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DARESBURY LABORATORY

INFORMATION QUARTERLY for MD & MC SIMULATIONS

An Informal Newsletter associated with Collaborative Computational Project No. 5 on Molecular Dynamics and Monte Carlo Simulations of Macroscopic systems.

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Contents

Editor: Dr. William Smith

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

Deputy Editor: Dr. David Heyes

Royal Holloway College,
University of London, Egham TW20 0EX
England

Editorial

Now that the newsletter has reached its eighth issue it is pleasing to report that interest in its contents remains high. The response to the recent CCP5 questionnaire revealed uniform appreciation of both its content and format. Such testimony is gratifying in view of the effort required to produce it! We hope that this new issue will be equally well received.

Our thanks once again go to the contributors listed below. Most of them have been contributors in the past and are partly the reason for the newsletter's popularity. We hope that our readers will be inspired themselves to contribute and we remind them that we are happy to consider any article they may wish to send. (We would be particularly pleased to hear from our overseas readers).

Lastly, we should thank the Reprographics Division at Daresbury Laboratory for their efforts in typing and producing the newsletter. Their flexibility and hard work greatly reduce the workload on your humble editor.

Contributors:

S.M. Thompson,	School of Chemical Engineering, Olin Hall, Cornell University, Ithaca, NY 14853, USA.
D.M. Heyes,	Department of Chemistry, Royal Holloway College, Egham, Surrey, TW20 0EX.
N. Corbin,	Department of Chemistry, University of Western Ontario, London, Ontario, Canada.
S.K. Mitra,	Computer Science Department, University of Reading, RG6 2AX.
R.W. Hockney,	" " " " " " " "
D. Fincham,	D.A.P. Support Unit, Queen Mary College, Mile End Road, London, E1 4NS.
K. Singer,	Department of Chemistry, Royal Holloway College, Egham, Surrey, TW20 0EX.
F. Gibb,	Library and Reprographic Services, SERC Daresbury Laboratory, Daresbury, Warrington, WA4 4AD.
W. Smith,	Theory and Computational Science Division, SERC Daresbury Laboratory, Daresbury, Warrington, WA4 4AD.

General News

1) The next CCP5 Meeting will be on the subject of "Phase Transitions" and is scheduled to occur in December, 1983. The location has not yet been decided. More details will be released in the next "Information Quarterly".

2) Our thanks go to all the CCP5 participants who completed and returned the CCP5 questionnaire, that was circulated recently. With this help an informed "Renewal Proposal" has been prepared and submitted to the SERC. At the time of writing there has been no discussion of the renewal of CCP5 within the SERC. We are, however, optimistic of the continuation of CCP5 beyond the 30th September, 1983!

3) Users of the Cray-1S at Daresbury will know that it is due to move to ULCC after Easter 1983. There are, however, potential sources of delay, principally the linking of the SERC network into the new ULCC telecommunications system and the completion of the ULCC building extension. Users should consult the ULCC Newsletter (No. 164 March, 1983) for details. The Cray-1S will be unavailable to users for approximately four weeks following the removal.

4) People who attended the seventh CCP5 meeting in Reading on "New Computers/The Simulation of Quantum Mechanical Systems" last December, were no doubt impressed by the organisation of the meeting as well as its content. Our thanks go to Professor R.W. Hockney of the Department of Computer Science and to the staff at Reading University for organising the meeting and to David Heyes of Royal Holloway College, for his assistance.

5) It has been suggested that the Newsletter could be used to announce forthcoming publications relevant to computer simulation. We would therefore be pleased to announce the imminent appearance of any such paper or document accepted for publication, provided thc the authors notify us in good time!

6) Readers are reminded of the existence of the CCP5 Program Library which is available to anyone interested in its contents. The programs may be obtained, free of charge, on submission of a magnetic tape to the program librarian (Dr. W. Smith, TCS Division, Daresbury Laboratory, Daresbury, Warrington, WA4 4AD). Listings, and documentation for individual programs are also available. A list describing the programs available is provided overleaf.

List of Programs in the CCP5 Program Library.

MDATOM by S. M. Thompson.

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

HMDIAT by S. M. Thompson.

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

MDLIN by S. M. Thompson.

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

MDLINQ by S. M. Thompson.

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

MDTETRA by S. M. Thompson.

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

MDPOLY by S. M. Thompson.

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

MDMIXT by W. Smith.

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

MDMULP by W. Smith.

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

MDMPOL by W. Smith & D. Fincham.

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

DENCOR by W. Smith.

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

CURDEN by W. Smith.

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

HLJ1 by D. M. Heyes.

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

HLJ2 by D. M. Heyes.

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

HLJ3 by D. M. Heyes.

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

HLJ4 by D. M. Heyes.

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

HLJ5 by D. M. Heyes.

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

HLJ6 by D. M. Heyes.

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

MCRPM by D. M. Heyes.

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

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

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

MDATOM by D. Fincham.

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

MDDIAT by D. Fincham.

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

MDDIATQ by D. Fincham.

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

MDIONS by D. Fincham & N. Anastasiou.

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

MDMANY by D. Fincham & W. Smith.

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

CARLOS by B. Jonsson & S. Romano.

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

MCN by N. Corbin.

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

SCN by N. Corbin.

M.C. simulation of atomic fluids. Standard (Rossky, Friedman and Doll) Monte Carlo program for atomic fluids.

SMF by N. Corbin.

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

REVIEW OF THE SEVENTH CCP5 MEETING: NEW COMPUTERS / THE SIMULATION OF QUANTUM MECANICAL SYSTEMS.

W. Smith.

The seventh CCP5 meeting, which was staged at Reading 16/17 th December 1982 was somewhat of a departure from previous CCP5 meetings. In recognition of the rapid developments in computer technology that have occurred over the last few years, part of the meeting was given over to the subject of new computers. The lectures on this theme were stongly indicative of the versatility and power of modern computers and managed a few surprises in an already surprising subject. Sharing with the topic of new computers was a collection of lectures on the quantum aspects of simulation work. This is a highly complicated area and the lectures clearly showed both the difficulties and the importance of this work.

The first speaker was Professor K. R. Wilson (University of California), who spoke on the subject of molecular mechanics. He began by describing existing interactive systems which permit the experimenter to participate in a molecular dynamics simulation. Through the use of manual controls the experimenter may exert forces and torques on a molecule and simultaneously feel the system response. Such systems are meant to enhance the experimenter's intuitive grasp of the dynamic processes within a liquid.

Professor Wilson has developed the graphical capability of his programs to produce motion pictures of simulated systems. One such film demonstrated the microscopic processes within such liquids as water, ethane and cyclohexane. The intramolecular motions were clearly visible. The film also showed the photodissociation of molecular chlorine in a selection of solvents. The processes of recombination and quenching and the influence of the solvents were revealed. The overlap of the vibrational frequency spectrum of the solvent with that of the excited chlorine molecule provided the explanation for the solvent quenching efficiency. A further demonstration of this graphical approach was given in a 3-D film of the mechanism of ion conduction in bacterial gramicidin.

Professor Wilson's principal research tool is a system he described as a molecular workstation, at the heart of which is an FPS AP 120B. Commenting on the use of this processor, he revealed that the block processing of data was necessary to reduce relative I/O overheads and that it was preferable to recalculate the data rather than reread them from storage. The AP 120B can be totally dedicated to one user, thus allowing long projects to be completed quickly, but its reliance on assembler language coding for optimal efficiency is a drawback. Professor Wilson sees the future in terms of extending the capability of the molecular workstation.

In the second lecture Dr. D. M. Heyes (Royal Holloway College) reported his investigations into the relative efficiency of the new computers in various MD simulations. Dr. Heyes has studied a broad range of computers, including serial (e.g. Amdahl 470/V8), pipeline (e.g. Cray-1S) and parallel processors (e.g. ICL DAP/2980). Each computer was used to simulate a Lennard-Jones fluid at different densities using a simple Verlet method initially and then extending to the more sophisticated 'neighbourhood table' and 'link cell' methods. The general superiority of the Cray-1S was apparent throughout, but it lost ground to the serial computers in the neighbour-listed methods due to the loss of vectorisation inherent in the SCATTER and GATHER operations. (Dr. Heyes's results are reported in the December issue of the CCP5 newsletter.)

The relative performance of serial, pipeline and parallel processors was also the subject of the lecture by Professor R. W. Hockney (Reading), who sought to provide a quantitative scheme both to classify and assess the performance of new computers. He began by defining the terms serial, pipeline and parallel as applied to processors and illustrated the differences by describing the central processing units of several available computers (Cray-1S, CDC Cyber 205, FPS AP 120B, ICL DAP).

To describe the performance of new computers Professor Hockney introduced two parameters; the half-performance vector length ($n1/2$) and the asympototic maximum performance (r_∞). The first parameter defines the length of a vector for which a computer achieves half of its maximum performance rate and is a measure of the hardware parallelism in the computer. The second parameter is the megaflop rate generally used to describe performance. Serial computers may be characterised by $n1/2 = 0$ and $r_\infty = 1/t1$, where $t1$ is the time for a single operation. Pipeline processors have: $n1/2 = (s+l-1)$ and $r_\infty = 1/T$, where s is the vector startup time, l is the length of the pipeline (i.e. the number of micro-instructions in the operation) and T is the computer's clock period. Array processors are described by $n1/2 = N/2$ and $r_\infty = n/t'$, where N is the number of processing elements and t' is the time for the parallel operation to be completed. When the number of processing elements exceeds the length of the array to be processed, (as in the case of a hypothetical paracomputer, where N is infinite), all operations are completed in a single step and r_∞ is then infinite.

Applying these constructs experimentally to specific computers Professor Hockney showed that the performance depended very much on the task alloted. The Cray-1 was shown to be least efficient when performing the SCATTER and GATHER operations, while the Cyber 205 was severly handicapped when processing non-contiguous array elements. The ICL DAP was extremely efficient at 1-bit operations as a consequence of being a bit processing computer. The results of these investigations were presented in the form of a 2-D chart of r_∞ vs. $n1/2$ for various operations. The Cray-1 operations occupied an area of high r_∞ and low $n1/2$; indicating its suitability as a general purpose computer. The Cyber 205 occupies a much larger area of the chart indicating a larger range of processing speeds and only reaching maximum rate for very long vectors. This tendency was even more marked with the ICL DAP. Both these computers can be operated in one of several modes, of differing speeds, depending on the precision required and they excel at specialised applications.

Professor Hockney's final contribution was to demonstrate how a knowledge of the r_∞ and n1/2 parameters for a given computer can assist with the selection of the most efficient algorithm for a given task.

