz. Met. and Metalloved. (USSR) 60 (1985) 1076-80.

Belyaev, A. and Palagashvili, E.
Clusters in binary alloy decay kinetics
Latv. PSR Zinat. Akad. Vestis. Fiz. Teh. Zinat. Ser. 2 (1986) 46-50.

Beniere, F. and Reddy, K.V.
Diffusion of heterovalent ions in ionic crystals
J. Phys. and Chem. Solids 47 (1986) 69-77.

Bergsma, J.P., Edelsten, P.M., Gertner, B.J., et al
Dynamics of the A+BC reaction in solution
Chem. Phys. Lett. 123 (1986) 394-8.

Berne, B.J.
Path integral Monte Carlo methods: static- and time-correlation functions
J. Stat. Phys. 43 (1986) 911-29.

Bernu, B., Hiwatari, Y. and Hansen, J.P.
Molecular dynamics simulation of the glass transition in binary mixtures of soft spheres
J. Phys. Colloq. 46 (1985) 323-7.

Bigot, B., Costa-Cabral, B.J. and Rivail, J.L.
Conformational equilibrium of 1,2-dichloroethane in methylchloride. A Monte Carlo simulation of the differential gauche-antisolvation
J. Chem. Phys. 83 (1985) 3083-94.

Billoire, A. and David, F.
Microcanonical simulations of randomly triangulated planar random surfaces
Phys. Lett. B 168B (1986) 279-83.

Binder, K.
Critical properties and finite-size effects of the five-dimensional Ising model
Z. Phys. B61 (1985) 13-23.

Binder, K., Landau, D.P. and Kroll, D.M.
Critical wetting with short-range forces: Is mean-field theory valid?
Phys. Rev. Lett. 56 (1986) 2272-5.

Binnig, G. and Rohrer, H.
Scanning tunnelling microscopic
Proc. 17th Int. Conf. on the Physics of Semiconductors (1985) 3-10.

Birshtein, T.M., Buldyrev, S.V. and Elyashevitch, A.M.
Monte Carlo simulation of the collapse transition of a two-dimensional polymer
Polymer 26 (1985) 1814-24.

Bishop, M. and Norcross, M.
The dispersion relation of the dynamic structure factor of one-dimensional Lennard-Jones fluids
Phys. Lett. A 115 (1986) 219-20.

Bishop, M., Michels, J.P.J and De Schepper, I.M.
The short-time behaviour of the velocity autocorrelation function of smooth, hard hyperspheres in three, four and five dimensions
Phy. Lett. 111A (1985) 169-70.

Blander, M., Saboungi, M.-L. and Rahman, A.
Molecular dynamics studies of complexing in binary molten salts. II. Molton M_3 Ax_6 and Ma_3X_{10}
J. Chem. Phys. 85 (1986) 3995-4004.

Boguslawski, P.
Electronic and crystal structure of semiconductors in pseudopotential theory
Acta Phys. Pol. A 69 (1986) 919-27.

Bohm, H.-J. and Ahlrichs, R.
The N_2-N_2 interaction - A theoretical investigation
Mol. Phys. 55 (1985) 1159-69.

Borstnik, B., Janezic, D. and Hadzi, D.
Monte Carlo study of ethanolamine-formic acid hydration. Effect of proton transfer
Theochem. 31 (1986) 341-52.

Branka, A. and Parrinello, M.
Free energy evaluation in the canonical molecular dynamics ensemble
Mol. Phys. 58 (1986) 989-93.

Bratko, D., Blum, L. and Luzar, A.
A simple model for the intermolecular potential of water
J. Chem. Phys. 83 (1985) 6367-70.

Bratko, D., Jonsson, B. and Wennerstrom, H.
Electrical double layer interactions with image charges
Chem. Phys. Lett. 128 (1986) 449-54.

Brey, J.J., Casado, J.M. and Morillo, M.
Spectral density for a non-linear Fokker-Planck model: Monte Carlo and analytical studies
Phys. Rev. A 32 (1985) 2893-8.

Brey, J.J., Casado, J.M. and Morillo, M.
Monte Carlo calculation of the asymptotic decay on the spectral density in a nonlinear stochastic system
Phys. Lett. A 112 (1985) 307-8.

Broughton, J.Q. and Gilmer, G.H.
Thermodynamic criteria for grain-boundary melting: a molecular-dynamics study
Phys. Rev. Lett. 56 (1986) 2692-5.

Broughton, J.Q. and Gilmer, G.H.
Molecular dynamics of the crystal-fluid interface. V. Structure and dynamics of crystal-melt systems
J. Chem. Phys. 84 (1986) 5749-58.

Broughton, J.Q. and Gilmer, G.H.
Molecular dynamics investigation of the crystal-fluid interface. IV. Free energies of crystal-vapor systems
J. Chem. Phys. 84 (1986) 5741-8.

Broughton, J.Q. and Gilmer, G.H.
Molecular dynamics investigation of the crystal-fluid interface. VI.
Excess surface free energies of crystal-liquid systems
J. Chem. Phys. 84 (1986) 5759-68.

Brown, D. and Clark, J.H.R.
Molecular dynamics computer simulation of polymer fiber microstructure
J. Chem. Phys. 84 (1986) 2858-65.

Bruce, A.D.
Universality in the two-dimensional continuous spin model
J. Phys. A 18 (1985) L873-7.

Buendia, G.M.
Comparative study of the discrete and the continuous Hubbard-Stratonovich transformation for a one-dimensional spinless fermion model
Phys. Rev. B 33 (1986) 3519-21.

Bug, A.L.R., Safran, S.A., Grest, G.S., et al
Do interactions raise or lower a percolation threshold?
Phys. Rev. Lett. 55 (1985) 1896-9.

Caffarel, M. and Claverie, P.
Treatment of the Schrodinger equation through a Monte Carlo method based upon the generalized Feynman-KAC formula
J. Stat. Phys. 43 (1986) 797-801.

Caillol, J.M. and Levesque, D.
Low-density phase diagram of the two-dimensional Coulomb gas
Phys. Rev. B 33 (1986) 499-509.

Caracciolo, S. and Glaus, U.
A new Monte Carlo simulation for two models of self-avoiding lattice trees in two dimensions
J. Stat. Phys. 41 (1985) 95-114.

Caracciolo, S. and Sokal, A.D.
Dynamic critical exponent of some Monte Carlo algorithms for the self-avoiding walk
J. Phys. A 19 (1986) L797-805.

Cardillo, M.J.
Helium diffraction as a probe of surface topography
Faraday Disc. Chem. Soc. No.80 (1985) 17-27.

Cardini, G., O'Shea, S.F. and Klein, M.L.
Gas-surface potential and the dynamics of overlayers
Faraday Disc. Chem. Soc. No.80 (1985) 227-38.

Ceccatto, H.A.
Effective discrete-time dynamics in Monte Carlo simulations
Phys. Rev. B 33 (1986) 4734-8.

Ceperley, D. and Alder, B.
Quantum Monte Carlo
Science 231 (1986) 555-60.

Ceperley, D.M.
The statistical error of Green's function Monte Carlo
J. Stat. Phys. 43 (1986) 815-26.

Ceperley, D.M. and Partridge, H.
The He_2 potential at small distances
J. Chem. Phys. 84 (1986) 820-1.

Chachaty, C.
Magnetic resonance spectra simulations applied to the molecular dynamics
of an anisotropic medium
J. Chim. Phys. and Phys. Chim. Biol. 82 (1985) 621-30.

Chaki, T.K. and Li, J.C.M.
Radiation damage in an amorphous Lennared-Jones solid. A computer
simulation
Phil. Mag. B51 (1985) 557-65.

Challa, M.S.S. and Landau, D.P.
Critical behaviour of the six-state clock model in two dimensions
Phys. Rev. B 33 (1986) 437-43.

Challa, M.S.S., Landau, D.P. and Binder, K.
Finite-size effects at temperature-driven first-order transitions
Phys. Rev. B 34 (1986) 1841-52.

Chapman, W. and Quirke, N.
Metropolis Monte Carlo simulation of fluids with multiparticle moves
Physica B and C 131B+C (1985) 34-40.

Cheng, H., Dutta, P., Ellis, D.E. et al
Molecular dynamics study a two-dimensional system with screened Coulomb interactions
J. Chem.Phys. 85 (1986) 2232-6.

Chen, S.-P., Egami, T. and Vitek, V.
Orientational ordering of local shear stresses in liquids: A phase transition
J. Non-Cryst. Solids 75 (1985) 449-54.

Chesnoy, J. and Weis, J.J.
Density dependence of the dephasing and energy relaxation times by computer simulations
J Chem. Phys. 84 (1986) 5378-88.

Ching, W.Y.
Electronic structures of crystalline Ni_3P and amorphous $Ni_{75}P_{25}$
J. Non-Cryst. Solids 75 (1985) 379-84.

Cieplak, P. and Geller, M.
Solvation of the tautomeric forms of 2-oxopyrimidine in carbon tetrachloride solution: A Monte Carlo simulation
Theochem. 25 (1985) 249-59.

Clarke, J.H.R. and Brown, D.
Molecular dynamics computer simulation of chain molecule liquids. I. The coupling of torsional motions to translational diffusion
Mol. Phys. 58 (1986) 815-25.

Clementi, E., Corongiu, G. and Detrich, J.H.
Parallelism in computational chemistry: applications in quantum and statistical mechanics
Physica B and C 131B+C (1985) 74-102.

Coker, D.F. and Watts, R.O.
Quantum simulation of systems with nodal surfaces
Mol. Phys. 58 (1986) 1113-23.

Collet, J. and Amand, T.
Model calculation of the laser-semiconductor interaction in subpicosecond regime
J. Phys. and Chem. Solids 47 (1986) 153-63.

Condon, J.H. and Ogielski, A.T.
Fast special purpose computer for Monte Carlo simulations in statistical physics
Rev. Sci. Instrum. 56 (1985) 1691-6.

Coniglio, A.
Droplet theory of phase transitions and metastability
Proc. Int. School of Physics 'Enrico Fermi'; Course LXXXIX. Highlights of condensed-matter theory.

Cordonnier, J.L., Romanetti, R. and Lesourd, J.-B.
On the hypotheses underlying molecular dynamics simulation models in ionic liquid systems
Math. Modelling 7 (1986) 83-90.

Cramer, S.N., Gonnord, J. and Hendricks, J.S.
Monte Carlo techniques for analyzing deep-penetration problems
Nucl. Sci. and Eng. 92 (1986) 280-8.

Creutz, M.
Deterministic ising dynamics
Ann. Phys. 167 (1986) 62-72.

Creutz, M., Mitra, P. and Moriarty, K.J.M.
Computer investigations of the three-dimensional ising model
J. Stat. Phys. 42 (1986) 823-32.

Croxton, C.A.
A Monte Carlo analysis of terminally attached self-avoiding polymer sequences in the vicinity of a rigid bounardy
J. Phys. A 19 (1986) 987-99.

Croxton, C.A.
The development of loops, trains and tails in a self-avoiding terminally attached molecule
J. Phys. A 19 (1986) 2353-67.

Croxton, C.A.
On the existence of a discontinuity in the segment profile for a terminally attached self-avoiding polymer
Phys. Lett. A 111 (1985) 453-6.

Danilov, V.I.
Application of the Monte Carlo method for studying the hydration of molecules: base stacking
Theochem. 31 (1986) 239-42.

Dasgupta, C.
Monte Carlo study of the nematic-to-smectic-A transition
Phys. Rev. Lett. 55 (1985) 1771-4.

Davydov, S.Yu. and Margolin, V.I.
Calculation of the thermal expansion of semiconductor crystals by the bonding orbitals method
Fiz.Tverd. Tela (USSR), 27 (1985) 3711-13.

Dayantis, J. and Sturm, J.
Monte-Carlo calculations on statistical chains enclosed inside a sphere
Polymer 26 (1985) 1631-7.

De Alcantara Bonfim, O.F. and Engelsberg, M.
Large-cell Monte Carlo renormalization-group method for a new type of environmental percolation
Phys. Rev. B 34 (1986) 1977-9.

De Las Rosa-Fox, N., Esquivias, L. and Villares, P.
Structural models of the amorphous alloy $Ge_{0\cdot24}As_{0\cdot40}Se_{0\cdot40}$ by a random technique
Phys. Rev. B 33 (1986) 4094-9.

