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.
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Contents

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Science & Engineering Research Council
Daresbury Laboratory, Daresbury,
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Editorial

We hear much these days about the potential for parallel processing in the art of molecular simulation. Just as the emergence of vector processors in the early 1980's promised (and delivered) a new level of performance, it is expected that parallel processors will provide the same, exciting advancement in capabilities. This is certainly the view we have all shared.

However, my own involvement in parallel processing over the last eighteen months or so has indicated that things are not as advanced as they could be. There are a number of reasons why I think this is so. Firstly, comparison of the new situation with the appearance of vector processors is misleading. The vector processors from the early '80s arrived as complete machines, at the forefront of a long line of development in computer architecture. In addition, most (if not all) came with good vectorising compilers, which made vectorisation relatively easy. Even so, it is interesting to note how few scientific programs actually achieve even a fraction of the full capability of the machines concerned. It would appear that most users are content with whatever performance is achieved by minimum effort. Such a half-hearted approach in the area of parallel processing would be fatal. In this context the wisdom of the establishment of the U.K. CCPs is manifest. Without them, one wonders, would there be as many truly vectorised programs in existence here?

The situation regarding parallel processors is more complex. Leaving aside the shared memory Crays and the like, which are essentially a continuation of the line of development from scalar to vector to parallel architectures. (Leaving aside too the DAP, which also grew up in a supportive environment which guaranteed that it fullfilled the needs of users). The parallel processors we are most likely to encounter, such as Transputer arrays, represent a radical departure from previous machines in having no fixed architecture and really do require a radical rethink if one is to program them successfully and efficiently. Coupled with this there is relatively little by way of software support. And how many scientists want to program in Occam? Few manufacturers offer parallel compilers that are as clever in parallel terms as the vectorising compilers for the vector machines. It is too early of course to expect a great deal here. The MIMD parallel machines are well in advance of the software developments that will get the best out of them. This will be so for some time to come, though we are all aware of the efforts being made to improve things in this regard.

These features of the problem are making life difficult for would be scientific users, but the problem is compounded by the user community itself. When I talk to colleagues about their work in this area, it seems clear that each group is working more-or-less in isolation. We are all solving problems which have been solved already by other groups. Why is this? The CCPs exist to improve the contact between groups and to enlighten everyone as to the best computational techniques and practice. CCP5 is no exception and has to date organised at least one workshop and has published some work on parallel algorithms in this newsletter. It is disappointing how little feedback has come from these. It is also significant that most of the effort of publicising the concepts of parallel processing have come from a very small group of people. We desperately need a stronger response from the CCP5 community here. There are many groups out there working on parallel algorithms that have presumably solved major problems or perhaps been defeated by them. We need to know what is going on and who is making progress. This newsletter is an excellent vehicle for this information and the CCP5 steering committee is well disposed to receive suggestions from the community. Please make use of both!

Contributors to the Current Issue.

Our thanks go to:

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General News.

1) The CCP5 workshop on "Novel Methods in Molecular Simulation" is to take place at Royal Holloway and Bedford New College on 3-4 July 1989. The final preparations are now being made, as the workshop is already nearly fully subscribed. A final announcement is made in the pages of this issue of the newsletter. Please respond urgently, if you have not already done so.

2) The CCP5 Annual Conference for 1990 will have the title "Grand Challenges in Molecular Simulation" and will be held December 18-19 1989 at Cambridge. We will provide more information in due course.

3) A conference is to be organised by CCP5 on the subject "Architecture and Algorithms in the Simulation of Condensed Phases" and is intended to take place in July 1990 at Edinburgh or St. Andrews. The organisers hope to invite several renowned U.K. and international scientists. The sessions will be on the subjects of SIMD, MIMD, General plus Special Purpose Machines and Future Trends in Simulation. An additional session is planned for manufacturers of hardware to lecture on the architecture and performance of various computers and to demonstrate the hardware on-site. Further news of this meeting will be given in this newsletter (and elsewhere) when plans are more concrete.

4) A number of scientists have been invited by CCP5 to vivit the U.K. in 1989, to give seminars and take part in discussions. The following have provisionally agreed to come.

- Prof. K. Binder (University of Mainz)
- Prof. D. Coker (University of Boston)
- Prof. M.L. Klein (University of Pennsyslvania)
- Prof. P. Wolynes (University of California)

Details of the proposed visits will be circulated to UK members of CCP5 when the itineraries have been finalised.

5) We have information about a number of conferences to take place in the near future, which may be of interest to CCP5 members. These are as follows:

- Royal Society of Chemistry,Faraday Symposium 25, "Large Gas Phase Clusters", 12-14 December 1989, University of Warwick. Enquiries Mrs Y. Fish, The Royal Society of Chemistry, Burlington House, London W1V 0BN, U.K..
- Gordon Conference on Chemistry and Physics of Liquids, 14-18 August, Holderness School. Chairman S.C. Greer. Enquiries Dr. A.M. Cruikshank, Director, Gordon Research Conferences, Gordon Research Center, University of Rhode Island, Kingston, RI 02881-0801, USA.
- Supercomputational Science Summer School, 18-29 September 1989, Rutherford and Appleton Laboratory, Coseners House, Abingdon. Limited participation: 40

people. Enquiries to The Secretary, Supercomputational Science Summer School, Atlas Centre, Rutherford and Appleton Laboratory, Chilton, OX11 0QX, U.K..

- Third World Conference in the Service of Man, 4-7 July, Barcelona, Spain. Topics covered: Simulation, Artificial Intelligence, Decision Making. Enquiries Jordi Romero, General Coordinator, Museu de lá Ciència, Teodor Roviralta, 55, 08022 Barcelona, Spain.

- 8th Summer School on Computing Techniques in Physics, "Man-machine Interface in the Scientific Environment",19-28 September 1989, Skalský dvour, Czechoslovakia. Enquiries Dr. J. Nadrchal, Insitiute of Physics, Czechoslovak Academy of Sciences, Na Slovance 2, 180 40 Praha 8, Czechoslovakia. Deadline for applications 30 June 1989.

We will be pleased to announce other conferences if our readers supply us with the necessary information.

6) Daresbury Laboratory: The NAS AS7000 computer that was the main central computer has departed. The CONVEX C220 that replaced it has already been upgraded to two processors. Meanwhile the INTEL iPSC/2 is fully functional and is showing much promise for scientific applications. It awaits an upgrade from a 32 to a 64 processor machine, a transformation we hope will happen soon! Concomitant with these changes, the central computer room is being reorganised to provide a user work area and self-service area.

7) The University of Manchester Regional Computer Centre (UMRCC) is no more! - at least, not in name. It is henceforth to be called the "Manchester Computing Centre", a name more accurately reflecting the centre's rôle nationally. As announced earlier the CYBER 205 has departed and has been replaced by an AMDAHL VP1200. Anyone still requiring old MVS/370 datasets, which have been stored on tape, is recommended to consult the UMRCC newsletter of February 1989 (No. 159).

8) The University of London Computing Centre has replaced the two Cray-1s computers with a single Cray XMP/28. They intend to put up UNICOS, the Cray version of UNIX, in the form of the operating system COS 1.17, at the end of 1989. To ease the problems of the overloaded Masstor storage device, a Storage Tek 4400 Automatic Cartridge System (ACS) is shortly to be installed. It is believed this will enable an effective and efficient archiving system. The system is briefly described in the January and February issues of the ULCC newsletter.

9) The Rutherford and Appleton Computer Centre has replaced the Forum and Arclight newsletters by a single glossy circular by the name of FLAGSHIP. In addition to providing news of computing matters, such as hardware and software, it also carries occasional descriptions of scientific work. Issue No.1 contains a report by B. Vessal and C.R.A. Catlow on MD simulations of glasses.

Readers are reminded that CCP5 has an allocation of Cray time on the RAL Cray XMP/48 for development of programs for the CCP5 community. Please apply to Dr. M. Leslie, TCS Division, SERC Daresbury Laboratory, Warrington WA4 4AD for further information.

Readers should know already, but users of E-mail in the UK wishing to communicate overseas, should use the address UK.AC.EARN-RELAY in place of UK.AC.RL.EARN when routing messages.

Program Libraries

The CCP5 Program Library.

The CCP5 Program Library provides programs and documentation 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.. Listings of programs are available if required but it is recommended that magnetic tapes (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.

Readers should also note that we are authorised to supply the example programs originally published in the book "Computer Simulation of Liquids", by M.P. Allen and D.J. Tildesley (Clarendon Press, Oxford 1987). These are supplied in the same manner as the resident CCP5 programs. We are grateful to Mike Allen and Dominic Tildesley for their permission.

We should also like to remind our readers that we would welcome further 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.

Please Note: For copyright reasons we are not able to supply the programs CASCADE, SYMLAT, THBFIT,THBPHON and THBREL free of charge to Universities outside the United Kingdom.

Program from the Book: "Computer Simulation of Liquids" by M.P. Allen and D. Tildesley. Clarendon Press, Oxford 1987.

These programs originally appeared on microfiche in the book "Computer Simulation of Liquids" by M. P. Allen and D. J. Tildesley, published by Oxford University Press, 1987. They are made freely available to members of CCP5, in the hope that they will be useful. The intention is to clarify points made in the text, rather than to provide a piece of code suitable for direct use in a research application. We ascribe no commercial value to the programs themselves. Although a few complete programs are provided, our aim has been to offer building blocks rather than black boxes. As far as we are aware, the programs work correctly, but we can accept no responsibility for the consequences of any errors, and would be grateful to hear from you if you find any. You should always check out a routine for your particular application. The programs contain some explanatory comments, and are written, in the main, in FORTRAN-77. One or two routines are written in BASIC, for use on microcomputers. In the absence of any universally agreed standard for BASIC, we have chosen a very rudimentary dialect. These programs have been run on an Acorn model B computer. Hopefully the translation of these programs into more sophisticated languages such as PASCAL or C should not be difficult.

M.P.Allen

THE CCP5 PROGRAM LIBRARY.

ADMIXT	[MD,LJA/MIX,LF,TH+MSD+RDF]	W. Smith
CARLOS	[MC,VS+Aquo,TH]	B. Jonsson S. Romano
CARLAN	[DA,CARLOS structure analysis]	B. Jonsson S. Romano
CASCADE	[LS,DIL,EM,TH+STR]	M. Leslie/ W. Smith
CURDEN	[DA,Current Density Correlations]	W. Smith
DENCOR	[DA,Density Correlations]	W. Smith
HLJ1	[MD,LJA,LF,TH+MSD+RDF]	D.M. Heyes
HLJ2	[MD,LJA,LF,TH+MSD+RDF+VACF]	D.M. Heyes
HLJ3	[MD,LJA,LF/LC,TH+MSD+RDF]	D.M. Heyes
HLJ4	[MD,LJA,LF/CP+CT,TH+MSD+RDF]	D.M. Heyes
HLJ5	[MD,LJA/SF,LF,TH+MSD+RDF]	D.M. Heyes
HLJ6	[MD,LJA,TA,TH+MSD+RDF]	D.M. Heyes
HMDIAT	[MD,LJD,G5+Q4,TH+MSD+QC]	S.M. Thompson
HSTOCH	[MD/SD,VS+BA,LF+CA,TH]	W.F. van Gunsteren/ D.M. Heyes
MCN	[MC,LJA,TH]	N. Corbin
MCLSU	[MC,LJA,TH]	C.P. Williams/ S. Gupta
MCMOLDYN	[MD/MC,LJS+FC+AQ, LF+QF/G5+QS,TH+RDF]	A. Laaksonen
MCRPM	[MC,RPE,TH+RDF]	D.M. Heyes
MDATOM	[MD,LJA,G5,TH+RDF+MSD+QC]	S.M. Thompson
MDATOM	[MD,LJA,LF,TH+MSD+RDF]	D. Fincham
MDDIAT	[MD,LJD,LF+CA,TH+MSD]	D. Fincham
MDDIATQ	[MD,LJD+PQ,LF+CA,TH+MSD]	D. Fincham
MDIONS	[MD,BHM,LF,TH+MSD+RDF+STF]	D. Fincham/ N. Anastasiou
MDLIN	[MD,LJL,G5+Q4,TH+MSD+QC]	S.M. Thompson.
MDLINQ	[MD,LJL+PQ,G5+Q4,TH+MSD+QC]	S.M. Thompson
MDMANY	[MD,LJS+FC,LF+QF,TH]	D. Fincham/ W. Smith
MDMIXT	[MD,LJS/MIX,LF+QF,TH]	W. Smith
MDMPOL	[MD,LJS+FC/MIX,LF+QF,TH]	W. Smith/ D. Fincham
MDNACL	[MD,BHM,LF,TH+MSD+RDF]	W. Smith
MDPOLY	[MD,LJS,G5+Q4,TH+MSD+QC]	S.M. Thompson
MDMULP	[MD,LJS+PD+PQ/MIX,LF+QF,TH]	W. Smith
MDSGWP	[MD,LJA/SGWP,LF,TH+VACF+RDF+QC]	W. Smith/ K. Singer
MDTETRA	[MD,LJT,G5+Q4,TH+MSD+QC]	S.M. Thompson
MDZOID	[MD,GAU,LF+QF,TH+MSD+RDF+VACF]	W. Smith
NAMELIST	[UT, Namelist emulation]	K. Refson