Dr. S. K. Mitra (Reading) described the steps he had taken to achieve a partial vectorisation of the PPPM program, which is a standard program for simulating large particulate systems (N > 1000), with long range forces. The PPPM (Particle - Particle - Particle - Mesh) algorithm separates the force into its long and short range components. The short range forces are handled by the 'link cells' method. The long range (electrostatic) forces are evaluated using a mesh charge sharing scheme and a fast Fourier transform technique to determine the potential. The electrostatic field is determined using a difference scheme. Vectorisation of these schemes was achieved using SCATTER and GATHER to prepare suitable arrays for processing in the treatment of the short range forces and a vectorised Fourier transform is used in the long range forces calculation. The program is now 2.14 times faster. Larger and more complicated systems are to be simulated because of these improvements.

Dr. D. Fincham (Queen Mary College) gave the first of three lectures dealing with the application of the ICL DAP in simulation work. He began by outlining the structure of the DAP and emphasised the 2-D arrangement of the processing elements as having importance in many applications. The DAP also functions as a storage module, which makes it commercially attractive. The DAP is a bit processor and this means that the user can define his his own precision, while such functions as EXP and SQRT are equally as fast as ordinary artihmetic. In addition the DAP has an extended FORTRAN language, which is quite simple to use, though some consideration of parallelism as a programming concept is required and this is translated into very efficient machine code. The DAP has found application in the MD simulation of solids and liquids, the former being the easier to implement because the mapping of 3-D lattices onto the 2-D array of processing elements within the DAP is particularly elegant. In the future Dr. Fincham sees the growth of microcomputers linked to powerful array processors and with enhanced graphics capabilities as a likely development and referred to Professor Wilson's molecular workstation as an example.

The application of the ICL DAP to specific problems was the concern of Dr. G. S. Pawley (Edinburgh) in his lecture. Dr. Pawley has applied the the DAP to the 3-D Ising model and to Quantum Chromo-Dynamics (QCD). There are some resemblances between the two applications in that both of them are lattice simulations and both require a great deal of calculation. These requirements are well fulfilled by the DAP. Three and four dimensional problems can be readily mapped onto the DAP 2-D array of processing elements. Also the low cost of the DAP means that it is available as a task dedicated computer. The 3-D Ising model was simulated using a 64*64*64 cube and the calculations proceeded at the rate of 2 million spin updates per second. Great care was needed to generate random numbers correctly for this application. The QCD model was simulated on an 8*8*8*8 lattice (representing the four dimensions of space and time) to which an SU(3) gauge field was added. The calculation rate was 100 updates per second. Very long calculations, lasting several hours, were necessary in order to achieve truly independent configurations. Dr. Pawley commented that the DAP was presently a very rudimentary computer and should see great improvements in performance in the future.

Dr. M. P. Allen (Oxford) has applied the DAP to a MD simulation of classical octupoles on a 2-D lattice. This problem maps particularly well onto the DAP as in other lattice applications. The representation of the quadrupole - quadrupole interactions made use of the quaternion orientation parameters to describe the angular dependence. The equations of motion were also couched in terms of these parameters, making the integration scheme particularly elegant. The simulated system consisted of 4096 particles and the calculation proceeded at the rate of 2000 timesteps in 15 minutes (10,000 particles per second). A number of correlation functions were calculated and the results were shown.

The last lecture of the day was followed by a demonstration of the ICL Perq microcomputer arranged by Dr. D. Fincham and Dr. D. Heyes. The Perq microcomputer has high resolution graphics and this was put to good use to demonstate the motions within a 16 particle MD simulation of a Lennard-Jones fluid. The Perq is believed to have considerable potential for simulation work and an attatched array processor is likely in the future.

The first speaker on the second day was Dr. A. F. Bakker (Delft). Dr. Bakker's interest is the construction of specialised computers for MD simulation work. Such computers have the advantage over conventional computers in that they can be precisely tuned to the task presented to them. Such factors as the choice of wordlength, an adapted instruction set, pipelined operations and the hardware utilisation of inherent parallelism provide great efficiency. To these must be added the modern conveniences of VLSI technology, computer aided design, advanced test equipment and microprocessors - all of which aid in the production.

The MD processor designed by Dr. Bakker and his colleagues is based on the Verlet integration algorithm and uses link-listing to enable the simulation of very large systems. However, unlike a conventional simulation of a Lennard-Jones system there is no computer program as such. The tasks normally defined by the software now find expression in the hardware construction of the MD processor. There were specific arithmetic units to update the particle positions and the momenta as well as to handle the link-list. There is no unique wordlength in the design, the particle positions have a 24 bit representation, the momenta a 32 bit representation and there is a 16 bit address representation. Interestingly, the periodic boundary condition is handled by a cyclic shift of the binary word storing the position. The processor makes as much use as possible of pipelining and parallelism to achieve maximum efficiency. Not only are x,y and z components of position (and momentum) updated in parallel, but quiescent data (i.e. data not otherwise being altered) are frequently tapped to calculate such quantities as the potential and kinetic energies. The current MD processor is configured with a HP 1000 minicomputer and an FPS AP 120B.

In the near future the MD processor will be capable of simulating 64,000 particles, of four diffent (Lennard - Jones) types together at a rate of 4 million particle pairs per second, which is equivalent to the Cray-1. The cost will be in the region of 15 to 20 thousand pounds, to which should be added 3 to 5 man-years of effort. Dr. Bakker conceded that the development of the MD processor raised many problems, not least the amount of new learning required by the developer, but the performance of the processor against the cost made it very attractive. He concluded his lecture with a description of the results of a 2-D Lennard-Jones simulation.

The section of the conference on new computers was concluded by a lecture by Professor C. Moser (CECAM). Professor Moser outlined the types of computing problems existing or imminent, such as plasma simulation, turbulence, spin glasses or the properties of materials and then described the types of computer that would be available to solve them. A current solution to such problems is the use of mainframe computers that possess vector registers or have attatched processors with this capability. Such computers are well known. A second solution is the production of special purpose computers. According to the design, these may have the advantages of large memory, cheapness and a freedom from software problems. Such computers have already been constructed, as for instance, the MD processor of Dr. A. F. Bakker. The disadvantages of such computers are the long period of development necessary to produce the finished model and the frozen nature of the program, which is embedded in the hardware design. The third solution is the design of new kinds of computer such as SIMD (Single Instruction Multiple Data-stream) and MIMD (Multiple Instruction Multiple Data-stream) computers. SIMD computers execute the same instruction on many data channels and thereby achieve high processing rates. The ICL DAP is an example of this. MIMD computers may perform many different instructions on many data channels and thus may be capable of ultra high speeds. Such MIMD computers are not yet available but are being studied, though they present considerable problems for the computer designers. In the future Professor Moser advocated a closer liaison between physicists and computer manufacturers to bring about the emergence of suitable computers.

The first lecture on the subject of quantum mechanical aspects of simulation was delivered again by Professor K. R. Wilson (California). Speaking on the application of quantum corrections to simulation of nuclear motions, Professor Wilson noted that on transforming the results into the frequency domain, high frequency motions tended to by harmonic while low frequency (diffusive) motions tended to be anharmonic. Harmonic motions are easily treated quantum - mechanically and hence the quantum correction is easy to determine. (i.e. construct the appropriate harmonic oscillator, solve the Schroedinger equation and take the limit as Planck's constant goes to zero). Anharmonic motions occur only in slower modes and are easily solved classically. Hence in these cases the quantum corrections are small. Using these ideas Professor Wilson was able to show how to correct I.R., Raman and electronic spectra as well as thermodynamic quantities. In cases where the frequency dependence showed contributions from several sources, the quantum correction appropriate to each source had to be weighted according to the peak intensity in the Fourier transform.

The simulation of true quantum systems (at zero temperature) by Monte Carlo, was the subject of the lecture given by Professor D.M. Ceperley (University of California). Professor Ceperley has applied the Monte Carlo method to both Boson and Fermion systems and his studies include small molecules (particularly Hydrogen), thin films, the electron gas and Helium-3 and Helium-4.

He began his lecture by describing the basic Monte Carlo method for Boson systems. The method is derived from the time dependent Schroedinger equation in imaginary time. This must be solved subject to the correct boundary conditions to obtain the groundstate of the system in question. On defining the probablity distribution function as a product of the unknown system wavefunction and a known trial wavefunction, the equation can be converted into a differental equation relating the time derivative of the distribution function to the 'local energy' and the 'quantum force', which are known quantities. This equation resembles a diffusion equation, with additional 'drift' and 'growth' terms and this permits the system to be evaluated by Monte Carlo methods.

The algorithm starts with an ensemble of systems, each comprised of 3N coordinates representing the N particle positions. The systems are chosen so that each has a probability given by the square of the trial wavefunction. A trial groundstate energy Vo is also chosen at the start. Each system in the ensemble is allowed to evolve in time. For a given timestep, a random displacement is added to the particle positions and the diffusion and drift terms computed. It is then that the importance sampling algorithm is applied. The new system is accepted with a weighting of 0,1 or 2, depending on the value of the computed local energy (e.g. if the local energy exceeds Vo, the step is unfavourable and the weighting will be zero). The number of systems is thus dependent on the value of Vo. To maintain a constant number of systems, (i.e. to keep the distribution function constant with time), Vo is increased or decreased via a feedback mechanism. After an equilibration period, Vo and the number of systems, remains fairly constant. The groundstate energy is ultimately given as a long time average of the local energy, and the corresponding variance is obtained from the square of the local energy.

(It should be noted however that, though presented as a finite timestep algorithm above, the actual algorithm used is the stochastic algorithm due to Kalos. This removes all errors due to the finite timestep.)

The simulation of Fermion systems is more difficult, since the trial and actual wavefunctions need not have the same sign everywhere and thus negative values of the distribution function may arise. This requires that the nodes in the wavefunction be known. There are two methods for dealing with such systems. In the 'fixed nodes' method the nodes of the wavefunction are considered to partition the 3N dimensional space into distinct volumes in each of which the problem is treated as a Boson problem. The generation of systems outside these volumes results in the wavefunction being set to zero. The process gives the upper bound to the Fermion energy, which is acceptable if the nodes given are accurate. The problem of the discontinuity of the solution across nodal boundaries remains however. The second method, known as the 'nodal relaxation method' is essentially a perturbation of the 'fixed nodes' method. In this method systems generated outside the 'fixed nodes' volumes are given negative weights. This effectively relaxes the nodal boundaries and is effective while the boundaries are relaxing.