De Leeuw, S.W., Kalia, R.K. and Vashishta, P.
On isosets of Brownian motion
Solid State Commun. 57 (1986) 749-52.

De Raedt, H and Lagendijk, A.
Comment on 'Monte Carlo studies of the quantum XY model in two dimensions'
Phys. Rev. B 33 (1986) 5102-3.

De Raedt, H.
Monte Carlo simulation of boson systems at finite temperature
Phys. Lett. A 112 (1985) 333-6.

de Scheper, I.M., Haffmans, A.F.E.M. and Van Beijeren, H.
Comment on 'Large long-time tails and shear waves in dense classical liquids'
Phys. Rev. Lett. 56 (1986) 538.

Debierre, J.-M. and Turban, L.
Monte Carlo study of linear diffusion-limited aggregation
J. Phys. A 19 (1986) L131-5.

Der, R. and Fritzsche, S.
Dynamical correlations and long-time tails in chemical reactions. A molecular dynamics study
Chem. Phys. Lett. 121 (1985) 177-81.

Desai, R.C. and Denton, A.R.
Fractal properties of clusters during spinodal decomposition
On Growth and Form - Fractal and Non-fractal Patterns in Physics. Proc. of the NATO Advanced Study Institute, 1986.

Deutsch, J.M.
Simulation of entangled polymer chains
J. Polym. Sci. Polym. Symp. 73 (1985) 161-73.

Dewitt-Morette, C., Low, S.G., Schulman, L.S., et al
Wedges. I
Found. Phys. 16 (1986) 311-49.

Dezsi, I.
Ion implantation in semiconductors investigated by nuclear spectroscopy methods
Hyperfine Interactions 26 (1985) 1051-67.

Dhanasekaran, R., Subramanian, C. and Ramasamy, P.
Statistical mechanical background of computer simulations for growth of crystals from solution
Indian J. Pure and Appl. Phys. 24 (1986) 134-6.

Dharma-Wardana, M.W.C., Aers, G.C., Levesque, D., et al
Comment on 'Pair interaction from structural data of dense classical liquids' by Levesque, Weis and Reatto, with their reply
Phys. Rev. Lett. 56 (1986) 1211-12.

Dickman, R. and Hall, C.K.
Equation of state for athermal lattice chains
J. Chem. Phys. 85 (1986) 3023-6.

Dietz, W. and Heinzinger, K.
A molecular dynamics study of liquid chloroform
Ber. Bunsenges. Phys. Chem. 89 (1985) 968-77.

Dixit, P.K.,Vaid, B.A. and Sharma, K.C.
Structural disorder model. Pressure-induced transitions in Sn and semiconducting compounds
Phys. Status Solidi B 135 (1986) 523-8.

Domany, E. and Gubernatis, J.E.
Critical dynamics, Lifshitz tricriticality, and supersymmetry: the Ising model on the HCP lattice
Phys. Rev. B32 (1985) 3354-7.

Dong, R.Y.
Molecular dynamics and spectral density determination in the smectic phases of a liquid crystal
J. Magn. Resonance 66 (1986) 422-33.

Dorfmuller, T., Samios, J. and Mittag, U.
Octupole and hexadecapole induction mechanisms in interaction-induced spectra: A molecular dynamics simulation of liquid CCl_4
Chem. Phys. 107 (1986) 397-403.

Drohm, J.K. and Schlijper, A.G.
Vapor-liquid equilibrium calculations by constrained free-energy minimization
Int. J. Thermophys. 7 (1986) 407-19.

Duarte, J.A.M.S.
On Monte Carlo generation of lattice trees
J. Phys. A19 (1986) 1979-81.

Dubi, A. and Elperin, T.
On the Markov chain analysis of source iteration Monte Carlo procedures for criticality problems. II.
Nucl. Sci. and Eng. 91 (1985) 77-83.

Dubi, A., Goldfeld, A and Burn, K.
Application of the single surface extended model of geometrical splitting in Monte Carlo
Nucl. Sci. and Eng. 91 (1985) 470-80.

Dunn, W.L.
The back-projection angular flux estimator
J. Comput. Phys. 61 (1985) 391-402.

Dymond, J.H., Easteal, A.J. and Woolf, L.A.
Experimental measurements, molecular dynamics simulations and application of a rough-hard-spheres model for tracer diffusion in octamethylcyclotetrasiloxane at 323K and pressure up .....
Chem. Phys. 99 (1985) 397-403.

Easteal, A.J. and Woolf, L.A.
Developments in the hard-sphere model of fluids: self-diffusion
High Temp.-High Pressures 17 (1985) 271-6.

Edberg, R., Evans, D.J. and Morriss, G.P.
Constrained molecular dynamics: Simulations of liquid alkanes with a new algorithm
J. Chem. Phys. 84 (1986) 6933-9.

Eid, M., Diop, C.M. and Nimal, J.C.
Gamma-ray streaming in straight pipes and bent ducts
Proc. Int. Meeting on Advances in Nuclar Engineering Computational Methods Vol. 2 (1985) 881-90.

Elango, M. and Kiv, A.
Radiation-induced electrostatic instability in nonmetallic solids
EESTI NSV Tead. Akad. Fuus, Inst. Uurim. (USSR) 57 (1985) 113-28.

Elofson, P.A., Rynefors, K. and Homlid, L.
Monte Carlo simulation of RRKM unimolecular decomposition in molecular beam experiments. IV. Product on angular and velocity distributions from $O(^1D)+H_2$
Chem. Phys. 100 (1985) 39-51.

Elperin, T. and Dubi, A.
On the Markov chain analysis of source iteration Monte Carlo procedures for criticality problems. I
Nucl. Sci. and Eng. 91 (1985) 59-76.

Elser, V.
Eliminating the minus sign in Monte Carlo simulations of fermions
Phys. Rev. A 34 (1986) 2293-301.

Ely, J.F.
A test of the mean density approximation for Lennard-Jones mixtures with large size ratios
Int. J. Thermophys. 7 (1986) 381-93.

El-Meshad, N. and Tahir-Kheli, R.A.
Diffusion in mixed A-B alloys in two and three dimensions
Phys. Rev. B 32 (1985) 6176-83.

Erpenbeck, J.J. and Cohen, E.G.D.
Note on the fractal dimension of hard sphere trajectories
J. Stat. Phys. 43 (1986) 343-7.

Erpenbeck, J.J. and Kincaid, J.M.
Calculation of the mutual diffusion coefficient by equilibrium and non-equilibruium molecular dynamics
Int. J. Thermophys. 7 (1986) 305-17.

Erpenbeck, J.J. and Luban, M.
Equation of state of the classical hard-disk fluid
Phys. Rev. A 32 (1985) 2920-2.

Espriu, D., Gross, M., Rakow, P.E.L. et al
Continuum limit on a 2-dimensional random lattice
Nucl. Phys. B: Field Theory and Stat. Syst. 265 (1986) 92-112.

Evans, D.J.
Rheology and thermodynamics from nonequilibrium molecular dynamics
Int. J. Thermophys. 7 (1986) 573-84.

Evans, M.W.
Molecular dynamical simulation of new auto and cross correlations in liquid water
J. Mol. Liq. 32 (1986) 173-81.

Evans, M.W.
Symmetry of cross-correlation tensors in molecular dynamics: Rotation and translation in condensed matter
Phys. Rev. A 33 (1986) 1903-12.

Evans, M.W.
Cross correlation between rotation and translation in spherical tops
Phys. Rev. A 34 (1986) 2302-6.

Evans, M.W.
The discovery by computer simulation of fundamental single molecule cross-correlation functions in the liquid state of matter
Physica B and C 131B+C (1985) 273-82.

Faas, M. and Hilhorst, H.J.
Hierarchical Monte Carlo simulation of the Ising model
Physica A 135A (1986) 571-90.

Fabbri, U. and Zannoni, C.
A Monte Carlo investigation of the Lebwohl-Lasher lattice model in the vicinity of its orientational phase transition
Mol. Phys. 58 (1986) 763-88.

Family, F., Meakin, P. and Vicsek, T.
Cluster size distribution in chemically controlled cluster-cluster aggregation
J. Chem. Phys. 83 (1985) 4144-50.

Fernandez, J.F., Ferreira, M.F. and Stankiewicz, J.
Critical behaviour of the two-dimensional XY model: A Monte Carlo simulation
Phys. Rev. B 34 (1986) 292-300.

Ferrario, M. and Tani, A.
A molecular dynamics study of the TIP4P model of water
Chem. Phys. Lett. 121 (1985) 182-6.

Ferrario, M., McDonald, I.R. and Klein, M.L.
Anion ordering in alkali cyanide crystals
J. Chem. Phys. 84 (1986) 3975-85.

Fincham, D.
Choice of timestep in molecular dynamics simulation
Comput. Phys. Commun. 40 (1986) 263-9.

Fincham, D., Quirke, N. and Tildesley, D.J.
Computer simulation of molecular liquid mixtures. I. A diatomic Lennard-Jones model mixture for $\mathrm{Co_2c_2H_6}$
J. Chem. Phys. 84 (1986) 4535-46.

Foiles, S.M.
Computer simulation of the surface segregation in binary alloys using the embedded atom method
J. Vac. Sci. and Technol. A 4 (1986) 761-2.

Fois, E.S., Gamba, A., Morosi, G., et al
Monte Carlo studies of aqueous solution of nitrogen using different potential energy surfaces
Mol. Phys. 58 (1986) 65-83.

Fornili, S.L., Migliore, M. and Palazzo, M.A.
Hydration of the hydronium ion. Ab initio calculations and Monte Carlo simulation
Chem. Phys. Lett. 125 (1986) 419-24.

Fox, G.C., Otto, S.W. and Umland, E.A.
Monte Carlo physics on a concurrent processor
J. Stat. Phys. 43 (1986) 1209-37.

Fracassi, P.F., Cardini, G., O'Shea, S., et al
Solid and liquid carbon monoxide studied with the use of constant-pressure molecular dynamics
Phys. Rev. B 33 (1986) 3441-7.

Fredrickson, G.H. and Brawer, S.A.
Monte Carlo investigation of a kinetic ising model of the glass transition
J. Chem. Phys. 84 (1986) 3351-66.

Fredricksson, H. and Svensson, I.L.
Computer simulation of the structure formed during solidification of cast iron
Physical Metallurgy of Cast Iron. Proc. of the Third Int. Symp. (1985) 273-84.

Freeman, D.L., Coalson, R.D. and Doll, J.D.
Fourier path integral methods: a model study of simple fluids
J. Stat. Phys. 43 (1986) 931-4.

Frenkel, D. and Mulder B.M.
The hard ellipsoid-of-revolution fluid. I. Monte Carlo simulations
Mol. Phys. 55 (1985) 1171-92.

Frenkel, D., Mulder, B.M. and McTague, J.P.
Phase diagram of hard ellipsoids of revolution
Mol. Cryst. and Liq. Cryst. 123 (1985) 119-28.

Frenkel, D., Vos, R.J., De Kruif, C.G. et al
Structure factors of polydisperse systems of hard spheres; a comparison of Monte Carlo simulations and Percus-yevic theory
J. Chem. Phys. 84 (1986) 4625-30.

Frobose, K. and Jackle, J.
Hopping and static correlations of higher order in a lattice gas
J. Phys. Colloq. 46 (1985) 141-3.

Frobose, K. and Jackle, J.
Static correlations of higher order and diffusion in an interacting lattice gas
J. Stat. Phys. 42 (1986) 551-66.

Fucito, F. and Solomon, S.
On the relation between the coulomb gas and the lattice XY model
J. Phys. A 19 (1986) L739-43.

Fukase, S., Takagi, R., Naito, S., et al
Estimation of contributions to the solubility of Ar gas in molten KCℓ by the molecular dynamics method
J. Phys. C 19 (1986) 3313-24.

Fye, R.M.
Study of Trotter-like approximations
J. Stat. Phys. 43 (1986) 827-9.

Fye, R.M.
New results on trotter-like approximations
Phys. Rev. B33 (1986) 6271-80.