SCN	[MC,LJA,RFD,TH]	N. Corbin
SURF	[MD,BHM/TF/2D,LF,TH+RDF]	D.M. Heyes
SYMLAT	[LS,PIL,EM+SYM,TH+STR]	Harwell
THBFIT	[LS,PIL,EM,Potential fitting]	Harwell
THBPHON	[LS,PIL/3B,EM,Phonon dispersion]	Harwell
THBREL	[LS,PIL,EM,TH+STR]	Harwell

Key:

Program types:	MD	Molecular dynamics
	MC	Monte Carlo
	LS	Lattice simulations
	SD	Stochastic dynamics
	DA	Data analysis
	UT	Utility package
System models:	LJA	Lennard-Jones atoms
	LJD	Lennard-Jones diatomic molecules
	LJL	Lennard-Jones linear molecules
	LJT	Lennard-Jones tetrahedral molecules
	LJS	Lennard-Jones site molecules
	RPE	Restricted primitive electrolyte
	BHM	Born-Huggins-Meyer ionics
	SGWP	Spherical gaussian wavepackets
	TF	Tosi-Fumi ionics
	VS	Variable site-site model
	BA	Bond angle model
	PD	Point dipole model
	PQ	Point quadrupole model
	MIX	Mixtures of molecules
	GAU	Gaussian molecule model
	FC	Fractional charge model
	PIL	Perfect ionic lattice model
	DIL	Defective ionic lattice model
	3B	3-body force model
	2D	Two dimensional simulation
	SF	Shifted force potential
	FC	Fractional charge model
	AQ	Aqueous solutions
Algorithm:	G5	Gear 5th order predictor-corrector
	Q4	Quaternion plus 4th. order Gear P-C
	LF	Leapfrog (Verlet)
	QF	Fincham Quaternion algorithm
	QS	Sonnenschein Quaternion algorithm
	LC	Link-cells MD algorithm
	CP	Constant pressure

	CT	Constant temperature
	TA	Toxvaerd MD algorithm
	CA	Constraint algorithm
	EM	Energy minimisation
	SYM	Symmetry adapted algorithm
	RFD	Rossky-Friedman-Doll algorithm
Properties:	TH	Thermodynamic properties
	MSD	Mean-square-displacement
	RDF	Radial distribution function
	STF	Structure factor
	VACF	Velocity autocorrelation function
	QC	Quantum corrections
	STR	Lattice stresses

Programs from the Book "Computer Simulation of Liquids"

F.1	Periodic boundary conditions in various geometries
F.2	5-value Gear predictor-corrector algorithm
F.3	Low-storage MD programs using leapfrog Verlet algorithm
F.4	Velocity version of Verlet algorithm
F.5	Quaternion parameter predictor-corrector algorithm
F.6	Leapfrog algorithms for rotational motion
F.7	Constraint dynamics for a nonlinear triatomic molecule
F.8	Shake algorithm for constraint dynamics of a chain molecule
F.9	Rattle algorithm for constraint dynamics of a chain molecule
F.10	Hard sphere molecular dynamics program
F.11	Constant-NVT Monte Carlo for Lennard-Jones atoms
F.12	Constant-NPT Monte Carlo algorithm
F.13	The heart of a constant μVT Monte Carlo program
F.14	Algorithm to handle indices in constant μVT Monte Carlo
F.15	Routines to randomly rotate molecules
F.16	Hard dumb-bell Monte Carlo program
F.17	A simple Lennard-Jones force routine
F.18	Algorithm for avoiding the square root operation
F.19	The Verlet neighbour list
F.20	Routines to construct and use cell linked-list method
F.21	Multiple timestep molecular dynamics
F.22	Routines to perform the Ewald sum
F.23	Routine to set up alpha fcc lattice of linear molecules
F.24	Initial velocity distribution
F.25	Routine to calculate translational order parameter
F.26	Routines to fold/unfold trajectories in periodic boundaries
F.27	Program to compute time correlation functions
F.28	Constant-NVT molecular dynamics - extended system method
F.29	Constant-NVT molecular dynamics - constraint method
F.30	Constant-NPH molecular dynamics - extended system method
F.31	Constant-NPT molecular dynamics - constraint method
F.32	Cell linked-lists in sheared boundaries
F.33	Brownian dynamics for a Lennard-Jones fluid
F.34	An efficient clustering routine
F.35	The Voronoi construction in 2d and 3d
F.36	Monte Carlo simulation of hard lines in 2d
F.37	Routines to calculate Fourier transforms

Situations Vacant

Superconductivity Research: Post-Doctoral Fellowship
University of Keele

Applications are invited for a 3-year SERC fellowship for a project which will use atomistic computer modelling techniques to investigate crystallographic and thermodynamic properties and phase relationships in high Tc superconducting oxides. The work which will make use of the CRAY XMP supercomputers at RAL and ULCC will be supervised by Profs. R. Catlow and M.J. Gillan and involves collaboration with Dr. S.C. Parker at Bath.

Applicants should have a Ph.D. degree in Chemistry, Physics, Materials Science or a relevant discipline; applications should be addressed to Prof. C.R.A. Catlow, Department of Chemistry, University of Keele, Keele, Staffs. ST5 5BG, from whom further details can be obtained.

EEC Funded PDRA on Computer Modelling of Zeolites
University of Keele

A PDRA for four years will be available from October 1989 for work on a project concerning molecular dynamics studies of structure and sorption in zeolites. The project is part of a larger EEC funded collaboration on theoretical and experimental studies of zeolites involving the universities of Keele, Eindhoven, Kiel and Turin. Applicants should have (or expect to have shortly) a Ph.D. or equivalent qualification and must be a citizen of an EEC country other than the U.K.. Applications should be addressed to Prof. C.R.A. Catlow, Department of Chemistry, University of Keele, Keele, Staffs. ST5 5BG, U.K..

FINAL ANNOUNCEMENT OF A CCP5 WORKSHOP ON: NOVEL METHODS IN MOLECULAR SIMULATION

at
Royal Holloway and Bedford New College,
Egham, Surrey TW20 0EX

3rd/4th July 1989

This workshop is intended to bring together researchers involved in new aspects of molecular simulation. Topics of discussion will include cellular automata, lattice simulations of long-range order, reverse monte carlo, Car-Parrinello, neural networks, percolation and Gibbs ensemble MC. The speakers include,

- Dr. M. P. Allen (University of Bristol)
- Prof. R. Cotterill (University of Lyngby, Denmark)
- Prof. M.J. Gillan (University of Keele)
- Dr. D.M. Heyes (RHBNC, University of London)
- Dr. R.L. McGreevy (University of Oxford)
- Dr. J. Naudts (University of Antwerp, Belgium)
- Dr. D. Nicolaides (University of Bristol)
- Prof. J.G. Powles (University of Kent)
- Dr. N. Quirke (BP Research, Sunbury-on-Thames)

Places are strictly limited. If you would like to attend please write to: Dr. D.M. Heyes, Department of Chemistry, Royal Holloway and Bedford New College, Egham, Surrey TW20 0EX. or electronic mail:

BITNET address is UHCA015@VAXB.RHBNC.AC.UK

or JANET address is UHCA015@UK.AC.RHBNC.VAXB.

Please describe your research interests and some recent publications if possible.

WORKSHOP ON PARALLEL ALGORITHMS IN MOLECULAR SIMULATION

Daresbury Laboratory

Provisional: 8th. November 1989

The purpose of this workshop is to bring together those groups currently working on real scientific problems and using parallel processing as the method of solution. The meeting will be an informal one-day affair, in which participants will present short (15 minute) talks on their methods. There will be opportunity for discussion and speculative suggestions. The number of participants will not exceed 30.

We hope to attract participants with interests the following areas:

- Systolic loop algorithms for MD and Monte Carlo.
- Hierarchical (master-slave) algorithms.
- Algorithms for multiple, independent simulations.
- Ewald sum and other methods for Coulombic Systems.
- Algorithms for heterogeneous systems (e.g. link-cells, neighbour lists etc.).
- Algorithms for macromolecules and polymers.
- Algorithms for biological molecules.
- Vectorisation on parallel machines.
- Parallel graphics in molecular simulation.
- Energy minimisation.
- Novel algorithms.

Readers interested in taking part in this workshop should contact Dr. W. Smith or Dr. F. Müller-Plathe, TCS Division, SERC Daresbury Laboratory, Warrington WA4 4AD, or via electronic mail WL@UK.AC.DL.DLGM, or FMP@UK.AC.DL.DLGM or FMP@UK.AC.RL (Bitnet). Please specify your area of work and subject of your talk (if any).

Atlas Centre
Rutherford Appleton Laboratory

SUPERCOMPUTATIONAL SCIENCE

Summer School

18th. - 29th. September, 1989.

The Coseners House, Abingdon and Rutherford Appleton Laboratory

Organized by : *R.G. Evans, P.C. Thompson & S. Wilson*

Scientific programme : The Summer School will consist of lecture courses on the effective exploitation of state-of-the-art supercomputers in science and engineering. The lectures will be largely in the areas of research associated with SERC Collaborative Computational Projects, which include:

Quantum Chemistry
Continuum states of atoms and molecules
Computational studies of surfaces
Protein crystallography
Molecular dynamics and Monte Carlo Simulation of Bulk Systems
Heavy particle dynamics
Analysis of Astronomical Spectra
Electronic Structure of Solids
Plasma Physics

The emphasis, however, will be on teaching generally useful numerical methods. Some practical work will also be undertaken.

Enrollment : The Summer School is intended to be at graduate and post-doctoral level and is open to participants from all disciplines. The number of participants is limited to about 40. Some financial support for SERC postgraduate students will be available. Further details can be obtained from The Secretary, Supercomputational Science Summer School, Atlas Centre Rutherford Appleton Laboratory, Chilton, OX11 0QX, U.K.

Report on the CCP5 Annual Conference: Computer Modelling of New Materials

W. Smith and M. Leslie,
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April 24, 1989

The CCP5 Annual Meeting this year took place in Bristol in January (4th-6th) and was organised by Dr. M.P. Allen of the University of Bristol. The meeting was jointly supported by CCP9, the sister project of CCP5 concerned with electronic structure calculations in solid materials. The subject of the meeting was "Computer Modelling of New Materials" which was intended to demonstrate the importance of simulation and modelling methods at the cutting edge of research in technologically important materials. The subject areas covered included polymers, ionic materials and semiconductors. A strong interest naturally arose in the re-invigorated science of high temperature superconductors, which have been treated by all the computational techniques available.

The meeting started with E.A. Colbourne of ICI Wilton, who spoke on the subject of "Molecular Modelling for Advanced Materials". Dr. Colbourne outlined the interest within ICI in the computer modelling of polymers. The motivation is the understanding of the molecular basis for the preparation and processing of polymers in an industrial context. ICI has an interest in both synthetic polymers and biopolymers, the former in the plastics industry and the latter in pharmaceutical development. These two kinds of polymer have some features in common, but largely the kinds of system being modelled, and the objectives of the work are different. The synthetic polymers are studied to understand their bulk properties and the biopolymers to gain insight into biological activity. Dr. Colbourne concentrated on synthetic polymers, with specific examples made of the polymers polyaryl-ether-ether-ketone (PEEK) and polyetheylene teraphthalate (PET).