Professor Ceperley concluded his lecture with a description of the results obtained for the electron gas (Jellium) and Hydrogen molecules. For the former he used a Jastrow trial wavefunction (the product of single particle wavefunctions and a pair correlation factor). The results for a system of about 250 electrons were compared with various many body theories, from which the 'coupled cluster method was found to give best agreement. Wigner crystallisation was also investigated.

The study of the Hydrogen molecule provided the equation of state of the element up to 4.5 Mb pressure, where there was evidence of the transition from molecular to atomic Hydrogen. Again a Jastrow wavefunction was used, but different single particle orbitals were used for the different phases.

Professor J.G. Powles (Canterbury, co-author J.L.F. Abascal, Madrid) spoke about the calculation of quantum corrections to the pair distribution function in atomic liquids. His technique uses the effective potential with perturbation theory and discrete statistical mechanics. A number of approximations are employed, which were suggested and justified by computer simulation methods. As expected, the corrections were small for liquid Argon, appreciable for liquid Neon and dominant for liquid Helium. The results show that if allowance is made for the quantum corrections, the Lennard-Jones 12/6 potential is quite adequate to describe Neon and is not anomalous, as had been reported earlier by Graaf and Moser (1971). Professor Powles suggested that the quantum corrections will be quite large for molecular liquids with low moments of inertia (e.g. $H2O$, HCl, $D2O$ and DCl) and this will throw doubt on the comparison of real data with classical simulations. The quantum corrections generally result in a smearing out of the pair distribution function, particularly for small radius, where penetration of the hard sphere radius is evident. The real data will exhibit less structure than the classical simulations, making interpretation difficult.

Dr. F. Barocchi (Instituto di Elettronica Quantistica del C.N.R., Italy) also spoke on the subject of quantum corrections in a Lennard-Jones fluid. He and his coworkers; M. Zoppi and M. Neumann, have shown how the Wigner $\hbar^2$ expansion can be applied to near classical systems to obtain series expansions of general correlation functions and the moments of their spectra, with respect to Planck's constant. They have obtained explicit terms up to the fourth power in h for zeroth, second and fourth moments for a many body system with the classical Hamiltonian and also the corresponding terms for variables that are functions of the momenta and coordinates. The quantum corrections for the many body system are then given in terms of averages over classical phase space.

Dr. Barocchi and his colleagues have successfully applied this method in a study of the interaction induced light scattering spectrum of a Lennard-Jones fluid in which the interaction induced pair polarisability anisotropy is given by the dipole - induced - dipole approximation. The first quantum corrections to the zeroth and second moments of the spectrum and the first and second quantum corrections to the pair distribution function and the neutron scattering factor were obtained. The computer simulation consisted of 108 atoms and required 200,000 timesteps to ensure convergence of the terms calculated.

Professor G. Jacucci (Trento) spoke about the path integral Monte Carlo method in quantum statistical mechanics. The path integral method, or Feynman - Kac method, is one of two methods currently available for the calculation of quantum statistics; the second method being the so called Green's Function Monte Carlo (GFMC) method. Both of these methods present formidable computational difficulty.

The calculation of quantum systems requires the determination of the eigenfunctions of the system. The average of a given function is then given as a product of the trace of the density matrix and the function operator. The Feynman - Kac method therefore requires a suitable approximation to the density matrix as the starting point.

Beginning with the quantum description of a system of free particles (in which the density matrix has a gaussian functional form), Professor Jacucci showed how a high temperature approximation to the density matrix for a general many body system could be obtained from a product of the free particle form and the exponential of the interaction potential (the so called 'primitive' approximation). This is the Feynman - Kac formulation, which is the starting point of the path integral method. It is integrable by the Metropolis Monte Carlo technique. A good approximation to the density matrix is paramount and the primitive approximation is inadequate when the short range potential is strongly repulsive as in the simulation of hard spheres. In these circumstances the 'image approximation', which is a familiar device in mathematical physics, is used. It ensures that the wavefunction at a discontinuous potential barrier has the correct functional behaviour. In the case of hard spheres, the image approximation is adapted to suit the spherical 'excluded volume' of the spheres by substituting a tangential plane for the surface of the sphere.

Professor Jacucci has applied the method to a quantum simulation of a system of hard spheres to determine the pair correlation functions.

The application of the Monte Carlo method to quantum spin systems was outlined by Dr. J.W. Lyklema (Institut fur Festkorperforschung der Kernforschunganlage Julich). Dr. Lyklema described an exact Monte Carlo method for calculating the thermodynamic properties of such a system, based on a generalisation of Handscomb's method for the ferromagnetic Heisenberg system. Using this method, the quantum mechanical expectation value for a given observable is expressed in terms of classical distributions. The Markov chain generation differs from Handscomb's method and enables a faster progression of the chain. The method was used to study one, two and three dimensional spin systems. The one dimensional results were compared with those of Bonner and Fisher (1964), who diagonalised the Hamiltonian for small systems numerically. In the ferromagnetic case the energy, susceptibility at zero field and specific heat were calculated and were in good agreement. Susceptibility for nonzero field also gave good agreement. Similar good results were obtained for the antiferromagnetic case,though the alternating signs in the expressions for the observables made matters more difficult. Results for higher dimensions were also reported.

Dr. N. Corbin (London, Ontario, formerly Royal Holloway College) spoke on the subject of the use of wave packets in molecular dynamics simulations. The time evolution of a wavefunction containing time dependent parameters has been described by Heller. There are two methods available, both resembling molecular dynamics, in each the atoms are represented by gaussian wave packets. The first method is severly limited by a locally harmonic approximation to the potential but nevertheless gives good results for low temperature solids such as Neon. The second method does not entail this approximation and is therefore more general. It has been successfully applied in simulations of liquid Neon at 30 K and 40 K. Other forms besides gaussian wave packet are possible, and are being studied. The potential energy expectation value is similar in form to that obtained by the path integral method, although the applications are very different in practice.

The final talk of the meeting was given by Professor Singer (Royal Holloway College) on the subject of molecular dynamics in semiclassical, many body systems. He began by outlining options available for simulating such systems, particularly the Gaussian wave packet method described previously by N. Corbin and a possible method based on the Miller stationary phase path integral techniques. While the former method appears promising, the latter requires considerable computational effort.

Professor Singer has attempted to base a dynamical simulation method on the Wigner - Kirkwood expansion in powers of $\hbar^2$. The method is computationally less expensive than the Gaussian wave packet method, but is less powerful and harder to justify theoretically. The derivation of the method was described. The method is stable when small timesteps are used (e.g. 2.5 fs for Nitrogen at 40 K). Preliminary results for Argon suggest that the negative lobe of the velocity autocorrelation function is deeper than that given classically.

Acknowledgement.

I am indebted to Prof. K. Singer and W.A.B. Evans as well as to the speakers themselves for their help in preparing this review.

Use of Neighbour Lists in Molecular Dynamics

S.M. Thompson

Introduction

The neighbour list is a device used in Molecular Dynamics simulations to increase execution speed by reducing the time taken to perform the most time consuming part of the calculation, the evaluation of the pair interactions. This article addresses the effect of some of the list parameters on the efficiency of utilisation of the list method. I will only consider systems of spherical molecules; the comments are general however and apply to other systems also.

Please note that all programming examples given here do not necessarily reflect the most efficient way of coding the particular sequence. The examples are for a system of Lennard-Jones atoms. The centre of mass coordinates are in the (-1,+1) system, which is probably the most efficient coordinate system for use in molecular dynamics simulations.

Some of the comments in the text apply only to serial processors. In addition, although the method is discussed in the context of Molecular Dynamics, it is equally applicable to Monte Carlo. In fact it is probably even more effective in Monte Carlo simulations since it removes some of the inefficiencies inherent in the MC scheme. That, however, is another story.

The Neighbour List Method

For a system of N particles interacting with a pairwise additive potential, the force acting on each particle at each step of the simulation is usually evaluated by calling a subroutine (call it FORCE; see Figure 1) that examines all pairs of particles and evaluates the force between those pairs separated by less than a specified cutoff distance, RCUT. A loop over particles, I=1,N-1, encloses a second loop over the possible neighbours of that particle, J=I+1,N. For every one of the N(N-1)/2 pairs, the interparticle separation is evaluated, taking into account the usual boundary conditions. If this separation is greater than RCUT (which must be less than half the width of the box), the interaction force is assumed to be zero. Hence the J-loop is terminated, J is incremented and the process continues. If the pair separation is less than or equal to RCUT, the force is calculated according to some specified pair potential.

This procedure can be divided into two parts. The first part, the identification of those pairs separated by less than the cutoff distance, requires examination of all pairs, and so the computer time taken is proportional to the square of the number of particles. The second part, the evaluation of the forces for those pairs separated by less than the cutoff distance, requires computer time roughly proportional to the number of particles and the cube of the cutoff distance. Thus, for a given cutoff distance, the time taken to perform the first part of the calculation outweighs that taken to perform the second part, when the number of particles is reasonably large.

The neighbour list method implements a scheme whereby the first part of the calculation is reduced one order so that the time taken is proportional to the number of particles. The force evaluation routine FORCE becomes two routines, FORCE1 and FORCE2 (see figures 2 and 3 respectively). FORCE1 proceeds in exactly the same way as FORCE, except that once the pair separations have been evaluated, they are compared with a chosen list parameter which we shall call the list radius, RLIST. The RLIST parameter is greater than the cutoff RCUT. If the separation is greater than RLIST, we can jump out of the J-loop as before. If it is less, then the subscript J is stored in a table called the neighbour list, and J is called a neighbour of I. The usual cutoff check then follows. Prior to entering the J-loop, the Ith entry of another table (call it NABIDX) is set with one more than the number of entries already made in the list at that point (the variable NELIST, which is initially zero). Each time an entry is made in the neighbour list, the number of entries is incremented. This scheme takes very little longer than the original force calculation in routine FORCE. If the maximum distance moved by any particle in the next, say, 10 steps is less than (RLIST-RCUT), then the neighbour list thus constructed contains all the required information about non-zero pair interactions for the next ten steps.

Subroutine FORCE2 calculates the pair forces using this list as follows. The usual I-loop is entered. The neighbours of I now have their subscripts (J) stored in locations NABIDX(I) through NABIDX(I+1)-1. The difference between these two numbers is usually much less than the number of particles in the system, and so the J-loop is less time consuming. The evaluation of forces now takes computer time proportional to the number of particles rather than to the square. If NABIDX(I) is greater than NABIDX(I+1)-1, then particle I has no neighbours and so the J-loop is not entered. This may be the case when stimulating certain inhomogeneous or dilute systems.