Galashev, A.E.
Thermodynamic stability of hexagonal closed packed (HCP) crystals in the molecular-dynamic argon model
Zh. Strukt. Khim. 25 (1984) 71-6.

Galashev, A.E. and Skripov, V.P.
Investigation on the disordering of argon hexagonal closed packed (HCP) crystals by the method of statistical geometry
Zh. Strukt. Khim. 25 (1984) 77-83.

Garcia Molina, J.J. and Garcia de la Torre, J.
The randomly broken chain as a semiflexible macromolecular model. Computer simulation of statistical properties
J. Chem. Phys. 84 (1986) 4026-30.

Garcia, A.L.
Nonequilibrium fluctuations studies by a rarefied-gas simulation
Phys. Rev. A 34 (1986) 1454-7.

Gardner, P.J. and Heyes, D.M.
Molecular dynamics computer simulations of molten zinc chloride
Physica B and C 131B+C (1985) 227-33.

Gawlinski, E.T., Kumar, S., Grant, M., et al
Breakdown of self-similar scaling in the two-dimensional random-field ising model: A Monte Carlo study
Phys. Rev. B 32 (1985) 1575-83.

Giege, R., Huong, P.V. and Moras, D.
Molecular dynamics in TRNA. crystallographic and Raman spectroscopic evidence
Spectrochim. Acta 42A (1986) 387-92.

Gillan, M.J. and Holloway, R.W.
Transport in the Frenkel-Kontorova model. III. Thermal conductivity
J. Phys. C 18 (1985) 5705-20.

Giro, A. Guardia, E. and Padro, J.A.
Langevin and molecular dynamics simulations of Lennard-Jones liquids
Mol. Phys. 55 (1985) 1063-74.

Glaus, U.
Monte Carlo simulation of self-avoiding surfaces in three dimensions
Phys. Rev. Lett. 56 (1986) 1996-9.

Goldman, S.
The convergence properties and stochastic characteristics inherent in force-biased and in metropolis Monte Carlo simulations on liquids
J. Comput. Phys. 62 (1986) 441-63.

Goldman, S. and Backx, P.
On water's ability to dissociate ion pairs
J. Chem. Phys. 84 (1986) 2761-5.

Gonzalez Miranda, J.M.
A molecular dynamics study of liquid potassium at 340 K
J. Phys. F 16 (1986) 1-10.

Grabow, M.H. and Andersen, H.C.
A comparison of the molecular dynamics method and energy minimization methods for modelling the structure of amorphous metals
J. Non-Cryst. Solids 75 (1985) 225-36.

Grady, M.
Fast algorithm for Monte Carlo simulations of systems with fermions
Phys. Rev. D 32 (1985) 1496-503.

Grassberger, P.
Spreading of percolation in three and four dimensions
J. Phys. A 19 (1986) 1681-9.

Grassberger, P.
On the hull of two-dimensional percolation clusters
J. Phys. A 19 (1986) 2675-7.

Gray,C.G., Sainger, Y.S., Joslin, C.G. et al
Computer simulation of dipolar fluids. Dependence of the dielectric constant on system size: a comparative study of Ewald sum and reaction field approaches
J. Chem. Phys. 85 (1986) 1502-4.

Grest, G.S.
Fully and partially frustrated simple cubic ising models: A Monte Carlo study
J. Phys. C 18 (1985) 6239-46.

Grest, G.S. and Kremer, K.
Molecular dynamics simulation for polymers in the presence of a heat bath
Phys. Rev. A 33 (1986) 3628-31.

Guardia, E., Giro, A. and Padro, J.A.
Nonadditivity effects in generalized Langevin dynamics simulation of interacting particles
J. Chem. Phys. 84 (1986) 4569-73.

Guha, A. and Roberts, L.
Generalised random paths in four dimensions
Phys. Lett. A 115 (1986) 45-8.

Guillope, M.
Allotropic transition in sigma=5(210) grain boundary at intermediate temperatures
J. Phys. 47 (1986) 1347-56.

Gupta, S. and Coon, J.E.
Structure and thermodynamics of molecular liquid mixtures
Mol. Phys. 57 (1986) 1049-61.

Gutierrez, G., Cadorin, D., Padilla, R. et al
Autoregressive model for 1-F noise. Noise in Physical Systems and 1-F Noise - 1985. Proc. 8th Int. Conf. on 'Noise in Physical Systems'.

Guttmann, A.J.
Validity of hyperscaling for the D=3 ising model
Phys. Rev. B 33 (1986) 5089-92.

Guttmann, A.J., Osborn, T.R. and Sokal, A.D.
Connective constant of the self-avoiding walk on the triangular lattice
J. Phys. A 19 (1986) 2591-8.

Haile, J.M.
On the use of computer simulation to determine the excess free energy in fluid mixtures
Fluid Phase Equilibria 26 (1986) 103-27.

Haile, J.M., Massobrio, C. and Torquato, S.
Two-point matrix probability function for two-phase random media: computer simulation results for impenetrable spheres
J. Chem. Phys. 83 (1985) 4075-8.

Hall, R.W. and Wolynes, P.G.
G.N. Lewis' atom and quantum Monte Carlo studies of liquids
J. Stat. Phys. 43 (1986) 935-48.

Hall, R.W. and Wolynes, P.G.
Quantum Monte Carlo study of a lattice-atom model for excitonic fluids
Phys. Rev. B33 1986 7879-81.

Harris, R.
A study of first- and second-order phase transitions using Monte Carlo simulations in the micro-canonical ensemble
Phys. Rett. A 111 (1985) 299-303.

Harten, P. and Suranyi, P.
Monte Carlo renormalization group study of the XY model
Nucl. Phys. B 265 (1986) 615-29.

Hashim, R., Luckhurst, G.R. and Romano, S.
Computer simulation studies of anisotropic systems. XIII. The orientational ordering of biaxial particles dissolved in a nematic liquid crystal
Mol. Phys. 56 (1985) 1217-34.

Hashim, R., Luckhurst, G.R. and Romano, S.
Computer simulation studies of anisotropic systems. XIV. Binary mixtures of liquid crystals
Liq. Cryst. 1 (1986) 133-46.

Hassold, G.N., Dreitlein, J.F., Beale, P.D., et al
Dynamics of the two-dimensional axial third-nearest-neighbour ising model: entrainment and diffusivity
Phys. Rev. B 33 (1986) 3581-4.

Haughney, M.,Ferrario, M. and McDonald, I.R.
Pair interactions and hydrogen-bond networks in models of liquid methanol
Mol. Phys. 58 (1986) 849-53.

Hayakawa, Y., Kondo, H. and Matsushita, M.
Monte Carlo simulations of the generalized diffusion limited aggregation
J. Phys. Soc. JPN 55 (1986) 2479-82.

Hee Lee, Y. and Lee, M.A.
Computer simulation of molecular orientational order: the Kerr effect in carbon disulphide
Superlattices and Microstruct. 1 (1985) 529-33.

Heermann, D.W.
Scaling and mean-field-like behaviour in phase separation processes
Z. Phys. B 61 (1985) 311-23.

Heinzinger, K.
Computer simulations of aqueous electrolyte solutions
Physica B and C 131B+C (1985) 196-216.

Henderson, J.R. and Van Swol, F.
On the approach to complete wetting by gas at a liquid-wall interface. Exact sum rules, fluctuation theory and the verification by computer simulation of the presence of long range .....
Mol. Phys. 56 (1985) 1313-56.

Hess, S.
Shear-induced melting and reentrant positional ordering in a system of spherical particles
Int. J. Thermophys. 6 (1985) 657-71.

Heydenreich, J.
Electron microscopical characterization of electronic materials
5th Int. Summer School on Crystal Growth and Materials Research (1985).

Heydenreich, J. and Breitenstein, O.
Characterization of defects in semiconductors by combined application of SEM(EBIC) and SDLTS
J. Microsc. 141 (1986) 129-42.

Heyes, D.M.
Tensile viscosities of the Lennard-Jones liquid
Phys. Lett. A 115 (1986) 42-4.

Heyes, D.M.
Some physical consequences of large shear rates on simple liquids
J. Chem. Phys. 85 (1986) 997-1008.

Heyes, D.M., Morriss, G.P. and Evans, D.J.
Nonequilibrium molecular dynamics study of shear flow in soft disks
J. Chem. Phys. 83 (1985) 4760-6.

Hirao, K. and Soga, N.
Molecular dynamic simulation of Eu^{3+}-doped sodium borate glasses and their fluorescence spectra
J. Am. Ceram.Soc. 68 (1985) 515-21.

Hirao, K. and Soga, N.
Molecular dynamics study of $2R_2O.SiO_2$ glasses
J. Non-Cryst. Solids 84 (1986) 61-7.

Holderna-Matuszkiewicz, K.
The influene of hydrostatic pressure on the molecular dynamics of DL-isoborneole
Acta. Phys. A69 (1986) 69-80.

Holt, D.B.
Microcharacterization of crystals using the scanning electron microscope
5th Int. Summer School on Crystal Growth and materials Research (1985).

Homma, S., Matsuda, H. and Ogita, N.
Decoupled cell method Monte Carlo simulation for quantum spin systems
Prog. Theor. Phys. 75 (1986) 1058-65.

Hoogland, A., Compagner, A. and Blote, H.W.J.
Smooth finite-size behaviour of the three-dimensional ising model
Physica A 132 (1985) 593-6.

Hooley, D.J.
Forth automates intrinsic viscosity determinations
J. Forth Appl. and Res. 3 (1985) 163.

Hooley, D.J.
System development via prototyping in the analytical laboratory
J. Forth Appl. and Res. 3 (1985) 165.

Hoover, W.G. and Kratky, K.W.
Heat conductivity of three periodic hard disks via nonequilibrium molecular dynamics
J. Stat. Phys. 42 (1986) 1103-14.

Hoppe, B. and Hirst, L.L.
Ordering in antiferromagnetic Potts model
J. Phys. A 18 (1985) 3375-80.

Houlrik, J.M. and Knak Jensen, S.J.
Phase diagram of the three-state chiral clock model studied by Monte Carlo renormalization-group calculations
Phys. Rev. B 34 (1986) 325-9.

Huller, A.
Order of the phase transition of a two-dimensional rotor system
Z. Phys. B 61 (1985) 289-97.

Imada, M.
Melting of the two-dimensional Wigner crystal in the quantum region
J. Stat. Phys. 43 (1986) 861-3.

Imafuku, M., Sasajima, Y., Yamamoto, R., et al
Computer simulations of the structures of the metallic superlattices Au-Ni and Cu-Ni and their elastic moduli
J. Phys. F 16 (1986) 823-9.

Impey, R.W., Sprik, M. and Klein, M.L.
Simulation of the cubic to orthorhombic phase transition in potassium cyanide
J. Chem. Phys. 83 (1985) 3638-44.

Isbister, D. and Morriss, G.P.
The dielectric constant of polar hard spheres
Chem. Phys. Lett. 122 (1985) 29-36.

Ito, T.
A pseudopotential approach to the disorder effects in III-V ternary semiconductor alloys
Phys. Status Solidi B 135 (1986) 493-502.

Jacobs, P.W.M. and MacDonaill, D.A.
Computer simulation of delta-bismuth oxide
Solid State Ionics Diffus. and React. 18-19 (1986) 209-13.

Jacucci, G., Ronchetti, M. and Schirmacher, W.
Computer simulation of the liquid Li_4 Pb alloy
J. Phys. Colloq. 46 (1985) 385-9.

Jagannadham, K. and Narayan, J.
The influence of a planar interface on the energy minimization principle
Mater. Sci. and Eng. 81 (1986) 127-39.

Jain, S.
Non-universality in the dynamics at the percolation threshold
J. Phys. A 19 (1986) L667-73.

Jain, S.
Breakdown of dynamic scaling at the percolation threshold
J. Phys. A 19 (1986) L57-61.

Janardan, K.G. and Gill, D.S.
A new test for hydrologic similarity
Modelling and Simulation. Proc. of the Sixteenth Annual Pittsburgh Conf., 1985, 1271-5.

Jancso, G., Heinzinger, K. and Bopp, P.
Molecular dynamics study of the effect of pressure on an aqueous NaCℓ solution
Z. Naturforsch. Teil 40A (1985) 1235-47.