The objective of the work on PEEK was to obtain an adequate description of the crystalline form using molecular mechanics methods. The difficulty here was obtaining a suitably accurate model potential, for which simple site-site pair potentials were used and tested by prediction of the lattice parameters. Several other possible structures were described, the key differences between them being expressed in terms of the disposition of the ketone and ether groups in adjacent polymer chains (referred to as the *register* of the two kinds of groups). Six structures were modelled by molecular mechanics and their relative thermodynamic stability (in terms of lattice energy) obtained. The energetics of different structures was important in the understanding of the mechanical properties of the polymer.

The study of PET was intended to discover the reasons for the improvement in the properties of this important plastic material as a result of mechanical processing (known as orientation). The normal extruded material is brittle, but becomes more flexible if stretched in the forward and transverse directions. The study, which included molecular orbital calculations, established that the stretching operation reduced the intramolecular stability of the chains, but that this was compensated for by intermolecular interactions. The calculations thus provided important clues to the observed properties of the material. In future studies, ICI intend to make use of molecular dynamics methods, which will provide methods of calculating stress-strain relationships and temperature and time dependent effects etc. They are however mindful of the greater expense implicit in this approach.

The second speaker, G. Goldbeck-Wood of Bristol University, also spoke on the subject of the polymer PEEK. His concern was to simulate the growth and melting behaviour of the crystalline solid using a a simple two dimensional model for the crystal growth process, due to Sadler and Gilmer, in which a slab of material grows along the top or side edges in a manner resembling a roughening transition. The preliminary results explain the isothermal growth rates, melting temperature and lamellar thickness of the crystal using parameters estimated from the enthalpy of fusion. The model has been extended to account for transient phenomena such as isothermal annealing.

T.K.H. Barron of Bristol University reported on studies of thermal expansion in idealised models of polyethylene. The underlying theory regards the thermal expansion as an elastic response to thermal stresses. A quasi-harmonic approximation is used in the first instance and the stresses are obtained from a perturbation calculation. A central force model is used for the interactions, which admits three distinct mechanisms for the thermal expansion. Firstly there is bond stretching due to assymmetry of the pair potential functions about the minimum. Secondly, there is contraction along bonds due to tension induced by transverse vibration. Thirdly there is bond rotation due to tension induced by both kinds of vibration. All of these are present to some degree in polymeric systems.

The different idealised models of polyethylene were described. All were contained within an orthorhombic unit cell. The most basic model consisted of parallel, straight flexible polymer chains, which underwent thermal contraction along the chain direction and expansion in the perpendicular direction. Zig-zag polymers (with a 90 degree bend at the carbon sites) showed the largest expansion perpendicular to the ribbon length. The effect was repeated in non-rectangular zig-zag chains, which were modelled by inclusion of second-neighbour interactions within the chains. A more realistic model of polyethylene, including explicit hydrogen atoms gave good agreement with experiment (X-ray diffraction) up to about 100 K; describing well the anisotropy of the vibration perpendicular to the chain direction, but gave large vibration magnitudes at higher temperatures.

D.A. Dunmur presented the first talk on the subject of liquid crystals under the provocative title of "Structure - Property Relationships in Liquid Crystals: Can Modelling do Better than Empiricism?". His primary concern was to determine the effect of molecular structure on the formation of liquid crystal (LC) phases, since it is well known that the LC phases are a small perturbation of the liquid state and minor molecular changes can have a substantial effect. He began with a brief description of the phenomenology of liquid crystals and the order parameters used to describe their anisotropic properties (i.e. the s, g_1 and g_2 parameters).

A general structure for molecules that give rise to the nematic/isotropic transition was outlined. It consisted of two ring systems with a bridging "link" group, terminal alkyl and other groups and laterally substituted groups. Various empirical "rules" have evolved, which indicate the favourability of the formation of a nematic phase. For example in the case of the ring system, the order: bicyclo-octane > cyclohexane > benzene is observed. Similar rules arise in regard to the linkage groups and the terminal alkyl group length (where an even/odd effect is also apparent). The importance of dipoles was also discussed: interestingly, no nematic dipole phases have yet been observed.

Professor Dunmur and his colleagues have investigated the subtle effects of molecular structure in these systems with the aid of molecular mechanics modelling. The MM2 force field was used to define the intramolecular effects and site-site forces used to describe the intermolecular effects. In addition a "nematic potential", which was a function of the LC order parameter, was introduced to incorporate the aligning effects of a very large system of molecules. The majority of the calculations dealt with a system of two molecules, for which the minimum energy of the dimer was sought, from many starting orientations. The objective was to find the favoured mode of alignment for the dimer as a precursor to liquid crystal formation. Several typical molecular structures were investigated, including dipolar species, disc-like and rod-like molecules, and molecules possessing chiral centres (such molecules give rise to chiral nematics, with a twist orientation). Overall the method shed some light on the formation of liquid crystals, with some disappointments, such as failure to predict stability trends in experimentally studied systems. However the model was admittedly basic in some respects and offered some hope for the future.

M.P. Allen of Bristol University described his simulations of liquid crystal films based on the Lebwohl-Lasher model, which is a lattice model incorporating nearest-neighbour interactions in the form of orientational coupling. The system had been studied by Fabbri and Zanoni and latterly by Luckhurst, Sluckin and Zewdie. The objective in Dr. Allen's work was to perform the necessarily long simulations to locate the nematic-isotropic phase transition in films of varying molecular thicknesses. The adaptation of the simulation (Monte Carlo) algorithm to suit the DAP massively parallel processor was described. This was an important aspect given the length of the simulation runs required. (It was estimated that an equivalent MD simulation for a non-lattice model, would require a complete microsecond simulation!.)

The location of the transition temperature (T_{NI}) was achieved by calculating the energy distribution function near the phase transition. For simulations at precisely T_{NI} two peaks should appear, at above or below this temperature the relative sizes of the peaks changes in favour of one of the structures. These considerations enable the accurate determination of the transition temperature (at the expense of very long runs). In these simulations it was found that the nematic/isotropic phase transition ceases to be of first order when the thickness of film reduced to 6 to 8 layers. Below this margin, it was not possible to separate out two peaks in the distribution function.

Dr. Allen went on to describe further work on the orientational wetting that occurs when the film is placed between fixed walls.

The first speaker on the second day was Dr. A.P. Sutton, of Oxford University, who spoke on the subject "Modelling Extended Defects in Silicon". He began by describing the "tight-binding" method that was used to calculate the electronic structure of silicon. In this prescription the bonding energy is written as sum of several terms: the covalent bond energy: the promotion energy (required to promote s^2p^2 occupancy to s^1p^3 prior to hybridisation); the change in electrostatic energy; the exchange and correlation energy and a correction term for the approximations employed. Each of these contributions are written in terms of the electron density matrix $\rho_{i,j}$ and empirical parameters are obtained from the literature or fitted to satisfy the bulk volume of silicon. The recursion method that is central to this treatment was described in detail.

A condition implicit in this treatment is "local charge neutrality", which is thought to be necessary to enable the interionic forces to be calculated with a degree of accuracy. To ensure this the on-site energy terms ($H_{i,i}$) are adjusted accordingly. In Dr. Sutton's work the method was tested by calculating the structural stability of silicon as a function of volume. The method gave good account of cubic phases but was significantly incorrect for the close packed fcc and bcc phases.

The method was then applied to several systems. The first was a stacking fault in crystalline tin. The method correctly indicated a wurtzite-like structure for the atoms at the defect. The next application was the 112 grain boundary in germanium, which structure was found to be graphite-like in the defect region with a significant peak in the band gap of the density of states - indicating "dangling bonds". In studies of silicon it was noted that the band gap contained little structure. The experiments indicate otherwise, but are probably contaminated with oxygen, which gives the band gap structure. In silicon it was believed that defects were likely to arise in preference to dangling bonds. A feature of the silicon 110 surface was the tilting of the atoms to remove degeneracy. This introduces strain in the system, but this was thought necessary to reduce the electronic energy. At this stage Dr. Sutton questioned the assumed need for local charge neutrality, since calculations without this ingredient gave equivalent results.

Finally, the tight-binding model was compared with the atomistic model potentials of Stillinger/Weber and Baskes. Both potential models failed to describe surface tilting, as expected in view of its quantum mechanical origin. However the Stillinger/Weber potential seemed to be adequate at describing a 112 interface within the bulk structure.

The application of the tight-binding method was further discussed by L. Goodwin of Imperial College in his talk entitled "Improved Tight Binding Parameters for Silicon". The tight-binding method was known to possess some significant failings, notably the incorrect energy-volume properties of the close packed crystal structures. An improved set of parameters were obtained by rescaling the tight-binding energy functional. The scaling procedure adopted was described. The new parameters were obtained by comparing the results with Yin and Cohen's density functional theory results for the diamond lattice structure. The transferability of the parameters was tested by application to silicon atomic clusters of 2-10 atoms (local charge neutrality was very important here!). The method gave satisfactory account of the bondlengths and structures of these clusters, including the intriguing deviation from octahedral symmetry of the 6-atom cluster.

The final talk on the tight-binding method was given by R. Davies of Imperial College and was on "An Efficient Algorithm for the Calculation of Interatomic Forces in the Tight-Binding Model". The central theme of this talk was a pronounced inconsistency between the analytical forces and the numerical derivatives of the energy within the tight-binding model. This is due to incompleteness in the recursion basis employed in the tight-binding method, which gives rise to an effective force (the Pulary force). This effect was examined in hcp and fcc transition metal atomic clusters of various sizes. It was found that the convergence of the forces and structural energy differences with cluster size, was poor at zero temperature. The problem with the convergence could be dramatically reduced if the discontinuity at the Fermi surface was thermally smoothed with the aid of the Fermi-Dirac function. This reduced the long ranged Friedel oscillations that caused the convergence difficulties.

Dr M. C. Payne (Cambridge) discussed the total energy pseudopotential technique of Car and Parrinello. This method is formulated in the language of molecular dynamics. Dr. Payne addressed the question of the extent to which the electronic degrees of freedom should be regarded as classical degrees of freedom. He stressed that the electronic degrees of freedom are heavily damped. If the ion positions are not evolved then the method is just an iterative matrix diagonalisation. Dr. Payne then considered the case where the ion positions move. Moving the ions feeds energy into the electronic degrees of freedom which then evolve as the energy is damped. The electronic degrees of freedom have 10^4 times the energy of the ions, so they act as a heat bath. However, they will be continually out of equilibrium with the ions which suggests that the ion dynamics will not be correct. Dr. Payne then went on to show that the errors in the Hellman-Feynman forces are self-cancelling. This introduces a constant error in the dynamics of the ions.

Dr Jordan (Birmingham) then described some of the experimental work which was currently being undertaken to look for new areas of common interest with the work of CCP5 and CCP9. He described the angle-resolved photoemission technique and discussed recent advances in the density functional theory which provide a test of the theory.

Dr Jones (Exeter) described some applications of Local Density Functional methods to calculations on solids. He described methods of evaluating the Hartree and exchange-correlation energies and potentials in such systems and introduced an approximation which had an n^3 dependence rather than n^4. Dr. Jones has used the method to study 5:3 semiconductors with the diamond structure. He has worked with cluster sizes of 56, 86 and 110 atoms terminated with hydrogen; for the 56 atom cluster there are approximately 200 orbitals and 150 basis functions to consider. Dr. Jones described defects in gallium arsenide. The defects were substitutional silicon or beryllium with hydrogen in the lattice. The pure GaAs was simulated with bond lengths correct to within 2% and a band gap of 3.5 eV compared with the experimental value of 1.5. A Ga atom was then replaced by Si and the structure relaxed. H was inserted in two trial positions. When bound to just the Si, the Si As bond length increased from 2.38Å to 2.73Å. The donor level dropped to the top of the valence band. With the H in the bond centered configuration, the Si As bond length increased to 3.4Å. This configuration did not passivate the defect in the same way as the first. The energy of this configuration was higher than the other, suggesting the first configuration as the correct one. Further confirmation came from the prediction of the vibration frequencies of the defect which are known experimentally. Some further work was described on the Beryllium defect, where the bond centered configuration is energetically preferred.

