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

Editor: Dr. William Smith
Deputy Editor: Dr. Maurice Leslie

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

Editorial

CCP5 Renewal

CCP5 has been renewed by SERC for a further two year period (i.e. until Sept 1990). The new grant will support Drs. Leslie and Smith at Daresbury plus funds for travel, collaborations and meetings. In addition it will be possible to run an extensive visitors programme.

The committees that reviewed our proposal were all complimentary about the science being done and being planned by the community. The future for the Project is therefore good.

The Executive Committee of CCP5 are very grateful to all who contributed to the successful Renewal Proposal.

Contributors to the Current Issue.

Our thanks go to:

C.R.A. Catlow B. Vessal	Department of Chemistry, University of Keele, Keele, Staffs ST5 5BG.
D. Fincham	Computer Centre, University of Keele, Keele, Staffs ST5 5BG.
M.J. Gillan	Department of Physics, University of Keele, Keele, Staffs ST5 5BG.
D.M. Heyes	Department of Chemistry, Royal Holloway and Bedford New College, Egham, Surrey TW20 OEX.
M. Leslie W. Smith	Theory and Computational Science Division, S.E.R.C. Daresbury Laboratory, Daresbury, Warrington WA4 4AD, Cheshire.
J. Moscinski J. Kitowski	Institute of Computer Science, AGH, 30-059, Cracow, Poland.
T. Nguyen	Massachusets Institute of Technology, Cambridge, MA 02139, U.S.A.

COMPUTER MODELLING OF NEW MATERIALS

A Joint CCP5 - CCP9 Meeting

4 January - 6 January 1989

This conference will bring together experts in two areas of condensed matter research: atomistic computer simulation methods and electronic structure calculations. These two communities are supported in the UK through the SERC Collaborative Computational Projects CCP5 and CCP9 respectively. The aim of this joint meeting is to encourage cross-fertilization of ideas and techniques in a variety of applications.

The theme of the conference will be the modelling of materials of current technological interest. These include the new high-Tc superconductors, semiconductors, polymers and liquid crystals. The following have agreed to give invited talks:

E. A. Colbourne	(ICI Wilton)
D. Dunmur	(Sheffield)
M. Gillan	(Keele)
B. L. Gyorffy	(Bristol)
R. Jones	(Exeter)
W. Mackrodt	(ICI Runcorn)
M. Payne	(Cambridge)
A. Sutton	(Oxford)

Time will be available for contributed papers and poster sessions.

The meeting will be held in Bristol University's Clifton Hill House, a comfortable hall of residence with integral conference facilities. For further details contact:

Dr. M. P. Allen
H. H. Wills Physics Laboratory
Royal Fort
Tyndall Avenue
BRISTOL BS8 1TL
United Kingdom

Tel: (0272) 303030 ext 3669
JANET: MPA @ UK.AC.BRISTOL.PVA

CCP5 WORKSHOP ON INTERIONIC POTENTIALS

March/April 1989

Most computer simulations assume that the interaction between ions may be expressed in terms of pair potentials. Some simulations assume three- or more-body potentials. Almost every imaginable approach (with the possible exception of human sacrifice) has been tried to obtain a suitable potential model. The majority of potentials have been obtained by some kind of fitting procedure. While this has had many successes, the shortcomings of fitting potentials to crystal data are becoming more and more evident. People are therefore turning to calculation, either by such simple methods as the electron-gas approximation or by more expensive (but hopefully more accurate) Hartree-Fock methods.

We therefore intend to hold a workshop on calculating interionic potentials. The main areas for discussion are intended to be:

1. Electron-gas methods; how and when to use them
2. Hartree-Fock potentials
3. Calculation of polarisabilities and dispersion
4. Wavefunctions for crystal environments.

Attendees will be asked to produce a potential (by whatever kind of calculation seems good to them) for TiO_2 and MgO so that we can discuss and compare methods.

Details are still to be decided, but we would like to hold the workshop late March or early April next year, probably at Cosenor's House. Would Those interested in attending please contact:

John Harding/Tony Harker
Theoretical Physics Division
Harwell Laboratory
Didcot
Oxon OX11 0RA

General News.

1) Preparations are well under way for the NATO ASI Summer School on "Simulation of Liquids, Polymers and Solids", which CCP5 is organising at the University of Bath for September 1988. The organisers received an enormous number of applicants and it has been necessary to give priority to students and scientists just commencing work in the simulation field. For this reason, late applications are very unlikely to be successful. For those unable to attend, we hope to provide some account of the meeting in the CCP5 Newsletter. The proceedings of the meeting will of course be published.

2) CCP5 in collaboration with CCP9 (the Collaborative Computational Project on the electronic structure of solids) is organising a meeting in Bristol for 4th-6th. January 1989 entitled "Computer Modelling of New Materials". Details of this meeting appear in the previous pages. The meeting constitutes the CCP5 Annual meeting.

3) A second meeting, on the subject of "Simulation of Biopolymers" is scheduled for late January 1989, and is also a collaborative effort, this time between CCP5 and CCP4 (the CCP devoted to protein crystallography). We will provide more details in our next newsletter.

4) A workshop on the Car-Parrinello Method is being planned for March 1989. It is intended that the workshop take a detailed look at the methodology and application of this technique. Enquiries should be made to Prof. M.J. Gillan, Department of Physics, Keele University, Keele ST5 5BG Staffs.

5) Other workshops in the pipeline include: Applications of simulation in synchrotron radiation experiments (Autumn 1988, enquiries to Prof. C.R.A. Catlow at Keele University); Interionic potentials from quantum mechanical and other methods (enquiries to J.H Harding and A.H. Harker, see announcement on previous page); and Potentials in biomolecules (1989, no further information yet).

A symposium on novel methods in simulation has been suggested, incorporating such methods as cellular automata, neural nets, fractals, maximum entropy, simulated annealing etc. We would be pleased to have some reactions to this suggestion, to gauge support for the idea.

Readers are asked to pass on any suggestions for suitable workshops to the CCP5 Executive Committee (Chairman: C.R.A. Catlow, Secretary: M. Leslie).

6) At Daresbury Laboratory significant changes in computer hardware are about to occur. The NAS AS7000 mainframe is to be replaced shortly by a CONVEX C220 mini-supercomputer, which currently stands in the computer room, somewhat ahead of schedule. The machine is a dual processor with vector capability (rated at about half Cray 1s performance), 256 Mbytes of main memory, 14 945 Mbytes of disc storage and a UNIX operating system. Its rôle will be as the main processor for theoretical calculations by the TCS division and analysis of Synchrotron experimental data.

On a less cheering note, and for rather comlicated reasons, Daresbury has seen the departure of the FPS T20 parallel processor. The machine was undoubtedly a powerful computer, if rather difficult to program optimally in its current configuration. The hypercube architecture and vector nodes probably anticipate a distinct line of development

heralding a new class of machines and for this reason its departure is to be regreted. However Daresbury's Advanced Research Computing Group will continue to work with other parallel processors and a replacement for the T20 is being sought.

6) The University of Manchester Regional Computer Centre will say goodbye to the CYBER 176 mainframe at the end of July. This is the last of the triumvarate of CDC machines using the SCOPE operating system and users are being asked to transfer their jobs elsewhere, such as to the VM/CMS domain of the Amdahl 5980. UMRCC has also taken steps towards the Common User Interface recommended by the Forty Report and VAX/VMS systems are being provided. The objective is to allow users access via common and familiar front-ends.

Via UMRCC we have learned that the important software library: Computer Physics Communications (CPC) Program Library, is available on-line from Queen's University Belfast. Users may access a data base, including an index, to locate programs. The programs of interest may be requested from the Library on-line and will receive them (plus invoice) by electronic mail. Further information is available via electronic mail to the address CPC@UK.AC.QUB.AMV1.

7) The University of London Computing Centre is currently looking into the possibility of replacing its two Cray 1s computers, with a view to reducing operational costs. The replacement system is expected to be able to cope with current workloads and deliver the same computational power. The possibility of a multi-node system exists, but the stipulations on the power of each node rule out massively parallel machines. A small groups has been set up to deal with this question and will report to the Computer Board in July. Users of the ULCC Crays are invited to send comments to the Head of Operating Systems; Dr. H. Kirkman. The same directive has also been given to UMRCC, with regard to the CYBER 205.

In common with UMRCC, London is also providing a VAX/VMS interface, to improve the Common User Interface.

A new version of the Amdahl 5890 operating system; known as MVS/XA, is being prepared for release. It is expected to enhance the service considerably, particularly in terms of memory usage.

Die-hard users of Phoenix 1 are being warned that it is to be withdrawn at the end of July.

8) The Rutherford and Appleton Computer Centre has replaced the Atlas 10 and IBM 3081 computers with a double processor IBM 3090-200E of the same combined power (the machine has vector processing capability). The disc space of the new system is 40 Gbytes (resulting in an increase of 23 Gbytes over the old system). Two 3480 cartridge tape drives have also been purchased. The operating system is a version of VM, known as VM/XA SF. This will be replaced eventually by MVS/XA SP, for those who know the difference!

RAL has announced that it is to take part in the IBM European Supercomputing Initiative, which could lead to considerable enhancements in the facilities RAL has available. Watch this space.

RAL has killed off its User Liaison Committee, so users with recommendations should now direct them to Paul Thompson, Head of User Support (PCT@RL.IB).

9) **Errata**: A few typographical errors have been discovered in the article "Coping with the Pressure ..." by W. Smith that appeared in the September 1987 issue of the newsletter. These are as follows.

In equation 9, there is a factor r_{ij}^2 missing from the numerator on the right hand side of the equation.

In equation 22, the definition of U_c is incorrect; it is a sum of erf terms, not erfc terms as presented.

We are grateful to D. Fincham and T. Nguyen for pointing out these errors and we apologise to our readers.

11) **The CCP5 Program Library.**

We are pleased to report the addition more programs to the library. The first program is MCMOLDYN, which was written by Dr. Aatto Laaksonen of the University of Stockholm. The program represents a very versatile package and can be used for molecular dynamics and Monte Carlo simulations of polyatomic molecules or ions in the liquid state or in aqueous solution. The program is fully documented in the journal "Computer Physics Communications", (Ref: A. Laaksonen, CPC (1986) 42 271).

The second package we have received is a utility for emulating the NAMELIST facility on machines not supporting this non-standard feature. The package is largely written in FORTRAN 77, with C support utilities. It was written and donated by Dr. Keith Refson of Oxford University.

We are grateful to Drs. Laaksonen and Refson for their contributions.

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 (to be supplied by the applicant) be used. It may also be possible to transfer a small number of programs over the JANET network to other computer centres in the U.K.. Please note that use of inappropriate packing for magnetic tapes (e.g. padded bags) may result in them being considered unusable by Daresbury Computing Division and returned without the required software. Please ensure that these forms of packaging are not used. A list of programs available is presented in the following pages. We should also like to remind our readers that we would welcome contributions to the Program Library. The Library exists to provide support for the research efforts of everyone active in computer simulation and to this end we are always pleased to extend the range of software available. If any of our readers have any programs they would like to make available, please would they contact Dr. Smith.

THE CCP5 PROGRAM LIBRARY.

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
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

SITUATIONS VACANT

(1) Short Term Postdoctoral Post

Quantum Simulations

A residue left on a SERC grant permits the employment of a postdoctoral research assistant for 3-4 months before the end of February 1989.

Topic: Methods of quantum mechanical computer simulation. (Reasonable flexibility concerning details).

Salary: According the SERC 1A scale i.e. depending on the age,but roughly £1000-1200 per month.

Enquiries (from U.K. or E.E.C citizens) to: Prof. K.Singer Department of Chemistry,RHBNC Egham Surrey TW20 0EX or by electronic mail: JANET

(2) Three Year Postdoctoral Position

Car-Parrinello Method

Professor Mike Gillan at the University of Keele has a 3-year postdoctoral research assistantship available to work on the Car-Parrinello method for calculating the properties of solids. Traditionally, the computer simulation of condensed matter has been based on pair-potential models for the interactions between atoms. As simulation expands into new areas, and attempts to tackle new materials, the limitations of the pair-potential approach is becoming increasingly evident, and there is a growing desire for something better. This 'something better' must come from an understanding of the electronic structure of the material. Recently, Car and Parrinello showed how simulation could be performed by solving Schrödinger's equation for the electrons for each configuration of the ions. This idea is part of the rapid general improvement that has taken place in *ab initio* electronic-structure methods in the last ten years.

What we plan to do in this project is to use techniques based on the Car-Parrinello idea to calculate the energy and structure of defects in a range of materials, including simple metals, transition metals and partially-covalent materials like Al_2O_3. The exploratory work that led up to this project has already given encouraging results. The problem chosen for exploratory purposes was the calculation of the vacancy formation energy in aluminium. The results obtained are in quite respectable agreement with experiment - and this is the first time this has been achieved. The prospects for extending the treatment to transition metals seem good, and if successful this would be an important 'first'. So the person appointed to this postdoctoral position would have a good chance of participating in really important developments.

As usual, applicants need to have a Ph.D. in an appropriate area, or expect to receive one soon. Formal enquiries can be made to The Registrar, University of Keele, Staffs, ST5 5BG (Tel: 0782-621111, ext. 3005). Informal enquiries to Professor M.J. Gillan (0782-621111, ext. 3911) are welcomed.

(3) SERC (Earmarked) Studentship

Applications of Transputers in Molecular Dynamics Simulations of Zeolites

This studentship is available from 1st October 1988 and will involve the exploitation of transputer systems in molecular dynamics simulations. The advent of transputer systems is probably the most exciting development in parallel processing, and the University of Keele has recently been awarded £ 100k to set up such a system. The project will include the development of molecular dynamics programs to run on the transputer system, and the application of these programs to simulations of zeolites, aluminosilicate minerals with important industrial applications. Among the problems that will be studied will be the behaviour of hydrocarbons in zeolites, and the development of potentials to describe hydrocarbon-zeolite interactions. The project will be carried out in close collaboration with Dr D Fincham in Keele Computer Centre.

Further details and an application form may be obtained from: Dr R A Jackson, Department of Chemistry, University of Keele, Staffs. ST5 5BG (telephone 0782 621111 ext 3185)

(4) Ph.D CASE Studentship

The Computer Simulation of Uranium Dioxide

Mike Gillan (Physics Department, University of Keele) has a CASE studentship available for a project on the molecular dynamics simulation of solid and liquid uranium dioxide (UO_2). Please draw this to the attention of new graduates who may be interested. The studentship is funded by the SERC and by Harwell Laboratory and is worth more than a normal PhD studentship, because Harwell expects to augment the grant by a special contribution. The student will be based at Keele, but will be expected to perform some of his/her research at Harwell (not less than 3 months in the 3 year period of the grant).

Uranium dioxide is an important and unusual material. It has anomalous thermodynamic and transport properties, which are believed to be related to the massive ionic disorder that occurs in the high-temperature solid and perhaps to electronic excitations (the material is a semiconductor). Harwell want to gain a fundamental understanding of these properties for reactor-safety reasons - UO_2 is the fuel normally used in nuclear reactors. Molecular dynamics simulation seems the ideal theoretical tool to get this understanding: with realistic models now available or under development for the interactions in UO_2, molecular dynamics should be able to do a very good job of interpreting the ionic disorder and other interesting effects.

The project will give an excellent training not only in simulation, but also in statistical mechanics, transport theory, interionic forces and many other aspects of condensed-matter theory. In addition, Keele has just been awarded a grant to buy a transputer system, and it is planned that this will be used to do some of the simulations. So there is a fine opportunity here for a computationally-minded student to be involved in some of the latest developments in computation.

Those interested can get application forms and further details from the Director of Academic Affairs, University of Keele, Keele, Staffordshire ST5 5BG, U.K., (Tel. 0782-621111, ext. 4007). Informal enquiries to Professor M.J. Gillan (same number, ext. 3911) are welcomed.

Review of the CCP5 Annual Meeting 6-8 January 1988: Industrial Applications of Molecular Simulation

D. Heyes, D. Fincham and W. Smith

July 1, 1988

The CCP5 Annual Meeting on the subject of "Industrial Applications of Molecular Simulations" was one of the most interesting meetings that CCP5 has organised. Over 130 people attended, making it also one of the largest. Not surprisingly, the subject attracted a substantial attendance from scientists working in industry and, as usual, there was strong support from scientists overseas, including the USA, Europe and China. The eight sessions of the meeting covered an enormous range of applications: bulk behaviour, solid state chemistry, macromolecules, biological materials and porous media, all of which demonstrated the challenges awaiting practitioners of molecular simulation. In the course of the meeting it emerged clearly, that molecular simulation has a very significant role to play in the industrial arena. In this regard the meeting was unquestionably a great success and a credit to the organisers; Prof. C.R.A. Catlow and Dr. N. Quirke.

The conference was opened by Prof. Catlow, who warmly welcomed the attendees. An overview of the role of simulation in the industrial environment was presented by Dr. N. Quirke. He pointed out that it is a cost effective route to solving some important applied problems, for example in the field of heterogeneous catalysis. He mentioned that collaboration between academics and industrialist was already well-established, especially through the CASE studentship scheme and, in his own company, BP's Venture Research Scheme.