When a new neighbour list is built using FORCE1, a vector for each particle is initialised to zero. At every subsequent step, this vector is incremented with the distance moved by each particle. The maximum distance moved, as determined at the end of every step, provides a guide as to when the list should be next updated. If the maximum distance moved is greater than FLUPD*(RLIST-RCUT), when FLUPD is a constant between zero and unity, then the list must be updated by calling FORCE1 again at the next step. If not, FORCE2 may be used again to calculate the forces.

Sometimes a constant list update interval, such as 10 steps, is used when implementing the neighbour list method. I do not recommend such a procedure, for two reasons. Firstly, if the simulation is performed at a state condition where particle motion is rapid, it is easy to get a condition where the list is used for a number of steps past the point where it should have been updated. This corrupts the particle trajectories and produces a discontinuous change in the energy of the system. Secondly, the list may well be used for less steps than it was possibly good for, with the result that a new neighbour list is built more times than is necessary. This slows down the program. It is better to let the program take full control over list management, in which case the list update interval is never of concern.

The parameter FLUPD deserves some thought. In cases where the list radius is only slightly greater than the cutoff, FLUPD will probably need to be in the region of 3/4. For larger list radii, a value up to about 0.95 can be used. In any event, FLUPD should be less than (1 - 1/(NSLU+1)), where NSLU is the shortest time (in steps) between successive updates of the list. Again, it is possible for the simulation to deal with this automatically, with the exception that an initial value is required, and would be used for the first few list cycles. This specification for FLUPD relies on the temperature remaining more or less constant and there being no phase changes.

Thus we are left with the list radius RLIST as the only unspecified parameter influencing the performance improvements obtainable from the neighbour list.

Effect of the Neighbour List Radius

The value of RLIST will have little effect on the time taken to construct the neighbour list, since all pairs of particles have to be examined anyway. The larger the value of RLIST, the more table space will be required (approximately proportional to RLIST**3), and the less often it will need to be updated. Using a large value of RLIST, however, can lead to performance degradation, since the large size of the list means that the FORCE2 routine now has to do more work to sort out which entries have non-zero interactions. Consequently, there is an optimum list radius which gives maximum performance. This radius will depend to some extent on your definition of performance. If you have to pay for memory usage, then the optimum RLIST will be smaller than if you are aiming for maximum execution speed, due to the increased costs for memory usage offsetting the increase in execution speed.

Simulations of 256 and 500 Lennard-Jones atoms at a reduced density of 0.8 and at a reduced temperature of 0.76 was run for 1000 steps with the self-maintaining list mechanism as described above. The potential cutoff radius RCUT was 2.5 diameters. Different values of RLIST were used to obtain the data shown in the table. This data is plotted in Figures 4 and 5, where RLIST is in units of collision diameters.

It can be seen that the optimum neighbour list radius, in terms of execution speed, is approximately 0.2 diameters larger than the cutoff radius for N=256, and approximately 0.4 diameters larger for N=500. The CPU time required per step falls steeply as the list is "turned on", and increases again, but more slowly, as the list radius becomes larger than the optimum. However, for list radii around the optimum, there is not very much effect of varying RLIST on the execution speed, especially for the N=500 system. It therefore appears from this data that 2.7 diameters would provide good performance for both systems. The optimum list radius increases execution speed by a factor of 1.54 for N=256, and by over a factor of 2 for N=500. For even larger systems, the effect on the execution time of introducing the list is much more dramatic. It remains to be seen what the effect of density is on these results.

List Radius	NSAVU (*)	N = 256	N = 500
			Time (**)
- no list -	n/a	3.33	10.00
2.60	5.78	2.24	4.93
2.70	12.50	2.17	4.55
2.90	26.32	2.28	4.51
3.10	43.48	2.47	4.79
3.43	83.33	2.89	-
3.50	100.00	-	5.86

Notes:

(*) NSAVU is the average number of steps between updates of the neighbour list. This data is for the N = 256 simulation (except for the last entry), but this figure is essentially independent of the system size. It does, however, depend on the value of the FLUPD parameters.

(**) "Time" is the CPU time required per step. These times were obtained using a PDP 11/70 minicomputer running the RSX-11M V4.0 operating system. The program was compiled with the PDP-11 FORTRAN-77 compiler, version 4.1, using the /NOTRACE option. This machine is approximately 18% the speed of an IBM 370/168. CPU times were measured using an in-house performance measurement package.

Figure 1. Extract from routine FORCE

```
    DO 100 I = 1,255
      JBEG = I + 1
      DO 200 J = JBEG,256
        XDIFF = XO(I) - XO(J)
        XDIFF = YO(I) - YO(J)
        ZDIFF = ZO(I) - ZO(J)
        XDIFF = XDIFF - 2*INT(XDIFF)
        YDIFF = YDIFF - 2*INT(YDIFF)
        ZDIFF = ZDIFF - 2*INT(ZDIFF)
        RSQ = XDIFF*XDIFF + YDIFF*YDIFF + ZDIFF*ZDIFF
        IF(RSQ.GT.RCUTSQ)GO TO 200
        RSQI = 1.0/RSQ
        R6 = SIGMA6*RSQI*RSQI*RSQI
        DUDRR1 = 48.0*RSQI*R6*(R6 - 0.5)
        FXIJ = XDIFF*DUDRR1
        FYIJ = YDIFF*DUDRR1
        FZIJ = ZDIFF*DUDRR1
        FX(I) = FX(I) + FXIJ
        FY(I) = FY(I) + FYIJ
        FZ(I) = FZ(I) + FZIJ
        FX(J) = FX(J) - FXIJ
        FY(J) = FY(J) - FYIJ
        FZ(J) = FZ(J) - FZIJ
200   CONTINUE
100 CONTINUE
```

Figure 2. Extract from routine FORCE1

```
      NELIST = 0
      DO 100 I = 1,255
        NABLOC(I) = NELIST + 1
        JBEG = I + 1
          DO 200 J = JBEG, 256
          XDIFF = XO(I) - XO(J)
          YDIFF = YO(I) - YO(J)
          ZDIFF = ZO(I) - ZO(J)
          XDIFF = XDIFF - 2*INT(XDIFF)
          YDIFF = YDIFF - 2*INT(YDIFF)
          ZDIFF = ZDIFF - 2*INT(ZDIFF)
          RSQ = XDIFF*XDIFF + YDIFF*YDIFF + ZDIFF*ZDIFF
          IF(RSQ.GT.RLSTSQ)GO TO 200
          NELIST = NELIST + 1
          NABTAB(NELIST = J
          IF(RSQ.GT.RCUTSQ)GO TO 200
          RSQI = 1.0/RSQ
          R6 = SIGMA6*RSQI*RSQI
          DUDRR1 = 48.0*RSQI*R6*(R6 - 0.5)
          FXIJ = XDIFF*DUDRR1
          FYIJ = YDIFF*DUDRR1
          FZIJ = ZDIFF*DUDRR1
          FX(I) = FX(I) + FXIJ
          FY(I) = FY(I) + FYIJ
          FZ(I) = FZ(I) + FZIJ
          FX(J) = FX(J) - FXIJ
          FY(J) = FY(J) - FZIJ
          FZ(J) = FZ(J) - FZIJ
200     CONTINUE
100   CONTINUE
      NABIDX(256) = NELIST + 1
```

Figure 3. Extract from routine FORCE2

```
      DO 100 I = 1,255
        JBEG = NABLOC(I)
        JEND = NABLOC(I+1) - 1
        IF(JBEG.GT.JEND)GO TO 100
        DO 200 JX = JBEG,JEND
          J = NABTAB(JX)
          XDIFF = XO(I) - XO(J)
          YDIFF = YO(I) - YO(J)
          ZDIFF = ZO(I) - ZO(J)
          XDIFF = XDIFF - 2*INT(XDIFF)
          YDIFF = YDIFF - 2*INT(YDIFF)
          ZDIFF = ZDIFF - 2*INT(ZDIFF)
          RSQ= XDIFF*XDIFF + YDIFF*YDIFF + ZDIFF*ZDIFF
          IF(RSQ.GT.RCUTSQ)GO TO 200
          RSQI = 1.0/RSQ
          R6 = SIGMA6*RSQI*RSQI*RSQI
          DUDRR1 = 48.0*RSQI*R6*(R6 - 0.5)
          FXIJ = XDIFF*DUDRR1
          FYIJ = YDIFF*DUDRR1
          FZIJ = ZDIFF*DUDRR1
          FX(I) = FX(I) + FXIJ
          FY(I) = FY(I) + FYIJ
          FZ(I) = FZ(I) + FZIJ
          FX(J) = FX(J) - FXIJ
          FY(J) = FY(J) - FYIF
          FZ(J) = FZ(J) - FZIJ
200     CONTINUE
100   CONTINUE
```