J. den Ouden described some work on the simulation of zeolites. He reviewed the importance of these materials in industrial processes. Zeolites contain Si, Al and O together with exchangable cations. They need to be selective for the shape of molecules which may be reactants, products or a transition state. He has been looking at Ni^{2+} in the two zeolites mordenite and silicalite. These have been modelled by distributing the aluminium randomly and investigating the preferred positions of the Ni^{2+}. The lowest energy configurations are those where the Ni^{2+} is bound to two Al^{3+} which have exactly one framework Si ion between them.

D. Heyes (Royal Holloway and Bedford New College) described some simulation work using Brownian dynamics on the electrorheological effect. This is the effect on the flow rate and viscous forces due to an electric field and has applications to the manufacture of clutches and damping devices. He considered 125μ glass spheres in an insulating oil. When an electric field is applied between two plates immersed in this fluid the spheres tend to align in strings between the plates. The strings oppose motion of the fluid when a shear is applied. He simulated this using standard Brownian dynamics but with a dipolar term on the spheres to reproduce the effect of the electric field.

Dr. W. Mackrodt (ICI) described some simulations of High T_c Materials. The techniques used were lattice statics and lattice dynamics using two-body potentials derived from the electron gas method. The shell model was used to simulate the polarizability of the ions. He stressed that this type of modelling should focus on the materials aspects of these compounds rather than attempting to answer detailed questions about mechanism. Using these potentials the structure of La_2CuO_4 may be simulated to within 1%. The orthorhombic phase is more stable than the tetragonal with a calculated transition temperature of $250K$. Dr. Mackrodt then suggested some other materials which may be worth investigation: Nd_2CuO_4 has CuO planes but does not have the same structure as La_2CuO_4. On the other hand, calcium and strontium cuprates have just 1 dimensional chains. Dr. Mackrodt had also calculated the phonon density of states of a number of these materials. In many cases a 10 meV peak is seen in the density of states. However the material $La_2SrCu_2O_6$ is not a superconductor and lacks the 10 meV peak. He then continued to suggest the effect of changing the oxidation state of the copper. Materials intermediate between La_2CuO_4 and $LaCuO_3$ could be investigated. One such compound is $La_3Cu_2O_7$ which is predicted to have the 10meV absorption . Some work has also been done on surface properties of these materials and on electronic defects.

Professor Catlow (Keele) then described some powder diffraction work performed on samples under pressure using the synchrotron at Daresbury. The material studied was La_2CuO_4. He found a $4 - 5\%$ reduction in a, b and c when the pressure was increased to 150 kbar and no evidence of a phase change. The predicted change in cell volume from the band structure calculations agrees well with the experiment.

The first speaker on the final day was Dr W. Temmerman of Daresbury Laboratory, who spoke on the subject "Computational Methods and Electronic Structure calculations for High T_c Materials". He began by describing the principal method he and his collaborators have used in this study, which is the LMTO-ASA or "Linear Muffin-Tin Orbitals in the Atomic Sphere Approximation". In this method, the atoms in the crystal are described by spherically symmetric potential fields in which the radial Schrödinger equation is solved. Use is made of the local density approximation to account for the electron exchange and correlation. The method is a self-consistent-field (SCF) method, in which the electron density is iterated until the lowest electronic energy is found in accordance with the Variation Principle. An important aspect of these calculations is the evaluation of the integrals in the Brillouin zone, which was described in detail. To stabilise the convergence of the SCF cycle, care is taken to produce a reliable progression to the energy minimum. This in practice amounts to mixing the electron densities of the previous two cycles at each cycle. In a typical application of the method (La_2CuO_9), the unit cell contains 14 atoms, giving rise to matrices 154x154 in size. 15 iterations are required for convergence and 150 k-points are obtained. On the Cray XMP/48 about 5 hours of cpu time are required.

The method has been applied to a number of crystal structures relevant to the study of high T_c superconductors. The electronic energy of the La_2CuO_4 structure was obtained as a function of volume and found to agree very well with experiment. However the method failed to explain that the structure is an antiferromagnetic insulator. Some light was shed on this problem in a study of La_2NiO_4. This material became metallic or insulating according to the ratio of the axial and planar $Cu-O$ bondlengths in the nominally octahedral structure. The generally good description of the electronic and bonding properties in this case suggests that an antiferromagnetic state in La_2CuO_4 may lie close to the groundstate.

Dr. D. Nicholaides of the University of Bristol described current progress in a "Molecular Dynamics Study of a 2D Gauge Glass". This work is in progress on the AMT DAP, which is employed in simulation studies at Bristol. The model is an idealisation of conduction through a random arrangement of superconducting grains, where each grain is assumed to have four nearest neighbours (to map onto the DAP architecture). The density of electron "Cooper Pairs" on each grain is assumed to be the same and the grains interact via the Josephson effect. An important feature of "glassy" models is the phenomenon called "critical slowing down", which implies the existence of long-lived metastable states and hence a costly simulation. Dr Nicholaides described his approach to this problem with a dynamical analogy of a many-particle system. The treatment required the introduction of a "mass matrix", the off-diagonal elements of which are dependent on the interaction terms in the system and are scaled by a control parameter. As this control parameter is reduced to zero, the eigenvalues of the mass matrix become the conventional system masses and normal dynamics applies. At nonzero values the eigenvalues may be very different from the natural masses and consequently the dynamics is different. This property may be used to alter the equations of motion to speed up the dynamics in regions where critical slowing down occurs. The method is currently undergoing development.

Professor Cormack (New York State College of Ceramics) described some of the pitfalls in using static simulation methods to model new materials. He defined new materials as ones whose properties fulfill a technological requirement. They are usually less ionic and have more complex structures than those which have been studied traditionally. The main difficulty in simulating these materials is to decide how transferrable the potentials are. Often materials of interest are ternary oxides where the potentials need to be transferred from binary oxides. In this case the short-range part of the potential transfers well but the shell model parameters do not.

Professor Cormack then gave some examples. The materials $MAl_{12}O_{19}$ (M = Sr, ...) and $LnMAl_{11}O_{19}$ (M = Mg, Mn, ...) are of interest as hosts for laser ions, as substrates for ferroelectric devices and in radioactive waste disposal. Simulation work on these materials is at an early stage, but the relaxed structures agrees well with experiment. Work is in progress on the point defect properties which are technologically important. Another example was $Gd_2Zr_2O_7$, which has a fluorite superlattice. A simulation using transferred binary oxide potentials failed because the shells polarized excessively. The remedy is to ensure that the shell model parameters are consistent with both the binary and ternary oxides.

Drs. Kenway and Parker (Bath) described some calculations on the segregation of

Ca and Mg ions to the surface of Al_2O_3. Two surfaces have been considered: a basal surface terminated by cations which contracts on relaxation and a prism surface which has rumpled Al – –O – –Al planes. Some calculations were presented on the segregation energies of defects at these surfaces.

Vectorized molecular dynamics algorithms

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1 On vector computation

The vector supercomputer [1] represents a compromise between the computer designer's desire to achieve maximal computation rate (within specified cost constraints) and the user's demand for the fastest possible computations over a broad range of problems. While this compromise has proved to have considerable benefit to both parties in a great many kinds of computation in science and engineering, there is no shortage of situations where the performance potential of the supercomputer is far from realized. What distinguishes algorithms that are effectively mapped onto a vector computer is the manner in which data is accessed and the nature of the processing carried out. Peak gains are achieved when the data is retrieved sequentially from storage, when only certain combinations of the basic arithmetic operations (preferably excluding division) are carried out, and when the results are returned sequentially to storage. Any deviation from a general operational pattern of this kind results in sub-optimal performance. However, with the exception of certain kinds of matrix and vector computation which manage to follow this prescription precisely, this state of perfection is unattainable. The issue then is how to achieve the best performance given the preferred manner of operation of the hardware.

In addition to the requirement that the data be sequentially ordered for vector processing, the processor design imposes a fixed startup overhead associated with each vectorized operation; this overhead is independent of the number of data items processed in the course of the operation. An immediate consequence of this overhead is that, if the vectors are too short, the somewhat paradoxical situation where vector processing is actually slower than the corresponding set of scalar operations (on the same computer) can be achieved; this is certainly something to be avoided. The minimal vector length requirements vary, depending on both the type of operation and the machine itself. But it is clear that in addition to rearranging the data to oblige the processor, it will also be necessary to ensure that the resulting data are organized into vectors that are of adequate length to guarantee that the fixed overheads do not nullify the expected performance gains. There is no promise that this can be achieved in all cases; there are indeed calculations for which effective vectorization is not possible.

To help the user tailor the computations for the vector processor the machine instruction set generally features the capability for reorganizing data at a fairly rapid rate, one that tends to be intermediate between vector and scalar processing speeds. There are different approaches to data rearrangement and selection, and not all approaches are to be found on all machines. Even when a particular scheme for rearranging data is implemented, the question of how fast such operations are carried out in comparison with the peak (vector) computation speed is something which must be taken into account.

The two principal schemes for selecting and reordering data are known as gather-scatter and compress-expand. The act of gathering data involves the use of a vector of indices to access some or all of the elements of a set of data items – in no particular order as far as the computer is concerned – and store them sequentially in another vector; the scatter operation is the converse, in which the index vector is used to store a sequential set of data items in some alternative order in another (possibly longer) vector (where some elements might be left unmodified). Compression involves selecting an ordered subset of data items from a vector and storing them as adjacent elements in another vector; expansion is just the reverse of this operation. Because the order of the data is preserved under the compress/expand operations, information concerning which of the elements are to be compressed, or where the elements resulting from an expansion are to be placed, can be represented in terms of a bit vector (where the ones and zeroes represent, respectively, the elements that are or are not involved), an extremely compact alternative to the more general vector of indices utilized by gather/scatter. The fraction of the total elements needed in operations that require ordered subsets of elements can determine whether gathering or compression is the more effective operation – provided the computer offers a choice; not all machines do.

Even if the computer has the flexibility for dealing with data that are arranged in a less than optimal manner, there is the issue of whether the compiler that translates the high-level source language program into the actual machine instructions is capable of recognizing the kinds of operations needed. Judging by the achievements to date, compiler efficiency is an even more complex issue than hardware efficiency, and the performance of different compilers exhibits a wide variation in this respect. Even if the compiler is very perceptive and competent at mapping the program onto the hardware, there are situations in which certain language constructs (for example the case of an algebraic statement which implies a recursive dependence on something that has only just been computed, which might be unvectorizable because of the manner in which pipeline processing restricts dependencies between individual data items involved) may prevent the compiler from dealing effectively with that segment of the program; in such situations further information – expressed in the form of directives that lie outside the programming language – may help the compiler perform its task (this might include information indicating that even though a recursive dependency has been detected it can still be safely vectorized). The capacity for aiding the compiler in this way also varies from one brand of computer to another.

The alternative to total dependence on the capability of the compiler is to directly invoke the machine instructions. This can be done by programming in assembly language, but there may exist a preferable alternative which facilitates accessing machine instructions by subroutine calls from the higher-level language. The advantage of the latter approach is that it need only be resorted to when the compiler cannot deal with the problem, and it leaves the text of the program in more intelligible form; for most of the program the compiler should prove up to the task, and only certain critical sections may need to be handled in this way. This feature too is not necessarily provided on all computers.

2 Reformulating molecular dynamics algorithms

The subject of molecular dynamics simulation – the techniques and the applications – have been described elsewhere [2, 3]. Here we deal with the question of reorganizing the molecular dynamics calculation into a form suitable for efficient vector processing. The most difficult instance of algorithm conversion is the one that deals with the case of a very large fluid system with only short-range interactions between particles. The discussion of this case will be deferred until last; the vectorization in other cases is much more readily carried out. We note that it is the details of the interaction computations on which the discussion is focused; the actual integration of the coupled equations of motion, as well as other relatively minor – from the point of view of computational effort – aspects of the simulations (such as establishing the initial conditions, or modifying particle coordinates to satisfy periodic boundary conditions) present no significant problems since these parts of the simulation constitute a relatively minor portion of the calculation that is readily (normally in a completely automatic manner) vectorized.