The first session dealt with simulations of bulk behaviour and began with Prof. K. Gubbins of Cornell, who described the methods currently employed in the simulation of phase equilibria. Prof. K. Gubbins developed the theme of the value of simulation in industry, by explaining the role of computer simulation in studying phase equilibria. The ability of simulation-aided-theory in predicting phase diagrams of three (or more) component mixtures is favourably competitive with experiment. He reviewed the methods for determining phase equilibria (especially near the critical point) of simulation fluids. Although it is feasible to model two phases in contact (for example, surface adsorption of Ar in a Kr/Ar liquid-vapour interphase), there are problems in establishing thermodynamic equilibrium. Finite size artifacts are also more prevalent in these two-phase simulations, when compared with the single phase cases. There are long (but natural) times needed to establish equilibrium, especially in the low and high density regimes. On balance, the so-called "indirect methods" are favoured. These involve separate evaluation of chemical potential in the two phases. There are several methods of performing this, which are all quite good at low and intermediate density but all become inefficient close to the liquid-solid coexistence line. These methods include, the "Test Particle" method, Grand Canonical Ensemble MC, and a new method, due to Panagiotopoulos

(the Gibbs ensemble), which simulates the two homogeneous phases in parallel and exchanges particles between the two simulation boxes. Simulations have been performed to help understand cosolvent-enhancement of solute solubility. The diverse methods often gathered together under the general label, "Thermodynamic Integration", were also discussed.

Dr. L.V. Woodcock, of the University of Bradford, discussed how the rheology of complex fluids can be predicted using the scaling properties of the hard- and soft-sphere fluids. This implies that the details of the potential are not too important. He showed that, making use of Ashurst and Hoover's empirical fit to the shear viscosity of the soft-sphere fluid, he could predict the viscosity of some very complicated molecular fluids (e.g., medium sized alcohols, alkanes and ethers) on average to better than 20% over their entire phase diagram. This is often more than adequate for engineering applications and is a more satisfying approach than the various modified van der Waals equations of state available. Admittedly both are fits to "experimental" data. The new approach, however, has parameters which are independently accessible and known for many molecules. The discussion moved onto methods for simulation of colloidal dispersions. His approach is to take the simplest model that will account for observed behaviour, concentrating often on hard-core potentials undergoing Stokesian or "drag" dynamics. The role of Brownian forces was considered generally unimportant for many rheological applications. Attempts were made to estimate its role in an approximate analytic manner. He also showed that there are substantial differences between the components of the self-diffusion coefficient under shear thinning flow.

The first session was concluded by Dr. D.M. Heyes, who reported some results of work performed with Dr. J.R. Melrose (both from Royal Holloway and Bedford New College). He showed how the shear thinning and thickening of gases, pure liquids and dispersions could be scaled onto the same "universal" curve. The shear rate needs to be made dimensionless be multiplication by a characteristic independently deriveable time. Having established a link between rheology and microscopic properties, the theme was broadened to establish a link between a transition in the density dependence of thermodynamic, mechanical and dynamical properties of simple fluids to the formation of percolation clusters. (These are clusters that span all space.) The separation between the particles used to determine percolation was just beyond the first peak in the pair radial distribution function, at a slightly supercritical state. He showed that the concept of percolation is a useful framework for developing theories of intermediate density fluids.

The second session was concerned with solid state chemistry. The opening speaker was Prof C.R.A. Catlow (Keele and Daresbury), who described the role of computer simulation in solid state chemistry. The range of applications of industial significance is vast and includes catalysis, solid electrolytes, ceramics, nuclear materials, silicates and most recently, high temperature superconductors. The principal methods available are energy minimisation, lattice dynamics, molecular dynamics and Monte Carlo.

Energy minimisation can be applied to both perfect and defective lattices and provides data on lattice (and defect) energies, elastic and dielectric constants, phonon dispersion and crystal structure prediction. The phonon data can also be used to calculate the free energy of the lattice and permits phase equilibrium studies. An example study of strontium zeolites was outlined. Studies of defects (vacancies and impurities) are made possible by a "two-region" strategy, which treats the lattice explicitly within the central region and employs the Mott-Littleton method for longer ranged effects. Free

energy calculations are possible with the "supercell" method, which embeds a defect within a large simulation cell with periodic boundaries.

The most common potential model for these methods is the Born model. In order of increasing difficulty, this entails; formal charges on the ions, short-range two body potential functions (e.g. Buckingham potential), the shell model for polarisation and additional bond-bending or three body terms. Parameterisation of these potentials may be done empirically; by least-squares fitting of structural, elastic, dielectric or lattice dynamical data. The parameters may also be fitted to non-empirical data such as electron gas and Hartree-Fock potentials.

Numerous example applications of these techniques were provided by Prof. Catlow. The reproduction of the structures of aluminosilicates, which are important in many industrial catalytic processes, were shown to be possible by the energy minimisation method, thus permitting theoretical deductions of the relative stability of zeolites. The work of Parker and Price in modelling the high temperature and pressure phase properties of $MgSiO_4$, which is of fundamental geological importance was described. The application of MD to studies of superionic conductors, such as the disordered fluorite structure $RbBiF_4$, showed the origins of the anomalous conductivity as being a concerted or cooperative F^- migration. A study of CeO_2, which also has a fluorite structure, using Monte Carlo simulations, went some way towards explaining the observed conductivity. Lattice dynamics studies of the superconducting oxides based on La_2CuO_4 revealed a soft phonon mode, thought to be of significance to their superconductivity. By such examples the power, versatility and industrial relevance of these methods was made manifest.

A new database for chemical structures was the subject of the talk by Dr. B. Collins of the IBM Scientific Centre. In a collaboration with Oxford University Press, IBM are attempting to combine the versatility of workstations with the data storage capabilities of optical discs. The objective is to produce a powerful database with extensive interrogation features. Some of these capabilities were demonstrated in a working model. Not only was it possible to search the database for specific molecular stuctures and text information, but it was also possible to manipulate 3-D projections of the molecules on screen. The cost of the final product was thought to be in the region of 10,000.

A.K. Cheetham of the University of Oxford described the use of computer graphics in studies of the chemistry of zeolites. Zeolites are extremely important industrially and accurate computer modelling of their properties and chemistry is very benefitial. By the method of molecular mechanics (energy minimisation) it is possible to calculate the global minimum energy of an adsorbed molecule. The example of methane in zeolite Y was considered. Good values of the adsorbtion energy are obtainable, but MC or MD is required to "sample" the system adequately, particularly at higher temperatures where more pronounced delocalisation of the adsorbed molecule is expected.

With the aid of some attractive graphics Dr. Cheetham showed the results of a number of interesting investigations. The migration of a pyridine molecule through channels of Potassium zeolite L was one. The pyridine slid along the walls of the channel; a result verified by experiment. More exact modelling; allowing the zeolite frame to relax, showed migration of the K^+ ions towards the pyridine molecule. Neutron diffraction is the means by which such predictions may be verified. In the case of benzene migration of the molecule down the channel was more central.

The use of zeolites as catalysts was highlighted by considering the catalytic conver-

sion of meta- to para-xylene in zeolite ZSM-5. The stucture of this zeolite is complex: straight vertical channels are crossed by horizontal "sinusoidal" channels to create a very porous structure. Modelling of this system shows that the para-xylene migrates much more freely through the pores than the meta-form; thus the zeolite is capable of distinguishing the two forms. The catalytic conversion involves protonation of the meta-xylene. Calculations of this process are complicated by structural factors and adequate modelling require recourse to quantum mechanical calculations of the whole molecular environment.

The use of zeolites in catalytic processes was taken up by Mr. R. Vetrivel of the University of Keele, in the final talk of the first day. Together with his collaborators he has studied the catalytic conversion of methanol to gasoline in zeolite HZSM-5, using a variety of simulation techniques. He began by describing the zeolite itself, which is an alumino- silicate in which aluminium and hydrogen atoms replace silicon in the skeletal structure. The structure is highly porous, with interconnecting straight and sinusoidal channels. The first step of the catalytic conversion is the conversion of methanol molecules to olefins, which then further react with methanol to produce gasoline. The process is highly efficient.

In the first (and rate determining) step, it is important to discover how the first C-C bond is formed, and what effects the channels of the zeolites have on the process. Two substantial programs have been expoited to help answer these questions: CASCADE, the CCP5 static and defective lattice program and GAMESS, a geometry-optimising quantum chemistry package (available through CCP1). The CASCADE study treated the methanol as a rigid molecule with fractional charges. The relaxation of the molecule location and the surrounding zeolite lattice revealed two sites suitable for initial adsorption. The GAMESS study for reasons of economy and practicality, removed the zeolite lattice, leaving a partial structure that was small enough to model quantum mechanically. The relaxed systems showed substantial differences in adsorption energy for the two probable sites. The more strongly bound (40kcal/mole versus 13 kcal/mole) showed significant chemical change; in particular strong evidence of protonation of zeolite oxygen by the methanol. The methods were clearly capable of providing deep insight into the catalytic processes.

The third session was devoted to macromolecules and was opened by Dr. J.T. Bendler (General Electric Corporate Research Center, N.Y.), who presented the results of a simulation study of chain packing in glassy (polycarbonate) polymers. (Polymers at room temperature are frequently in the glassy state.) He gave an overview of the challenges presented by this phenomenon to the simulator. The glass transition temperature (measured by a change in the frequency dependent modulus) can depend very sensitively on the the nature and number of substituents on backbone aromatic rings. Of particular interest is to understand the microscopic origin of the low frequency mechanical loss peak, which is quite distinct from that of the lattice vibrations at higher frequency. Is it some form of travelling local conformational change (e.g., cis-trans going to trans-cis) ? How well does it agree with the theories of Flory, Rouse and Zimm, and de Gennes? His simulation contained a single polymer trapped in a box with graphite walls. The polycarbonate form was chosen because it can be obtained experimentally in the pure amorphous or crystalline states. This is in contrast to polyethylene, which is not easily made in a homogeneous state. The simulations were run for 10 picosec at 850 K on a VAX. He looked at energy versus density.

Dr. J.H.R. Clarke (U.M.I.S.T.) presented some simulation results obtained with Dr. D. Brown, of dense amorphous polymethylene chains. The motivation for this was to determine, and thereby understand, the effects of monomer-level chain interactions on its extensional behaviour. These effects are not accounted for in statistical mechanical theories. He pointed out that there are considerable difficulties in fully representing a material containing a wide range of dynamical relaxation times (from 1 picosec to ca. 1 sec). Nevertheless, the high frequency response accessible to MD is still of great interest. Using a constrained chain (although no rigid bond angles) and the Steele dihedral potential, they explored the stretching of a chain under stress, using their constant stress algorithm. The MD box contained a single chain of 500 LJ monomer units. The ratio of trans to cis was close to ideal (mostly trans). They looked at 1 and 2 kbar pressure ramps, above the glass transition temperature. At the higher stress the chain yielded and showed domains of local parallel alignment of the chain segments, with only a small change in the trans-gauche ratio.

Dr. B. Smit (Shell Research, Amsterdam), presented the results of some ingenious MD simulations, performed with R. Reijnhart, of model surfactant systems. The model was of amphiphilic molecules at a liquid-liquid interface. The immiscible liquids were represented by LJ particles with the same like-interactions but repulsive cross-interactions. The surfactant was a diatomic. They found phase separation of the two liquids, with the surfactant occupying the interphase region. The amphiphile substantially reduced the surface tension (as predicted by the Gibbs Adsorption Isotherm). There was no evidence of micelle formation. It was suggested that a larger simulation box could remedy this.

The fourth session dealt with simulations of biological materials and commenced with a lecture by David White of the University of Glasgow. Dr White and his collaborators have developed transputer based systems for applications in the molecular mechanics of biological molecules. Typically these molecules are very large (10,000 atoms) with a proportionate number of functional groups and consequently require a large number of force constants for the energy minimisation procedure. Optimising molecular geometries in this way generally requires a supercomputer, but even then there exists a graphics "bottleneck", since it is usual to place molecules into appropriate initial configurations "manually" and this requires interactive graphics. This is the rationale for exploiting the cheapness and versatility of transputers, which allow the construction of processors specific to the molecular mechanics problem. The Glasgow group have constructed their own parallel processors. Each board has eight transputers, with 4Mbytes per node. It is reckoned that approximately four boards provide the equivalent of 1 Cray 1s computer. This equivalence has been calculated using the linear dependence of the processing power with the number of transputers employed, a dependence which has been observed in the development stages.

The availablity of good hardware however, is not the only requirement for successful molecular modelling. Dr White's group has also been developing potential functions for biological systems. The contributions that must be considered include: harmonic bond stretching; valence angle stretching; tortional terms; 3- and 4-body contributions; coulombic interaction; short ranged interactions (Lennard Jones) and trigonal planar terms. All of these interactions require parameterisation and a vast number of force constants are necessary. Dr. White has attempted to reduce the number of parameters by discovering empirical relationships between the parameters for different systems and devising data tables from which the full parameters for any given case may be deduced.

Experience has shown that hydrogen potentials depart from the general relationships and separate tables are required for them. Overall the strategy has been successful.

Dr. White concluded his talk with a description of how the molecular mechanics program was optimised for parallel processing: initially each transputer was assigned the task of working out individual second derivative terms, but this strategy diminished in effectiveness as the system grew. Later on more effort was directed into partitioning the work more evenly between processors.

Dr. D.S. Moss of Birkbeck College, in a talk on the molecular dynamics of proteins, looked into the problem of comparing results from simulations with the results provided by X-ray diffraction analysis. Both methods, it was claimed, had their limitations, since both were based on an inevitably imperfect model. For example, in MD there were approximations in the potential, whereas the process of fitting X-ray data was complicated by substituents of proteins that possessed high conformational freedom ("floppiness"), which implied a departure from the harmonic model used in the analysis of the X-ray data. The anharmonicity of the model protein makes molecular dynamics an attractive method of modelling it. It is interesting that both methods assume rigidity of the substituents to facilitate the modelling process, though for different reasons.

A comparison was made between the structure of ribonuclease as obtained by MD simulation and that obtained from X-ray analysis. The MD simulation was performed using the Groningen GROMOS package. The starting configuration was based on the X-ray data, relaxed using a Monte Carlo initialisation. The simulation was over 24 ps and equilibration lasted 8 ps. The average structure of the "backbone" resembled that obtained by the X-ray analysis, but the side chain conformations showed greater differences. This is exactly where the two methods were expected to differ most. An advantage of the MD simulation is that it is able to show the differences in mobility between parts of the same molecule and thus offer clues to the biological activity of certain sites. An example of this is the motion observed in one of the histadine side chains near an active site. The conclusion of the study was that the differences between the methods arose from the potential parameterisation, boundary conditions and equilibration in the case of the molecular dynamics, and from the assumed sterochemical structure and harmonic approximation in the case of the X-ray analysis.

Dr. O.H. Olsen of the Novo Research Institute, Denmark described how simulation has been used to model excitations in proteins in the common α - helix structure. The problem is significant in determining the mechanism of energy transport in biological systems. A 3-D model of simple protein, based on empirical data, has been simulated using molecular dynamics program CHARMM. The data has been subjected to a spectral analysis, which revealed the strong amide-I vibrations. Excitation of the molecule is long-lived. The results suggest that a linear model of the system is possible. Dr. Olsen and his colleagues have constructed a model based on coupled linear oscillators, the parameters of which are obtained by fitting the phonon dispersion curves. This model gave a good account of the time dependence of the intramolecular vibrations of the α - protein and had the additional advantage of being inexpensive in computer time.

The biological activity of proteins is usually dependent on the presence of water, to such an extent that the water is retained in the crystallised protein. Dr. Julia Goodfellow of the Crystallography Department at Birkbeck described a detailed anaysis of the distribution of water molecules in protein crystals, using sixteen accurate protein structures obtained by high resolution X-ray crystallography. The analysis took the form

of a statistical enumeration of the grouping of water molecules around the main chains of proteins and particular side chains and atoms. Superposition of the distributions about identical side chains in different locations and proteins were used to determine "idealised" distribution functions and the results were displayed graphically. An analysis such as this provides insight into a number of interesting phenomena, such as the role of hydrogen bonding and the effect of hydrophilic and hydrophobic attributes of side chains on the overall protein conformation. The results showed that the grouping of water molecules about main-chain atoms was not particularly sensitive to the hydrophobic nature of the side chains associated with them. However there was a clear preference for water molecules to cluster about the side chains with low hydrophobicity. The results thus showed that clustering of water molecules in crystalline proteins was clearly non-random and was consistent with hydrogen bonding and stereochemical expectations. Futher analysis of these data, including energy minimisation, is expected to yield a more accurate method for modelling crystal stuctures, including the solvent environment.