Janke, W. and Kleinert, H.
Thermodynamic properties of a three-dimensional defect system
Phys. Rev.B33 (1986) 6346-51.

Janke, W. and Kleinert, H.
How good is the Villain approximation
Nucl. Phys. B. 270 (1986) 135-53.

Janke, W. and Kleinert, H.
Tricritical points in three-dimensional XY model with mixed action
Phys. Rev. Lett. 57 (1986) 279-82.

Janke, W. and Toussaint, D.
Laplacian roughening on a triangular lattice
Phys. Lett. A 116 (1986) 387-91.

Jankowski, D.G.
Diffusion-recombination phenomena from paired initial conditions
Phys. Rev. A33 1986 4415-18.

Jaric, M.V. and Tuthill, G.F.
Thermodynamic polydispersity and the Flory exponent
Phys. Rev. Lett. 55 (1985) 2891-4.

Jasnow, D., Mon, K.K. and Ferer, M.
Interfacial tension and correlation lengths for the three-state Potts model in two dimensions
Phys. Rev. B 33 (1986) 3349-52.

Jellinek, J., Beck, T.L. and Berry, R.S.
Solid-liquid phase changes in simulated isoenergetic Ar_{13}
J. Chem. Phys. 84 (1986) 2783-94.

Jing-Den Chen and Wilkinson, D.
Pore-scale viscous fingering in porous media
Phys. Rev. Lett. 55 (1985) 1892-5.

Jodrey, W.S. and Tory, E.M.
Computer simulation of close random packing of equal spheres
Phys. Rev. A 32 (1985) 2347-51.

Jonsson, B., Edholm, O. and Teleman, O.
Molecular dynamics simulations of a sodium octanoate micelle in aqueous solution
J. Chem. Phys. 85 (1986) 2259-71.

Jorgensen, W.L. and Madura, J.D.
Temperature and size dependence for Monte Carlo simulations of TIP4P water
Mol.Phys. 56 (1985) 1381-92.

Jorgensen, W.L. and Ravimohan, C.
Monte Carlo simulation of differences in free energies of hydration
J. Chem. Phys. 83 (1985) 3050-4.

Joshi, Y.P. and Tildesley, D.J.
Molecular dynamics simulation and energy minimization of O_2 adsorbed on a graphite surface
Surf. Sci. 166 (1986) 169-82.

Jurkiewicz, J., Krzywicki, A. and Petersson, B.
A numerical study of discrete Euclidean polyakov surfaces
Phys. Lett. B 168B (1986) 273-8.

Kabadi, V.N.
Moleular dynamics of fluids: the Gaussian overlap model. II.
Ber. Bunsenges. Phys. Chem. 90 (1986) 327-32.

Kabadi, V.N. and Steele, W.A.
Simulation study of rotational and translational dynamics of diatomic molecules with quadrupolar interactions
J. Phys. Chem. 89 (1985) 1467-73.

Kalia, R.K. and Vashishta, P.
Microscopic structure of two-dimensional electron glass
Mater. Sci. Forum 4 (1985) 99-103.

Kalia, R.K., De Leeuw, S.W. and Vashishta, P.
Fractal dimensionality of Brownian motion in two dimensions
J. Phys. C 18 (1985) L905-8.

Kalinichev, A.G.
A Monte Carlo study of dense supercritical water
Teplofiz. Vys. Temp. 23 (1985) 683-6.

Kalinichev, A.G.
Monte Carlo study of the thermodynamics and structure of dense supercritical water
Int. J. Thermophys. 7 (1986) 887-900.

Kantor, Y.
Three-dimensional percolation with removed lines of sites
Phys. Rev. B 33 (1986) 3522-5.

Kapaev, V.V.
Laser-induced formation of a periodic structure on the surface of semiconductors
Zh. Tekh. Fiz. 55 (1985) 2244-7.

Karowski, M. and Rys, F.S.
Critical behaviour of the loop gas model on the square lattice
J. Phys. A 19 (1986) 2599-609.

Karpuzov, D.S.
Profile evolution in high-dose ion implantation: a computer simulation study
Phys. Status Solidi A 94 (1986) 365-70.

Kasai, T., Ohashi, K., Ohoyama, H. et al.
Formation and characterization of an SH($^2\pi_{3/2,1/2}$) radical beam produced by the F + H_2S reaction using a sectupole electric field
Chem. Phys. Lett. 127 (1986) 581-4.

Kawabata, C., Takeuchi, M. and Bishop, A.R.
Monte Carlo molecular dynamics simulations for two-dimensional magnets
J. Stat. Phys. 43 (1986) 869-71.

Kerstein, A.R. and Edwards, B.F.
Crossover from contact propagation to chemical propagation in first-passage percolation
Phys. Rev. B 33 (1986) 3353-69.

Kertesz, J., Czerti, J. and Szep, J.
Monte Carlo simulation programs for microcomputers
Eur. J. Phys. 6 (1985) 232-7.

Khalatur, P.G., Papulov, Yu.G. and Pavlov, A.S.
The influence of solvent on the static properties of polymer chains in solution. A molecular dynamics simulation
Mol. Phys. 58 (1986) 887-95.

Khalatur, P.G., Papulov, Yu.G. and Pletneva, S.G.
Monte Carlo simulation of the liquid-crystalline ordering of semiflexible polymers
Mol. Cryst. and Liq. Cryst. 130 (1985) 195-202.

Kielpinski, A.L., Mansour, K. and Murad, S.
Equilibrium and non-equilibrium computer simulation studies of polar fluids and non-polar mixtures
Int. J. Thermophys. 7 (1986) 421-30.

Kikuchi, M. and Okabe, Y.
A simple method of Monte Carlo renormalization group
Prog. Theory. Phys. 75 (1986) 192-4.

Kikuchi, M. and Okabe, Y.
Monte Carlo study of critical relaxation near a surface
Phys. Rev. Lett. 55 (1985) 1220-2.

Kim, K.S. and Clementi, E.
Hydration analysis of the intercalated complex of deoxydinucleoside phosphate and proflavin: computer simulations
J. Phys. Chem. 89 (1985) 3655-63.

Kincaid, J.M. and Erpenbeck, J.J.
The mutual diffusion constant of binary, isotopic hard-sphere mixtures: molecular dynamics calculations using the Green-Kubo and steady-state methods
J. Chem. Phys. 84 (1986) 3418-31.

Kirkpatrick, T.R. and Nieuwoudt, J.C.
Mode-coupling theory of the large long-time tails in the stress-tensor autocorrelation function
Phys. Rev. A 33 (1986) 2651-7.

Kjellander, R. and Marcelja, S.
Perturbation of hydrogen bonding in water near polar surfaces
Chem. Phys. Lett. 120 (1985) 393-6.

Kjuntsel, I.A., Mokeeva, V.A. and Soifer, G.B.
A phase transition and molecular dynamics in crystaline $C_6H_5CHCl_2$ by ^{35}Cl NQR investigations
Z. Naturforsch. Teil 41A (1986) 275-8.

Kline, L.E.
Electron and chemical kinetics in the low-pressure rf discharge etching of silicon in SF_6
IEEE Trans. Plasma Sci. 14 (1986) 145-55.

Klots, C.E.
Evaporative Cooling
J. Chem. 83 (1985) 5854-60.

Klyavin, O.V. Likhodedov, N.P. and Orlov, A.N.
Computer simulation of the atomic mechanism for migration and interaction of interstitial impurities with the core of a screw dislocation in a BCC lattice
Fiz. Tverd. Tela (USSR), 28 (1986) 156-62.

Klyushnik, B.N., Marchenko, G.N., Khalatur, P.G.
Computer simulation of interaction of polymer chains with the liquid-crystalline matrix
Vysokomol. Soedin. Ser. A (USSR) 27 (1985) 1468-74.

Koch, S.W. and Abraham, F.F.
Temperature-induced commensurate-incommensurate transition of submonolayer krypton on graphite
Phys. Rev. B 33 (1986) 5884-5.

Kogut, J. and Polonyi, J.
Microcanonical study of the planar spin model
Nucl. Phys. Field Theory and Stat. Syst. 265 (1986) 313-23.

Kohring, G., Shrock, R.E. and Wills, P.
Role of Vortex strings in the three-dimensional O(2) model
Phys. Rev. Lett. 57 (1986) 1358-61.

Kolinski, A., Skolnick, J. and Yaris, R.
Monte Carlo dynamics of diamond-lattice multichain systems
aip Conf. Proc. 137 (1985) 241-5.

Kolinski, A., Skolnick, J. and Yaris, R.
On the short time dynamics of dense polymeric systems and the origin of the glass transition: a model system
J. Chem. Phys. 84 (1986) 1922-31.

Koonin, S.E.
Auxiliary-field Monte Carlo Methods
J. Stat. Phys. 43 (1986) 985-90.

Koura, K.
Monte Carlo simulation of electron swarm in a model gas: transverse and longitudinal diffusion coefficients
J. Phys. Soc. JPN 55 (1986) 2500-3.

Kou-Chang Su, Ohnaka, I., Yamauchi, I., et al
Computer simulation of solidification of nodular cast iron
Physical Metallurgy of Cast Iron. Proc. of the Third Int. Symp. (1985) 181-9.

Kovalenko, L.G., Goncharov, E.G. and Krasovskii, E.I.
Analysis of the characteristics of parallel- and diverging-beam schlieren instruments using the data of a computer statistical modelling
Opt. Mekh. Prom. St. 52 (1985) 1-4.

Kremer, K.
Critical exponents and scaling functions of a self-avoiding walk interacting with a defect plane
J. Chem. Phys. 83 (1985) 5882-7.

Kremer, K.
Dynamics of entangled polymer melts in two and three dimensions
J. Polym. Sci. Polym. Symp. 73 (1985) 157-60.

Krishan, K., Purniah, B. and Srinivasan, S.
Computer simulation of defects and radiation damage
Bull. Mater. Sci. 8 (1986) 155-67.

Kruger, P., Strassburger, W., Wollmer, A., et al
A comparison of the structure and dynamics of avian pancreatic polypeptide hormone in solution and in the crystal
Eur. Biophys. J. 13 (1985) 77-88.

Kubota, N., Kawakami, T. and Tadaki, T.
Calculation of supercooling temperature for primary nucleation of potassium nitrate from aqueous solution by the two-kind active site model
J. Cryst. Growth 74 (1986) 259-74.

Kumar, S., Vinals, J. and Gunton, J.D.
Monte Carlo renormalization-group study of the dynamics of the kinetic ising model
Phys. Rev. B 34 (1986) 1908-17.

Kunc, J.A. and Shemansky, D.E.
The potential curve of the He-alpha-quartz surface interaction
Surf. Sci. 163 (1985) 237-48.

Kung, D.S.
Quantum Monte Carlo of coupled fermion chains
J. Stat. Phys. 43 (1986) 873-4.

Kutner, R.
Correlated hopping in honeycomb lattice: tracer diffusion coefficient at arbitrary lattice gas concentration
J. Phys. C 18 (1985) 6323-39.

Kutner, R. and Van Beijeren, H.
Tracer diffusion in a one-dimensional lattice gas in the presence of a drift force
Solid State Ionics Diffus. and React. 18-19 (1986) 229-31.

Laakkonen, J. and Nieminen, R.M.
Molecular dynamic studies of quenching
J. Non-Cryst. Solids 75 (1985) 237-42.

Laaksonen, A. and Clementi, E.
Theoretical study of some gas, liquid and crystal properties of sodium chloride using ab initio potentials
Mol. Phys. 56 (1985) 495-524.

Lam, P.M.
On Monte Carlo generation and study of anisotropy of lattice animals
J. Phys. A 19 (1986) L155-9.

Lam, P.M.
Monte Carlo study of lattice animals in D dimensions
Phys. Rev. A 34 (1986) 2339-45.

Lam, P.M., Bao, W. and Yang, Y.S.
Renormalization group study of anomalous acoustic behaviour in critical percolation network
Z. Phys. B 61 (1985) 283-7.

Landman, U., Luedtke, W.D., Barnett, R.N. et al
Faceting at the silicon (100) crystal-melt interface: Theory and experiment
Phys. Rev. Lett. 56 (1986) 155-8.

Larsson, K.-E. and Gudowski, W.
Generalized viscosity, pair potential, and memory functions from $S(Q,\Omega)$ measurements for liquid metals
Phys. Rev. A 33 (1986) 1968-83.