For relatively small systems, typically up to a few hundred particles, the quickest method for a vector processor is generally the simplest one, namely to consider all pairs of particles, even if they lie beyond the interaction range. The interaction computation can easily be altered to return a zero value if the cutoff separation is exceeded. If the pairing is carried out in a suitable manner that ensures that interacting pairs are organized as vectors associated with the particles concerned in an equitable manner [4] (since the interactions between pairs of particles can be regarded as a triangular matrix, the simplest scheme of processing a row or column at a time is not the most efficient way to approach the problem) the data to be processed can be organized into vectors of adequate length to avoid serious problems with the fixed startup overheads. The additional computations required to evaluate interactions between particles lying outside the interaction range are, in this case, not of sufficient quantity that the alternative techniques described below would yield any improvement in performance.

If the molecules of the fluid are complex, in the sense that there are several interactions sites at fixed relative positions within the molecule, then the amount of computation required normally precludes consideration of systems larger than about a thousand particles. In order to vectorize such a computation it is again worth considering the possibility of treating all pairs of molecules in the system (and subsequently discarding those pairs separated by more than the cutoff range – where the separation now refers to the centers of mass), but this time the calculation is broken into several sections (at the conceptual level, although the implementation itself may involve treating all these sections in a uniform manner as parts of a single 'outer' loop) each of which deals with a distinct pair of interaction sites in all the molecule pairs; for each pair of site types the innermost loop of the program evaluates the contributions from just those site pairs for all molecules of the system. This is the opposite of the usual approach in which all site pairs belonging to a particular pair of molecules are treated together; it also requires additional storage to hold interim data for the coordinates of the interaction sites on all of the molecules as well as the forces acting at each of the sites, but the rearrangement of the order of the computational loops results in an algorithm which vectorizes with no difficulty.

The computations associated with two other types of system are also readily vectorized. If the interaction is long-ranged, all pairs of particles interact and there is little opportunity for any shortcuts; the necessarily heavy computation will be carried out in fully vectorized fashion. Ewald sums [5] or particle-in-cell methods [6] may be applicable. Simulation of solids also presents an ideal situation for vector processing. The fact that the interacting pairs remain the same throughout the computation means that there is little problem in rearranging the computations in an appropriate way; this might be done by ordering the processing of interacting pairs according to the direction and range by which they are offset in the lattice.

This leaves the problem of a fluid with short-range interactions, where 'short' is defined relative to the length of the region occupied by the fluid. On a scalar computer there are two techniques in use, preferably both together, which reduce the size-dependence of the computation from quadratic to linear. The first is based on the introduction of a fictitious space-filling array of cells to which the particles are assigned. There is then no difficulty in determining which particle pairs interact using an amount of computation proportional to system size. If the linear dimensions of the cell are chosen so that they exceed the interaction range then only particle pairs that lie in the same or in neighboring cells are possible interaction candidates. The second is the construction of a list containing those neighboring pairs of particles that actually interact [7]. Since the earlier subdivision into cells overestimates the number of potentially interacting pairs that must still be examined to determine if they really do interact, there is clearly something to be gained from this approach, although there is a substantial penalty to be paid in terms of storage requirements for the extra information generated. Since the rearrangement of particles in the fluid is a gradual process it may not necessary to update this list at every time step; the frequency of updates can be reduced if the list includes particle pairs whose separation exceeds the maximum range of interaction by a prescribed small amount – there is a tradeoff involved with the work needed for generating the neighbor list and the increased size of list if additional non-interacting pairs are included. By monitoring the maximum particle displacements at each time step it is possible to ensure that the neighbor list is recomputed as infrequently as possible, while at the same time guaranteeing that no interactions are missed.

This represents the most effective approach to dealing with this kind of problem on a scalar computer; the question is how to achieve a similar reduction in computational effort in a vector environment. Quite obviously one would not want to completely abandon the approach which leads to a linear rather than quadratic size dependence since there is no way the gains resulting from vectorization can compensate for this loss. But to achieve this dependence requires representing the information embodied in the cell subdivision, and possibly the neighbor list as well, in a form that can be handled in vectorized fashion. As will become apparent, the solution is basically a simple one, although the implementation can become somewhat awkward.

On a scalar computer, the information concerning which particles belong to which cells is stored in set of linked lists, one such list per cell. A linked list [8] is a way of structuring data that is not intended to be accessed sequentially; with each data item there is associated a pointer to the next data item (if any – otherwise the pointer is given a special 'null' value). Starting from the head of the list, which is merely a pointer associated with the cell itself, the contents of the cell can be determined by following the chain of pointers. The reason for using a linked list is the fact that no a priori limits are imposed on cell occupancy, as would be the case if a fixed amount of storage were reserved for each cell; the result is a considerable saving in storage – often as important a factor in software implementation as the speed of the computation. Unfortunately the linked list concept is totally incompatible with the vector approach and so must be sacrificed in the interest of overall performance, even if the storage requirements increase as a consequence. The question is the choice of an effective alternative.

The technique actually used – described in greater detail in [9] – requires that the identity of the cell occupied by each particle be determined as a first step. Then the data reorganization is carried out by placing the particle serial numbers in one of a set of 'layers'. There are enough such layers to accommodate the maximum possible cell occupancy, and each layer contains a single storage element for each cell. The first particle in a particular cell is assigned to the first layer (the order of particles within cells is of course arbitrary), the second particle in the cell – if present – to the second layer, and so on. Assigning a particle to a layer requires knowing how many particles in that cell have already been assigned. A simple scheme which scans the complete set of particles just once is obviously not vectorizable, since the number of layers that must be examined in order to assign each particle varies, depending on cell occupancy. The alternative, vectorizable scheme, involves filling the layers one at a time, even thought it implies scanning the entire set of particles several times. This technique is not as bad as it might seem however, because once a particle has been assigned to a layer it can be eliminated from the set of particles yet to be assigned. The processing involved in the construction of each such layer is fully vectorized, and all but the final layers corresponding to the tail of the cell-occupancy distribution provide sufficiently long vectors to yield effective vector-processing performance (assuming a large enough system).

Once a layer has been populated, the data it contains can be compacted if storage is at a premium. A particularly effective method for those machines which support the operations of compression and expansion is to pack the layer data in an ordered manner and use a bit vector to indicate which of the cells are actually occupied. When the data is later required by the interaction computations the layer contents can be re-expanded. A further extension of this idea, that plays an important role in the computations for extremely large systems (a hundred thousand particles or more), is that the region of space occupied by the system can be divided into a number of subregions, and only the particular portion of the layer associated with the part of the system actually being considered need be expanded. In the case of a subdivided system, additional effort is required to ensure that interacting particles located in distinct subregions of the system are dealt with properly, but the extra bookkeeping is not unmanageable and does not add significantly to the workload.

The interaction computations that follow the layer assignment involve the treatment of all pairs of occupied layers; for each pair of layers, the pairs of particles at locations in the layers corresponding to the cells for which interactions are possible are considered – but only if the cell locations in both layers are occupied by particles; a particular case that requires special attention is that of a layer paired with itself – each pair of particles appears twice and so only half the pairs should be treated. This calculation also vectorizes readily, although effort is wasted when sparsely occupied layers are paired; it is quite possible to have no interaction terms emerging from the processing of such layer pairs. Despite the wasted effort, this scheme is probably the most efficient on machines that support the compress/expand operations at the hardware level.

An alternative approach is to use the layers to construct neighbor lists. The neighbor lists produced in this manner will have the property that in the list segment corresponding to a given layer no particle can appear more than once. Thus the interaction computations can again be vectorized, and the additional saving is that the neighbor list construction, together with the prerequisite layer assignment, need not be carried out at every time step. There is a heavy storage penalty associated with neighbor lists, especially if the interaction range allows many interacting neighbors per particle; it is unlikely that the approach would be useful for the extremely large systems that are now being studied – an example of the sacrifice in speed to economize on storage.

More of the bookkeeping mentioned earlier is needed to take periodic boundaries into account, as well as to deal with the interactions if the subdivision technique is employed. In particular, the conditional tests associated with periodic boundaries when computing interactions (the interparticle forces wrap around the 'edges' of the system, so that particles at opposite ends interact if both are sufficiently close to their respective boundaries) can be avoided by replicating the particles near the boundaries; these dummy particles are used only for computing the interactions and are then discarded.

Since layer assignment requires significantly less work than the interaction computations themselves, the assignment can be carried out afresh at each time step; thus there is no need, for example, to monitor particle displacements (as was done when using neighbor lists) to avoid the possibility that cell occupancies may no longer be correct. Finally, another shortcut that can be used if an efficient gather operation is available is to employ tabulated interactions and to perform a table lookup (possibly supplemented by interpolation) rather than evaluate the interactions from scratch; again the decision as to which technique is preferable depends on the machine.

3 Summary

It should be clear from the foregoing that there is no single technique that can be used for implementing all molecular dynamics simulations on all vector supercomputers. There are a broad variety of problem types, and an almost equally broad range of supercomputer architectures. By way of an exercise the reader should examine both the similarities and differences between well-known kinds of machine, typically the Cray X-MP and the ETA-10 (which in most respects is equivalent to the Cyber 205). A particular kind of computation which runs efficiently on one brand, or even model, of machine may not perform as well on another. The storage requirements can also differ significantly between machines, and there is often a need to determine an optimum balance between speed and memory needs. This is not the place to go into further details of the techniques which have appeared in print elsewhere (ref. [9], and to be published); suffice it to say that the methods have made possible production type simulations of 200,000 particle systems over a similar number of time steps, and are capable of dealing with even larger systems as suitable computers become available (tests on systems containing as many as 500,000 particles have been carried out). Such enormous (by usual standards) systems appear to be necessary for the study of classes of hydrodynamic instability at the microscopic level [10], and could well turn out to be necessary in other contexts as well.

Acknowledgements

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Preliminary Results of Molecular Dynamics Simulations of Yttria Doped Ceria

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Abstract

Preliminary results of molecular dynamics (MD) simulations of the super-ionic system $(CeO_2)_{1-x}(YO_{1.5})_x$ are reported. Analysis of diffusion in the O^{2-} sub-lattice, as determined from study of the mean square displacement as a function of the time, suggest that the magnitude of diffusion is strongly dependent on the dopant configuration.

Introduction

Studies of fluorite oxides doped with yttria and rare earth oxides show the conductivity to depend markedly on the concentration of dopant [1,2]. The most characteristic feature is the conductivity maximum, which, in the case of yttria doped ceria, occurs at approximately 5-8% dopant. This maximum has been found to be closely related to the activation enthalpy which goes through a minimum at approximately the same concentration [1,2].

Studies by Murray [3] and Murray, Murch and Catlow [4] using the combined HADES Monte-Carlo technique have been quite successful in reproducing this conductivity maximum. Among the more interesting results was the observation that a fully ordered Y^{3+} distribution (at 14.28 mole %) yielded a conductivity 1.5 orders of magnitude lower than that for a random distribution [3]. However, this approach takes no explicit account of kinetic effects which one would expect to be important in a superionic conductor. Accordingly, MD calculations were performed in order to take a direct look at diffusion in doped CeO_2.

Table 1: Comparison of calculated and experimental properties H_σ is the effective Arrhenius enthalpy. H_m is the activation enthalpy to free O^{2-} migration. H_A is the effective association enthalpy.