The fifth session, and the first on the simulation of materials began with a talk by W.C. Mackrodt of ICI, Runcorn, on atomistic simulations of ceramics. Simulation is a valuable asset to research in ceramics; it provides additional information on such diverse properties as bulk structure, surface structure, crystal morphology, point and extended defects, grain boundaries, electronic defects, transport properties, phonon dispersion etc., in all of which, computer simulation is a genuine practical tool augmenting the skills of experimentalists. As a topical example of these methods, Dr. Mackrodt outlined the progress that has been recently made in understanding the properties of high temperature superconductors.

There are two classes of high temperature superconductors; those based on the $La_{2-x}M_xCuO_4$ with $M = Ca, Sr, Ba$ and $x = 0.1 \ldots 0.2$ and those based on $MN_2Cu_3O_{7-\delta}$ with $M = Ca, Sr, Ba$, $N = Y, La, Yb$ etc. and $\delta = 0.1 \ldots 0.2$. They are highly defective materials, and the superconductivity is dependent upon the process of manufacture, but there is evidence of Cooper pairing of electrons in the superconductivity. Much recent attention has been spent on measurement of the properties, manufacture and the search for new superconducting materials. These activities have gone together with a deepening theoretical understanding, in which simulation has played an essential part.

Concentrating on the first kind of material, Dr. Mackrodt described the results of simulation studies, begining with the structure of the pure material. (A necessary condition for modelling superconductivity is the correct deduction of the properties of the basic material.) Experiments show that below 500K it is orthorhombic and above 500K it is tetragonal. Electronic structure calculations suggested the tetragonal phase was 2-D metallic. Experiments however show that the doped materials are orthorhombic and the transition between the two cannot be electronically driven. Lattice calculations give the relative stabilities of the two structures correctly ($E_{ortho} < E_{tetrag}$) and the phase transition is now thought to be entropically driven.

The evidence is that the superconductivity is phonon driven. Freeman has suggested high energy phonon modes are significant, while Weber suggests coupling of low phonon modes is involved. Atomistic simulations of the density of phonon states give a peak at 4meV, ie a soft phonon mode, which is significant for entropy driven phase transitions. (Neutron scattering shows a strong peak at 10 meV.) Doping of the orthorhombic lattice causes the acoustic peak to become more prominent. It was pointed out that the calculated and experimental phonon modes were very close.

The importance of dopants in the superconducting material implies that defects play an important role. There is evidence for both La and equatorial-O vacancies, which simulations show to have similar defect energies. There is also the possibility of electronic defects and there is evidence of electron holes, either in the copper 3d band or the oxygen sp band. Atomistic simulations show valence band holes and the large and small polaron energies are very similar. This implies strong electron hole - lattice coupling, independent of the superconductivity. The density of states (electronic) shows a band gap at 4.2 eV and the lowest charge transfer exciton is at 5.5 eV.

Stoichiometry plays an important role in determining superconductivity. The oxygen stoichiometry has a significant effect on the critical temperature T_c. There is evidence for sodium and potassium impurities in superconductors. Calculations show where the impurities are substituted. Substitution at a copper site destroys the superconductivity, while substitution at a Lanthanum site enhances it. Granularity of the ceramic reduces conductivity, this implies weak links between grains and requires an explanation, possibly in terms of the surface properties of the crystal faces.

Ceramics were also the subject of a talk by S. Parker of Bath University; this time on ceramic oxide surfaces. The aims of his work, in collaboration with several colleagues, was to predict the properties of the surfaces by atomistic simulations. The properties of interest being: the surface structure; surface energy; defect formation and migration and the segregation of impurities. These properties being of particular interest in corrosion and catalysis studies.

The method employed is due to Tasker. The system is modelled as a stack of crystal planes, with 2-D periodicity in the xy-plane. In the vertical plane the crystal is divided into two regions; in Region 1 the ions are allowed to relax to resolve stresses, while in Region 2 the ions are fixed at the bulk positions. The thickness of these regions is optimised to ensure convergence. The general strategy of the method is energy minimisation to achieve the lowest energy structure. The model is fully ionic (with Ewald sum) and includes short ranged forces modelled either by empirical or non-empirical potentials. The modelling of the potential is checked by comparing predicted properties (crystal structure, dielectric constant, elastic constants etc.) with known values. A given model potential is assumed transferable to other crystal phases.

An example application given by Dr. Parker, was the modelling of the defect surface of Chromia (Cr_2O_3). The energy of formation of a vacancy in the 0001 surface was shown to converge on the bulk value as depth below the surface was increased. However, for this surface it was apparent that vacancies were most likely to form 3-5 atom planes below then surface; a result that differed for different surfaces. Another interesting calculation showed that the isovalent impurity ion Al^{3+}, which might be expected to dissolve in the bulk (on account of the small ionic radius) in fact segregated on the surface. This was opposite to the result for unrelaxed surfaces. Contrariwise, the large Y^{3+} ion dissolved readily. A second study considered the segregation of silicon ions in magnesium oxide, in which it was shown that the favoured structure is tetrahedrally coordinated; the silicon forming SiO_2 sheets rather than chains or clusters.

Further studies in this field will include dynamical simulations, studies of defect concentrations as a function of depth and grain boundary diffusion.

In a talk which introduced the concept of fractals, Dr. J. Kieffer of Purdue University descibed his studies of low density silica aggregates. These surprising materials are produced experimentally by hydrolysis under nonequilibrium conditions and can have a

density as low as one twentieth of the silica glass. They are produced computationally from a molecular dynamics simulation of SiO_2 by isotropically expanding the simulation cell to the point where the network of the silicon-oxygen bonds break. Beyond this point voids develop in the system, which grow with the expansion, though initially retaining sufficient connectivity to span the cell. Finally, at the percolation threshold, the system breaks down into isolated clusters, which restructure to a more efficient coordination. The primary concern of Dr. Kieffer was to provide a quantitative description of the distended nature of these materials with the aid of statistical fractals. Studies of the radial distribution functions at different densities (i.e. at different degrees of connectivity) provided a relationship with the fractal dimension. Studies of the phonon density of states also showed manifestations of the fractal behaviour. The simulation results may be compared with experiment, particularly neutron diffraction and light scattering.

Silica, this time in the form of a glass, was the subject of a talk given by B. Vessal of Keele University. Together with his collaborators, he has been studying the properties of this material by the method of molecular dynamics. Previous workers have successfully simulated the thermodynamic properties of silica, however the probability distribution of the $O - Si - O$ bond angle in these simulations departed substantially from the experimental determinations. Dr Vessal has attempted to correct for this deficiency by including 3-body (bond bending) forces in the molecular dynamics simulation.

The bond bending potential used consisted of a harmonic term in the angle between $O - Si - O$, with an additional scaling by exponential terms diminishing with the lengths of the $Si - O$ distances. (This is a model using point ions, with molecular entities identified as clusters of ions.) Special care was taken to define the short ranged potentials, which consisted of several functions, defined over specific ranges, and spline fitted at the junctions. The potential was fitted to α-quartz using the CCP5 static lattice programs. The 648 ion simulation in other respects resembled a normal ionic simulation. The simulation gave the correct radial distribution functions (and coordination numbers) and provided a good description of the bond angle distribution.

The second session on the simulation of materials (and sixth overall) began with Dr. S. Clarke of Imperial College, who presented the results of a microscopic model of epitaxial growth (with D.D. Vvedensky). The model represented the relaxation of adatom structure following subjection to molecular beam ("epitaxy"). (The surface structure is characterised experimentally by RHEED electron scattering.) The solid-on-solid Monte Carlo model used nearest neighbour interactions. It revealed an initial rapid decay of dendritic growth followed by a slower compaction of the clusters, and evening out of the step-density . This promises to be an important "growth" area for simulation.

Dr. C.C. Matthai from University College Cardiff presented the results of MD simulations of transition metal silicide growth on a silicon substrate, again with epitaxy in mind. The accommodation of Ni on a silicon substrate was modelled as a function of temperature. The Si substrate had bond stretching and bending terms, using the Dodson and Stillinger-Weber potentials. Two layers of Ni were considered. Interestingly the Ni does not sit attached to a "dangling" Si bond but spans at least two Si atoms. After quenching there is considerable mixing of the species observed.

Dr. J.D. Sherwood of Schlumberger Cambridge Research presented "hydrodynamic dynamics" simulation results of model plate-like particles. The simulations were two-dimensional, and therefore represented the particles "thin side on" as lines. Inertial

effects were ignored. An approximate solution of the Stokes equations was obtained using boundary element methods. Dr. Sherwood raised some well-focussed current problems in conclusion. How important are inertial effects? What are the relative magnitudes of viscous and clay particle - clay particle stresses? What are the effects of Brownian motion?.

The session was concluded with a highly entertaining and enlightening talk by Prof. J. W. Perram (Odense University). He is planning to use the ideas behind constrained molecule MD to guide "seeing" robots, so that they avoid colliding with other objects (principally humans!). His idea is to decompose the robot's armed segments into jointed hard ellipsoids. Making use of Wertheim's solution of hard ellipsoid dynamics the MD program would specify the trajectory of its arms . (The humans would also be ellipsoids!) These methods, though far removed from their origin in molecular dynamics, present practical solutions to real problems arising in robotic engineering.

In the seventh session, on porous media, all the speakers emphasised the industrial importance of an improved understanding of the behaviour of fluids in pores, of relevance to adsorption, catalysis and separation. The first speaker was J M D MacElroy (with S-H Suh), from the University of Missouri-Rolla, who studied the Lennard-Jones fluid inside cylindrical pores, the main aim being to distinguish between the two cases of smooth walls and of walls given a structure by lining them with Lennard- Jones atoms. Grand canonical Monte Carlo simulation was used and the results compared with various theories and experiment.

In the case of smooth walls the results for the density and density profile of the fluid agree with the "superposition" approximation to the YBG equation rather better than with the more sophisticated solution of Fisher. There was disagreement with theory as far as diffusion in narrow pores is concerned, but this is to be expected since the bulk RDF is used in evaluating the integrals in the theories. The simulations disagree completely with experiment, and this is because the wall structure is ignored.

In the case of structured walls it was found that the mean density was close to the bulk value (except for very narrow pores), in agreement with a well-known empirical rule. (With structureless walls a lower density had been observed.) The density profiles agreed well with Fisher's theory. Diffusion constants are smaller than with structureless walls, and the VACFs show this is due to back-scattering from wall atoms.

Jeremy Walton (with N Quirke, both from the BP Research Centre) used Grand Canonical Monte Carlo to study the Lennard-Jones fluid in a gap between parallel planar attractive walls. His interest was in the phase transition known as capillary condensation, in which a vapour condenses to a liquid inside the pores of an adsorbent at a pressure below that of the bulk SVP. The main quantity studied was the adsorption as a function of pressure (obtained in the constant chemical potential simulation from the equation of state), for various sizes of pore up to mesopores (20 molecular diameters). The reduced temperature was 0.8, compared with a critical temperature of 1.1.

Large slits showed capillary condensation with coexisting liquid and vapour branches over a range of pressures. One of these phases must be metastable, and the grand potential was used to determine the pressure at which the actual phase transition takes place. The point of condensation shifts to lower pressures as the slit is made smaller, and below a critical separation (about seven molecular diameters) no separate phases are seen. Both the gas and liquid phases showed enhanced density compared with the bulk, because of the attraction from the walls, and both showed simular structure near

the walls, with evidence of five distinct layers just before condensation.

Keith Gubbins (with G S Heffelfinger) considered mixtures of Lennard-Jones molecules inside cylindrical pores with walls composed of similar molecules. This type of system is of interest because mixtures show differences in the relative volatility of the components between the bulk and pore cases. The model system was an Ar/Kr mixture: the diameters of the two molecules are similar, but Kr is more strongly adsorbed by the walls. Molecular dynamics simulation was used and the system quenched from a supercritical temperature, so that spinodal decomposition into liquid and vapour phases, separated by menisci, took place. This enabled the liquid- vapour coexistance to be studied directly, for various compositions. It was found that the difference in volatility between the two components was reduced in the capillary case compared with the bulk. In small pores the adsorption of Ar was very small. The relative adsorption of the two components was strongly dependent on temperature.

The eighth and final session, and the third to deal with the simulation of materials, began with a description of the molecular dynamics simulation of some technologically important materials by M. Gillan of Harwell. Special emphasis was given to uranium IV oxide, which is extremely important in the nuclear industry. It is particularly important to know about the high temperature and pressure properties of this material, but it is difficult to do the appropriate experiments. Simulation is therefore one of the best means of satisfying this need. It is also a material with some unusual properties. An example is the increase in the constant pressure specific heat, by a factor of two, as the melting point is approached. Structurally UO_2 has the fluorite structure, and hence has high ionic disorder at high temperatures. Effectively one of the sublattices melts, and the material becomes superionic. An added complication is that the material becomes a semiconductor at higher temperatures, when the 2eV band gap is breached. Also, in the reactor, the sample is contaminated by nuclides.

In modelling UO_2, reference is often made to CaF_2 and $SrCl_2$ as idealised models e.g. in $SrCl_2$ conductivity grows with temperature, the specific heat shows a peak value and the anions move easily through the high temperature crystal. MD simulations on these systems are straightforward; they are fully ionic and easily modelled with Born-Meyer potentials, this was first done by Rahman in 1976. (More recent simulations have included the shell model of polarisability.) Dr. Gillan showed some results from simulations of CaF_2. In some revealing slide views, the low temperature crystal was ordered, but the high temperature crystal revealed substantial anion migration, while the cations remained localised. The diffusion coefficient for the anion compared well with experiment, as did the prediction of the onset of superionic conductivity. Closer examination of single anions showed the "hopping" of the ions from site to site. Neutron scattering will show the direction of the hopping and calculation of the fraction of hops to nearest and next-nearest neighbour sites is possible (79% to 21% respectively). The results of simulation and neutron studies agree.

More recent work has concentrated on UO_2 itself. Again the material is fully ionic and Born-Meyer potentials have been used. The superionic conductivity has been reproduced yet again and the predicted melting point closely resembles the experimental value (3250K vs. 3100K). Anion disorder begins at 2100K as predicted. The molar volume at constant temperature also compares favourably with experiment. Thus there is good reason to trust the deductions based on this model. Thus the disparity between experimental and predicted specific heat strongly suggests the importance of electronic

excitations. It was concluded that realistic simulations of UO_2 are possible and valuable information may be drawn from them.

Dr. M. Heggie (University of Exeter) described the recent progress the Exeter group has made in the atomistic modelling of advanced research materials, including materials significant to the nuclear industry, such as graphite. Their work is aimed at replacing purely empirical potentials by potentials fitted to *ab initio* calculations of suitable fragments of solid systems. Dr Heggie believes that we have reason to be optimisitic about the capabilities of computer modelling in this area. The reasons are the growth of readily available computing power and the emergence of ever-more powerful techniques. This latter aspect is demonstrated by the predictive power of ab initio methods, which can even be called upon to correct misleading experimental results.

Dr. Heggie also described his work on the modelling of defects with atomistic methods. The aim was to account for the effects of the defects (cracks, dislocations, dopants etc.) on the mechanical strength of silicon and quartz. The methods available; static lattice methods, *ab initio* methods (density functional theory, norm-conserving pseudopotentials etc) were togther capable of explaining the observed effects. It was in this work that the ability of computer modelling to correct erroneous experimental results was made manifest. Other properties that were described included phonon spectra and the hydrogen atom concentration at a model of a surface defect in silicon.

The final speaker of the meeting was Dr. A.N. Cormack of Alfred University N.Y., who spoke on the subject of the role of atomistic simulations in the control of microstructure-property engineering. The aim of this work is to employ atomistic simulation methods to gain understanding, and hence control, of the microstructure of important materials such as ceramics. Control of the microstructure is essential, since the bulk properties of these materials is defined by the microstructure. Ultimately, the intention is to be able to define a microstructure for a given ceramic property and to specify the manufacturing process to achieve that microstructue. The properties that are of interest are the thermal, electrical and mechanical properties, for which ceramics are signally important. The controls available to the manufacturer are the stoichiometry, firing temperature, rate of crystallisation etc. Dr. Cormack described the computing models currently being employed or are being developed (e.g. Johnson-Mehl model of nucleation and grain growth) to predict the microstructure of industrially important materials and indicated the importance of accurately modelling the granularity of the material.

The meeting was brought to a close by Professor Catlow, who summarised the contents of the meeting and the role to be played by CCP5. He highlighted the breadth and diversity of the simulation methods and the realism of the results obtained. The high industrial relvance of this work was self-evident. On the hardware side, the emergence of new kinds of processors; particularly parallel processors, augured new directions and methods of application. Looking forward, there was a need for more structured collaboration, particularly between university and industrial based research groups and CCP5 was already well-disposed towards this end. The future activities of CCP5, as defined by its recent SERC Renewal Proposal, included a determined commitment towards industrial collaboration in the subject areas that had been so fully expounded in the meeting.