Laviolette, R.A. and Stillinger, F.H.
Multidimensional geometric aspects of the solid-liquid transit ion in simple substances
J. Chem. Phys. 83 (1985) 4079-85.

Lee, D.H., Joannopoulos, J.D., Negele, J.W. et al
Symmetry analysis and Monte Carlo study of a frustrated antiferromagnetic planar (XY) model in two dimensions
Phys. Rev. B 33 (1986) 450-75.

Lee, K.-H., Sandler, S.I. and Monson, P.A.
Local compositions and the square-well fluid
Int.J. Thermophys. 7 (1986) 367-79.

Lee, K.-H., Sandler, S.I., Patel, N.C.
The generalized Van der Waals partition function. III. Local composition models for a mixture of equal size square-well molecules
Fluid Phase Equilibria 25 (1986) 31-49.

Legrand, B., Treglia, G., Desjonqueres, M.C. et al
A 'quenched molecular dynamics' approach to the atomic stability of the (100) face of BCC transition metals
J. Phys. C19 (1986) 4463-72.

Levesque, D., Weiz, J.J. and Loubeyre, P.
Phase transitions in high-pressure ^{4}He: a study using molecular-dynamics and Monte Carlo methods
Phys. Rev. B 34 (1986) 178-88.

Levine, S.M. and Garofalini, S.H.
Molecular dynamics simulation of PT on a vitreous silica surface
Surf. Sci. 163 (1985) 59-66.

Levy, R.M. and Keepers, J.W.
Computer simulations of protein dynamics: theory and experiment
Comments Mol. and Cell. Biophys. Comments Mod. Biol. Part A 3 (1986) 273-94.

Levy, R.M., Sheridan, R.P., Keepers, J.W. et al
Molecular dynamics of myoglobin at 298K. Results from a 300-PS computer simulation
Biophys. J. 48 (1985) 509-18.

Lie, G.C. and Clementi, E.
Molecular-dynamics simulation of liquid water with an ab initio flexible water-water interaction potential
Phys. Rev. A 33 (1986) 2679-93.

Linse, P. and Andersen, H.C.
Truncation of Coulombic interactions in computer simulations of liquids
J. Chem. Phys. 85 (1986) 3027-41.

Lin, J. and Chiu, L.C.
Treatment of broadening in Monte Carlo calculations of quantum transport
Appl. Phys. Lett. 47 (1985) 1304-6.

Loh, E., Jr., Scalapino, D.J. and Grant, P.M.
Monte Carlo simulations of the quantum XXZ model in two dimensions
Phys. Scr. 32 (1985) 327-33.

Loh, E., Jr.
Monte Carlo method for quantum spins using boson world lines
Phys. Rev. Lett. 55 (1985) 2371-4.

Loh, E., Jr.
A Monte Carlo method for quantum spins using boson world lines
J. Stat. Phys. 43 (1986) 875-6.

Loh, E., Jr., Scalapino, D.J. and Grant, P.M.
Reply to 'Comment on 'Monte Carlo studies of the quantum XY model in two dimensions''
Phys. Rev. B 33 (1986) 5104.

Longa, L.
Equilibrium properties of linear diatomic chain
Acta Phys. A68 (1985) 803-13.

Lu Wei, Ye Hongjuan, Tao Fengxiang, et al
Kramers-Kronig relations and far infrared optical constants of semiconductors
Chin. J. Infrared Res. 5A (1986) 33-42.

Lucas, A.A., Vigneron, J.P., Lambin, P.H., et al
Electron energy loss spectroscopy of surface and interface phonons of insulators, semiconductors, and superlattices
Int. J. Quantum Chem. Quantum Chem. Sym. 19 (1985) 687-705.

Luckas, M., Deiters, U. and Gubbins, K.E.
Integrals over pair- and triplet-correlation functions for the Lennard-Jones (12-6)-Fluid
Mol.Phys. 57 (1986) 241-53.

Luk'yanov, M.N., Darinskii, A.A., Gotlib, Yu.Ya. et al
Simulation by molecular dynamics method of polymer systems oriented with the aid of external field
Vysokomol. Soedin. Ser. A (USSR) 27 (1985) 1506-12.

Lyklema, J.W. and Kremer, K.
Monte Carlo series analysis of irreversible self-avoiding walks. II. The growing self-avoiding walk
J. Phys. A 19 (1986) 279-89.

MacGowan, D. and Evans, D.J.
Heat and matter transport in binary liquid mixtures
Phys. Rev. A 34 (1986) 2133-42.

Mackenzie, N.D.
The 2D random-field ising model-Monte Carlo simulations
J. Phys. C 19 (1986) 563-7.

Madden, P.A. and Tildesley, D.J.
Interaction-induced contributions to Rayleigh and allowed Raman bands-A simulation study of CS_2
Mol. Phys. 55 (1985) 969-98.W

Malyutenko, V.K., Liptuga, A.I., Moin, M.D. et al
Kinetics of thermal emittance of finite-dimension semiconductors
UKR. Fiz. Zh. 30 (1985) 1854-6.

Manz, J.
Molecular dynamics along hyperspherical coordinates
Comments At. and Mol. Phys. 17 (1985) 91-113.

Marchese, F.T. and Beveridge, D.L.
Thermal motion from Monte Carlo simulations of aqueous ionic solutions
Int. J. Quantum Chem. 29 (1986) 619-25.

Marro, J., Labarta, A. and Tejada, J.
Critical behaviour of ising models with static site dilution
Phys. Rev. B 34 (1986) 347-9.

Martin, O.
Lyapunov exponents of stochastic dynamical systems
J. Stat. Phys. 41 (1985) 249-61.

Martin, W.R., Rathkopf, J.A. and Nowak, P.F.
Vectorized Monte Carlo photon transport on the CRAY-XMP
Trans. Am. Nucl. Soc. 50 (1985) 278-9.

Masri, P., Tasker, P.W., Hoare, J.P. et al
Entropy of segregation of isovalent impurity cations at the surface of an ionic crystal: MGO(100)Ca^{2+}
Surf. Sci. 173 (1986) 439-54.

Mazenko, G.F. and Valls, O.T.
Slow equilibration in systems undergoing diffusion-controlled phase separation on a lattice
Phys. Rev. B 33 (1986) 1823-9.

Mazzone, A.M.
Modelling of disorder induced by thermal spikes in ion bombarded silicon
Radiat. Eff. Lett. Sect. 87 (1985) 91-9.

Mazzone, A.M. and Finetti, M.
Monte Carlo simulation of mixing of a multilayered target
Radiat. Eff. Lett.l Sect. 87 (1986) 155-61.

Mazzone, A.M., Servidori, M. and Cembali, G.
Monte Carlo simulation of the annealing kinetics of oxygen recoils formed in through-oxide implants on silicon
Phys. Status Solidi A 94 (1986) 171-6.

McGreevy, R.L., Baranyai, A. and Ruff. I.
A less arbitrary determination of coordination numbers in disordered systems
Phys. and Chem. Liq. 16 (1986) 47-54.

Meakin, P.
Computer simulation of growth and aggregation processes
On Growth and Form - Fractal and Non-fractal Patterns in Physics. Proc. of the NATO Advanced Study Institute, 1986.

Meakin, P. and Deutch, J.M.
Fractal structures from an evaporation-condensation model
J. Chem. Phys. 83 (1985) 4086-92.

Meirovitch, H.
Computer simulation of the free energy of polymer chains with excluded volume and with finite interactions
Phys. Rev. A 32 (1985) 3709-15.

Meirovitch, H. and Scheraga, H.A.
Computer simulation of the entropy of continuum chain models: the two-dimensional freely jointed chain of hard disks
J. Chem. Phys. 84 (1986) 6369-75.

Mercier, B.
Non-statistical Monte-Carlo
Transp. Theory and Stat. Phys. 15 (1986) 565-96.

Metsch, P., Spit, F.H.M. and Bakker, H.
Computer simulation of simultaneous bulk, grain-boundary, and surface diffusion
Phys. Status Solidi A 93 (1986) 543-7.

Meyer, M. and Ciccotti, G.
Molecular dynamics simulation of plastic adamantane. I. Structural properties
Mol. Phys. 56 (1985) 1235-48.

Michel, G.
Dispersion in first passage time for biased diffusion
J. Phys. A 19 (1986) 2461-3.

Migliore, M., Fornili, S.L., Spohr, E., et al
A molecular dynamics study of the structure of an aqueous KCℓ solution
Z. Naturforsch. Teil 41A (1986) 826-34.

Mikhailin, A.I. and Romanov, A.E.
Amorphization of a disclination core
Fiz. Tverd. Tela (USSR), 28 (1986) 601-3.

Mikhailov, G.A.
Vector representation of bilinear estimates in the Monte Carlo method and the realization of special iterative processes
Dokl. Akad. Nauk 285 (1985) 803-7.

Milchev, A. and Binder, K.
Monte Carlo study of a lattice gas model with nonadditive lateral interactions
Surf. Sci. 164 (1985) 1-18.

Mills, M.F., Reimers, J.R. and Watts, R.O.
Monte Carlo simulation of the OH stretching spectrum of solutions of KCℓ, KF, LiCℓ and LiF in water
Mol. Phys. 57 (1986) 777-91.

Mills, P., Anderson, C.F. and Record, M.T., Jr.
Monte Carlo studies of counterion-DNA interactions. Comparison of the radial distribution of counterions with predictions of other polyelectrolyte theories
J. Phys. Chem. 89 (1985) 3984-94.

Mills, P., Paulsen, M.D., Anderson, C.F., et al.
Monte Carlo simulations of counterion accumulation near helical DNA
Chem. Phys. Lett. 129 (1986) 155-8.

Minnhagen, P.
Empirical evidence of a non-universal Kosterlitz-Thouless jump for frustrated two-dimensional XY models
Phys. Rev. B 32 (1985) 7548-51.

Mohanty, U.
Inferences from a microscopic model for the Stokes-Einstein relation
Phys. Rev. A 32 (1985) 3055-8.

Moller, W.
A computer study of the collisional mixing of Pt in Si
Nucl. Instrum. and Methods. Phys. Res. Sect. B 15 (1986) 688-91.

Mon, K.K.
Self-similarity and fractal dimension of a roughening interface by Monte Carlo simulations
Phys. Rev. Lett. 57 (1986) 866-8.

Mon, K.K. and Jasnow, D.
Surface tension and universality in the three-dimensional ising model
J. Stat. Phys. 41 (1985) 273-80.

Moody, M.C., Ray, J.R. and Rahman, A.
Free energy difference calculations comparing FCC and HCP structures using molecular dynamics computer simulations
J. Chem. Phys. 84 (1986) 1795-802.

Morales, J.J., Toxvaerd, S. and Rull, L.F.
Computer simulation of a phase transition at constant temperature and pressure
Phys. Rev. A 34 (1986) 1495-8.

Morgan, W.L.
Molecular dynamics simulation of geminate recombination by electrons in liquid methane
J. Chem. Phys. 84 (1986) 2298-303.

Morgenstern, I. and Wurtz, D.
Monte Carlo procedure for 2-dimensional fermion systems
Z. Phys. B61 (1985) 219-22.

Mori, Y. and Miura, I.
Computer simulation study on the morphology of two-phase alloy structures using the model of random nucleation and grain growth
J. Jpn. Inst. Met. 49 (1985) 832-8.

Moscinski, J. and Jacobs, P.W.M.
Molecular dynamics simulation of defect motion
Physica B and C 131B+C (1985) 175-95.

Mulder, B.M. and Frenkel, D.
The hard ellipsoid-of-revolution fluid. II. The Y-expansion equation of state
Mol. Phys. 55 (1985) 1193-215.

Murad, S., Papaionannou, A. and Powles, J.G.
A computer simulation for model fluid hydrogen chloride
Mol. Phys. 56 (1985) 431-43.

Murch, G.E.
Diffusion-limited evaporation - A Monte Carlo approach
High Temp. Sci. 20 (1985) 75-85.

Murray, A.D., Murch, G.E. and Catlow, C.R.A.
A new hybrid scheme of computer simulation based on Hades and Monte Carlo: Application to ionic conductivity in Y^{3+} doped CEO_2
Solid State Ionics Diffus. and React. 18-19 (1986) 196-202.