	Shell Model [3]	Rigid-Ion Model	Experiment
H_m	0.49 eV	0.55 eV	(0.49 [7] - 0.61 [1] eV)
H_A	0.53 eV	0.46 eV	—
H_σ	1.02 eV	1.01 eV	1.04 eV
Static dielectric constant	20.6	8.4	—

Short-range potentials

In their simulations Murray et al. [3,4] used Buckingham potentials, coupled with the shell model for ionic polarizability. Their potentials were based on electron-gas calculations. However, the restriction of MD to the rigid-ion approximation results in migration energies which are too high. The following adjustments were therefore made:

1. The $Ce^{4+} - O^{2-}$ short-range (rigid-ion) potential was adjusted to give correct migration energies, as calculated using the HADES code [5]. It was not possible to simultaneously fit both the static dielectric constant and the barrier to migration.
2. The potential was also fitted to the 0 K lattice constant of 0.5397 nm. The latter was determined by extrapolation of thermal expansivity data [6].
3. The rigid-ion model also results in too large a binding energy for a dopant-vacancy nn cluster. Accordingly, the hardness parameter in the $Y^{3+} - O^{2-}$ potential was adjusted from its electron-gas value to yield a nn binding energy of 0.46 eV (Table 1).

In other respects the short-range potentials used are the same as those used by Murray et al. [3,4]. Experimental and calculated properties are compared in Table 1. It can be seen that the rigid- ion potentials appear to predict reliable values for those features which one expects to dominate the diffusion of oxygen vacancies.

Simulation Conditions

The simulation conditions are detailed below:

1. The simulation box consisted of a 4x4x4 cubic arrangement of Ce_4O_8 cells yielding a total of 768 atoms in the undoped lattice.
2. The initial configuration assumed the perfect fluorite structure. The HADES / Monte-Carlo technique found that an ordered distribution of yttrium resulted in a lowering of the conductivity by 1.5 orders of magnitude [3]. Accordingly, Y^{3+} and O^{2-} vacancies were positioned randomly.
3. A target temperature of 833 K was employed in order to facilitate direct comparison with the work of Murray, Murch and Catlow [3,4].

4. A lattice constant of 0.5443 nm at 833 K was calculated from thermal expansivity data [6]. The lattice constant was assumed to be independent of dopant concentration.
5. Constant volume conditions were used.
6. A time step of $\Delta t = 2 \cdot 10^{-15}$ seconds was employed.
7. The simulation ran for a total of 3000 time steps (6 ps) of which 800 were for thermal equilibration. This would normally be considered quite short for an MD simulation. However, it is statistically equivalent to a 48 ps run with a 2x2x2 cubic box containing 8 Ce_4O_8 cells. Moreover, in this preliminary investigation of CeO_2, we are interested only in the qualitative/semi-quantitative behaviour of diffusion in the O^{2-} sublattice. Diffusion, as determined from the time dependence of the mean square displacement (MSD), is normally determined adequately in about 2 ps. Analysis of the diffusion over the final 2000 time steps (4 ps) should, therefore, be sufficient for the purposes of this study.

Results

Simulation runs were performed at a variety of dopant concentrations two or more times. Each run at a given concentration corresponds to a different random distribution of dopants and vacancies. The calculated oxygen diffusion is detailed in Table 2. In the HADES/Monte-Carlo calculations [3,4] a simulation box of 8x8x8 (512) Ce_4O_8 cells was employed. The MD simulations were restricted to a 4x4x4 box for reasons of expense. In the light of evidence that an ordered distribution of dopants can dramatically lower the conductivity [3] we were a little concerned about the effect of the periodic boundary conditions. Averaging over time origins was not performed as this might serve to hide such effects. Instead, diffusion was calculated by a least squares fitting of MSD time dependence.

The magnitude of the diffusion is what one would expect for a superionic conductor of this sort. The calculated diffusion is surprisingly sensitive to the initial distribution of vacancies and dopants. Moreover, there appears to be an upper limit to diffusion at any given concentration. This limit is approximately linear in the mole % dopant (* in Table 2).

Diffusion continues to rise with increasing dopant concentration. Clearly, therefore, the simulation is failing to model some feature of the system which would increase the migration enthalpy. One such feature is the contraction of lattice with increasing mole % dopant. Unfortunately, data for the high-temperature lattice constant dependence on mole % dopant was not available to us. Consequently, we assumed the same % contraction as at 298 K for 20% dopant [8]. Deviations from Vegard's rule were ignored and the lattice constant was determined from the 0% and 20% dopant values by interpolation or extrapolation as appropriate.

Calculations were repeated using the modified lattice constants. This resulted in some improvement, namely a maximum in the conductivity; however, it is too shallow and occurs at too high a concentration of dopant. The diffusion data remain strongly sensitive to the configuration of dopants and vacancies.

Moreover, in both sets of simulations it was found that the O^{2-} diffusion for a given dopant configuration sometimes varied significantly with time. That is, it was

Table 2: Oxygen diffusion as a function of the dopant concentration

%dopant	Diffusion 10^5 cm^2 sec^{-1}			
	run 1	run 2	run 3	run 4
0.78	0.0190*	0.0163	0.0032	0.0000
2.34	0.1419	0.1492*	———	———
3.91	0.4215*	0.2257	———	———
6.25	0.2479	0.2526*	———	———
7.81	0.3743*	0.0202	———	———
10.16	0.4692	0.0627	0.1406	0.8718*
15.63	0.3131	0.7351*	0.6777	———
23.44	1.4122*	0.2126	0.4052	0.1288
31.25	0.2164	1.2429	1.5639*	0.2169

observed that diffusion, proceeding with a particular value of D, might suddenly adopt a different D value, or indeed stop altogether (D = 0). This phenomenon might be related to trapping of vacancies. The observation that vacancy migration occasionally stops altogether may indicate correlated vacancy motion.

Discussion

The results of these preliminary simulations are in poorer agreement with experiment that might have been expected. Clearly, the diffusion process is more complicated that at first envisaged. A number of possible explanations may be advanced:

1. The short-range potentials were fitted to the energy barrier to vacancy migration and to the an dopant-vacancy binding energy. There may be more complicated structures of clusters which are not correctly modelled by this potential.
2. In this type of MD we are limited to approximately 1000 atoms. In this simulation we had 768 atoms in the undoped system - 256 Ce^{4+} and 512 O^{2-}'s. The conductivity maximum occurs at roughly 6% dopant. For 6.25 mole % dopant we have only 16 Y^{3+} dopant ions and 8 O^{2-} vacancies. This is hardly a representative selection of Y^{3+} and O^{2-} vacancy environments. This analysis suggests that either bigger simulation boxes are employed or that averages of many simulations for every concentration are taken.
3. A third possibility is that of artificial ordering due to the periodic boundary condition. Murray [3] found using the HADES/Monte-Carlo model that diffusion differs dramatically between ordered and random distributions of dopants. The Y^{3+} were distributed randomly within the simulation box. However the periodic boundary condition might result in a migrating O^{2-} vacancy experiencing a pseudo-ordered environment. This consideration also points towards the use of a larger simulation box.

We are currently pursuing these calculations with a view to determining the approximation(s) responsible for the unusual diffusion data.

Conclusions

1. Yttria doped ceria yields diffusion with sensible values.
2. Results are sensitive to dopant configuration.
3. Poor statistics for dopant ions and vacancies suggest (i) the use of much larger simulation boxes or (ii) averaged results of numerous independent simulations for each concentration
4. The periodic boundary condition may result in artificial ordering, indicating again the use of a larger simulation box.

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The Minimum Image Convention in Non-Cubic MD Cells

W. Smith

March 29,1989

Introduction

In molecular dynamics simulations of liquids the most common (but not the only [1, 2]) periodic boundary conditions employed are those of the simple cube. However in simulations of crystalline ionic systems, these periodic boundary conditions are not generally suitable and an alternative is required which matches the natural periodicity of the crystal. The most obvious choice under these circumstances is a parallelepiped MD cell, which may be defined simply as a multiple of the unit cell for the crystal lattice (Figure 1). Thus if the unit cell has vectors $\underline{a}$, $\underline{b}$ and $\underline{c}$, the MD cell is defined analogously by vectors $\underline{A}=l\cdot\underline{a}$, $\underline{B}=m\cdot\underline{b}$ and $\underline{C}=n\cdot\underline{c}$ respectively (l,m and n being integers). The volume of the MD cell is then $l\cdot m\cdot n$ times the unit cell volume. The advantages of this approach, particularly when constructing the initial lattice or analysing the simulated structural properties, are obvious.

Two questions that immediately arise from this are: (a) how does one go about formulating such a scheme? and (b) is it an efficient way to proceed? The purpose of this note is to discuss some aspects of these questions.

Formulating the Scheme

Since the problem arises most commonly in simulations of crystalline systems, it is natural to resort to the methods of crystallographers. In crystallography, the crystal structure is defined by the unit cell vectors $\underline{a}$, $\underline{b}$ and $\underline{c}$ and the so-called fractional coordinates $\underline{s}_i$ of the ions within the unit cell [3]. The components s_{xi}, s_{yi} and s_{zi}, of the vectors $\underline{s}_i$ range in value from 0 to 1, hence their name. The positions $\underline{r}_i$ of the ions in the crystal are given by:

$$\underline{r}_i = s_{xi}\underline{a} + s_{yi}\underline{b} + s_{zi}\underline{c}$$

or in matrix notation:

$$\underline{r}_i = \underline{\underline{h}}\,\underline{s}_i$$

Where the columns of the matrix $\underline{\underline{h}}$ are composed of the vectors $\underline{a}$, $\underline{b}$ and $\underline{c}$. It therefore appears that we have two ways of defining the location of an ion in the cell: the location in *real* space defined by $\underline{r}_i$ and the location in *dimensionless* space defined by $\underline{s}_i$. It turns out that we need to use both of these coodinate systems to formulate a periodic boundary condition for MD simulations. In what follows, to reduce verbiage, I refer to $\underline{r}_i$ as vectors in R space and $\underline{s}_i$ as vectors in S space.

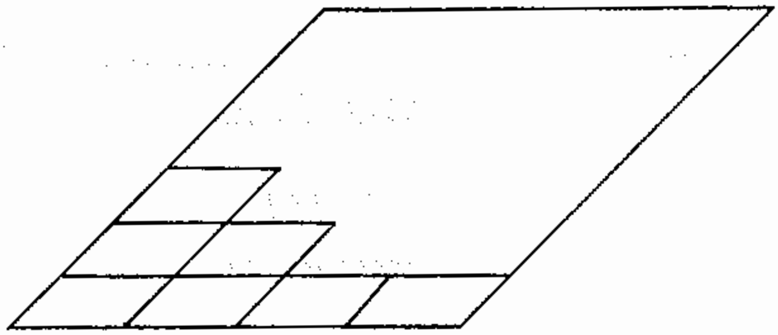

Figure 1

The relationship between the unit cell and the MD cell (in 2D).

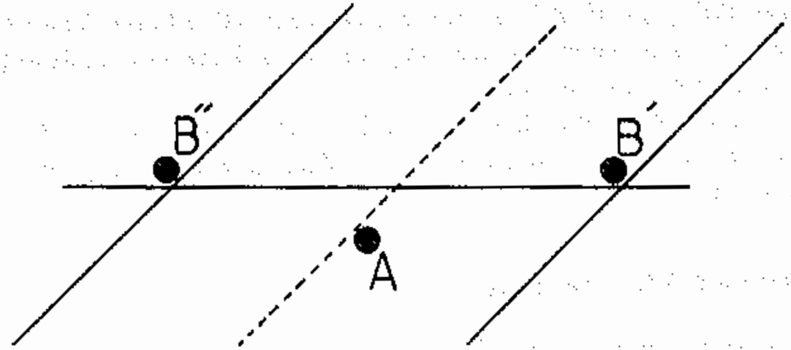

Figure 2

A problematic arrangement of ions in the proposed periodic boundary scheme (a 2D analogy). Ion A is near the centre line of the cell. The scheme will select the image B' in preference to B", which is actually the nearer of the two images. The use of an appropriate spherical cutoff removes this difficulty (see text).

In this formulation we therefore think of the MD cell as being a kind of "unit cell" defined by the vectors $\underline{A}$, $\underline{B}$ and $\underline{C}$ described above. The locations of the ions within the cells are therefore defined in matrix notation by:

$$\underline{r}_i = \underline{\underline{H}}\, \underline{s}_i$$

Where matrix $\underline{\underline{H}}$ is composed of the vectors $\underline{A}$, $\underline{B}$ and $\underline{C}$ analogous to the unit cell case. We may perform the simulation in either R or S space, though if we use the latter we will have to use the Lagrangian formulation of mechanics in place of the more common Newtonian [4]. Despite this apparent additional complexity I have found this option advantageous in dealing with ionic systems, since then the Ewald sum is more easily dealt with [5]. However to avoid a lengthy digression I will assume that we are to work in S space, but note that the alternative is equally acceptable. I will use the relationship between the $\underline{r}_i$ and $\underline{s}_i$ coordinates to refer back to the *real* world where necessary.