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- British Petroleum

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Review of the CCP5 Workshop on "Parallel Computers in Molecular Simulation"

W. Smith and D. Fincham

June 15, 1988

The first session of the meeting was devoted to the Distributed Array Processor, commonly known as the DAP. The first speaker on this occasion was Mike Allen of Bristol University. He began by describing the current AMT DAP, which the Bristol Physics Department now possesses courtesy of the SERC Computer Science Initiative. This model DAP has a 32x32 array of bit processors and is eminently suitable for Ising model simulations. Dr. Allen's recent research has concentrated on liquid crystals; in particular the Lebwohl-Lasher model. In this model the interactions are between nearest-neighbours, which couple according to their relative orientations. The system consisted of 32x32xN molecules, forming layers of depth N. Previous workers have studied systems 10x10x10 (Luckhurst et al) and 30x30x30 (Fabbri and Zannoni). As in previous studies, the objective was to study the nematic/isotropic phase transition as a function of the thickness (N) of the "slab". The simulations used standard Metropolis MC adapted for parallel simulation on the DAP. Thus the method employed a "checkerboard" model with 1024 parallel spin updates each step. Very long simulations were necessary in this work, up to 500 times those required by Luckhurst et al, in order to locate the phase transition accurately.

Another application of the DAP is as a graphics processor. Dr Allen has performed substantial simulations of hard ellipsoids using the algorithm of Frenkel and Mulder. These simulations were performed on the Cyber 205 (the DAP not being particularly suited for this kind of simulation), but the graphics processing capabilities of the DAP have been exploited, with assistance from John Quinn of AMT, to produce motion pictures of the ellipsoids in motion. Examples of these were shown, revealing the spontaneous ordering and disordering that occurs in these systems in the course of the simulation. The pictorial information appeared complicated (to beginners!) but was aided by an adjacent plot of a nematic ordering parameter, which revealed spontaneous ordering as a departure from a spherical surface (isotropic ordering) to an ellipsoid (nematic ordering) as the dynamical simulation proceeded.

Dr. D. Nicolaides, also from Bristol, outlined his work on phase transitions in confined lattice gas systems. The essential computational feature of this work was that the model could be couched as a spin model like the 3D Ising model. This meant that the high efficiency of the DAP for simulating spin systems (10 million spin updates per second were quoted) could be exploited. The model included wall effects, in addition to the spin-spin coupling which gave a 4D phase diagram for the parameters concerned. Characterisation of this model by means of simulation was under way. The location of the thick/thin film boundary by simulation and comparison of results with predictions by mean-field theories were aspects of the work that were mentioned.

Prof. G.S. Pawley from Edinburgh described his experiences of the DAP architecture, which now goes back several years. He too began by outlining the structure of the DAP3, but paid particular attention to two specific features not commonly described. The first of these was a "bit plane" in the array of processors which had been inserted to provide fast output. This feature offered the possibility of real-time graphics as the simulation was in progress. The second feature of note was "redundancy", which was an essential part of the error-correction on the DAP. It consisted of a duplicate set of processors, which duplicated the calculation in progress and checked for errors. This was one of the reasons for the high reliability for the DAP, but alas, the duplicate processors were not available for additional computation! Prof. Pawley reported that the software provided by AMT was of good quality and included a useful debugger.

Research at Edinburgh included work on the Ising model. Prof. Pawley showed several slides which revealed the growth of domains as a function of temperature, applied field etc. and he pointed out features of the model, such as "square domains", which had been unnoticed before the use of the graphical facility. He concluded that the graphical capability was likely to be of great educational value in the future.

Other work that had been performed by the Edinburgh group included neural networks, molecular clusters and rotator phases, all of which were efficiently performed on the DAP. Prof. Pawley described how the dimensionality of a given problem could be reduced to suit the dimensionality of the DAP processing array. The current work of the group was on cellular automata; specifically to explore the tertiary structure of proteins.

The second session dealt with Transputer based parallel processors. The first speaker was Prof. S. Fornili of Palermo, Italy. Prof. Fornili's group are interested in biological systems, such as Gramicidin A, and the nature of the protein-water interaction. They have also studied hydrogen bonding and solvation of the H^+ and HO^- ions. These calculations require a great deal of processing power and they have turned to Transputers as a cost-effective alternative. The computer system they have developed consists of an IBM PC, Inmos B003 and B004 boards and a Micropolis Winchester 150 Mbytes drive.

On the software side, they began with a simple Vax MD program, which they converted to Occam. They tried different methods of achieving parallelism, namely: particle mapping (PM); interaction mapping (IM) and a method they described as "bustrophedonic" mapping (BPM) [1] The objective was to find the most efficient partitioning of the work amongst the processors (load balancing). The BPM method proved to be the most efficient and Prof. Fornili described the method in some detail. In the implementation described four transputers performed the computation of the forces and a fifth acted as a control processor. The particles were alloted to processors in the bustrophedonic manner and circulated systolically as the forces were accumulated. A comparison was made between T414 and T800 Transputer performances and between Transputer performance and mainframes.

Andrew Raine of York University described the development of systolic loop algorithms for molecular dynamics simulations, in a collaboration with D. Fincham and W. Smith. He began by describing the nature of systolic loops, which, in the current development, assume a ring topology for the processors. Data flows around the ring of the processors, so that none of them necessarily has all the data defining the dynamical

[1] This name derives from a primitive writing mode in which the text direction reverses at the end of each line, rather than reverting to the start of of a new line.

system. In all these algorithms each particle has at least one packet of data consisting of its position and its force accumulators. These packets are passed between the processors as the forces are calculated.

Mr Raine described three basic algorithms: SLS (systolic loop single) in which each particle has a single data packet; SLD (systolic loop double) in which each particle has two data packets and SLB (systolic loop bidirectional), which is a version of SLD in which data flows in both directions around the ring of processors. Each of these algorithms has its own advantages, but the most efficient is SLS.

Greater efficiency in these algorithms can be achieved in two ways. Firstly, it is possible to overlap the computation of the forces with the passing of packets between processors. Provided the calculation of the forces takes more time than the communication, the passing of data is free of cost. The SLS and SLB algorithms gain most from this strategy, since they have fewer occasions when processing must wait for communication, than SLD. The second method to improve efficiency is to pass data packets that specify several particles at once. The coding of this is more complicated, but it offers the best way forward for more advanced systems, where molecules rather than Lennard-Jones atoms constitute the particles.

David Brindle of Sheffield University described his studies of the micellar phase of amphiphiles. The original work concentrated on a two dimensional lattice model, but is now being extended to three dimensions. The problems associated with load balancing of the simulation over several processors were raised.

M. Saqi of Birkbeck described the work he and his collaborators intend to undertake in calculating the free energy of amino acids, with the aid of a Meiko M40 Parallel processor. (This consists of a local host transputer, T800 quad boards with 8 Mbytes of RAM. The front end will be a MicroVax II and 300M bytes of disc space will be available.) The methods they intend using include the perturbation method and thermodynamic integration. The theoretical basis of these methods was descibed in detail. The Monte Carlo method is their favoured simulation technique. The proposed parallel implementation allocated a single transputer as a main processor, which performed the Monte Carlo 'move' and several 'slave' processors to calculate the energy change.

The first day concluded with two short talks on the FPS T20 parallel processor at Daresbury Laboratory. The T20 consists of 16 processors connected in a hypercube or "tesseract" topology. Each node consists of a T414 Inmos Transputer plus an FPS vector processor and 1 Mbytes of dual-ported RAM. In addition to the 16 processing nodes, there are two system nodes to handle internode communication and I/O. The programming language is FORTRAN with system utilities to provide the communications.

Dr. M. Leslie of Daresbury described his adaptation of the Fourier component of the Ewald summation method for the T20. The Fourier component is readily vectorisable, and Dr. Leslie has couched the entire calculation in the form of matrix multiplication, thereby gaining maximum efficiency of the vector processors. The changes to the basic algorithm to obtain parallel processing were described. Altogether the Fourier component ran at approximately half Cray 1s speed. He is now working on the Real-space component of the Ewald sum, with a view to matching this performance. Once again, a matrix multiplication approach is being adopted.

Dr. W. Smith described two simple parallel molecular dynamics algorithms, which he termed 'replicated data' algorithms, because all of the nodes of the parallel processor

carry a replica of the configuration data. The first algorithm described was a pralle version of the well-known Brode/Ahlrichs MD algorithm, which he hoped would be particularly suited to the vector processors of the T20. Parallelisation of this algorithm is straightforward. However, there is potentially a severe bottleneck in the communication of the pair forces between processors. (Overlapping the communications with computation is a possiblity, but this seems likely to disrupt the vectorisation.) Further work on this is being undertaken. The second algorithm adopted the simple expedient of neglecting Newton's third law in the calculation of the pair forces. This allowed the convenient decomposition of the pair force matrix to achieve ideal load balancing. The additional cost of computing each pair force twice was offset by the great reduction in the data passed between the processors. The algorithm was thus a good candidate for systems with many processing nodes.

The second day began with a talk by Prof. J. Moscinski of the Institute of Computer Science, Krakow. He described the current aims of this institute with regard to parallel processing. The intention is to construct a 64 node "hypercube" processor, hosted by an IBM PC and exploiting currently available Intel microprocessors. The programming language will be PASCAL, with extensions for parallelism (PARLAN-86). They intend to design a method for decomposing molecular dynamics simulations for execution on a multinode system. The intention being to provide an automatic decomposition with dynamic load balancing.

Prof. Moscinski went on to describe a scheme for vectorising molecular dynamics simulations of particles in cylinders, for the CYBER 205 computer. The method requires sorting of the particles in the direction of the cylinder axis and makes use of the excellent capabilities of the 205 in sorting (33000 numbers in $\sim$ 1 seconds). He also described the likely adaptations for extending the method to bulk systems, a method he named the "linked strip" method. Again, sorting of the particles in one dimension was employed and the appending of neighbouring strips to achieve long vector lengths was described.

Professor J. Perram of Odense University, Denmark also described a new molecular dynamics algorithm, which was especially suited to vector and parallel processors. At the heart of the method is the Ewald transformation, which is conventionally used to simulate Coulombic systems, but is easily adapted to suit any force law. The advantage of this approach stems from the fact that the Fourier component of the resulting Ewald sum is highly vectorisable and is extremely efficient. The strategy is to set up the simulation so that the real space component is dealt with by a link-cells method, which implies a short cut-off in real space. This throws much of the calculation into the reciprocal space, where the computation is already very efficient. Thus in both real and reciprocal space the calculations are handled by efficient methods. In real space, the time (T_R) to compute the forces (to a given accuracy) is proportional to N^2/m^3, where N is the number of particles and m^3 is the number of link-cells. Meanwhile, in reciprocal space the time (T_C) to compute the forces (to a given accuracy) is proportional to K^3N, where K^3 is the number of reciprocal vectors required. The number K is related to the convergence parameter α, which in turn is related to the width of the link-cells in real space. In fact T_C can be shown to be proportional to m^3N. Thus the total time to compute the forces is of the form $T = AN^2/m^3 + BNm^3$ (where A and B are constants). Minimizing this expression with respect to the number of link-cells shows that the computing time for this method scales as $N^{3/2}$, while still achieving the desired accuracy.

Mr N. Ruddock of the Chemistry Department at the University of Glasgow described the use of Tranputers in energy minimization calculations of protein structures. The Glasgow group has been using Transputers in this area for some time. Initially, with only a few Transputers available they achieved parallelisation of their programs by allocating one Transputer to each dimension (X,Y,Z) of the problem, with a central Transputer as the main processor. Later developments were more sophisticated and allocated to each Transputer a specific task or subtask. The logical relationship between Transputers was thus delegative and heirarchical, and load balancing was achieved by addition of more Transputers where computation was most expensive. In effect, the parallel processor became a "special purpose" machine, specifically designed to deal with the problem of molecular structure. (Adaptations to molecular dynamics are possible and are under development). Mr Ruddock described in detail the nature of the problems of molecular structure determination, the basic methods employed and the partitioning of the problem over the network of Transputers.

The Glasgow group have designed and constructed their own compute cards based on the T800 Transputer, and which have application in molecular graphics and molecular modelling. A protein modelling system is planned.

The meeting was concluded by four commercial presentations from manufacturers of computing hardware. The companies concerned were SENSION, SEQUENT, ACTIVE MEMORY TECHNOLOGY (makers of the DAP) and ARROW COMPUTERS (U.K. distributors of the NCUBE massively parallel computer).

SENSION Ltd. decscribed their Transputer-based PARALLAX system. A module holds five boards, and a variety of boards are available; e.g. quad compute boards with 4 T800 Transputers; a graphics board; an input/output motherboard. Modules may be linked by fibre optics. Software includes the INMOS TDS and 3L FORTRAN compiler; other transputer software will be offered when it is in a robust state.

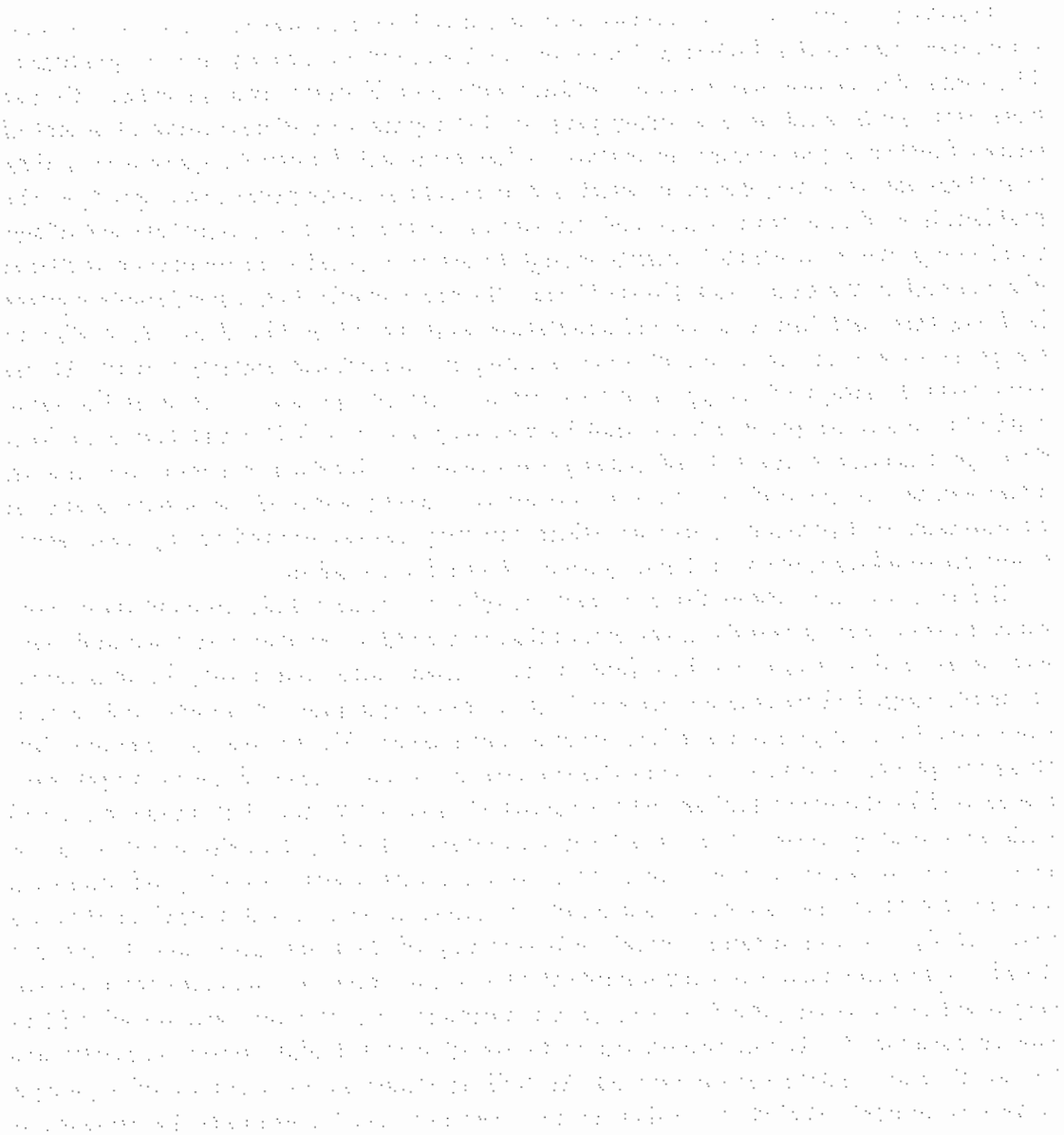
SEQUENT (Europe) Ltd. described their shared-memory multi processor SYMMETRY. A number of INTEL 80386 microprocessors are linked to the common memory by a very fast bus, and the UNIX operating system maintains a single queue of processes which it distributes to available processors. The machine appears to the user as a time-sharing system. Two British Universities have ordered systems for the central service. However the SYMMETRY is also a true parallel processor because it is possible for individual programs to utilise more than one processor. This is achieved either by introducing compiler directives into a program, or by an automatically parallelising FORTRAN compiler.

ACTIVE MEMORY TECHNOLOGY Ltd. described the current generation of DAPs, which were mentioned above. These are programmed in FORTRAN PLUS, a version of FORTRAN extended so that operations on vectors and matrices can be handled in single statements. They showed videos of some of their demonstrations, including the Ising model, which revealed the impressive power of the machine for interactive graphics.