Murthy, G. and Shankar, R.
Tests for Monte Carlo renormalization studies on ising models
J. Stat. Phys. 42 (1986) 275-88.

Muser, H.E. and Rys, F.S.
Use of microcomputers for fast Monte Carlo calculations
JPN J. Appl. Phys. Suppl. 24 (1985) 192-4.

Muser, H.E. and Rys, F.S.
Influence of the line stiffness on the critical properties of 2D domain walls and polymer systems
Z. Phys. B61 (1985) 153-7.

Muser, H.E., and Siems, R.
Statistical mechanics of a finite ferroelectric with a constant interaction
JPN J. Appl. Phys. Suppl. 24 (1985) 195-7.

Naghizadeh, J. and Kovac, J.
Temperature-dependent cubic-lattice-model simulation of polymer-chain dynamics
Phys. Rev. B 34 (1986) 1984-6.

Nakanishi, H.
Some remarks on diffusion on fractals
Mater. Sci. Forum 4 (1985) 129-43.

Nakanishi, H.
Some remarks on diffusion on fractals
Diffus. and Defect Data 42 (1985) 41-56.

Nakanishi, H. and Family, F.
Large-cell Monte Carlo renormalization of irreversible growth processes
Phys. Rev. A 32 (1985) 3606-17.

Nakanishi, K.
Effect of pressure on the internal energy of Lennard-Jones mixtures
Physica B and C 139 (1986) 148-50.

Naraghi, M.H.N. and Chung, B.T.F.
A stochastic approach for radiative exchange in enclosures with directional-bidirectional properties
Trans. Asme. J. Heat Transfer 108 (1986) 264-70.

Neumann, M.
Dielectric relaxation in water. Computer simulations with the TIP4P potential
J. Chem. Phys. 85 (1986) 1567-80.

Nezbeda, I. and Vortler, H.L.
MC simulation results for a hard core model of carbon tetrachloride
Mol. Phys. 57 (1986) 909-18.

Nguyen, H.L., Khanmohammadbaigi, H. and Clementi E.
A parallel molecular dynamics strategy
J. Comput. Chem. 6 (1985) 634-46.

Nicolaides, D. and Bruce, A.D.
Universal local dynamics
J. Phys. A 19 (1986) 1753-6.

Nizzoli, F.
Theory of Brillouin scattering from surface waves in semiconductor supported films and layered structures
Proc. 17th Int. Conf. on the Physics of Semiconductors, (1985) 1145-50.

Nose, S.
An extension of the canonical ensemble molecular dynamics method
Mol. Phys. 57 (1986) 187-91.

Nose, S. and Yonezawa, F.
Isobaric-isothermal molecular dynamics study on the glass transition of a Lennard-Jones system
Solid State Commun. 56 (1985) 1005-8.

Nose, S. and Yonezawa, F.
Isothermal-isobaric computer simulations of melting and crystallization of a Lennard-Jones system
Solid State Commun. 56 (1985) 1009-13.

Nose, S. and Yonezawa, F.
Isothermal-isobaric computer simulations of melting and crystallization of a Lennard-Jones system
J. Chem. Phys. 84 (1986) 1803-14.

Nymeyer, A.
A Monte Carlo analysis of the two-dimensional modified step model
J. Phys. A19 (1986) 2183-93.

Nymeyer, A. and Irving, A.C.
A Monte Carlo analysis of the two-dimensional planar and step models
J. Phys. A 19 (1986) 1745-52.

Ochoa, R. and Simmons, J.H.
High strain rate effects on the structure of a simulated silica glass
J. Non-Cryst. Solids 75 (1985) 413-18.

Ohdomari, I., Mihara, T. and Kai, K.
Computer simulation of high-resolution transmission electron microscopy images of Si SiO_2 interfaces
J. Appl. Phys. 59 (1986) 2798-802.

Ohmine, I.
Energy dissipation mechanism of the optically excited molecules in solvents: A trajectory study for a photoisomerization process of the π-conjugated molecular in Ar and water
J. Chem. Phys. 85 (1986) 3342-58.

Okai, B.
Mechanism of B1-B2 transition of ionic crystals under pressure
Physica B and C 139 (1986) 221-3.

Ottinger, H.C.
Monte Carlo renormalisation group for the true self-avoiding walk
J. Phys. A 19 (1986) 961-71.

Pabst, W.
Radiative transfer calculation by Markov statistics
J. Illum. Eng. Soc. 15 (1985) 29-39.

Padro, J.A., Guardia, E. and Sese, G.
On the reliability of Langevin dynamics: simulation of liquid isotopic mixtures
Phys. Lett. A 115 (1986) 132-4.

Palenskis, V.P., Laucius, J. and Mykolaitis, H.
Simulation and statistical properties of flicker noise
Litov. Fiz. SB. (USSR) 24 (1984) 32-41.

Palinkas, G. and Heinzinger, K.
Hydration shell structure of the calcium ion
Chem. Phys. Lett. 126 (1986) 251-4.

Pandey, S. and Trikha, S.K.
Computer simulation studies of the phase transition in compressible deuteroammonium chloride
Aust. J. Phys. 38 (1985) 733-40.

Paniagua, M., Garcia, de la Vega, J.M., and Alvarez Collado, J.R.
Two-configuration MC potential energy surface for the reaction of Mg with HF
Chem. Phys. 101 (1986) 55-65.

Paolini, G.V., Ciccotti, G. and Massobrio, C.
Nonlinear thermal response of a Lennard-Jones fluid near the triple point
Phys. Rev. A 34 (1986) 1355-62.

Parlinski, K. and Grimm, H.
Molecular-Dynamic study of the molecular glass model for
$RB_{1-x}(ND_4)_x xD_2PO_4$
Phys. Rev. B 33 (1986) 4868-79.

Parsonage, N.G.
Size-effects on simulations in the grand canonical ensemble
Chem. Phys. Lett. 127 (1986) 594-9.

Partiti, C.S.M., Piccini, A. and Rechenberg, H.R.
Quadrupole interaction and molecular dynamics in $A_2FeC\ell_5.H_2O$(A=K, RB, BH_4): evidence for a structural phase transition in $(NH_4)_2FECL_5$.H....
Solid State Commun. 56 (1985) 687-91.

Paskal, Yu.I. and Domrachev, V.E.
Computer simulation of vacancy-controlled phase separation of binary solid solution
Metalbfizika (USSR) (1984) 959-66.

Pasterny, K. and Kocot, A.
Application of the confined rotator model for calculation of higher-order orientational correlation functions
J. Chem. Soc. Faraday Trans. II 82 (1986) 485-94.

Pavlovich, V.N.
Diffusion in semiconductors, stimulated by resonant laser radiation and heat pulses
Energy Pulse Modification of Semiconductors and Related materials. Proc. of Conf., Vol. 1 (1985) 72-6.

Pearson, E.M., Halicioglu, T. and Tiller, W.A.
Laplace-transform technique for deriving thermodynamic equations from the classical microcanonical ensemble
Phys. Rev. A 32 (1985) 3030-9.

Pechenik, A., Susman, S., Whitmore, D.H., et al
Ionic conductivity in glasses: a Monte Carlo study of ordered and disordered one-dimensional models
Solid State Ionics. Diffus. and React. 18-19 (1986) 403-9.

Pechenik, A., Whitmore, D.H. and Ratner, M.A.
Conductivity and ordering on the planar honeycomb lattice: A Monte Carlo study of transport and order parameters in betaseconds aluminas
J. Chem. Phys. 84 (1986) 2827-36.

Peterson, B.K., Walton, J.P.R.B. and Gubbins, K.E.
Microscopic studies of fluids in pores: computer simulation and mean-field theory
Int. J. Thermophys. 6 (1985) 585-93.

Petroff, P.M.
Role of electron microscopy in semiconductor electronic defects analysis
Microscopic Identification of Electronic Defects in Semiconductors (1985) 433-40.

Pollmann, J., Kalla, R., Kruger, P., et al
Atomic, electtonic and vibronic structure of semiconductor sufaces
Appl. Phys. A41 (1986) 21-38.

Posselt, M.
A short overview on Monte Carlo simulations of ion beam penetration into amorphous solids
Phys. Status Solidi A 94 (1986) 337-41.

Radkowitsch, H., Prielmeier, F.X., Lang, E.W., et al
Density dependence of the molecular dynamics of fluid Ch$_3$F and Cf$_3$H studied by NMR
Physica B and C 139 (1986) 96-9.

Raedt, H.D. and Lagendijk, A.
Monte Carlo simulation of quantum statistical lattice models
Phys. Rep. 127 (1985) 233-307.

Raff, L.M., Nooreatcha, I. and Thompson, D.L.
Monte Carlo variational transition-state theory study of recombination and description of hydrogen on Si(111)
J. Chem. Phys. 85 (1986) 3081-9.

Rahman, A.
Molecular dynamics studies of structural transformation in solids
Mater. Sci. Forum 1 (1984) 211-22.

Rangaswamy, M. and Farkas, D.
Prediction of high dose ion implantation profiles as influenced by radiation transport and sputtering
Ion Beam Processes in Advanced Electronic materials and Device Technology, 1985, 91-6.

Rapaport, D.C.
Cluster number scaling in two-dimensional percolation
J. Phys. A 19 (1986) 291-304.

Remerie, K., Engberts, J.B.F.N. and Van Gunsteren, W.F.
A molecular dynamics computer simulation study of the temperature dependence of hydration of 1,4-dioxane and 1,3-dioxane
Chem. Phys. 101 (1986) 27-44.

Remerie, K., Van Gunsteren, W.F. and Engberts, J.B.F.N.
A molecular dynamics computer simulation study of the hydration of bis(methylsulphonyl)methane in water
Mol. Phys. 56 (1985) 1393-409.

Ribeiro, A.C. and Martins, A.F.
Molecular dynamics in a columnar D_{HO} liquid crystal-NMR study
Port. Phys. 16 (1985) 117-23.

Rodmacq, B., Billard, L., Mangin, P., et al
Computer simulation of hydrogenated and deuterated CuTi amorphous alloys
J. Phys. Colloq. 46 (1985) 415-19.

Rojas, O.L., Levy, R.M. and Szabo, A.
Corrections to the quasiharmonic approximation for evaluating molecular entropies
J. Chem. Phys. 85 (1986) 1037-43.

Romano, S.
Computer simulation study of a simple cubic dipolar lattice
Nuovo Cimento 7D (1986) 717-33.

Romano, S.
Computer simulation of a long-ranged ising antiferromagnet in one dimension. II. Inverse-square-power law
Nuovo Cimento B 89 (1985) 1-13.

Romano, S.
Computer simulation study of the singlet orientational distribution function for a model antiferroelectric nematic
Europhys. Lett. 2 (1986) 431-6.

Rosato, V., Ciccotti, G. and Pontikis, V.
Molecular-dynamics study of surface premelting effects
Phys. Rev. B 33 (1986) 1860-70.

Rosenman, I., Batallan, F., Magerl, A. et al
Molecular dynamics and phase transitions in HNO_3 graphite intercalation compound studied by quasi-elastic neutron scattering
Synth. Met. 12 (1985) 117-23.

Ruff, I., Baranyai, A., Palinkas, G. et al
Grand canonical Monte Carlo simulation of liquid argon
J. Chem. Phys. 85 (1986) 2169-77.

Rujan, P., Uimin, G. and Selke, W.
Commensurate-incommensurate phase transitions and wetting in a lattice-gas model with axially competing interactions
Phys. Rev. B 32 (1985) 7453-68.

Rull, L.F., Morales, J.J. and Cuadros, F.
Isothermal molecular-dynamics calculations
Phys. Rev. B 32 (1985) 6050-52.

Russell, J.E.
Analysis of the reaction $He^{+}+He+He=He_2{}^{+}+He$. II. Improved sampling.
J. Chem. Phys. 84 (1986) 4394-400.

Russell, J.E.
Analysis of the reaction $He^{+} + He + He = He_2{}^{+} + He$
J. Chem. Phys. 83 (1985) 3363-89.

Ryckaert, J.-P. and Ciccotti, G.
Andersen's canonical-ensemble molecular dynamics for molecules with constraints
Mol. Phys. 58 (1986) 1125-36.