It is a characteristic of S space coordinates that the location of the periodic images in the infinite crystal of an ion labeled i is accomplished by the simple addition of an integer to each of the components of $\underline{s}_i$. If we are concerned only to find those image ions in the immediately adjacent cells, they can all be found by adding or subtracting unity. This is all we need to know to formulate the periodic boundary scheme in the MD simulation!.

In MD the periodic boundary is employed in two circumstances. Firstly, it is used to relocate ions, that have moved out of the MD cell in the course of the simulation, back into the cell at its image point, to maintain the total number of ions in the cell. Secondly, for a given ion, it is used to find the nearest image of each other ion in the MD cell, in order to calculate the pair forces and energies.

The first case is easy to describe and, if we are working in S space, easy to apply; we simply replace each $\underline{s}_i$ by its corrected vector $\underline{s}_i^c$:

$$\underline{s}_i^c = \underline{s}_i - INT(2\underline{s}_i - \underline{1})$$

Where $\underline{1}$ is a vector with unit components. (Note that the MD cell has faces at $s_x = 0$ and $s_x = 1$ in this case, and not at $s_x = -1$ and $s_x = +1$ as is commonly used in MD. The same comment applies in the y and z directions also.) The second case is more complicated, because we do not wish merely to locate an image ion, but we must be sure it is the *nearest* image and this necessitates working in both S and R spaces. To be specific, we have an ion pair labelled i and j and we wish to calculate their separation in both S and R spaces (i.e. $\underline{s}_{ij}$ and $\underline{r}_{ij}$), such that the $\underline{r}_{ij}$ *is the smallest possible.* It turns out to be simpler than may be anticipated. Working in S space we calculate

$$\underline{s}_{ij} = (\underline{s}_i - \underline{s}_j) - INT(2(\underline{s}_i - \underline{s}_j) - \underline{1})$$

Which is essentially the same as the above equation for relocating wayward ions. Our next step is even simpler:

$$\underline{r}_{ij} = \underline{\underline{H}}\, \underline{s}_{ij}$$

Where $\underline{\underline{H}}$ is the matrix defining the MD cell. This is all we need!

An argument I have heard opposing this scheme is that it may not pick out the correct nearest image for ions separated by distances close to half the width of the MD cell. That such a suggestion is made is understandable when one realises that the selection of the nearest image is made in S space, where the anisotropy of the real MD cell has been removed. (The kind of circumstances where problems are most easily seen are shown in Figure 2.) However, the procedure is safe if one is using a spherical cutoff in R space, the radius of which *is not greater than half the smallest perpendicular width of the MD cell.* In mathematical terms: If we define the perpendicular widths of the cell as:

$$W_A = |\underline{A} \bullet \underline{B} \times \underline{C}|/|\underline{B} \times \underline{C}|$$

$$W_B = |\underline{B} \bullet \underline{C} \times \underline{A}|/|\underline{C} \times \underline{A}|$$

$$W_C = |\underline{C} \bullet \underline{A} \times \underline{B}|/|\underline{A} \times \underline{B}|$$

(This is, of course, merely the shortest distance between opposing faces of the MD cell). Then the condition for non-violation of the minimum image convention is:

$$R_c < 0.5 * MIN(W_A, W_B, W_C)$$

The proof of this simple. In the appendix I show that an ion at the centre of a sphere of radius R_c defined as above, can only interact with one of the images of the other ions in the MD cell and that this image must necessarily be the nearest.

Efficiency

The algorithm described above has the merit of simplicity, but something should be said about its efficiency. The main point I should raise is that the requirement of a spherical cutoff to guarantee the minimum image can result in lower efficency than for simple cubic boundary conditions. There is not only the matter of the additional computation associated with the matrix operations described above and which may or may not matter much if the forces being calculated are relatively expensive. There is also the fact that volume of the sphere enscribed by the cutoff *at best* can only contain approximately half the ions that the cell contains. Therefore if one choses to use a parallelepiped MD cell that is far removed from a cube, one should recall that much effort will go into calculating the distance between ions which subsequently will be deemed to be non-inteacting. In such circumstances the use of a 'Neighbour List' method [6] may be essential. Alternatively, one could consider an alternative unit cell for the system, which is more like a cube. Fortunately this is often easier than it sounds.

Readers who have their own methods for dealing with the problem outlined in this note are invited to contribute their solutions!

Acknowledgments

I am indebted to B. Vessal and M. Leslie for raising the questions this note discusses. D. Fincham is thanked for reading the draft. All mistakes remaining are mine alone.

Appendix

Proof of Validity of Minimum Image

The proof given here is not rigorous in the mathematical sense, but I hope the argument is sufficiently clear to warrant its acceptance. Basically, it goes as follows:

1. Each ion has a fractional coordinate $\underline{s}_i$ in S space that is related to its coordinate in R space by the relation:

   $$\underline{r}_i = \underline{\underline{H}}\,\underline{s}_i$$

   where $\underline{\underline{H}}$ is the matrix defining the MD cell.
2. Since the system is infinitely periodic the location of the cell origin is immaterial. Suppose we chose the origin to be at the location of one of the ions. I call this the shifted cell, to distinguish it from the original cell.
3. The shifted cell will, by definition, contain *unique* images of all the ions. i.e. within this cell no two ions will be periodic images of each other. The shifting procedure is best carried out in S space, using the integer arithmetic described above.
4. Even though the shift of the cell origin is performed in S space, the same ion will be at the origin of the corresponding cell in R space. Furthermore, there will be a one-to-one correspondence between all the ions in the S space cell and those in the R space cell. Hence the ions in the R space cell also form a unique set - none is the periodic image of another in the same cell.
5. A sphere drawn in R space around the central ion of radius less than the minimum width of the cell *cannot include ions that are periodic images of each other.* This must follow because the sphere is contained within the cell and the cell has no internal periodic images.
6. *Therefore all pair interactions between the central ion and the other ions within the same sphere are unique and necessarily represent the nearest image interactions of the central ion.*
7. Clearly, we may now consider any other ion as being at the centre of the cell and repeat the argument. This proves that all the interactions calculated in this scheme satisfy the minimum image convention.

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Minimum Image Calculations on IBM-3090 VF

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Keeping the computing requirements of minimum image calculations low can be important in order to keep the overall CPU requirements of molecular dynamics and Monte Carlo simulations low. In this regard, the review paper of Fincham and Heyes (Adv. Chem. Phys., 63, 493, (1985)) discusses some of the minimum image methods applicable to different vector processing computers. In the past (Comp. Phys. Comm., 48, 197, (1988)), we have tested one of these methods (developed by Fincham and Ralston),

$$\underline{t} = \underline{t}(i) - \underline{t}(j)$$

$$\underline{r} = (L/2.) * (\underline{t} - 2. * INT(\underline{t}))$$

on an IBM-3090 E series computer with vector facility using the IBM VS-FORTRAN 2 vectorizing compiler. Here $\underline{t}$ represents coordinates of molecular centers in the (-1,1) system, L is the side length of the cubic box, and $\underline{r}$ is the distance between the centers of molecules i and j. This method was shown to work quite well with vectorization.

Recently, it was suggested to us by the IBM Kingston (New York) specialists to use the AINT function instead of the INT function in the above calculations. Our test Monte Carlo simulations of 108 LJ sphere systems show further savings of nearly 8% using the VS-FORTRAN 2 compiler on IBM-3090 with VF after switching on the vectorization option (savings were not observed during the scalar-only runs) when the AINT function was used. We believe that such savings can also be obtained in molecular dynamics simulations.

We are grateful to the staff of IBM Kingston Laboratory for their suggestions. We point out that this discussion is limited only to the use of the particular software and hardware discussed here.

Yet Another Gaussian Quadrature Generator

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1. Introduction

There seems to be an ongoing interest in the development of computational procedures for the generation of abscissas and weights for Gaussian integration rules as is illustrated by a number of programs published recently in the Computer Physics Communications Program Library [1-3]. For special integration schemes very fast methods have been devised (see [3]).

Here, an algorithm is presented that is based on the three-term recurrence relation for orthogonal polynomials and that is similar to one previously used in moment theory (for a review see [4]). Its advantages are that it applies to any Gaussian quadrature rule, that it is very easy to implement, that the burden of numerical computation may be transferred to existing optimized software, and that it is very stable also for a large number of quadrature points, while it is still reasonably fast.

In a quadrature a definite integral over a function $f(x)$ is approximated by an appropriate summation

$$\int_{x_l}^{x_u} f(x)w(x)dx = \sum_{i=1}^{n} w_i f(x_i)$$

where x_l and x_u are the lower and upper limits of the integration interval, $w(x)$ is a nonnegative weight function, the x_i are the abscissas and the w_i the weights of the quadrature rule associated with x_l, x_u and $w(x)$. In the Gaussian quadrature scheme, see e.g. [5], which is the most accurate for a given number of quadrature points n the abscissas are taken to be the roots of the orthogonal polynomial $P_n(x)$ of degree n and the weights may be calculated from

$$w_i = \left[\sum_{m=0}^{n-1} \frac{P_m^2(x_i)}{N_m}\right]^{-1}$$

the $P_m(x)$ satisfying the orthogonality relation

$$\int_{x_l}^{x_u} P_n(x)P_m(x)w(x)dx = N_m\delta_{mn}$$

Given the x_i the w_i may therefore be calculated rapidly. The main computational problem is to determine the x_i.

2. A general algorithm for abscissas and weights

Let each orthogonal polynomial $P_n(x)$ be normalized in such a way that the coefficient of the highest power x^n is $(-1)^n$. For any such set of orthogonal polynomials the following recurrence relation holds [6]

$$P_n(x) = (a_n - x)P_{n-1}(x) - b_{n-1}P_{n-2}(x)$$

with the special cases

$$P_0(x) = 1$$

$$P_1(x) = -x + a_1$$

The recurrence coefficients a_n and b_{n-1} are given by

$$a_n = \frac{\int_{x_l}^{x_u} xP_{n-1}^2(x)w(x)dx}{\int_{x_l}^{x_u} P_{n-1}^2(x)w(x)dx}$$

$$b_{n-1} = \frac{\int_{x_l}^{x_u} P_{n-1}^2(x)w(x)dx}{\int_{x_l}^{x_u} P_{n-2}^2(x)w(x)dx} = \frac{N_{n-1}}{N_{n-2}}$$

A set of orthonormal polynomials $\{Q_n(x)\}$

$$\int_{x_l}^{x_u} Q_n(x)Q_m(x)w(x)dx = \delta_{mn}$$

is related to $\{P_n(x)\}$ by

$$P_n(x) = N_n^{1/2}Q_n(x)$$

Inserting the $\{Q_n(x)\}$ into the recurrence relation yields after rearrangement

$$xQ_{n-1}(x) = -\sqrt{b_n}Q_n(x) + a_nQ_{n-1}(x) - \sqrt{b_{n-1}}Q_{n-2}(x)$$

with the special case

$$xQ_0(x) = -\sqrt{b_1}Q_1(x) + a_1Q_0(x)$$

The recurrence relations for all polynomials up to degree n may be summarized in a matrix equation

$$\begin{pmatrix} a_1 & -\sqrt{b_1} & & & & \\ -\sqrt{b_1} & a_2 & -\sqrt{b_2} & & & \\ & -\sqrt{b_2} & a_3 & -\sqrt{b_3} & & \\ & & \ddots & \ddots & \ddots & \\ & & & -\sqrt{b_{n-2}} & a_{n-1} & -\sqrt{b_{n-1}} \\ & & & & -\sqrt{b_{n-1}} & a_n \end{pmatrix} \begin{pmatrix} Q_0(x) \\ Q_1(x) \\ Q_2(x) \\ \vdots \\ Q_{n-2}(x) \\ Q_{n-1}(x) \end{pmatrix}$$

$$= x \begin{pmatrix} Q_0(x) \\ Q_1(x) \\ Q_2(x) \\ \vdots \\ Q_{n-2}(x) \\ Q_{n-1}(x) \end{pmatrix} - \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ -\sqrt{b_n} Q_n(x) \end{pmatrix}$$

For x_i being a root of $Q_n(x)$ and hence a root of $P_n(x)$ the last vector vanishes completely and the equation becomes an eigenvalue equation

$$\begin{pmatrix} a_1 & -\sqrt{b_1} & & & & \\ -\sqrt{b_1} & a_2 & -\sqrt{b_2} & & & \\ & -\sqrt{b_2} & a_3 & -\sqrt{b_3} & & \\ & & \ddots & \ddots & \ddots & \\ & & & -\sqrt{b_{n-2}} & a_{n-1} & -\sqrt{b_{n-1}} \\ & & & & -\sqrt{b_{n-1}} & a_n \end{pmatrix} \begin{pmatrix} Q_0(x_i) \\ Q_1(x_i) \\ Q_2(x_i) \\ \vdots \\ Q_{n-2}(x_i) \\ Q_{n-1}(x_i) \end{pmatrix} = x_i \begin{pmatrix} Q_0(x_i) \\ Q_1(x_i) \\ Q_2(x_i) \\ \vdots \\ Q_{n-2}(x_i) \\ Q_{n-1}(x_i) \end{pmatrix}$$

The quadrature abscissas x_i may thus be obtained as the eigenvalues of the real symmetric tridiagonal matrix formed by the recurrence coefficients. Computationally, this diagonalization is the most time-consuming part of the calculation, but it can be performed stably, reliably and efficiently by standard subroutines [7].