ARROW COMPUTERS Ltd. described the NCUBE massively parallel computer, for which they are UK agents. The NCUBE processor has floating point hardware on-chip, and eleven communication channels. Ten of these channels can be used to build hypercubes of orders up to 10 (i.e. 2^{10} nodes); the eleventh provides direct connection to i/o boards for conventional communication or graphics. The operating system is a version of UNIX in which multiprocessor programs can be developed and run. FORTRAN

programs may call library routines for inter-node communications. Time sharing on the hypercube is possible in sense that separate subcubes may be allocated to different users.

The organisers of the meeting gratefully acknowledge the support of the above mentioned companies towards the cost of this workshop.



A SHORT VISIT TO COPENHAGEN

M.J. Gillan,
Physics Department,
University of Keele,
Keele,
Staffordshire, ST5 5BG.

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Thanks to CCP5, who generously provided travel funds, I was recently able to make a two-day visit to the Technical University of Denmark at Lyngby near Copenhagen. The main idea of this was to make contact with Jens Norskov and his group. He has been very much involved over many years in developing an understanding of potential energy functions, particularly in metals. It has been well known for quite a long time that there are very few metals in which a pair potential description is any good; so the problem is to derive from a physical description of the electronic structure a realistic total energy function which is simple enough to use in conventional simulation methods like molecular dynamics and Monte Carlo. He has recently had considerable success in doing this, and has also started simulation work based on his ideas. So a visit to his group to find out more about what is going on seemed particularly timely. At the same time, I bring back snippets of news from Cotterill's group, which is at the same institute - many people will know that he was very active in MD simulation for a long time, particularly in the field of melting mechanisms. Finally, I was able to spend an afternoon at the Oersted Institute in Copenhagen itself, where there is work going on on problems of hydrogen in metals, which are very closely related to my own recent quantum-simulation work on these systems. More details below.

Before I say more about the visit itself, maybe it will be helpful to mention its relevance to some recent trends in the simulation community. As simulation expands into new fields, and attempts to shed light on more complicated materials, the limitations of simple empirical interaction models become more apparent. Actually, such limitations have been apparent for a long time in some areas. Metals are one example, but there are plenty of others: covalent compounds are another case. Even in simple ionic materials like the alkali halides, where empirical models like the shell model have had such outstanding success, there has been a widespread feeling that the situation is not satisfactory. In all these areas, then, there is a growing desire to go beyond empirical descriptions of the energy as a function of configuration and seek descriptions that are more solidly based on a fundamental understanding of electronic structure. In the last decade or so there have been remarkable strides in the ability to calculate the total energy of solids by solving the Schroedinger's equation for the electrons within well-defined approximations [1]. It has turned out to be possible to calculate basic quantities like the equilibrium lattice parameter and the bulk modulus to an accuracy of a percent or two, to predict reliably the stable crystal structure, and for example the pressure at

which structural transformations occur, for a wide range of different materials. A recent development that has attracted a lot of attention is the Car-Parrinello method [2]. This gives a method of performing molecular-dynamics simulation with the total energy and interionic forces calculated at each time step by this kind of ab initio electronic-structure calculation. However, these ab initio calculations are still very demanding in computer time, except for rather small systems, and there has been a lot of interest in seeking something intermediate between the completely ab initio approach and unbridled empiricism - something that would incorporate the essential physics of the electronic structure, and yet would be not much more complicated than pair potentials. This brings me back to the Copenhagen visit. Norskov has been one of the inventors and developers of an idea that goes under the name of the 'effective medium' theory [3], called by some the 'embedded-atom method' [4]; it is also closely related to the Finnis- Sinclair potential recently proposed for the description of transition metals [5]. The theory embodies the principles of the ab initio electronic- structure calculations, but makes approximations which lead to a very simple expression for the total energy as a function of configuration. One of the aims of the visit, then, was to find out more about these developments.

The main idea of the effective-medium theory is that the total energy of a collection of atoms can be considered as a sum of energies, which have the significance of 'embedding' energies. An embedding energy means the energy change when a free atom is embedded in a uniform electron gas of a given density. This works by saying that each atom in the system sits in the electron density distribution due to the neighbouring atoms, this distribution being approximated as locally uniform. This idea was proposed a number of years ago for the description of impurities in metals [3]. More recently, it has been realised that the same concept can be used to describe pure metals themselves, including defects like surface and vacancies. Recently, Norskov, together with his collaborators Jacobsen and Puska [6], have developed a systematic derivation of this theory, starting from fundamental principles, and I will try to summarise some of the main points.

The whole approach depends crucially on density-functional theory, which also provides the foundation for most of the recent ab initio work, so I must remind you what this is. The main idea is that the total ground-state energy of the system of atomic nuclei and electrons is a functional of the electron density [7] - in other words a specification of the electron-density distribution $\rho(r)$ uniquely determines the ground-state energy. It is useful to write the energy as:

$$E[\rho] = Q[\rho] + \int d\underline{r} v(\underline{r})\rho(\underline{r}) + E_i, \qquad (1)$$

where $v(\underline{r})$ is the Coulomb interaction between nuclei and electrons and E_i is the Coulomb interaction between the nuclei; the functional $Q[\rho]$, which accounts for the kinetic energy of the electrons and their Coulomb interaction energy, is a universal function of $\rho(r)$. A key point of this density-functional formalism is that the true ground-state energy for a given $v(\underline{r})$ is the minimum of $E[\rho]$ over all $\rho(r)$ for a given number of electrons - this is a consequence of the usual Rayleigh-Ritz variational principle. The condition for E to the stationary with respect to variations of $\rho(r)$ is:

$$\delta Q/\delta\rho(\underline{r}) + v(\underline{r}) = \mu \qquad (2)$$

where μ is the chemical potential. It is usual to write $Q[\rho]$ as the sum of the kinetic energy E_K, the Hartree energy E_H, and the exchange-and-correlation energy E_{xc}:

$$Q[\rho] = E_K[\rho] + E_H[\rho] + E_{xc}[\rho], \tag{3}$$

and to make the local approximation for E_{xc}:

$$E_{xc} = \int d\underline{r}\rho(\underline{r})\epsilon_{xc}(\rho(\underline{r})) \tag{4}$$

where $\epsilon_{xc}(\rho)$ is the exchange-correlation energy per electron in the uniform electron gas of density ρ. The stationarity condition can then be written:

$$\delta E_K/\delta\rho(\underline{r}) + v(\underline{r}) + \int d\underline{r}' \frac{\rho(\underline{r}')}{|\underline{r} - \underline{r}'|} + \frac{d}{d\rho}[\rho\epsilon_{xc}(\rho)] = \mu \tag{5}$$

But this is exactly the same as we would get for non-interacting electrons, except that the true 'external potential' $v(r)$ is now replaced by the effective potential $v_{eff}(r)$ given by:

$$v_{eff}(\underline{r}) = v(\underline{r}) + \int d\underline{r}' \frac{\rho(\underline{r}')}{|\underline{r} - \underline{r}'|} + \frac{d}{d\rho}[\rho\epsilon_{xc}(\rho)], \tag{6}$$

The consequence is that the ground-state energy of the interacting-electron system can be determined by solving the effective single-particle Schroedinger equations:

$$[-\frac{1}{2}\nabla^2 + v_{eff}]\psi_\lambda(\underline{r}) = \epsilon_\lambda\psi_\lambda(\underline{r}), \tag{7}$$

with the density given in terms of the occupied wavefunctions by:

$$\rho(\underline{r}) = 2\sum_\lambda |\psi_\lambda(\underline{r})|^2. \tag{8}$$

These equations are to be solved self-consistently.

What I have sketched here is the standard density-functional theory that is usually employed for full ab initio calculations. It gives the very accurate results for lattice parameter etc. referred to above. But the practical solution of these equations is a major undertaking, because a large number of wavefunctions must be handled, and these must be iterated to self-consistency. The aim of the effective-medium theory of Norskov et al [3] is to introduce approximations so that the simple expression for the total energy is reduced to a much simpler form.

One of the key points in doing this is to remark that since the energy expression is variational, we commit only small (and hopefully negligible) errors if we use a density distribution that differs slightly from the true ground-state density. Now it has long been known from practical experience that the electronic density distribution in condensed matter systems can often be well represented as a superposition of atomic density distributions. So what is suggested is that it is good enough to represent the density $\rho(r)$ for a superposition of the densities for each atom sitting in a uniform electron gas. This uniform density is taken to be an average of the density distribution due to the neighbouring atoms. This Ansatz still does not quite determine the total energy, because the kinetic energy associated with the superposition of densities is not known. This kinetic energy can also be reformulated in terms of the single-particle energies of the effective Schroedinger equation (equation (7)). But in certain cases (for example a

perfect solid) it can be argued that this single-particle contribution changes only by a negligible amount as one goes from the atom in the uniform electron gas to the atom in the solid. With this and some other minor approximations, the total energy can be written in a remarkably simple form:

$$E = \sum_i E_{c,i}(n_i), \tag{9}$$

where $E_{c,i}(n_i)$ is the embedding energy of atom i in the uniform electron gas of density n_i. Norskov and co. have shown that this formula gives a very satisfactory account of the equilibrium lattice parameter, bulk modulus and cohesive energy of the simple metals. The theory can also be extended to treat surfaces, defects and impurities. They have shown that a fairly good account is given of the relaxations at different crystal surfaces of aluminium.

Very recently, they have used their theory in Monte Carlo simulations of crystalline aluminium. The main object here has been to study whether their 'effective medium' approach, in addition to giving the correct lattice constant, also gives a successful account of the lattice expansion. Since they are using classical simulation, a meaningful comparison can, of course, only be made above about the Debye temperature (i.e. above about 300K). The predictions are quite impressive: above 300K, the simulated expansion coefficient is $2 \times 10^{-5} K^{-1}$, which is to be compared with the experimental value of $2.4 \times 10^{-1} K^{-1}$.

Everything in the garden is not lovely, unfortunately. They are currently struggling with the problem of calculating the formation energy of the vacancy in aluminium. Their effective medium approach gives a value of about 1.2eV, which is considerably higher than the experimental value (0.66eV). They have been sufficiently puzzled by this to ask whether the various experiments - which converge on about the same value - could all be wrong. Monte Carlo work is now in progress to see whether the temperature variation of the formation energy is large enough to account for the discrepancy. It should be added that this problem of the vacancy in aluminium is a notoriously hard one - there have been many previous attempts at calculating the formation energy, none of which have been very convincing. I have my own calculations on this in progress, based on density functional theory plus pseudopotentials. The calculations are still being refined, but appear to be settling down at about 0.5eV.

An area where the effective medium approach is particularly illuminating is in the calculation of impurity energies in metals. Norskov and co. have shed much light recently on hydrogen in metals, a subject dear to my own heart. They have shown that the energy of hydrogen as a function of position in a metal is very well accounted for by saying that it depends only on the host electron density at that position. This argument predicts that the binding energy of hydrogen to a metal surface will be essentially the same for all metals, which is what is found experimentally. The theory also gives good values for the heat of solution of hydrogen in the bulk metal, and the binding energy to vacancies. It seems certain that this approach will have an important unifying effect on our understanding of hydrogen in metals.

Another important area of work, which unfortunately I had not enough time to hear about properly, concerns the theory of catalysis at metal surfaces. here too, effective medium ideas have given important insights. They have been successful recently in predicting the rate of NH_3 synthesis from N_2 and H_2 at transition metal surfaces,

and the influence on this rate of enhancers (electropositive atoms like the alkalis) and poisoners (electronegative atoms like oxygen and sulphur).

While I was in Lyngby, I also had a chance to catch up with news of Rodney Cotterill. He and his group are now very much into neural networks. One of the fascinating things they have been busy with is setting up networks that can learn the relationships between patterns of information. They have applied this to the problem of the relationship between amino-acid sequence and secondary structure in proteins. Basically the network is presented with both the sequence and the structure of a large number of proteins. It gets to work on this and, by a process of trial and error, does the best job it can of constructing the connection between the two. This connection can then be used to predict the unknown secondary structure of a protein whose sequence has been determined. Tests suggest that a success rate of around 80% is achievable, which is considerably better than other methods. I felt that the day when computers put us all out of a job seemed a little nearer.

Finally, my discussion with Per Hedegard at the Oersted Institute, though all- too-brief, was extremely instructive. He and his collaborators have been busy recently in two main areas: (i) quantum effects of hydrogen in metals; (ii) high T_c. Ignorance prevents me from commenting intelligently on the second of these. At low temperatures, hydrogen passes between interstitial sites in a metal entirely by quantum tunnelling. At very low temperatures, the tunnelling frequency can be directly measured in some metals by quasielastic neutron scattering. The theoretical interpretation of this tunnelling frequency though, is highly non-trivial, because the hydrogen is coupled to the vibrational and electronic degrees of freedom. Both the phonons and the electrons have the effect of renormalizing (in fact reducing) the tunnelling frequency. This is an example of the controversial problem of tunnelling of a particle coupled to a thermal bath. In this kind of problem, Feynman's path- integral formulation of quantum mechanics is extremely powerful. There are two reasons for this. Firstly, it provides the basis for quantum simulation [8]. Secondly, it gives a means of 'integrating out' the bath degrees of freedom and reducing the problem to an effective single-particle problem, with the bath effects appearing as a retarded self interaction of the particle.

Concerning the phonons, Hedegard [9] has been able to use the path-integral approach to give a justification for a rather ad hoc approach that has been used in previous theoretical work. The effect of the electrons is much more subtle, and progress is somewhat hampered by he fact that there is some uncertainty about the size of the effect to be expected. But the progress he is making will undoubtedly help to clarify this tricky but fascinating area of the subject.

All in all, this was an extremely rewarding and instructive couple of days, and I am grateful to CCP5 for making it possible.

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MOLECULAR DYNAMICS SIMULATION OF ALKALISILICATE GLASSES

B. Vessal, M. Leslie, and C.R.A. Catlow

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In this note we report on the molecular dynamics (MD) simulation of several alkalisilicate glasses. The computational details are reported elsewhere [1] , but briefly the MD simulation is undertaken using a monoclinic simulation box with a volume of 7538.9 cubic Angstroms and containing 576 ions.

In all cases we have 128 silicon ions, 320 oxygen ions, and 128 alkali ions. Newton's equations of motion are integrated using Beeman's algorithm and a time step of three femtoseconds. The glasses were prepared by melting a system of 576 ions having the crystal structure of sodium disilicate with the sodium ions replaced by the appropriate alkali ions at 6000 K, and then cooling successively to 2500 K, 1200 K, 625 K, and 293 K for seven and a half picoseconds, giving a total annealing time of thirty seven and a half picoseconds. The velocities were rescaled during the first three picoseconds at each temperature to equilibrate the system.

The long range coulomb part of the potential is evaluated using Ewald's method. A four range Buckingham potential is used to model the short range interactions between different ions.

An essential feature of our new potential model is the inclusion of a three body potential between the O-Si-O triads. Consider the three ions i, j, and k interacting according to the following potential

$$E_{ijk} = \frac{1}{4} A_{ijk} B_{ijk} B_{ijk} exp(-r_{ij}/\rho_1) exp(-r_{ik}/\rho_2) \tag{1}$$

where

$$A_{ijk} = \frac{1}{2} k_{ijk} (\theta_0 - \pi)^2$$

$$B_{ijk} = (\theta_0 - \pi)^2 - (\theta - \pi)^2$$

k_{ijk} is the three body spring constant and θ_0 is the equilibrium bond angle, i.e. 109.45 degrees, and θ is the calculated bond angle.

The parameters for the short range and three body potentials are determined using our THBFIT code which uses a least-squares fitting method to get the best agreement between the observed and the computed properties of alpha quartz. The alkali oxygen potentials are taken from reference [2]. The relevant parameters in the short range and the three body potentials are listed in Table 1.

The radial distribution functions (RDF), and the bond angle distributions (BAD) were calculated after running for six picoseconds at 293 K and were accumulated every ten timesteps for three hundred timesteps. The RDF for cesium disilicate glass,

Table 1: Potential Parameters

Parameter	$Si-O$ Potential	$O-O$ Potential
A_{ij}/eV	1005.1563	497896.9000
ρ_{ij}	.3277	.149
$C_{ij}/(eVA^6)$	25.	52.12
$k_{ijk}/(eV/rads^2)$	729.0189	
$A_1/(eV/A^5)$	-15.6911723	-.7894742
$B_1/(eV/A^4)$	165.2261909	13.0952378
$C_1/(eV/A^3)$	-697.1112644	-86.6996290
$D_1/(eV/A^2)$	1484.1446300	286.4412780
$E_1/(eV/A)$	-1611.8417758	-472.3745705
$F_1/(eV)$	724.2200617	311.1788448
$P_1/(eV/A^3)$	-.0233139	-.0251198
$Q_1/(eV/A^2)$	.2214821	.3052061
$R_1/(eV/A)$	-.6702747	-1.2208242
$S_1/(eV)$	.6187898	1.5952103
r_1/A	1.5	2.9
r_2/A	2.5	3.6
r_3/A	3.5	4.2
r_c/A	7.6	7.6

potassium disilicate glass, 33.3% potassium + 66.7% cesium disilicate glass, and 66.7% potassium + 33.3% cesium disilicate glass are shown in Figs. 1-8.