Rynefors, K., Elofson, P.A. and Holmlid, L.
Monte Carlo simulation of $O(^1D)+H_2$ and $O(^1D)+HC\ell$-rotational excitation of product OH radicals
Chem. Phys. 100 (1985) 53-63.

Ryzhov, V.V., Turchanovsky, I.Yu. and Shemyakina, S.B.
Dynamics of pulsed electron-beam annealing of ion-implanted semiconductors
Energy Pulse Modification of Semiconductors and Related Materials. Proc. of Conf., Vol. 1 (1985) 42-7.

Saetre, T.O., Hunderi, O. and Nes, E.
Computer simulation of primary recrystallisation microstructures: the effects of nucleation and growth kinetics
Acta Metall. 34 (1986) 981-7.

Sagarik, K.P., Ahlrichs, R. and Brode, S.
Intermolecular potentials for ammonia based on the test particle model and the coupled pair functional method
Mol. Phys. 57 (1986) 1247-64.

Sahimi, M.
Phenomenological renormalisation of Monte Carlo data for percolation
J. Phys. A 18 (1985) 3597-603.

Saito, K. and Moriuchi, S.
Development of a Monte Carlo code for the calculation of gamma ray transport in the natural environment (dosimetry application)
Radiat. Prot. Dosim. 12 (1985) 21-8.

Sakuma, T. and Miyazaki, T.
Theory of the surface acoustic soliton. III. Effect of the anharmonic loss and surface inhomogeneities
Phys. Rev. B 33 (1986) 1036-46.

Samios, J., Mittag, U. and Dorfmuller, T.
A molecular dynamics simulation of interaction-induced FIR absorption spectra of liquid CS_2
Mol. Phys. 59 (1986) 65-79.

Sanchez, A., De Miguel, J.J., Martinez, E., et al
Phase diagram of sulphur on Mo(110)
Surf. Sci. 171 (1986) 157-69.

Sang Bub Lee and Nakanishi, H.
Crossover scaling in biased self-avoiding walks
Phys. Rev. B 33 (1986) 1953-62.

Sang-Rak Kim and Jong-Jean Kim
Molecular dynamics study on simple liquids. I. Comments on the computer programs
New Phys. (Korean Phys. Soc.) 24 (1984) 341-52.

Sank-Rak Kim and Jong-Jean Kim
Depolarized light scattering from simple liquid under shear flow: nonequilibrium molecular dynamics study
Phys. Lett. A 114 (1986) 43-6.

Santoro, R.T., Barnes, J.M. and Alsmiller, R.G., Jr.
Monte Carlo and discrete ordinates calculations of 14-MeV neutrons streaming through a stainless steel duct: Comparison with experimental. I
Nucl. Sci. and Eng. 92 (1986) 584-95.

Sasagawa, F., Miyashita, S. and Suzuki, M.
Monte Carlo simulation of nonlinear stochastic processes: noise-induced long-time tail and its universality
Prog. Theor. Phys. 74 (1985) 1013-21.

Saxena, A., Gawlinski, E.T. and Gunton, J.D.
Structural phase transitions on the Si(100) surface
Surf. Sci. 160 (1985) 618-40.

Scalapino, D.J.
Simulations: A tool for studying quantum condensed matter systems
J. Stat. Phys. 43 (1986) 757-70.

Schafer, L. and Baumgartner, A.
Internal correlations of a single polymer chain
J. Phys. 47 (1986) 1431-4.

Schiferl, S.K. and Wallace, D.C.
Statistical errors in molecular dynamics averages
J. Chem. Phys. 83 (1985) 5203-9.

Schmelzer, J.
The curvature dependence of surface tension of small droplets
J. Chem. Soc. Faraday Trans. I 82 (1986) 1421-8.

Schmidt, V., Hillebrand, R., Albrecht, R., et al
Computer simulation of HREM images of network models of Si-O_2 glass
Ultramicroscopy 17 (1985) 357-64.

Schneider, M., Rahman, A. and Schuller, I.K.
Vapor-phase growth of amorphous materials: A molecular-dynamics study
Phys. Rev. B 34 (1986) 1802-5.

Schobinger,M. and Abraham, F.F.
Energetics of the incommensurate phase of krypton on graphite: a computer simulation study
Structure of Surfaces, (1985) 334-40.

Schoen, M. and Hoheisel, C.
The shear viscosity of a Lennard-Jones fluid calculated by equilibrium molecular dynamics
Mol. Phys. 56 (1985) 653-72.

Schoen, M. and Hoheisel, C.
Static and dynamic cross correlation in thermodynamically stable and unstable mixtures. II. Molecular dynamics studies on Lennard-Jones systems consisting of particles of unequal size
Mol. Phys. 57 (1986) 65-79.

Schoen, M. and Hoheisel, C.
Computation and analysis of the total dynamic structure factor $S(K,\Omega)$ for small wave vectors: A molecular dynamics study for Lennard-Jones liquid mixtures
Mol. Phys. 58 (1986) 181-92.

Schoen, M., Hoheisel, C. and Beyer, O.
Liquid CH_4, liquid CF_4 and the partially miscible liquid mixture CH_4CF_4. A molecular dynamics study based on both a spherically symmetric and a four-centre Lennard Jones potential
Mol. Phys. 58 (1986) 699-709.

Schoen, M., Vogelsang, R. and Hoheisel, C.
Computation and analysis of the dynamic structure factor $S(K,\Omega)$ for small wave vectors. A molecular dynamics study for a Lennard-Jones liquid
Mol. Phys. 57 (1986) 455-71.

Schommers, W.
Structural and dynamical behaviour of noble-gas surfaces
Phys. Rev. B 32 (1985) 6845-52.

Schrader, R.
String tension and glueball mass in a lattice theory of disconnected, selfintersecting random surfaces
Commun. Math. Phys. 102 (1985) 31-46.

Schranz, H.W., Nordholm, S. and Freasier, B.C.
A test of RRKM theory against numerical simulation for classical chain molecules. I. Method and preliminary results
Chem. Phys. 108 (1986) 69-91.

Schrobinger, M., Koch, S.W. and Abraham, F.F.
Langevin dynamics simulations of phase separation in a one-component system
J. Stat. Phys. 42 (1986) 1071-89.

Schulten, K. and Bittl, R.
Probing the dynamics of a polymer with paramagnetic end groups by magnetic fields
J. Chem. Phys. 84 (1986) 5155-61.

Schuttler, H.-B., and Scalapino, D.J.
Monte Carlo studies of the dynamics of quantum many-body systems
Phys. Rev. Lett. 55 (1985) 1204-7.

Seaton, N.A. and Glandt, E.D.
Monte Carlo simulation of adhesive disks
J. Chem. Phys. 84 (1986) 4595-601.

Selke, W. and Szpilka, A.M.
Monte-Carlo study of a model for the roughening transition of high-index crystal faces
Z. Phys. B 62 (1986) 381-6.

Shankar, R.
Truncation errors in the Monte Carlo renormalization group: A comparative study
Phys. Rev. B33 (1986) 6515-18.

Shankar, R. and Gupta, R.
Clear evidence of redundant operators in Monte Carlo studies of the ising model
Phys. Rev. B 32 (1985) 6084-6.

Shankar, R., Gupta, R. and Murthy, G.
Dealing with truncation in Monte Carlo renormalization - Group calculations
Phys. Rev. Lett. 55 (1985) 1812-15.

Shapir, Y.
Comment on 'Monte Carlo test of dimensional reduction for branched polymers in three dimensions'
J. Phys. A 19 (1986) 825.

Shegelski, M.R.A.
New result for the chemical potential of intrinsic semiconductors: Low-temperature breakdown of the Fermi-Dirac distribution function
Solid State Commun. 58 (1986) 351-4.

Sheikhet, I.I. and Simkin, B.Ya.
Monte Carlo calculations on the structure and energetics of aqueous methylformamide, including the enolic form
Zh. Strukt. Khim. 25 (1984) 91-7.

Shen-Shu Sung and Jordan, P.C.
Structures and energetics of monovalent ion-water microclusters
J. Chem. Phys. 85 (1986) 4045-51.

She, R.S.C., James C. and Evans G.T.
Orientational correlations in fluids of convex bodies. II. Explicit results for two- and three-dimensional systems
J. Chem. Phys. 85 (1986) 1525-33.

Shreve, A.P., Walton, J.P.R.B. and Gubbins, K.E.
Liquid drops of polar molecules
J. Chem. Phys. 85 (1986) 2178-86.

Shteinberg, A.S.
Short-range order in binary alloys
Fiz. Met. and Metalloved. 61 (1986) 657-65.

Shteinberg, A.S.
Influence of correlation on the temperature of an ordering phase transition in a binary alloy
Fiz. Met. and Metalloved. 60 (1985) 444-8.

Shukla, R.C. and Heiser, G.A.
Mean-square atomic displacement of alkali-metal atoms: a comparison of the lattice-dynamics and molecular-dynamics results
Phys. Rev. B 33 (1986) 2152-7.

Silverberg, M., Ben-Shaul, A. and Rebentrost, F.
On the effects of adsorbate aggregation on the kinetics of surface reactions
J. Chem. Phys. 83 (1985) 6501-13.

Simmons, A.D. and Cummings, P.T.
Non-equilibrium molecular dynamics simulation of dense fluid methane
Chem. Phys. Lett. 129 (1986) 92-8.

Simonen, E.P.
Theory of amorphization kinetics in intermetallics
Nucl. Instrum. and Meths. Phys. Res. Sect.B, B16 (1986) 198-202.

Sinder, M.I.
Theory of impurity diffusion profiles with concentration-dependent diffusion coefficients
Fiz. and Tekh. Poluprovodn. (USSR), 20 (1986) 373-5.

Singer, K. and Smith, W.
Semiclassical many-particle dynamics with Gaussian wave packets
Mol. Phys. 57 (1986) 761-75.

Singh, S and Goldman, S.
Some practical considerations in the use of metropolis and force biased Monte Carlo simulations on liquids
J. Comput. Phys. 62 (1986) 464-71.

Skotniczny, Z., Moscinski, J. and Rycerz, Z.
Computer simulation studieds of cation migration mechanisms in sodium beta-alumina
J. Phys. C 19 (1986) 4781-96.

Smilauer, P.
Percolation theory
Cesk. Cas. Fyz. Sekce A (Czechoslovakia), 36 (1986) 220-48.

Sogo, K. and Kimura, N.
A Monte Carlo computation of the entropy, the free energy and the effective potential: use of distribution functions
Phys. Lett. A 115 (1986) 221-4.

Sokolic, F., Guissani, Y. and Guillot, B.
Molecular dynamics simulations of thermodynamic and structural properties of liquid SO_2
Mol. Phys. 56 (1985) 239-53.

Spielberg, J.I. and Gelerinter, E.
EPR probe study of the molecular dynamics of the supercooled liquid, the glass state, and the glass transition in liquid-crystalline MBBA (N-(P-methoxybenzylidene)-P-butylaniline)
Phys. Rev. A 32 (1985) 3647-60.

Spohr, E. and Heinzinger, K.
Molecular dynamics simulation of a water-metal interface
Chem. Phys. Lett. 123 (1986) 218-21.

Spohr, E. and Heinzinger, K.
A molecular dynamics study of an aqueous LiI solution between Lennard-Jones walls
J. Chem. Phys. 84 (1986) 2304-9.

Sprik, M., Impey, R.W. and Klein, M.L.
Study of electron solvation in liquid ammonia using quantum path integral Monte Carlo calculations
J. Chem. Phys. 83 (1985) 5802-9.

Sprik, M., Impey,R.W., and Klein, M.L.
Electron-ion interactions and ionization in a polar solvent
Phys. Rev. Lett. 56 (1986) 2326-9.

Sprik, M., Klein, M.L. and Chandler, D.
Simulation of an excess electron in a hard sphere fluid
J. Chem. Phys. 83 (1985) 3042-9.

Stancioff, P., Willis, C., El-Batanouny, et al
Sine-Gordon kinks on a discrete lattice. II. Static properties
Phys. Rev. B 33 (1986) 1912-20.