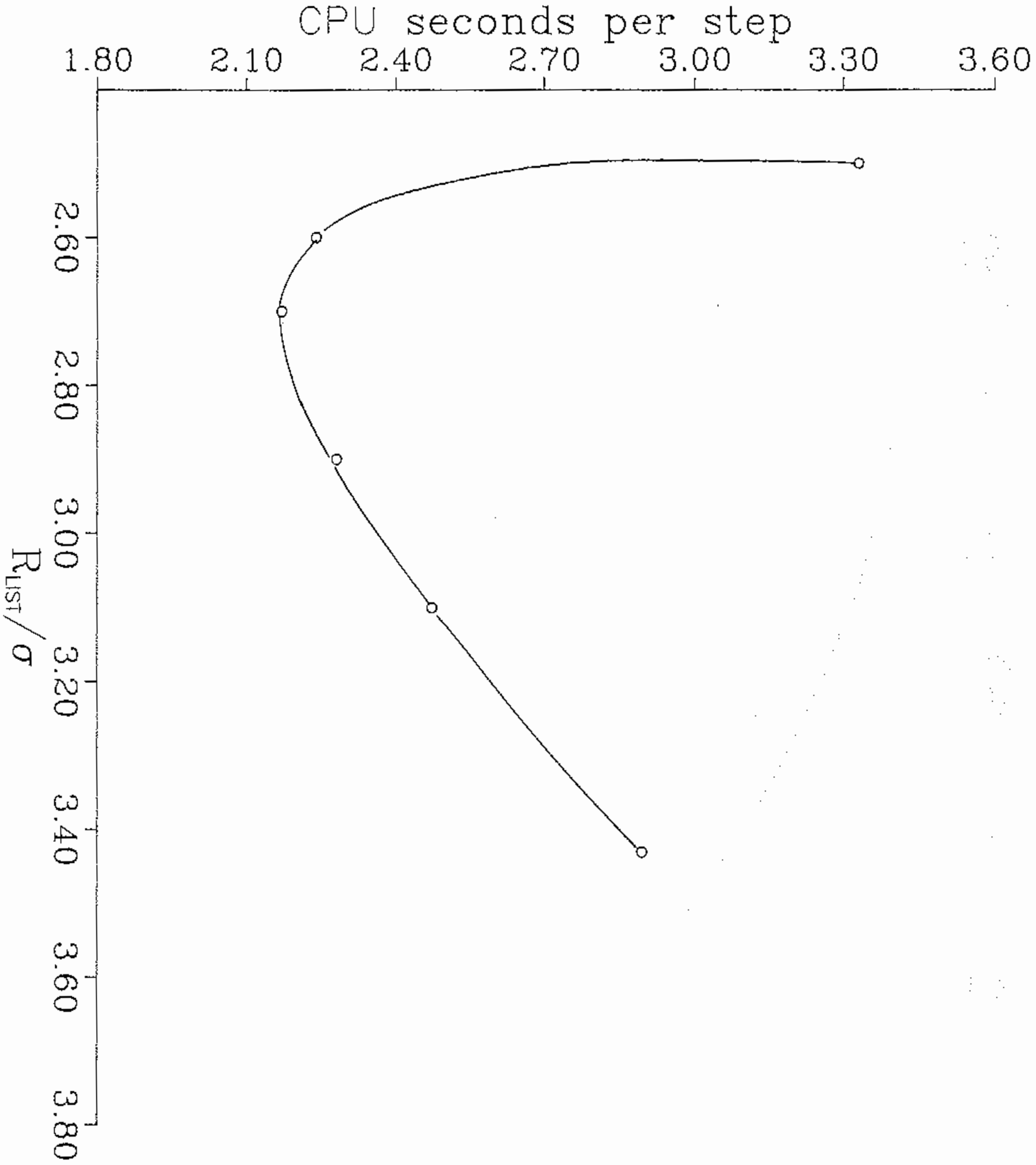


Figure 4. CPU time vs. list radius, N = 256.

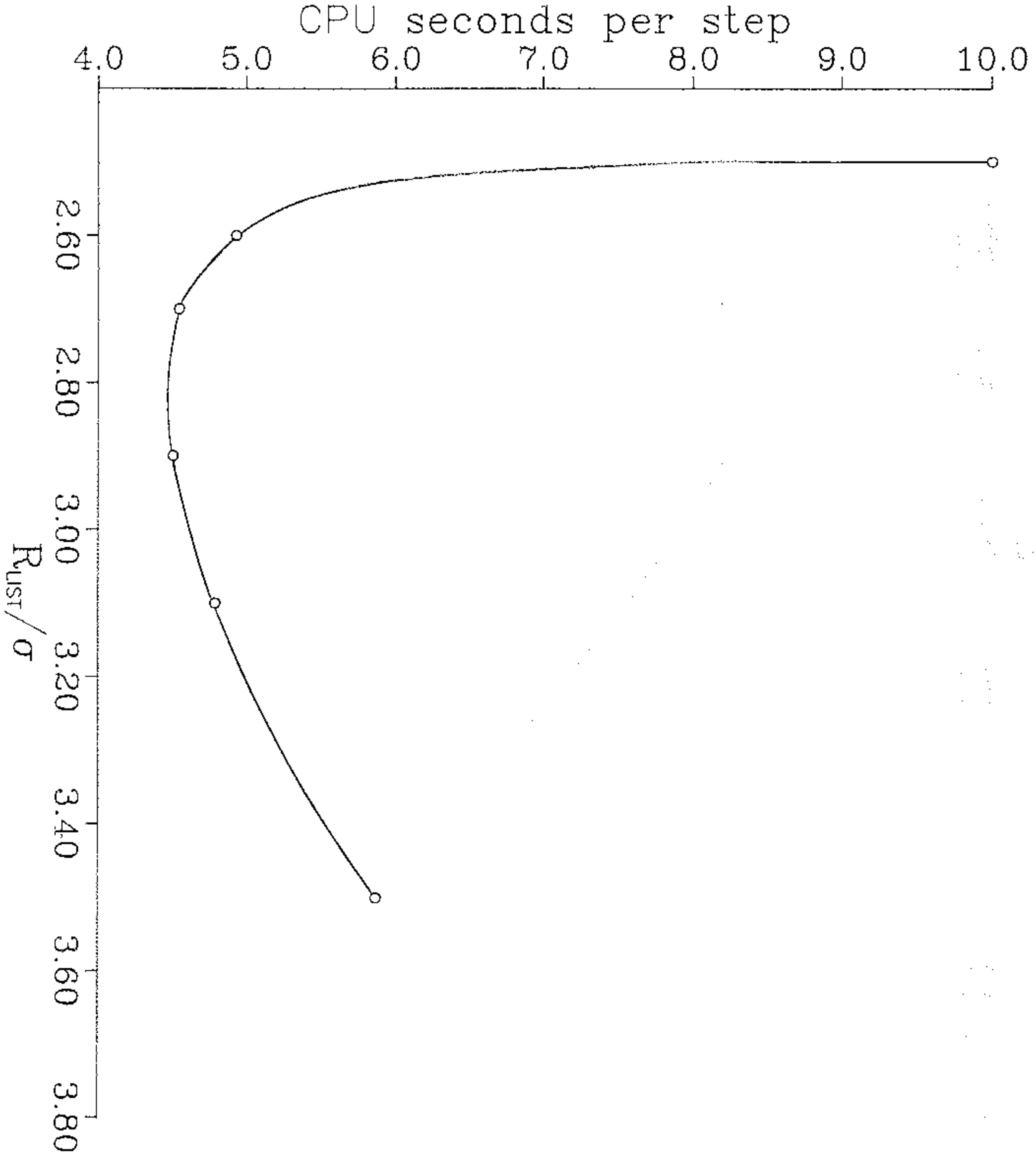


Figure 5. CPU time vs. list radius, N = 500.

MD Incorporating Ewald Summations on Partial Charge Polyatomic Systems

by

D.M. Heyes

This note is intended as a warning to those workers involved in simulating partially charged polyatomic systems by MD. It is usual to employ the Ewald method to treat the long range Coulomb interactions for bulk systems.[1,2] It is perhaps obvious to state that the useful configuration electrostatic potential energy does <u>not</u> include interactions between fractional charges on the <u>same</u> composite unit. A "blind" application of the Ewald transformation can, unfortunately, incorporate these irrelevant potential components. In response, Ewald formulae for this problem are derived below which have the correct terms to avoid such self-interactions. This conveniently reduces to a modified self-energy term within a conventional Ewald formalism.

Consider N polyatomic units which can be ions or molecules. Each unit, i, has an arbitrary number, n_{pi}, of partial charges which have magnitude q_{ik} where $1 \leq k \leq n_{pi}$. The monopolar potential at partial charge site $\mathbf{r}_{ik}$ is

$$V_{ik} = \begin{array}{l} \text{a)}\ \sum\limits_{\substack{j\neq i\\(\mathbf{n}=0)}}^{N} \\ \text{b)}\ \substack{j=1\\(\mathbf{n}\neq 0)} \end{array} \sum_{\ell=1}^{n_{pj}} \frac{q_{j\ell}}{|\mathbf{r}_{ik}-\mathbf{r}_{j\ell}+\mathbf{n}|} \qquad (1)$$

Here,

$$\mathbf{n} = i_x\mathbf{L}_x + i_y\mathbf{L}_y + i_z\mathbf{L}_z\ , \qquad (2)$$

which is the real lattice vector. $\underset{\sim}{L}_x$, $\underset{\sim}{L}_y$ and $\underset{\sim}{L}_z$ are the MD cell sidelength vectors. i_x, i_y and i_z are integers that can independently range between ± ∞. As usual, quantities with wavy underlines denote vectors. Note that charge interactions from within the same polyatomic unit have been correctly omitted. A restriction is,

$$\sum_{i=1}^{N} \sum_{k=1}^{n_{pi}} q_{ik} = 0 , \qquad (3)$$

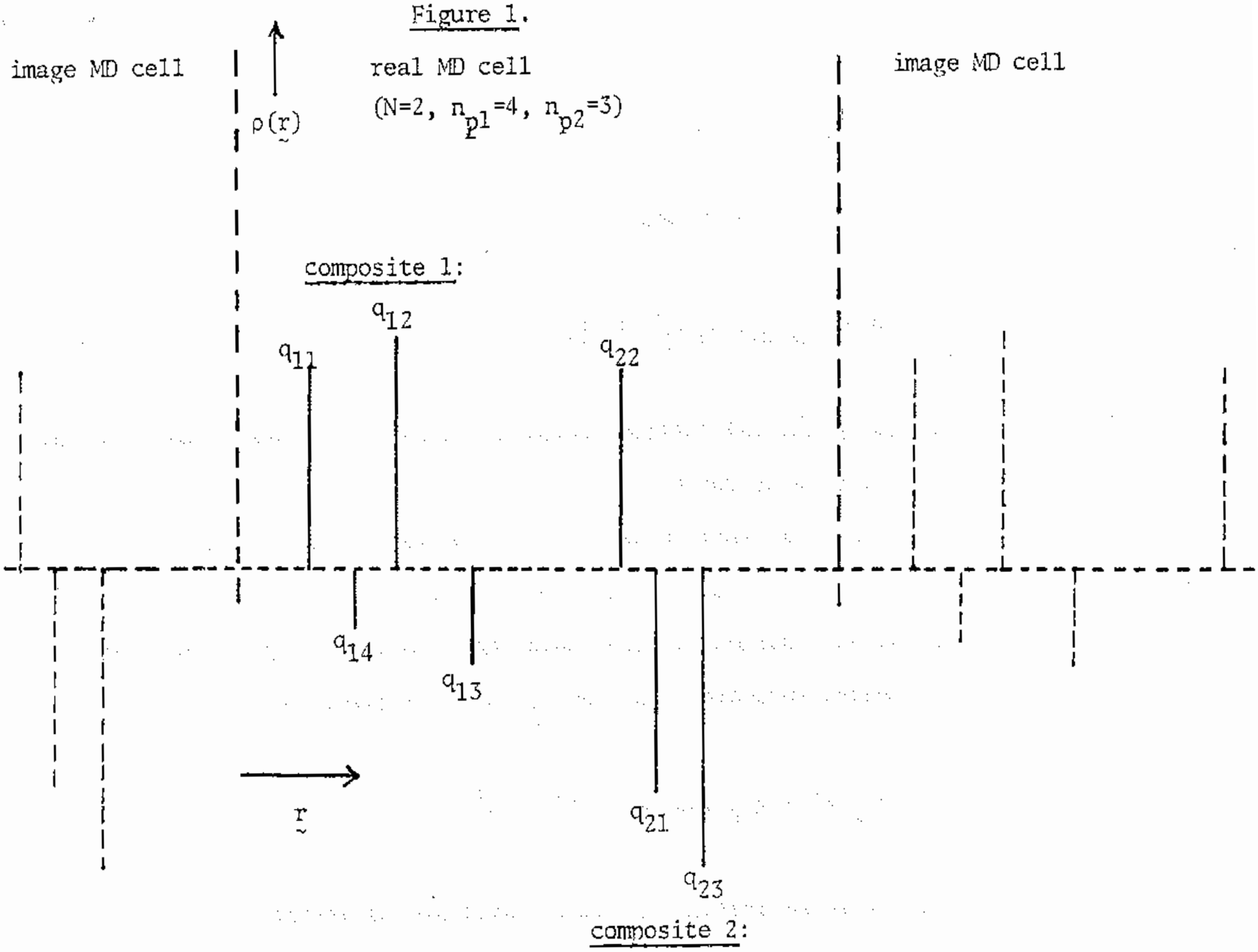
i.e. the system must be overall neutral. The potential at any neutral point, $\underset{\sim}{r}_{i\ell}$, in a polyatomic unit can be obtained by setting $q_{i\ell} = 0$.