The Si-O RDF are essentially similar with two peaks at 1.55 A, and 2.2 A. The second peak is due to the five coordinated silicon atoms. The Cs-O peak in Fig. 2 is at 2.9 A which is quite close to the sum of the cesium , and the oxygen ionic radii (1.67 A, and 1.21 A respectively). Also the K-O npeak in Fig. 4 is at 2.75 A which is not in good agreement with the sum of the potassium, and the oxygen ionic radii (1.33 A, and 1.21 A respectively). This could be due to the deficiencies in the K-O potential which is used.

The BAD for lithium disilicate glass are shown in Figs. 9-11. The O-Si-O BAD has a maximum at the tetrahedral angle with a shoulder at 98 degrees which is again due to five coordinated silicon atoms. The Si-O-Si BAD has a wide distribution with a maximum at 161.5 degrees.

The coordination numbers of the alkali ions are determined using a cutoff of 2.7 A for lithium, 3.0 A for sodium, 3.4 A for potassium, and 3.7 A for cesium. The coordination numbers of the alkali ions are l listed in Table 2, while the coordination numbers of the silicon ions are gathered in Table 3. It can be seen from Table 2 that the smaller the alkali ion the lower is the coordination number, something which is expected. Also the smaller the alkali ion the sharper is the distribution of the coordination numbers. Also it is evident from Table 2 that in all of the glasses that are studied most of the silicon atoms are four coordinated, and the coordination number distribution of silicon in glasses containing smaller alkali ions are sharper.

As can be seen from the RDF, the BAD, and the coordination numbers we have a relatively high percentage of five coordinated silicons which should not be there according

Table 2: Coordination Number of Alkali Ions

Coord. No.	$Li_2Si_2O_5$	$Na_2Si_2O_5$	$K_2Si_2O_5$	$Cs_2Si_2O_5$
1	.93%	0.0%	0.0%	0.0%
2	24.42	.78	0.0	0.0
3	44.13	15.80	.86	0.0
4	22.84	33.56	6.42	2.51
5	6.24	27.38	24.05	5.04
6	1.40	14.87	29.14	16.37
7	.03	6.39	21.19	26.01
8	.00	1.18	13.86	25.28
9	.00	.05	3.57	14.78
10	.00	.00	.85	6.20
11	.00	.00	.05	2.90
12	.00	.00	.00	.82
13	.00	.00	.00	.08

Table 3: Coordination Number of Silicon Ions

Coord. No.	$Li_2Si_2O_5$	$Na_2Si_2O_5$	$K_2Si_2O_5$	$Cs_2Si_2O_5$
2	0.0%	.34%	.20%	.19%
3	11.3	13.81	15.56	11.71
4	79.50	72.26	66.7	64.59
5	8.61	11.31	16.01	21.65
6	.59	2.28	1.53	1.86

to the experiment. So we are refining our potential model currently to overcome this problem.

Acknowledgements

We want to thank Bill Smith, M. Amini, and David Fincham for fruitful discussions.

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[1] B. Vessal, M. Leslie, and C.R.A. Catlow, Molecular Simulation, submitted.

[2] S.C. Parker, Ph. D. Thesis, University College London (1982).