Stillinger, F.H. and Laviolette, R.A.
Sensitivity of liquid-state inherent structure to details of intermolecular forces
J. Chem. Phys. 83 (1985) 6413-18.

Straatsma, T.P., Berendsen, H.J.C. and Stam, A.J.
Estimation of statistical errors in molecular simulation calculations
Mol. Phys. 57 (1986) 89-95.

Straley, J.P.
Effect of topological frustration on the freezing temperature
Phys. Rev. B 34 (1986) 405-9.

Strekalov, V.N.
Diffusion in semiconductors under laser annealing conditions
Fiz. and Tekh. Poluprovodn. (USSR), 20 (1986) 361-3.

Stump, D.R.
Application of the projector Monte Carlo method to the transfer matrix of the classical XY model
Nucl. Phys. B: Field Theory and Stat. Syst. 265 (1986) 113-28.

Styer, D.F., Phani, M.K. and Lebowitz, J.L.
Multiatom interactions in the FCC Ising binary alloy: low-temperature behaviour and Monte Carlo simulation
Phys. Rev. B34 (1986) 3361-70.

Sugiyama, G. and Koonin, S.E.
Auxiliary field Monte Carlo for quantum many-body ground states
Ann. Phys. 168 (1986) 1-26.

Suh, S.-H. and Macelroy, J.M.D.
Molecular dynamics simulation of hindered diffusion in microcapillaries
mol. Phys. 58 (1986) 445-73.

Susuki, M.
Quantum statistical Monte Carlo methods and applications to spin systems
J. Stat. Phys. 43 (1986) 883-909.

Suzuki, M.
New Methods to study critical phenomena-systematic cluster mean-field approach, and thermofield dynamics of interacting quantum systems
Quantum field theory. Proc. Int. Symposium in Honour of Hiroomi Umezawa (1986) 505-31.

Suzuki, M.
Thermo field Monte Carlo and transfer-matrix methods in quantum systems
Phys. Rett. A 111 (1985) 440-4.

Szabo, Gy. and Kertesz, J.
Lattice gas model on tetrahedral sites of BCC lattice: anisotropic diffusion in the intermediate phase
Hungarian Acad. Sci. Budapest Report: KFKI-1986-06-E, 1986.

Szabo, G. and Kertesz, J.
The lattice gas model on tetrahedral sites of a BCC lattice: Anisotropic diffusion in the intermediate phase
J. Phys. C19 (1986) L273-7.

Szczesniak, E.
Molecular dynamics and phase transitions in solid 2-methyl-2-propanethiol studied by ^{1}H NMR relaxation
Mol. Phys. 58 (1986) 551-60.

Tachiya, M.
Influence of the mean free path of reactant particles on the kinetics of diffusion-controlled reactions. II. Rate of bulk recombination
J. Chem. Phys. 84 (1986) 6178-81.

Tahir-Kheli, R.A. and El-Meshad, N.
Particle motion in a mixed dynamic alloy: binary system in one dimension
Phys. Rev. B 32 (1985) 6184-9.

Tahir-Kheli, R.A. and El-Meshad, N.
Correlated diffusion in two-dimensional systems
Phys. Rev. B 32 (1985) 6166-75.

Tahir-Kheli, R.A., Elliott, R.J. and Holdsworth, P.C.W.
Correlated random walks on two-sublattice systems. II. Monte Carlo simulations
Phys. Rev. B34 (1986) 3233-7.

Takagi, R., Fukase, S., Naito, S., et al
Growth of aggregate of Cl^- ions in the molten $K_{0\cdot 8}$ $(KCL)_{0\cdot 2}$ system simulated by molecular dynamics
Trans. Jpn. Inst. Met. 26 (1985) 855-60.

Takagi, R., Fukase, S., Naito, S., et al
Computer simulation of the molten $K_{0\cdot 8}(KC\ell)_{0\cdot 2}$ system at 1073K
Trans. Jpn. Inst. Met. 26 (1985) 615-21.

Takahashi, M.
Effective potential method in path-integral Monte Carlo calculation and application to ^{4}He at T>4K
J. Phys. Soc. Jpn. 55 (1986) 1952-60.

Takasu, M. and Suzuki, M.
Monte Carlo simulation of relative diffusion in stochastic fields
Physica A 137 (1986) 454-63.

Takasu, M., Miyashita, S. and Suzuki, M.
Monte Carlo simulation of quantum Heisenberg magnets on the triangular lattice
Prog. Theor. Phys. 75 (1986) 1254-7.

Talbot, J., Lebowitz, J.L., Waisman, E.M. et al
A comparison of perturbative schemes and integral equation theories with computer simulations for fluids at high pressures
J. Chem. Phys. 85 (1986) 2187-92.

Tallon, J.
Layerwise structure in the FCC(111) solid-liquid interface
Phys. Rev. Lett. 57 (1986) 1328-31.

Tanaka, M. and Kawabe, T.
On the spin-one Ising model for an adsorbed monolayer
J. Phys. Soc. Japan 55 (1986) 1873-9.

Tang, S., Mahanti, S.D. and Kalia, R.K.
Ferroelastic phase transition in two-dimensional molecular solids
Phys. Rev. Lett. 56 (1986) 484-7.

Tang,. S. and Mahanti, S.D.
Vortices and strings: phase transition in anisotropic planar-rotor systems
Phys. Rev. B 33 (1986) 3419-22.

Tapia, O. and Lluch, J.M.
Solvent effects on chemical reaction profiles. I. Monte Carlo simulation of hydration effects on quantum chemically calculated stationary structures
J. Chem. Phys. 83 (1985) 3970-82.

Thirumalai, D.
Path-integral Monte Carlo simulations of electron localization in water clusters
J. Stat. Phys. 43 (1986) 973-84.

Tobochnik, J., Gould, H. and Klein, W.
Early-time instabilities in a dynamic percolation model
Phys. Rev. B 33 (1986) 377-84.

Todd, J., Merlin R., Clarke, R. et al
Synchrotron x-ray study of a fibonacci superlattice
Phys. Rev. Lett. 57 (1986) 1157-60.

Vinals, J. and Gunton, J.D.
Fixed points and domain growth for the Potts model
Phys. Rev. B 33 (1986) 7795-8.

Vovelle, F., Genest, M. Ptak, M.
EMPWI Monte Carlo simulation of liquid water
Theochem. 32 (1986) 1-12.

Vrbik, J. and Rothstein, S.M.
Optimal spacing and weights in diffusion Monte Carlo
Int. J. Quantum Chem. 29 (1986) 461-8.

Vrbik, J. and Rothstein, S.M.
Quadratic accuracy diffusion Monte Carlo
J. Chem. Phys. 63 (1986) 130-9.

Walker, A.B., Smith, W. and Inglesfield, J.E.
Phase diagrams of simple metals from molecular dynamics
J. Phys. F 16 (1986) L35-41.

Wang Jing-Han, Li De-Xiu and Chen Jin-Chang
Computer simulation of the structure of amorphous alloy $Ni_{64}B_{36}$. I. The chemical short range order in the alloy
Acta Phys. Sin. 35 (1986) 482-8.

Warshel, A. and King, G.
Polarization constraints in molecular dynamics simulation of aqueous solutions: the surface constraint all atom solvent (SCAAS) model
Chem. Phys. Lett. 121 (1985) 124-9.

Watson, B.P.
Percolation at the surface of semi-infinite two-dimensional lattices
Phys. Rev. B33 (1986) 6446-50.

Weber, M.J.
Computer simulations of rare earth sites in glass: experimental tests and applications to laser materials
Cryst. Lattice Defects and Amorphous Mater. 12 (1985) 527-40.

Weber, T.A. and Stillinger, F.H.
Interactions, local order, and atomic-rearrangement kinetics in amorphous nickel-phosphorous alloys
Phys. Rev. B 32 (1985) 5402-11.

Wejchert, J., Weaire, D. and Kermode, J.P.
Monte Carlo simulation of the evolution of a two-dimensional soap froth
Phils. Mag. B 53 (1986) 15-24.

Wielopolski, P.A. and Smith, E.R.
Dihedral angle distribution in liquid N-butane: Molecular dynamics simulations
J. Chem. Phys. 84 (1986) 6940-2.

Wilkinson, M.K., Gaunt, D.S., and Lipson, J.E.G.
Lattice models of branched polymers: statistics of uniform stars
J. Phys. A 19 (1986) 789-96.

Wilson, M.A., Pohorille, A. and Pratt, L.R.
Molecular dynamic test of the Brownian description of Na^+ motion in water
J. Chem. Phys. 83 (1985) 5832-6.

Wojcik, M. and Clementi, E.
Molecular dynamics simulation of liquid water with three-body forces included
J. Chem. Phys. 84 (1986) 5970-1.

Wu Dacheng, Zhao Delu and Qian Renyuan
Monte Carlo simulation of a confined random-walk chain
Polymer 27 (1986) 1087-90.

Xu Chi, Chen Nianyi, Jiang Naiziong, et al
Computerized simulation of structure of cryolite melt
Acta Metall. Sin. (China), 22 (1986) B68-74.

Yamaguchi, T., Okada, I., Ohtaki, H., et al
X-ray and neutron diffraction and molecular dynamics simulation of molten lithium and rubidium nitrates
Mol. Phys. 58 (1986) 349-64.

Yamamoto, T. and Hara, T.
X-ray and Monte Carlo studies on the 19 degrees C transition of poly(tetrafluoroethylene)
Polymer 27 (1986) 986-92.

Yang, Y.S. and Lam, P.M.
Contant fugacity Monte Carlo enumeration method for linear and branched polymers
Commun. Theor. Phys. 4 (1985) 497-501.

Yanushkevich, V.A., Poyaninov, A.V. and Prutskov, E.G.
Mechanism of formation and ionization of point-type defects in
semiconductors on pulsed laser irradiation
Izv. Akad. Nauk SSSR Ser. Fiz. 49 (1985) 1146-52.

Yashonath, S. and Rao, C.N.R.
An investigation of solid adamantane by a modified isothermal-isobaric
ensemble Monte Carlo simulation
J. Phys. Chem. 90 (1986) 2552-4.

Yashonath, S. and Rao, C.N.R.
Structural changes accompanying the formation of isopentane glass
J. Phys. Chem. 90 (1986) 2581-4.

Yin, M.T.
Theory of structural properties of covalent semiconductors
Proc. 17th Int. Conf. on the Physics of Semiconductors (1985) 927-32.

Yu, K.W. and Hui, P.M.
Random walks in one-dimensional disordered systems: A Monte Carlo study
Phys. Rev. A 33 (1986) 2745-8.

Zabolitzky, J.G.
Monte-Carlo solution to the many-body Schrodinger equation
Prog. part and Nucl. Phys. 16 (1986) 103-38.

Zannoni, C.
A cluster Monte Carlo Method for the simualtion of anisotropic systems
J. Chem. Phys. 84 (1986) 424-33.

Zhang, Y.C. and Shapir, Y.
Kinetic growth of polyelectrolytes: long-range true self-avoiding walks
Phys. Rev. B 33 (1986) 4941-3.

Zhao-Bin Su, Ya-Xin Wang and Lu Yu
Quantum fluctuation of the order parameter in polyacetylene
Mol. Cryst. and Liq. Cryst. 118 (1985) 75-9.

Zichi, D.A. and Rossky, P.J.
Solvent molecular dynamics in regions of hydrophobic hydration
J. Chem. Phys. 84 (1986) 2814-22.

Ziff, R.M.
Test of scaling exponents for percolation-cluster perimeters
Phys. Rev. Lett. 56 (1986) 545-8.

Zogal, O.J., Galewski, Z., Grech, E., et al
Molecular dynamics in solid 1,4-Diazabicyclo(2.2.2)octane perchlorate and hemiperchlorate
Mol. Phys. 56 (1985) 673-81.

Zoppi, M. and Spinelli, G.
Interaction-induced translational Raman scattering of liquid argon: the spectral moments
Phys. Rev. A 33 (1986) 939-45.

Computer simulation of condensed matter. Proceedings of the NATO advanced research workshop
Physica B and C 131B+C (1985).

Fifth International Conference on Dynamical Processes in the excited states of solids
J. Phys. Colloq. 46 (1985)

Proceedings of the Conference on Frontiers of Quantum Monte Carlo
J. Stat. Phys. 43 (1986)

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