At each MD time step, new positions are found for the molecules. As these configurations are replicated by periodic boundary conditions, MD produces a new lattice every time step. The charge density at point $\underset{\sim}{r}$ in space is $\rho(\underset{\sim}{r})$ where,

$$\rho(\underset{\sim}{r}) = \sum_{i=1}^{N} \sum_{\ell=1}^{n_{pi}} q_{i\ell}\, \delta(\underset{\sim}{r}-\underset{\sim}{r}_{i\ell}) , \qquad (4)$$

where $\underset{\sim}{r}$ only needs to range within the origin MD cell. This is a valid constraint because of the periodic nature of the charge density and potential. The charge density is pictorially represented in figure 1. It can be considered to be a repeating series of charge spikes, represented as usual[2] by a Kronecker Delta symbol notation, $\delta(\ldots)$.

Figure 1.



The Ewald representation of equation (1) is

$$V_{ik} = \sum_{\substack{j\neq i\\(\mathbf{n}=0)\\ j=1\\(\mathbf{n}\neq 0)}}^{N} \sum_{\ell}^{n_{pj}} \sum_{\mathbf{n}} q_{j\ell} \frac{\operatorname{erfc}(\alpha|\mathbf{r}_{ikj\ell} + \mathbf{n}|)}{|\mathbf{r}_{ikj\ell} + \mathbf{n}|}$$

$$+ \frac{1}{\pi V} \sum_{j}^{N} \sum_{\ell}^{n_{pj}} \sum_{\mathbf{h}\neq 0} q_{j\ell} \exp(-\pi^2|\mathbf{h}|^2\eta^2)$$

$$\times \cos(2\pi\mathbf{n}.\mathbf{r}_{ikj\ell}) \, |\mathbf{h}|^{-2} - V'_{ik} \, , \qquad (5)$$

where erfc(x) is the complementary error function[3] of x,

$$\mathbf{r}_{ikj\ell} = \mathbf{r}_{ik} - \mathbf{r}_{j\ell}, \qquad (6)$$

$$V = \underset{\sim}{L}_x \times \underset{\sim}{L}_y . \underset{\sim}{L}_z \ , \tag{7}$$

is the MD cell's volume.

$$\underset{\sim}{h} = (i_x/\underset{\sim}{L}_x,\ i_y/\underset{\sim}{L}_y,\ i_z/\underset{\sim}{L}_z), \tag{8}$$

is the reciprocal lattice vector in which i_x, i_y and i_z have the same significance as for $\underset{\sim}{n}$.

The first term in equation (5) is the potential due to the original point charge lattice minus that of a coincident lattice of spread out charges of equal total magnitude and sign. The form of the charge spreading function $P_{j\ell}(u)$ is a gaussian

$$P_{j\ell}(\underset{\sim}{u}) = q_{j\ell}\ \exp(-u^2/\eta^2)/\pi^{3/2}\eta^3 \ , \tag{9}$$

where η is an arbitrarily chosen distance parameter.

Note that,

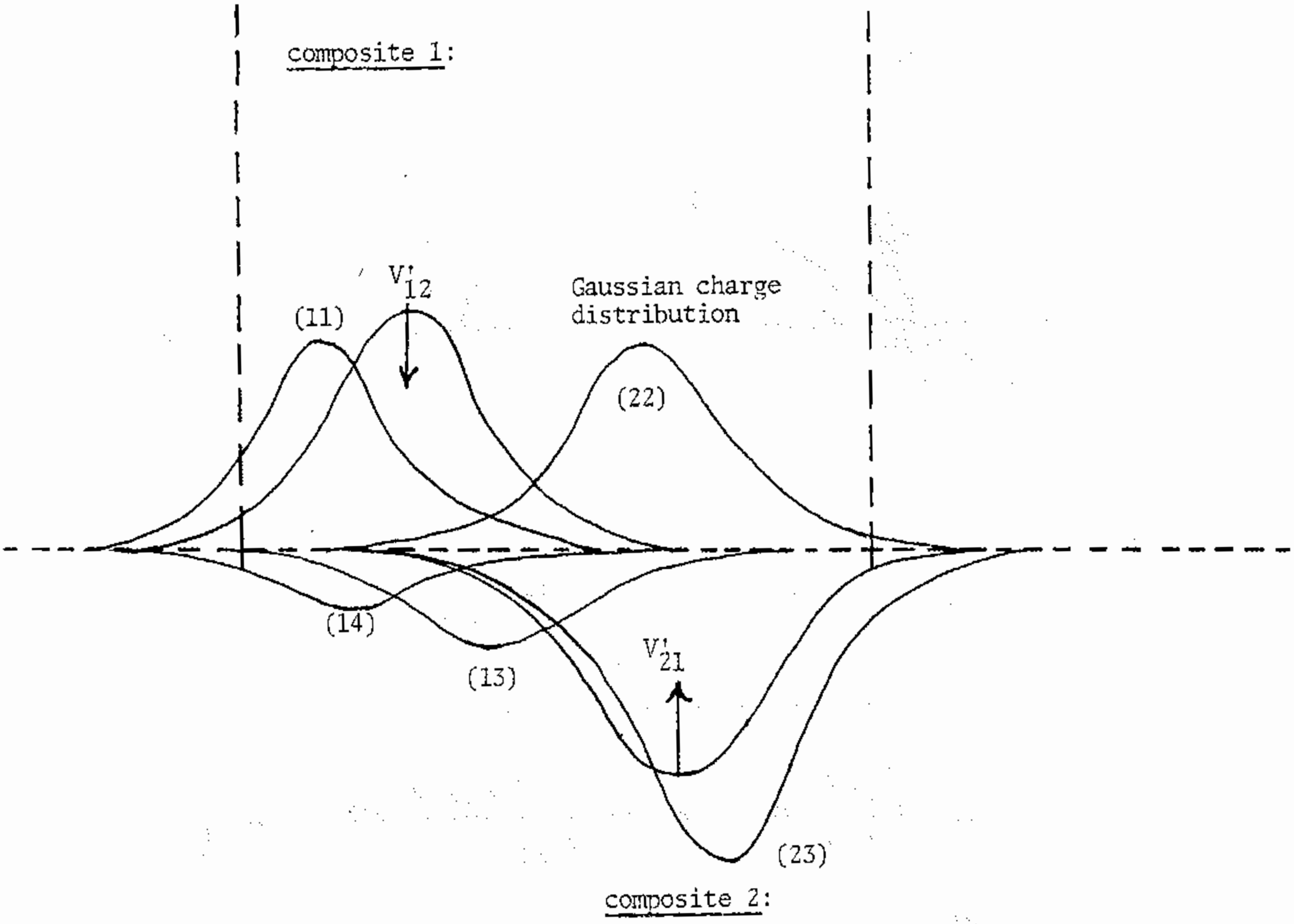
$$\int_{\text{all space}} P_{j\ell}(\underset{\sim}{u})\ d^3\underset{\sim}{u} = q_{j\ell} \ ; \tag{10}$$

a necessary normalisation condition.

The second series in equation (5) is the potential arising from the spread-out charge lattice of sign equal to that of the original point charge lattice. The third contribution to the potential, V'_{ik}, subtracts the so-called self-potential terms which are the main new point of interest in this note. The second series in equation (5) includes the potential at $\underset{\sim}{r}_{ik}$ due to the charge distribution centred on $\underset{\sim}{r}_{ik}$ and those other partial charges, $q_{i\ell}$ where $1 \leq \ell \neq k \leq n_{pi}$, which are to be found on the same composite polycharge unit. The term V'_{ik} removes these unnecessary terms, which are pictorially represented in figure 2.

Figure 2.

Self potentials at partial charge sites (12) and (21)



Now,

$$V'_{ik} = \sum_{\ell=1}^{n_{pi}} \frac{\int \rho_{i\ell}(\underset{\sim}{u})\, d^3\underset{\sim}{u}}{|\underset{\sim}{u} - \underset{\sim}{r}_{ik\ell}|} \quad . \tag{11}$$

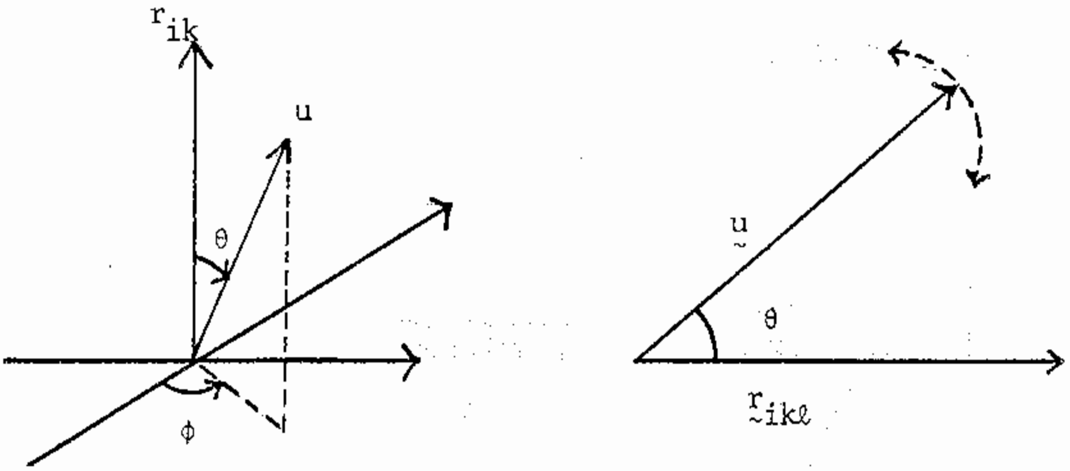
Here ℓ is the subscript for a partial charge on the polyatomic species i and,

$$\underset{\sim}{r}_{ik\ell} = \underset{\sim}{r}_{ik} - \underset{\sim}{r}_{i\ell} \; . \tag{12}$$

It is convenient to perform the integral in equation (11) by transforming to spherical co-ordinates[4] as outlined in figure 3,

Figure 3.