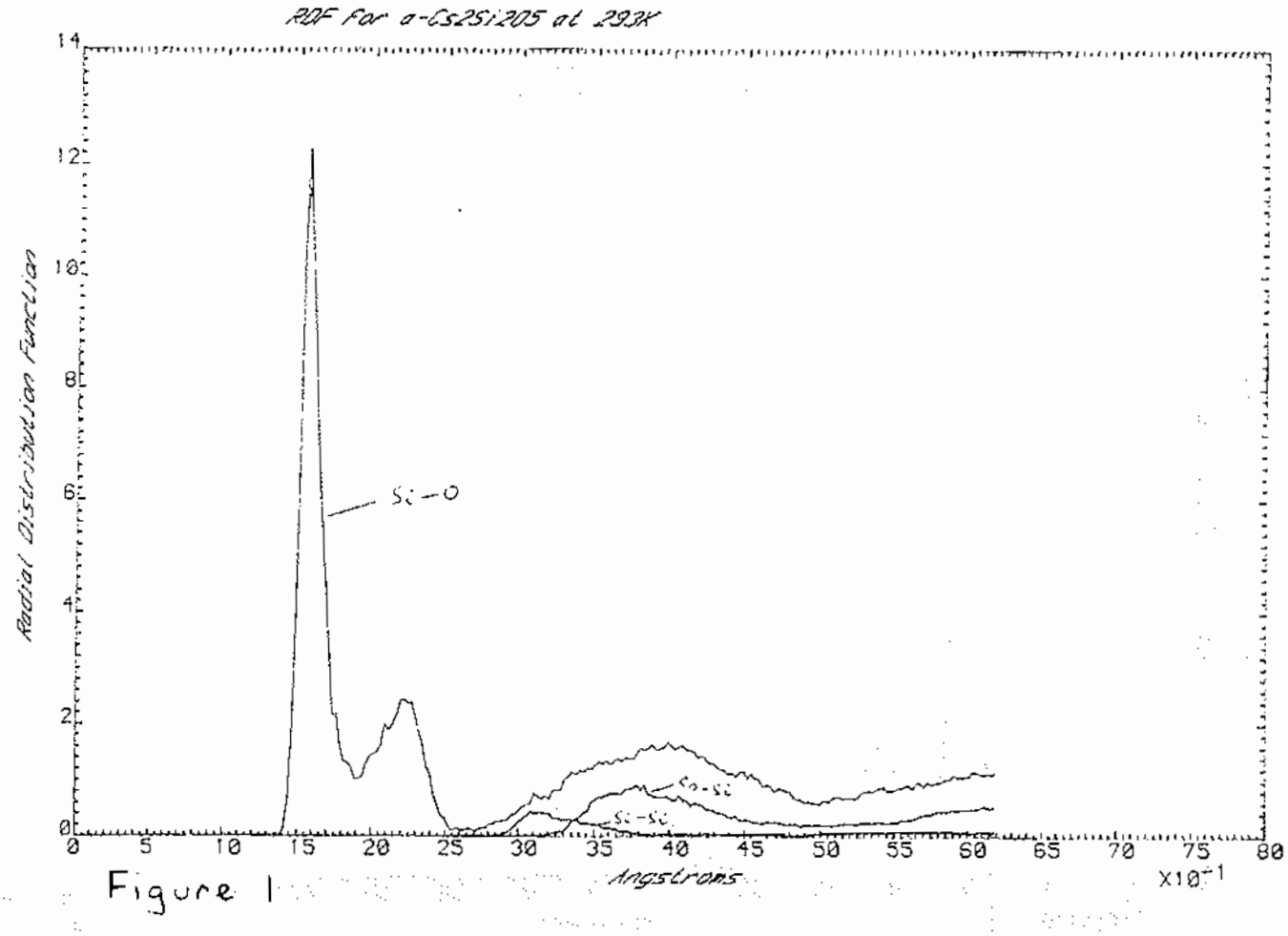

Figure 1

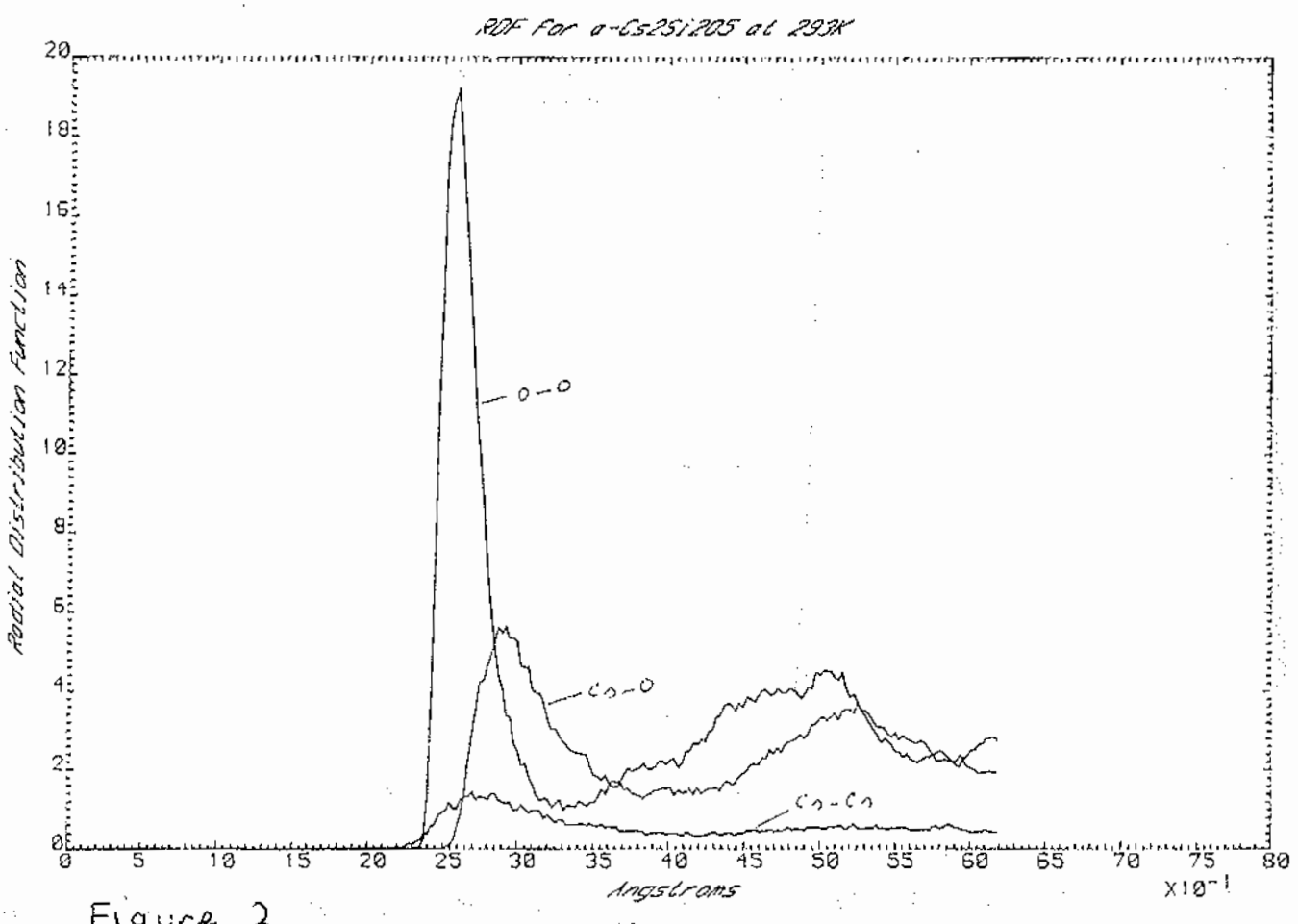

Figure 2

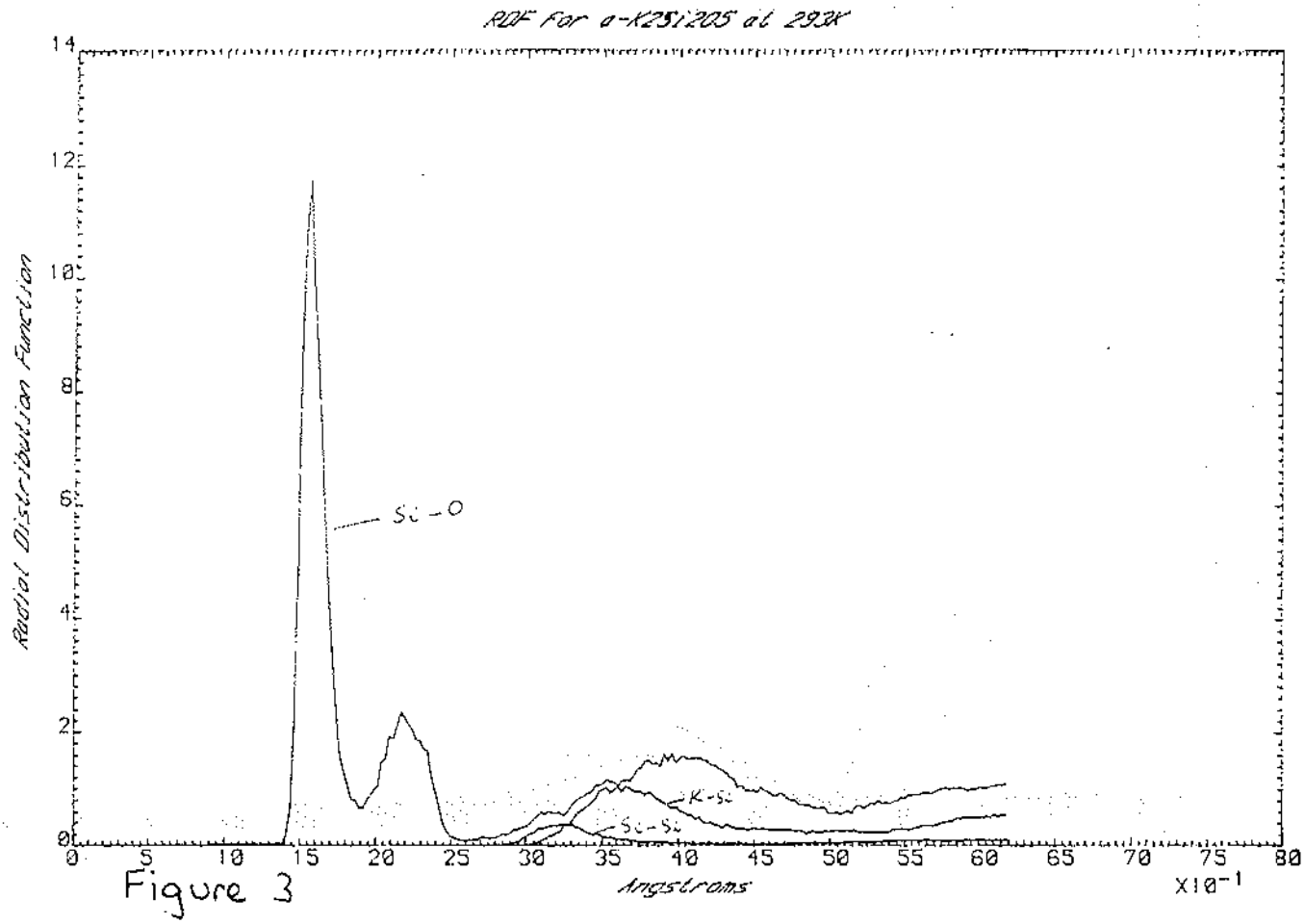

Figure 3

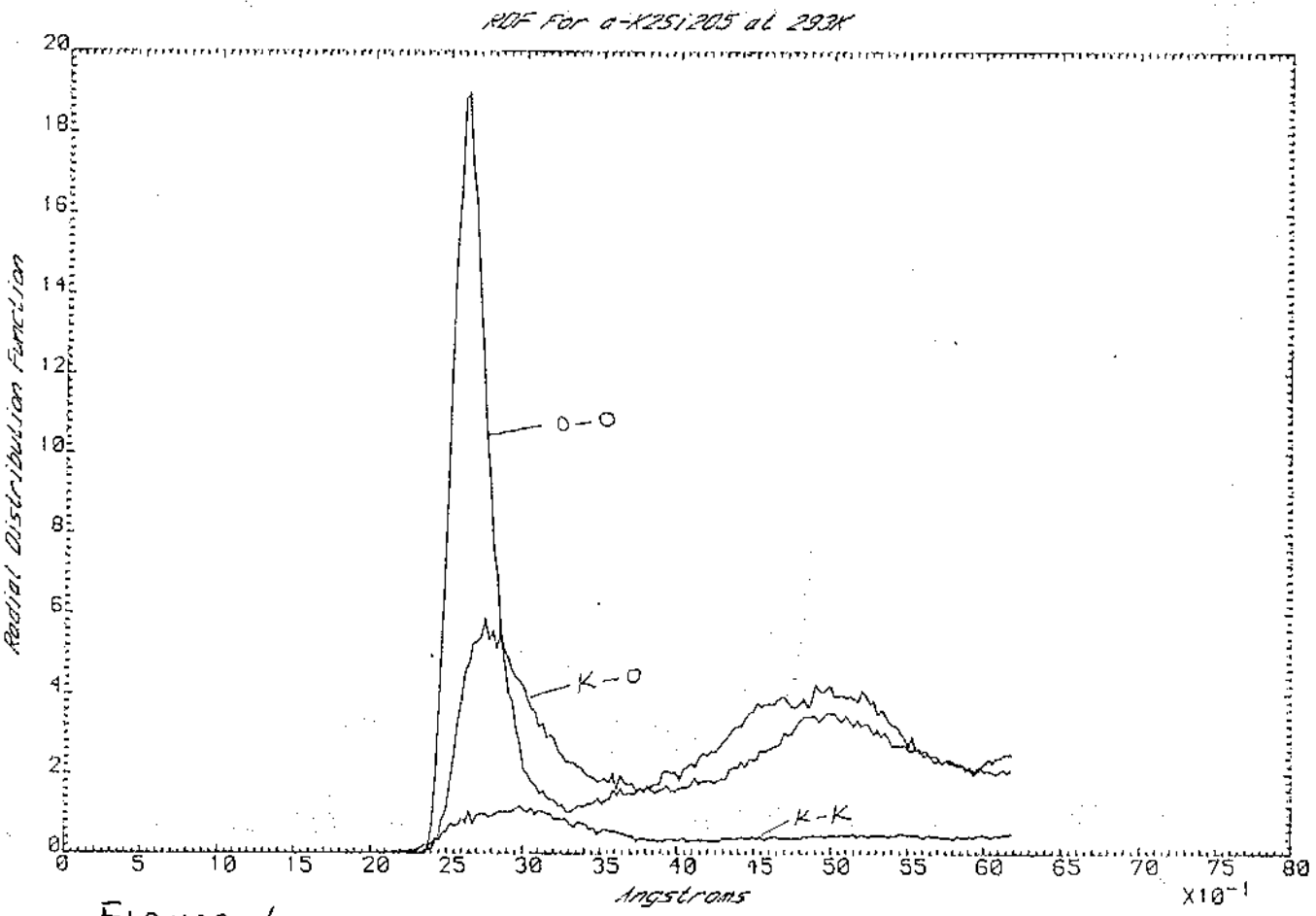

Figure 4

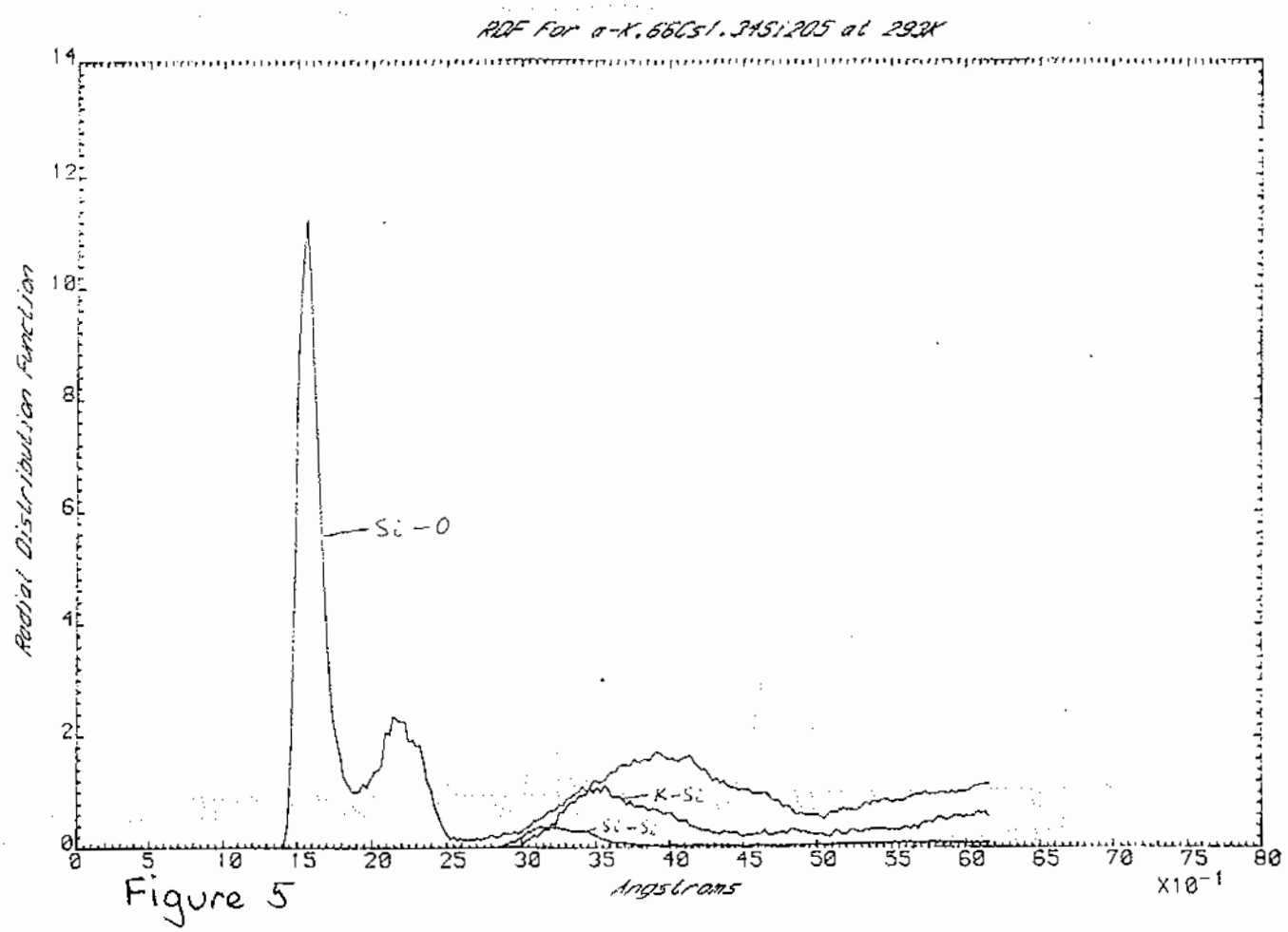

Figure 5

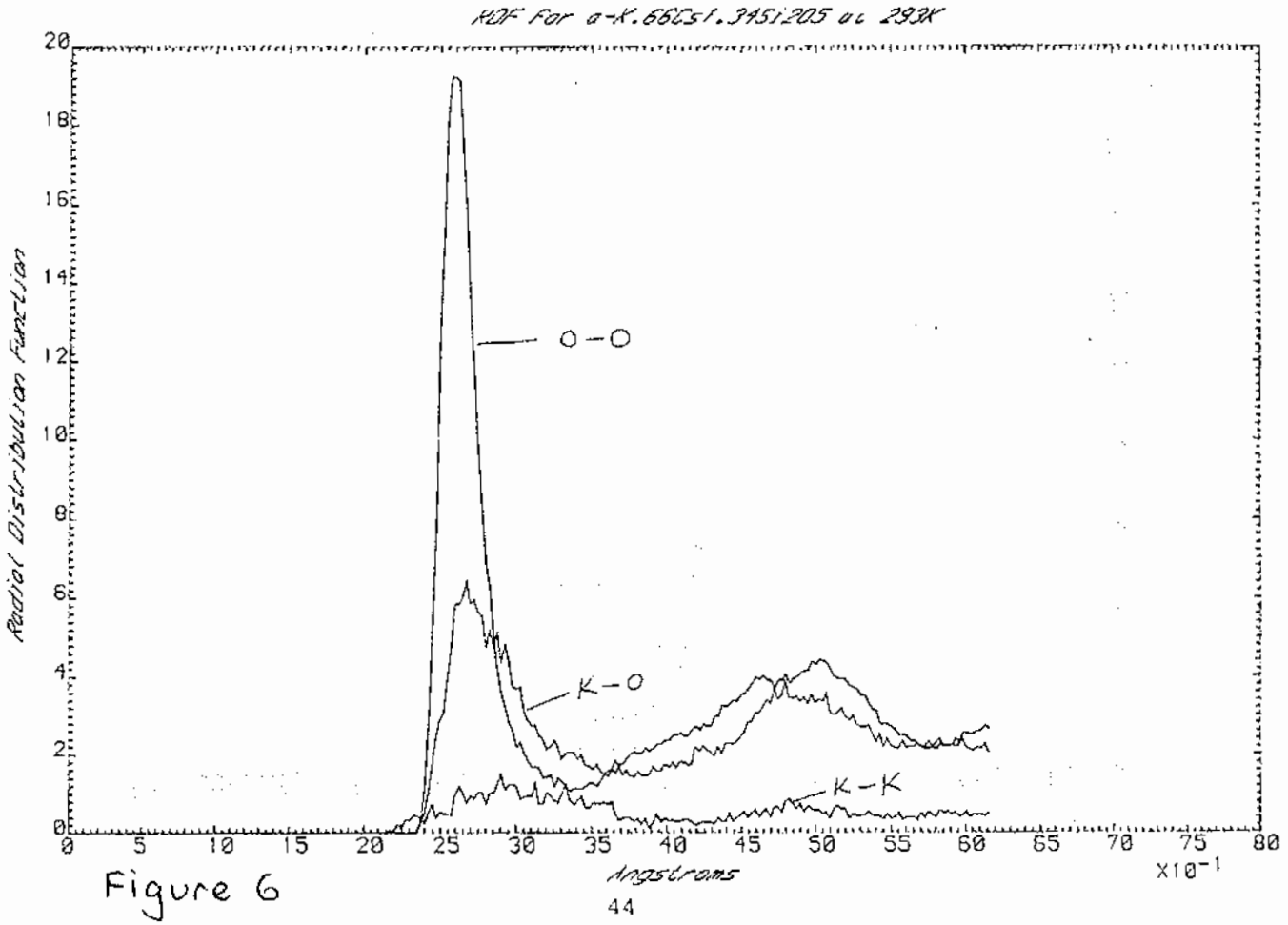

Figure 6

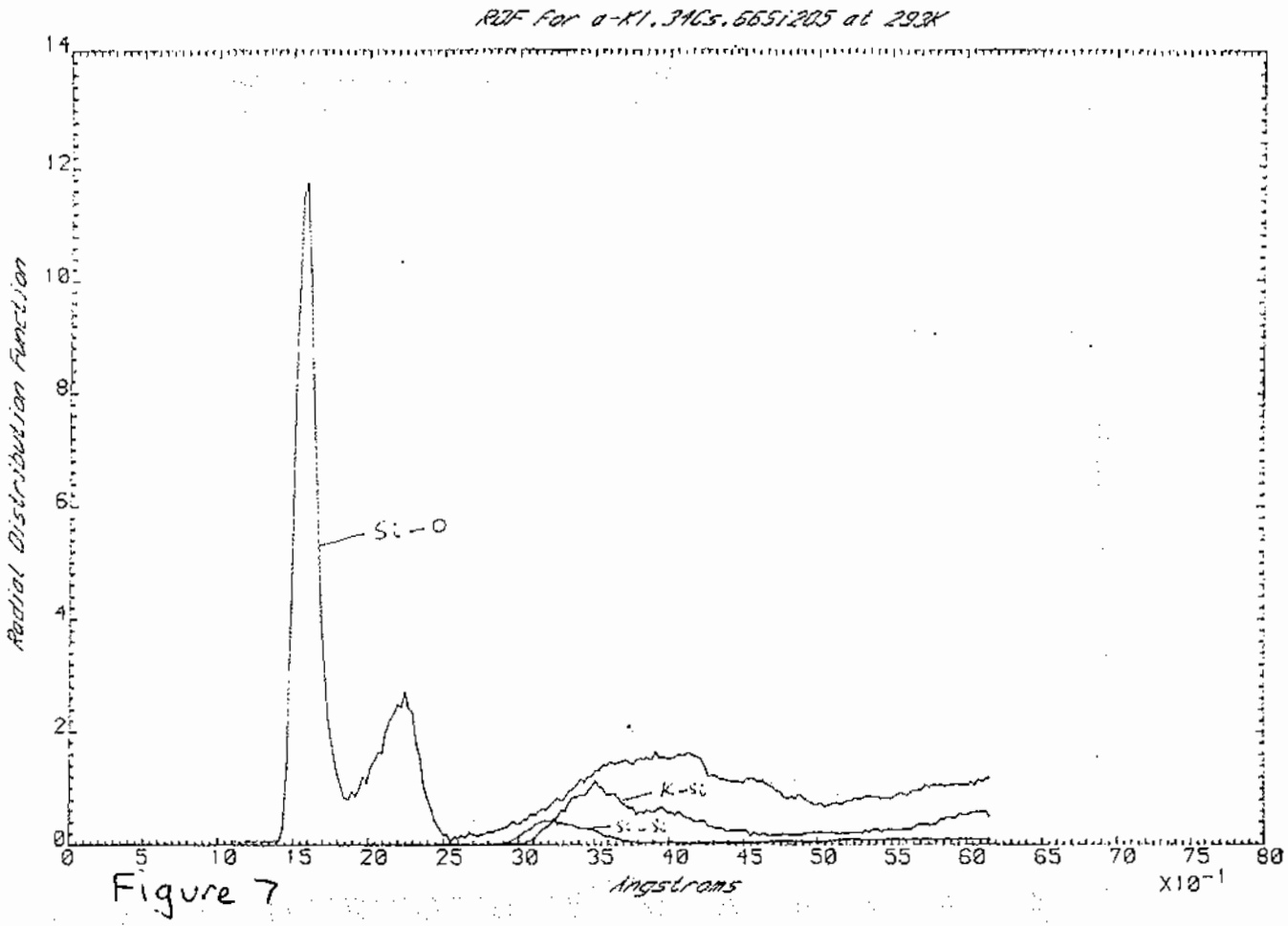

Figure 7

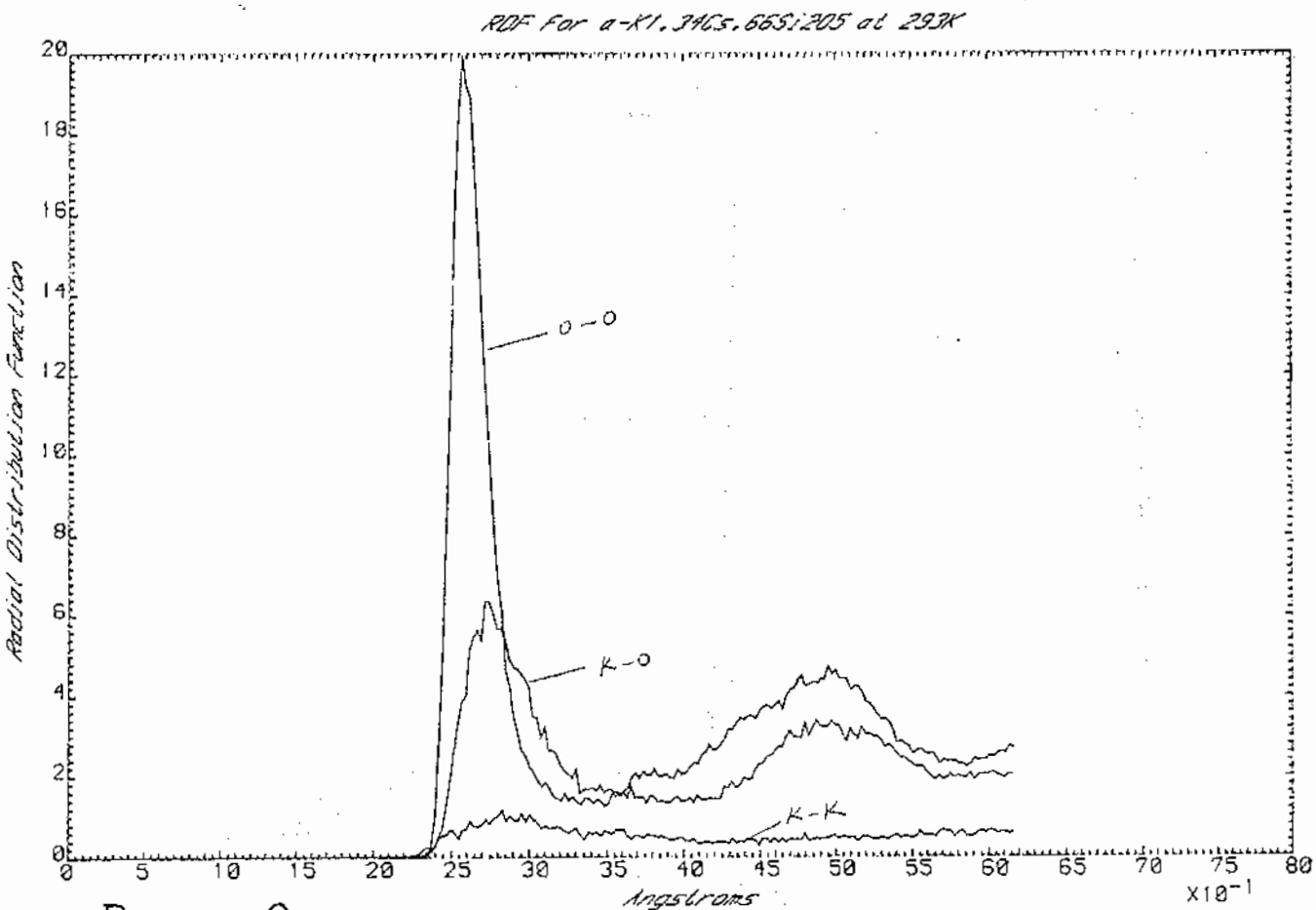

Figure 8

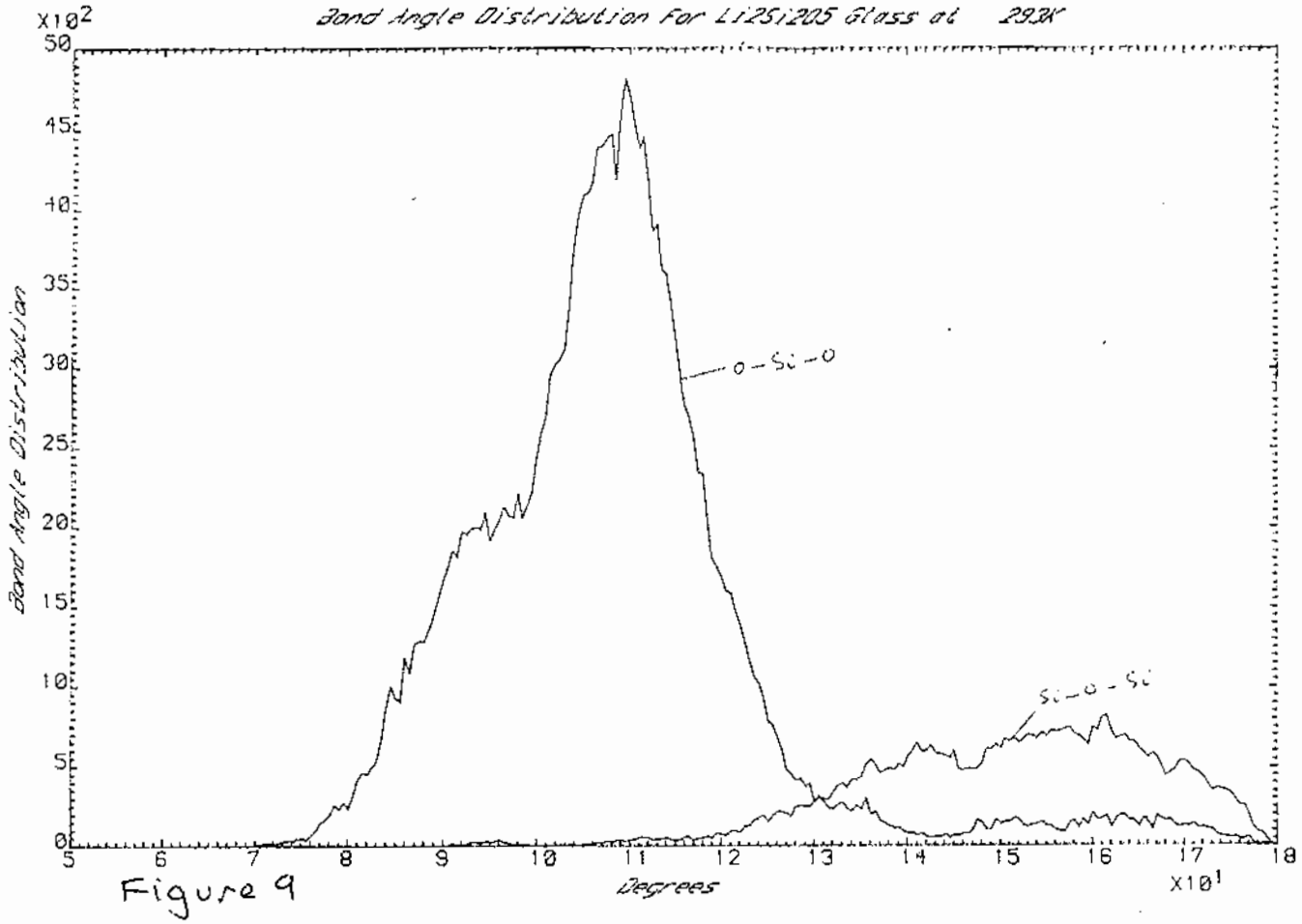

Figure 9

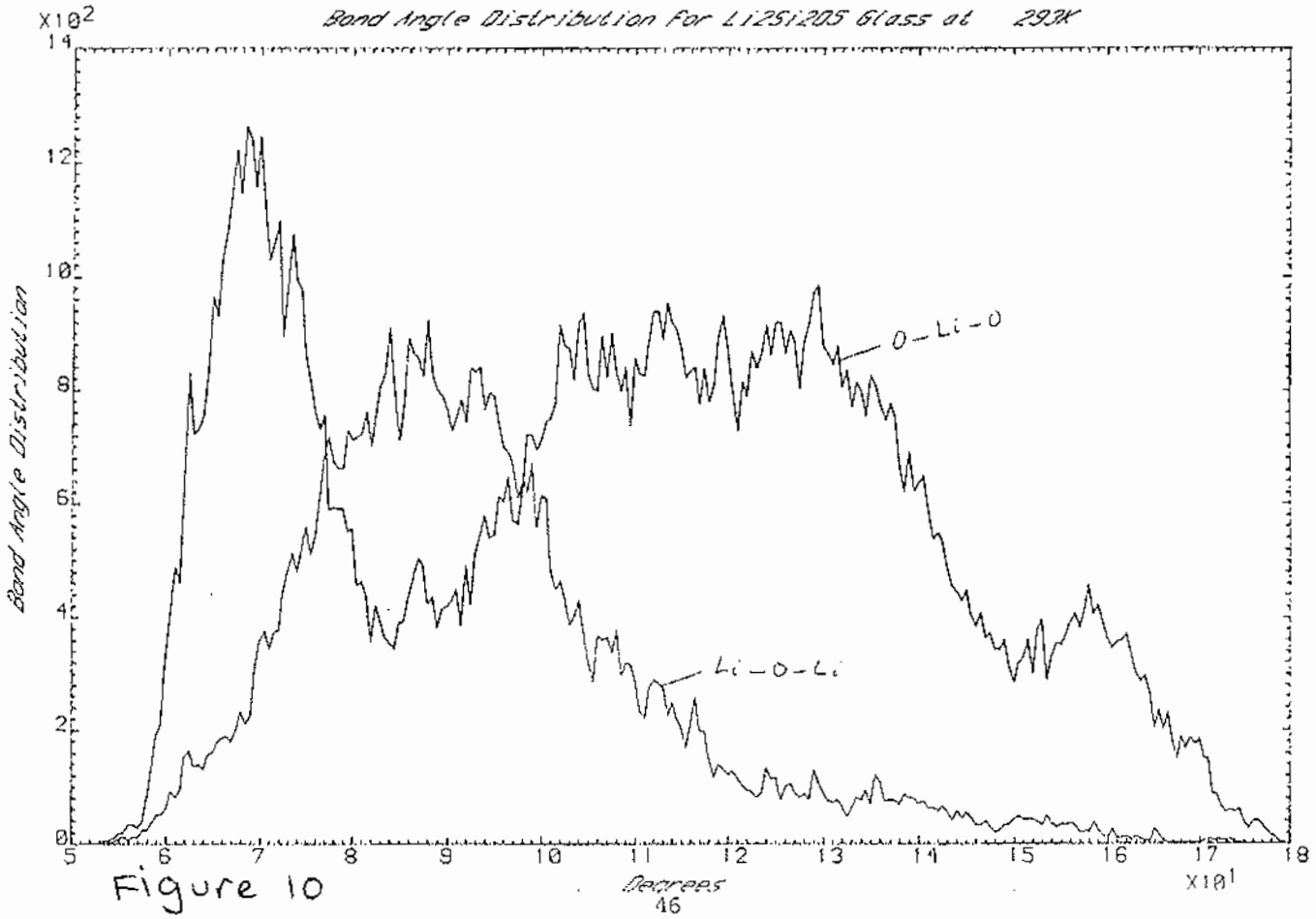

Figure 10

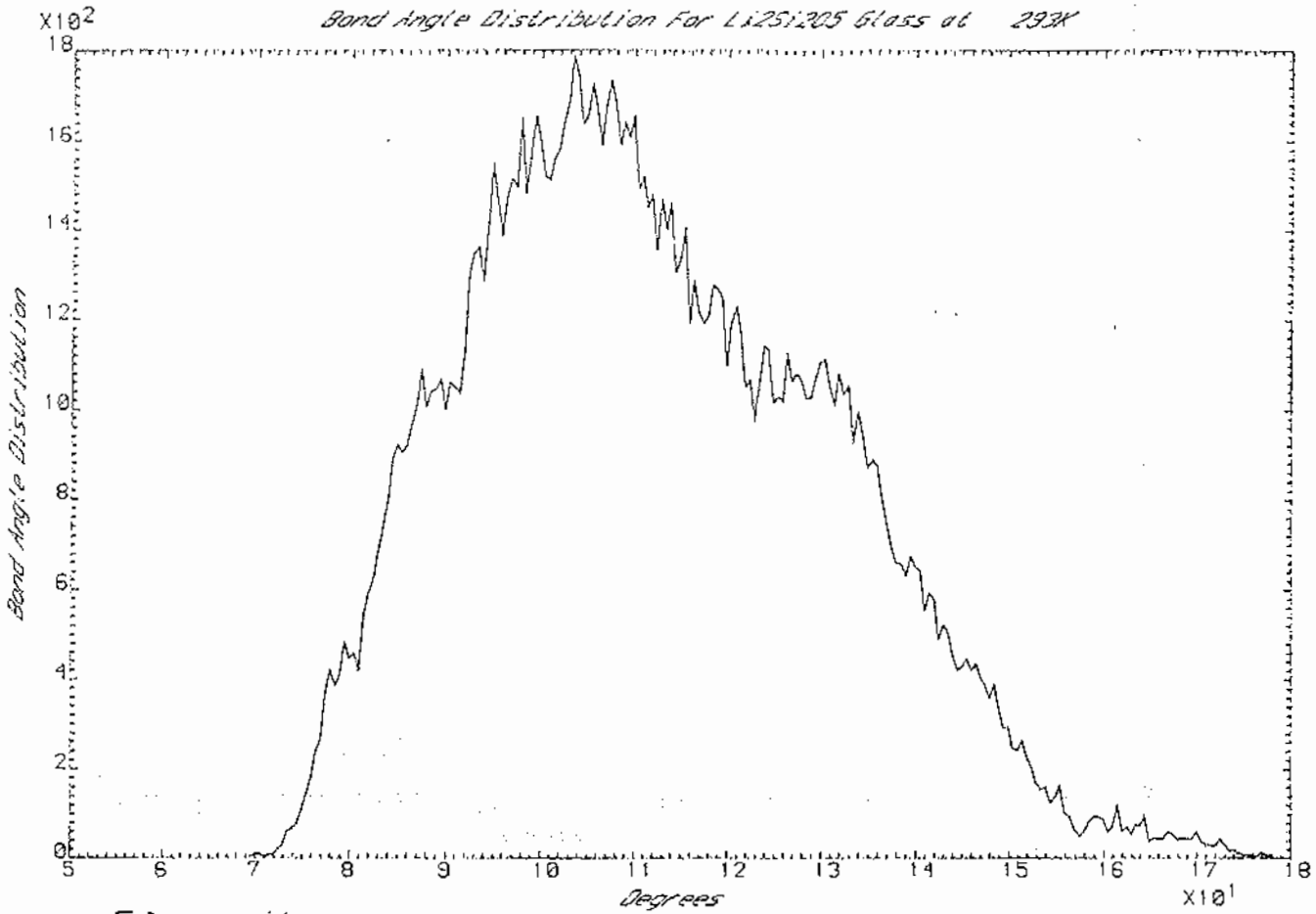
Bond Angle Distribution For Li2SiO5 Glass at 293K
X10^2
18
16
14
12
10
8
6
4
2
0
Bond Angle Distribution
5
6
7
8
9
10
11
12
13
14
15
16
17
18
Degrees
X10^1

Figure 11

CONSTANT PRESSURE SIMULATION WITH COULOMBIC INTERACTION

Tue Nguyen

Massachusetts Institute of Technology, Cambridge, MA 02139, U.S.A.

1. Introduction

Constant pressure simulation (Parrinello-Rahman technique [1]) is very useful in studying structural phase transition in solids. This note discusses the application of the method to the long range Coulombic potential.

2. Equations of motion for constant pressure simulation

This section summarizes the technique presented in the Parrinello-Rahman paper [1]. The reader is referred to [1] for more details. For the sake of simplicity, only the case where hydrostatic pressure is applied is considered here.

We start with the Lagrangian (eq. 2.8 of [1])

$$L = \frac{1}{2} \sum_{i=1}^{N} m_i \, \dot{\underline{s}}_i' \, \underline{G} \, \dot{\underline{s}}_i - U + \frac{1}{2} W \, \mathrm{Tr} \, \dot{\underline{h}}' \dot{\underline{h}} - p\Omega \qquad (1)$$

where the dots denote time derivatives, the apostrophe denotes matrix transpose, m_i is the mass of atom i, $\underline{h}$ is the transformation matrix connecting real coordinates $\underline{r}$ with reduced coordinates $\underline{s}$ ($\underline{r} = \underline{h}\underline{s}$), $\underline{G}$ is $\underline{h}'\underline{h}$, U is the

potential energy of the whole system, W is the wall mass, p is the external hydrostatic pressure, Ω is the volume (= det $\underline{h}$). The equation of motion for $\underline{s}_i$ is

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\underline{s}}_i}\right) - \frac{\partial L}{\partial \underline{s}_i} = 0$$

This gives

$$m_i G_{\delta\alpha} \ddot{s}_{i\alpha} + m_i \dot{G}_{\delta\alpha} \dot{s}_{i\alpha} + \frac{\partial U}{\partial r_{i\epsilon}} h_{\epsilon\delta} = 0$$

or

$$\ddot{s}_{i\beta} = -\frac{1}{m_i} h^{-1}_{\beta\epsilon} \frac{\partial U}{\partial r_{i\epsilon}} - G^{-1}_{\beta\delta} \dot{G}_{\delta\alpha} \dot{s}_{i\alpha}$$