Numerical diagonalization procedures usually yield eigenvectors $\mathbf{u}_i$ of unit length so that the quadrature weights can not be extracted from them directly. However, for the weights the following equations hold

$$1 = w_i \sum_{m=0}^{n-1} Q_m^2(x_i) = \mathbf{u}_i \cdot \mathbf{u}_i$$

A sufficient condition for the second equation to hold is

$$w_i Q_m^2(x_i) = u_{mi}^2$$

Table 1. Recurrence coefficients for commonly used Gaussian quadrature rules.

Name	x_l, x_u	$w(x)$	a_n	b_n	N_0
Gauss-Legendre	$-1, 1$	1	0	$\frac{n^2}{(2n+1)(2n-1)}$	2
Gauss-Laguerre	$0, \infty$	$\exp(-x)$	$2n - 1$	n^2	1
generalized Gauss-Laguerre	$0, \infty$	$x^k \exp(-x)$	$2n + k - 1$	$n(n + k)$	$k!$
Gauss-Hermite	$-\infty, \infty$	$\exp(-x^2)$	0	$\frac{n}{2}$	$\sqrt{\pi}$
Gauss-Chebyshev	$-1, 1$	$(1 - x^2)^{-1/2}$	0	$\frac{1}{4}$	π

for every $m = 0, 1, \ldots, n-1$ (let the elements of $\mathbf{u}_i$ also be numbered from 0 to $n - 1$), and particularly

$$w_i Q_0^2(x_i) = u_{0i}^2$$

or

$$w_i = N_0 u_{0i}^2$$

which is the desired expression for the quadrature weights.

3. Special cases

The algorithm outlined in section 2 for finding the x_i and w_i holds for any set of orthogonal polynomials. For a given Gaussian quadrature rule the corresponding orthogonal polynomials have to be transformed from their standard normalization to a normalization so that the coefficient of the highest power in x is 1 and -1 for even and odd degree, respectively, and the a_n and b_n that appear in the recurrence relation have to be determined. For the common Gaussian quadrature rules analytical formulas for the recurrence coefficients may be derived.

The Gauss-Hermite quadrature may serve as an example. The Hermite polynomials $H_n(x)$ in their standard normalization [8]

$$\int_{-\infty}^{+\infty} H_n^2(x) \exp(-x^2) dx = 2^n n! \sqrt{\pi}$$

satisfy the following three-term recurrence

$$H_n(x) = 2xH_{n-1}(x) - 2(n-1)H_{n-2}(x)$$

The renormalized polynomials $P_n(x)$ are linked to the standard Hermite polynomials by $H_n(x) = (-2)^n P_n(x)$ and the recurrence relation becomes

$$P_n(x) = -xP_{n-1}(x) - \frac{n-1}{2}P_{n-2}(x)$$

which yields

$$a_n = 0 \qquad b_n = \frac{n}{2}$$

Note that in general the a_n are zero if $-x_l = x_u$ and $w(x)$ is an even function.

The recurrence coefficients for other Gaussian integration schemes may be derived in a similar fashion. For a few of the most commonly used quadratures they are listed in table 1.

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Book Reviews

W. Smith

April 4, 1989

Here for the first time in the CCP5 newsletter we publish some reviews of books relevant to the science of molecular simulation. We would welcome other independent reviews from our readers.

An Introduction to Computer Simulation Methods: Applications to Physical Systems, by H. Gould and J. Tobochnik

This book comes in two volumes and represents a valuable addition to the pedagogy of computational science. The authors clearly recognise that simulation is a coherent branch of science in its own right and augments scientific progress rather than merely appends to it. Together the two volumes comprise a structured introduction to the science of computer simulation, which would take an undergraduate student from the modelling of simple systems to applying fundamental techniques to real projects close to the frontiers of research. The book is stimulating and informative and is sufficiently well thought out that it is possible for a student with access to a microcomputer to learn a great deal unsupervised. If coupled with an imaginative undergraduate course, one could envisage an enthusiastic student making very impressive progress.

Part one of the book starts with simple models, such as Newton's law of cooling and vertical motion and progresses to more difficult subjects such as planetary motion, molecular dynamics, chaos and wave motion. From the beginning the book is at pains to draw out the physics of the problems, while maintaining good computational practice. The treatment is not overtly mathematical and the numerical equations are dealt with clearly and concisely. The simple beginnings should not be scoffed at; a complete novice can begin with this book and learn facts that more experienced simulators may have overlooked. Even for the "old hands" at the subject, some of the problems would be greatly entertaining.

Part two is more demanding. The book launches into numerical integration (Monte Carlo), random walks, percolation and fractals, cellular automata, the microcanonical and canonical ensembles and concludes with the simulation of quantum systems. It must be said that none of these topics is treated in profound depth, but this is not the objective. The authors intention is to provide insight into the subjects through the direct application of the basic principles. It is a far remove from labouring over mathematical texts and is more akin to learning about science through experiment. There is much to be said for this approach, provided one doesn't fall into the trap of computing instead of thinking. It is perhaps the most important aspect of this book that the reader is encouraged to think about the subject and design appropriate computational experiments. The objective always is to learn about science, not to generate numbers. It is to be hoped that this book, and others like it, will become commonplace.

An Introduction to Computer Simulation Methods: Applications to Physical Systems (Parts 1 and 2), by H. Gould and J. Tobochnik, published by Addison-Wesley 1988.

Simulation of Liquids and Solids: Molecular Dynamics and Monte Carlo Methods in Statistical Mechanics. Edited by G. Ciccotti, D. Frenkel and I.R. McDonald

This useful volume consists of a collection of seminal papers in the development of molecular simulation, with corrections and additional footnotes provided by the editors. Altogether it is a valuable reference for anyone active in the ever-broadening subject and particularly for postgraduates newly embarking on a research career. Several of the early founding papers are present, including papers by Metropolis *et al*, Alder and Wainwright, Rahman, Verlet etc. all of which are a delight to read.

It is not the function of this volume merely to provide a historical reference however. Each of the papers presented marks a point in the development in the science of simulation from which new and still active areas of research have opened up. It is therefore an essential starting point for anyone commencing work in these areas.

Several of the papers describe the powerful algorithms currently being used: the rigid body algorithm of Evans and the constraint method of Ciccotti, Ryckaert *et al*; the constant pressure algorithms of McDonald (Monte Carlo) and Andersen and Parrinello & Rahman (MD); the ensemble methods of Evans, Hoover and Nosé and methods for calculating free energy and entropy by Bennet, Romano and Singer. In addition there are classic applications of simulation such as Stillinger and Rahman's study of water. It is good to have so useful a source at hand.

If the book has a weakness, it is that the subject matter threatens to outstrip it. In five or ten years time, one suspects, it will be very difficult to put together a similar volume and still retain a sense of commonality and completeness. Towards the end of the book one encounters the work of Brooks, Karplus, Klein, Ceperley, Car and Parrinello and others. One begins to see how this prediction will be fulfilled. This is a very timely book!

Simulation of Liquids and Solids: Molecular Dynamics and Monte Carlo Methods in Statistical Mechanics, Edited by G. Ciccotti, D. Frenkel and I.R. McDonald, published by North Holland 1987

The Fast Fourier Transform and its Applications by E.O. Brigham

This book is a sequel to an earlier volume by the same author entitled "The Fast Fourier Transform" and it is written in the same style and with much material in common. It does however take the subject substantially further. The value of the book stems from its style; the author has chosen to develop the subject for its own intrinsic worth and leaves the reader to exploit its potential. The author favours a pedagogic approach, relying much on graphical demonstrations rather than abstract theorems (though central concepts are also treated mathematically) and as a result one is able to progress rapidly through the subject, without losing contact with its subtlety and yet gaining a clear grasp of the basics.

Among the topics covered by the book are: the basic mathematical properties of the Fourier transform; convolution and correlation; the discrete Fourier transform (which is the *real* subject of the book; the fast Fourier transform is after all merely an algorithm!); discrete convolution and correlation; the Fast Fourier Transform algorithm of Cooley and Tukey; the two dimensional Fourier transform; the use of window functions and much else besides. All of it is discussed in the same accessible style.

Molecular dynamicists would probably not think of buying this book; it is after all much more the stuff of electrical engineers and the omission of even a mention of molecular dynamics would be taken as a serious deficiency. This however would be mistake; a molecular dynamicist would learn much from reading it. Despite the lack of reference to MD the reader would feel strongly encouraged to exploit the efficiency of the FFT in simulation work, which would be no bad thing! (A very good example would be the use of the FFT in the calculation of correlation functions or perhaps the time dependent methods for simulating quantum systems that have appeared recently.) However, as anyone who has attempted to exploit the FFT will reveal, it has sometimes surprising properties, which can confuse the unwary. The value of this book is that one will be able to anticipate these and will be able to deal with them as they arise.

The Fast Fourier Transform and its Applications by E.O. Brigham, published by Prentice Hall, 1988.

The CCP5 Literature Survey 1988

W. Smith

April 4, 1989

Readers with a discerning eye for these things will notice that the literature survey this year has a slightly different flavour from previous years. The reason for this is the unfortunate termination of the CAN/SDI INSPEC service at the University of London Computing Centre, which took place approximately half way through the year. This service formerly provided the bulk of our references and its termination necessitated a search for an alternative.

Thanks to the advice of Dr. J. Altmann, the former manager of the ULCC INSPEC services, we were able to transfer our requirements quickly to the SDI service of INSPEC in Hitchin, Hertfordshire, and continue the survey with their facilities. We are grateful to Dr. Altman for her assistance in this matter and thank her and her colleagues for their past service. We are grateful too to Geoff Jones, the Head of Selective Services at INSPEC for his patient assistance during the transfer.

All references included in the list below are selected from the INSPEC database and are reproduced with the permission of INSPEC, the Institution of Electrical Engineers. The INSPEC database covers all areas of physics, electronics and computing.

As in the past, by reason of the large volume of material the survey is capable of generating, we have deliberately constructed a search profile to narrow down the search drastically. The number of references we have obtained represents the optimum we are able to process through the newsletter. We cannot guarantee therefore that we have gathered all the papers that are relevant to CCP5 members. Readers are invited to send us a list of their own papers if they are missing from our survey. We will publish them in the next issue. Despite the aforementioned difficulties, we believe that the survey produced is a valuable contribution. We hope that our readers find it to be so.

Our final note of gratitude goes to Miss A.P. Haskayne, of the Daresbury Reprographic Service, who patiently typed and sorted the list. Your editor reserves the sole responsibility for any errors appearing.

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