Polar coordinate transformations.



$$V'_{ik} = \sum_{\ell=1}^{n_{pi}} \int_0^{2\pi} d\phi \int_0^{\infty} u^2 du \int_0^{\pi} \frac{P_{i\ell}(u) \sin\Theta \, d\Theta}{(u^2 + r_{ik\ell}^2 - 2ur_{ik\ell} \cos\Theta)^{\frac{1}{2}}} \quad \cdot \qquad (13)$$

First, perform the integral with respect to Θ,

$$V'_{ik} = 2 \sum_{\ell=1}^{n_{pi}} \int_0^{2\pi} d\phi \int_0^{\infty} u^2 du \left. \frac{P_{i\ell}(u) . (u^2 + r_{ik\ell}^2 - 2ur_{ik\ell} \times \cos\theta)^{\frac{1}{2}}}{2ur_{ik\ell}} \right|_0^{\pi} \cdot \qquad (14)$$

Now,

$$\left. (u^2 + r_{ik\ell}^2 - 2ur_{ik\ell} \cos\Theta)^{\frac{1}{2}} \right|_0^{\pi}$$

$$= (u + r_{ik\ell}) - (r_{ik\ell} - u) = 2u, \text{ for } u < r_{ik\ell},$$

$$= (u + r_{ik\ell}) - (u - r_{ik\ell}) = 2r_{ik\ell}, \text{ for } u > r_{ik\ell}. \qquad (15)$$

as this integral must always be positive.

Hence,

$$V'_{ik} = \sum_{\ell=1}^{n_{pi}} 4\pi\{ \int_{o}^{r_{ik\ell}} u^2 du \frac{P_{i\ell}(u)}{2ur_{ik\ell}} .2u$$

$$+ \int_{r_{ik\ell}}^{\infty} u^2 \frac{du\ P_{i\ell}\ (u)}{2u\ r_{ik\ell}} .2r_{ik\ell}\} ,$$

$$= \sum_{\ell=1}^{n_{pi}} \frac{4\pi}{r_{ik\ell}} \{ \int_{o}^{r_{ik\ell}} u^2 du\ P_{i\ell}(u)$$

$$+ \int_{r}^{\infty} r_{ik\ell}\ u\ du\ P_{i\ell}(u)\} ,$$

$$= \frac{4\pi^{-\frac{1}{2}}}{\eta^3} \sum_{\ell=1}^{n_{pi}} \frac{q_{i\ell}}{r_{ik\ell}} \{ \int_{o}^{r_{ik\ell}} u^2 \exp(-u^2/\eta^2) du$$

$$+ \int_{r}^{\infty} r\ u\ \exp(-u^2/\eta^2)\ du\} ,$$

$$= \frac{4\pi^{-\frac{1}{2}}}{\eta^3} \sum_{\ell=1}^{n_{pi}} \frac{q_{i\ell}}{r_{ik\ell}} .- \frac{\eta^2}{2} \{u\exp(\ -u^2/\eta^2) \Big|_{o}^{r_{ik\ell}}$$

$$- \int_{o}^{r_{ik\ell}} \exp(-u^2/\eta^2)\ du + r_{ik\ell} \exp(-u^2/\eta^2) \Big|_{r_{ik\ell}}^{\infty} \}$$

$$= \frac{2}{\pi^{\frac{1}{2}}\eta} \sum_{\ell=1}^{n_{pi}} \frac{q_{i\ell}}{r_{ik\ell}} \{ \int_{o}^{r_{ik\ell}} \exp(-u^2/\eta^2)\ du\} . \qquad (16)$$

Hence,

$$V'_{ik} = \sum_{\ell=1}^{n_{pi}} \frac{q_{i\ell}}{r_{ik\ell}} \mathrm{erf}(r_{ik\ell}/\eta) . \qquad (17)$$

The component in equation (17) arising from the gaussian charge distribution centred on partial charge k at $\underset{\sim}{r}_{ik}$ involves taking the limit of $r_{ik\ell} \rightarrow 0$ (i.e. $k = \ell$). As,

$$\mathrm{erf}(r_{ik\ell}/\eta) = \frac{2}{\sqrt{\pi}\eta} r_{ik\ell} + O(r_{ik\ell}^3) \ \ldots , \qquad (18)$$

then

$$\boxed{V'_{ik} = 2\pi^{-\frac{1}{2}}\eta^{-1}\, q_{ik} + \sum_{\ell\neq k}^{n_{pi}} q_{i\ell}\, \frac{\mathrm{erf}(r_{ik\ell}/\eta)}{r_{ik\ell}}\,,} \qquad (19)$$

Equation (19) takes on the form of the normal Ewald self-potential if $n_{pi} = 1$.

To conclude, equations (4) and (19) are the Ewald expressions to evaluate electrostatic interactions between molecules or ions containing arbitrary distributions of point fractional charges within them.

These correction terms are incorporated in CCP5 program MDMPOL.

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The use of Monte Carlo methods other than the well-known Metropolis algorithm, described by Quirke (1), does not seem to be widespread although their methods have definite advantages. The availability of dynamical properties through molecular dynamics is an advantage, but there are many problems where MD is not applicable, or where the dynamics is not real, (eg. path integral problems).

As usually implemented, the Metropolis algorithm moves 1 particle to a new position randomly chosen to be in a small cube centred on the particle's previous position, calculates the consequent charge in energy, and accepts or rejects the move accordingly. The size of the cube is a parameter of the method, and is usually selected such that about 50% of the moves are accepted. If the cube is too large, essentially all moves are rejected, if too small, all are accepted, in either case the system is essentially frozen in one configuration.

Two algorithms are available for biasing the moves so that the particle is preferentially moved in the direction most likely to lead to acceptance, that is in the direction of the force acting on it. These are known as "force-bias", (2), and "Smart", (3), methods, and have been described at some length in the literature (4-7). Programs for "Metropolis" or "Smart" simulation of atomic systems are in the CCP5 library, molecular or "force-bias" versions are easily developed. The calculation of forces (and torques) adds slightly to the computational cost of the simulation, although not much, if the pressure is being calculated! The major expense is in the calculation of normally-distributed random numbers, which are not as easily obtained as numbers uniform on (0,1).

The RMS displacement, per particle, per step, has been suggested as a measure of computational efficiency, and this quantity has been calculated for a simple L-J liquid, using either the "Metropolis" or "Smart" algorithm. For this simple potential, the best "Smart" simulation was 30% more efficient than the best "Metropolis" run, but cost about 30% more computer time, because of the extra computation in the random number generation. For more complicated potentials, this difficulty would be less important, and the advantage in the use of the "Smart" technique would be clear.

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The vectorised code of the P^3M algorithm on Cray-1S

S.K.Mitra and R.W.Hockney

Computer Science Department, Reading University, Reading

(U.K.)

ABSTRACT

The molecular dynamics program for ionic systems, P^3M, has been modified to run on Cray-1S. By vectorising the code for force calculations and some other subroutines we have reduced the computational time considerably. The vectorised code of P^3M on Cray-1S (for a test system containing 3000 ions) is 4.5 times faster than the CDC 7600 code.

In the molecular dynamics (MD) calculation, a large part of the computer time is spent in calculating the force on a given particle due to all other particles. In a system, where the interparticle forces are long range , a direct summation of these forces up to the required range is prohibitively expensive.

The particle-particle and particle-mesh (P^3M) algorithm [Eastwood, Hockney and Lawrence 1981] is especially designed to handle such computations effeciently. In common with the Ewald method this algorithm also relies on separating the interparticle forces into a short range part, f_{sr} and a long range part, R (e.g. see figure 1), where f_{sr} is non zero for particle separations less than a cutoff distance, r_e , and R is a smoothly varying function of interparticle distance, i.e. R can be Fourier transformed to give non zero values for a limited range of k vectors.

The total short range force on a given particle , i, is obtained by summing over all the short range interparticle forces due to surrounding particles lying within the range of the cutoff distance. An efficient scanning procedure is required to find the neighbours of the particle i. In the P^3M a chaining mesh of the size > r_e is used to divide the entire volume into coarse cells, and a linked list of particles within each cell is prepared before invoking the force calculation. From this linked list all the neighbours of a particle within r_e can be obtained by scanning the cell (containing the particle) and all the nearest neighbouring cells. In the subroutine SRFORC of the P^3M code, the neighbours of the particle, i, are identified from the linked list, their coordinates are gathered from the the central array CORE and the squares of their distances from the particle, i, are calculated. The interparticle short-range force for the each pair is then obtained from the short-range force table prepared in the beginning of the calculation.

From the above description we find that the short-range force calculation is by nature not vectorisable. Consequently in the vectorised version of P^3M , we have adhered to the chain cell and linked list method, and modified the program by using partially vectorised code for gathering the coordinates of the neighbours and for scattering the the updated momenta into the array, CORE. Random-gather and random-scatter routines are not very cost effective because in a typical system there are only 10 to 16 neighbours within the cutoff radius of a particle.

the total long range part of the force on particle i, is calculated by using the particle-mesh (PM) method which consists of the following steps:

1. Charge is assigned to the charge-potential mesh (subroutine QSHARE);
2. the fast Fourier transform technique is used to solve for the potential due this charge distribution (subroutine POTP3M);
3. Mesh defined fields are calculated using a difference scheme, and the forces on the particle i, are calculated from the field by using a suitable interpolation scheme (subroutine MESHFC).

Some segments of the charge assignment and the force interpolation subroutines (QSHARE and MESHFC) readily vectorise. Potential evaluation by Fourier transforms, POTP3M, can be made much faster by using the fast Fourier transform routine, FFT77, specially design to handle multidimensional periodic arrays efficiently on Cray-1S [Temperton 1980].

In addition to these, the subroutine NEWENX, where the positions of the the ions are updated and various thermodynamic properties are calculated, can also be vectorised.

For the sake of comparison we have simulated three identical systems, one on the CDC 7600 using the serial-code of P^3M and other two on the Cray-1S using the serial code and the partially vectorised code of P^3M respectively. Each system is a multicomponent system and contains 3000 ions. The long-range force calculation is performed by using 32^3 mesh and 10^3 chaining cells are used for the short-range force calculation. The program timings for various subroutines for these three simulations are shown in Table I. First of all we note here that the CDC 7600 code is portable to the Cray-1S and that a straight forward transfer of the code to the Cray-1S makes it about two times faster.

There is only very limited scope for the the use of vector operations in the short-range force calculation (SRFORC) consequently the modified code improved its efficiency by only 20%. In this subroutine a major part of the computer time is used in sorting the neighbours and gathering their coordinates. An efficient random-gather and random-scatter procedure will make it more efficient.

In the particle-mesh force calculation most of the subroutines atleast partially vectorise. e.g. QSHARE and MESHFC, and each takes only half the time of the unvectorised code. The vectorised POTP3M is almost seven times faster than its serial-version. The same is true for subroutine NEWENX. Overall the vectorised code of P^3M is 2.14 times faster than the serial code.

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TABLE I

PROGRAM TIMINGS IN MILISECONDS			
Subroutine	CDC7600	Scalar-Cray	Vector-Cray
SRFORC	2000	860	660
QSHARE	386	218	118
POTP3M	1418	853	125
MESHFC	1552	621	305
NEWENX	79	36	6
CLASS-2	5436	2588	1214

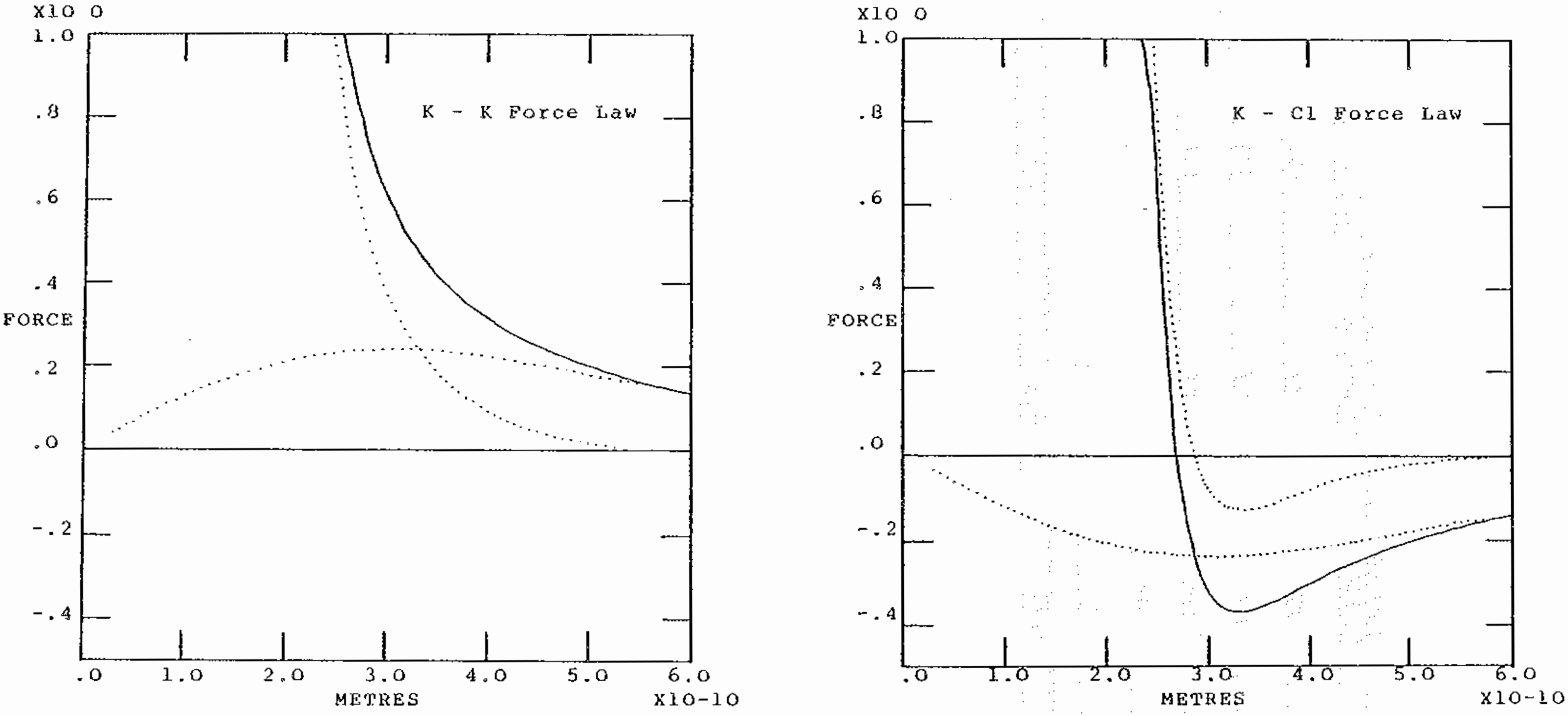

FIGURE 1. A typical form of interparticle force law. Total force (solid line), mesh force (dotted line going to origin) and short range force (other dotted line). From Eastwood et al. (1981)

RDF ON THE DAP: EASIER THAN YOU THINK!

D. Fincham

Calculating the radial distribution function in a liquid simulation is an example of the general histogram problem. Suppose the array VALUES() contains NVALUES real numbers, and we wish to sort them into a histogram i.e. form a count in the array NUMBER() telling us how many of the values fall into each of a series of sub-ranges of the real number space.

Usually the sub ranges have equal width, and let us suppose for simplicity that all the elements of VALUES lie in the range 0 to $N\Delta x$. The obvious serial solution is:

```
      DO 1 J=1,NVALUES
      IBIN=VALUES(J)/DELTAX+1
    1 NUMBER(IBIN)=NUMBER(IBIN)+1
```

This is an example of what is known as the 'random addressing' problem since the elements of NUMBER are not accessed in a regular manner. Since it is clear that the above loop does not 'vectorise', many people assume that the histogram problem must be unsuitable for parallel processing. To overcome this mental block some lateral thinking is required; the solution is to loop over <u>bins</u> of the histogram rather than over the <u>values</u> to be sorted. The DAP code then looks like:

```
      LOGICAL BIN(,),ALREADY(,)
                ..
                ..
                ..
      ALREADY=.FALSE.
      DO 1 JBIN=1,N
      BIN=(VALUES.LE.X(JBIN)).AND.(.NOT.ALREADY)
      NUMBER(JBIN)=SUM(BIN)
    1 ALREADY=ALREADY.OR.BIN
```

Here, to avoid slowing down the loop with scalar arithmetic, I assume that:

```
      X(JBIN)=JBIN*DELTAX
```

has been precomputed, which only needs to be done once. (presumably the histogram loop will be called many times, for example, in the RDF case, on successive steps of the simulation). I have also assumed that there are 4096 values to be sorted so that VALUES is a DAP matrix; the extension to less than or more than this number of values is trivial.

BIN is a logical matrix which is set .TRUE. in positions where the corresponding element of VALUES falls into the current bin;

these elements are the ones which are smaller in value than the upper limit of the bin, and have not already been considered. The SUM function applied to a logical matrix returns the number of .TRUE. elements, thus giving directly the appropriate entry in the histogram.

An important point to notice is that this code contains no arithmetic, only logical comparisons and logical operations, which are extremely fast on the DAP because of the bit-serial nature of the processors. This is a perfect example of how parallel processing is very different from conventional computing. The random addressing problem has gone away because we are accessing the DAP store by content rather than using an address in the conventional sense. This is possible because the DAP can search through its memory locations in parallel on a bit-by-bit basis.

A Fast Method for the Evaluation of Square Roots in Computer Simulation

K. Singer

In MC or MD codes where the box length is set $<$ = 2.0, the cut-off length is (almost always) $<$ 1.0. A square root routine can take advantage of the limited range - except for the very large systems or very small particles $0.1 < r^2_{ij} < 1.0$. If this is so, the algorithm described below, which is about 20 times faster than the standard SQRT function available on the CDC 7600, can be used.

Construct a least squares polynomial

$$\int_{0.1}^{1} \Big[\sum_{j=0}^{n} a_j x^{2j} - x^{\frac{1}{2}} \Big] \, dx = \min \qquad 1.$$

For n = 3 one finds

a_3	a_2	a_1	a_o
.430526	-1.097209	1.428264	0.1882532

If $y = x^{\frac{1}{2}}$ and $y^{(o)}$ the value obtained from this polynomial, closer approximations are obtained by means of

$$y^{(i+1)} = y^{(i)} - \tfrac{1}{2}\Delta/y^{(i)}, \ \Delta = (y^{(i)})^2 - x \qquad 2.$$

With j = 3, two steps lead to 6 figure accuracy. Satisfactory, albeit slightly less accurate (5 figures) results may be obtained from j = 3 and one refinement steps 2) or from j = 2 or even 1 with 2 or 3 refinement steps.

A possible coding is

(RSQ = r_{ij}^2)

```
Y  =  ((.430526*RSQ - 1.097209)*RSQ + 1.428264)*RSQ + 0.1882532)

DY =  Y*Y-RSQ

Y  =  Y-0.5*DY/Y

DY =  Y*Y-RSQ

Y  =  Y-0.5*DY/Y
```

This algorithm can be advantageous when an odd power of r_{ij} occurs in the pair potential or when it is desired to evaluate the r_{ij} histogram at every step.

CCP5 Literature Survey

F. Gibb, W. Smith

On the suggestion of Profesor J.G. Powles, the CCP5 Chairman, we have conducted a search of the scientific literature over the last three or so years to provide our readers with a list of publications relevant to CCP5 computer simulation work.

The search was conducted on the current INSPEC file on Lockheed Dialog's Information Retrieval System in Palo Alto, California. This data file covers the period 1977 to date and includes all records in the "Physics Abstracts" publication.

"Computer Simulation" is a broad category and it was therefore necessary to define strict parameters for the search. We have chosen to provide references from 1980 onwards that are relevant to any of the categories, "Monte Carlo", "Molecular Dynamics" and "Computer Simulation" and which have appeared with the PACS classification codes 61.20-p to 61.20.Qg. The result is a list of some 270 references representing classical, semiclassical and quantum theories of liquid structure.

While we believe that all the references obtained will be relevant to CCP5, it is highly possible that we have not included all those of interest in the period concerned. We would be pleased to hear of any areas seriously neglected. In this context it would help if appropriate keywords or PACS classification codes were provided.

The reference list is provided with the eighth issue of the CCP5 newsletter "Information Quarterly". It covers the period from 1st January, 1980, to (approximately) September, 1982. The list is in approximate chronological order. We hope to provide a further update on a later occasion.

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