or

$$\ddot{\underline{s}}_i = \frac{1}{m_i} \underline{\underline{h}}^{-1} \underline{F}_i - \underline{\underline{G}}^{-1} \dot{\underline{\underline{G}}} \dot{\underline{s}}_i \qquad (2)$$

where $\underline{F}_i = -\frac{\partial U}{\partial \underline{r}_i}$.

The equation of motion for the $\underline{h}$ matrix is

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\underline{\underline{h}}}}\right) - \frac{\partial L}{\partial \underline{\underline{h}}} = 0$$

This gives

$$W \ddot{h}_{\alpha\beta} = \sum_i m_i h_{\alpha\gamma} \dot{s}_{i\gamma} \dot{s}_{i\beta} - \frac{\partial U}{\partial h_{\alpha\beta}} - p \Omega h^{-1}_{\beta\alpha}$$

where the identity $\frac{\partial \Omega}{\partial h_{\alpha\beta}} = \Omega h^{-1}_{\beta\alpha}$ is used. Thus

$$W \ddot{\underline{\underline{h}}} = \sum_i m_i \underline{v}_i \underline{v}_i \underline{\underline{h}}'^{-1} - \frac{\partial U}{\partial \underline{\underline{h}}} - p \Omega \underline{\underline{h}}'^{-1} \qquad (3)$$

with the approximation $\underline{v}_i = \underline{\underline{h}} \dot{\underline{s}}_i$.

These equations of motion, (2) and (3), are general and can be applied to any interaction potential, including Coulomb or three body potential.

3. Coulombic interaction

Using the Ewald method, the Coulombic potential can be expressed as [2]

$$U = \frac{2\pi}{\Omega} \sum_{k\neq 0} A_k \sum_{j,m} Q_{jm} + \frac{1}{2} \sum_{j,m} \frac{q_j q_m}{r_{jm}} \operatorname{erfc}(\alpha r_{jm}) - \frac{\alpha}{\sqrt{\pi}} \sum_j q_j^2 \qquad (4)$$

where

$$A_k = \exp(-k^2/4\alpha^2) \,/\, k^2$$

$$Q_{jm} = q_j q_m \exp(i \underline{k}.\underline{r}_{jm}) = q_j q_m \exp(2\pi i \underline{n}.\underline{s}_{jm})$$

with $\underline{n} = (n_x, n_y, n_z)$ where n_x, n_y, n_z are integers and the reciprocal vector $\underline{k}$ is

$$\underline{k} = 2\pi \underline{\underline{h}}'^{-1} \underline{n}$$

The first term of (4) is called the Fourier space term U_F, the second term is called the real space term U_R, and the third term is the self term U_S. The self term U_S does not contribute to the equation of motion.

The equation of motion for the atom coordinates $\underline{s}_j$ requires the calculation of the force $\underline{F}_j$ which can be obtained from (4) by differentiation

$$\underline{F}_j = -\frac{4\pi}{\Omega} q_j \sum_k A_k \, i\underline{k} \exp(i\underline{k}.\underline{r}_j) \sum_m q_m \exp(-i\underline{k}.\underline{r}_m)$$

$$+ \sum \frac{q_j q_m}{r_{jm}^3} \underline{r}_{jm} \left[\operatorname{erfc}(\alpha r_{jm}) + \frac{2\alpha}{\sqrt{\pi}} r_{jm} \exp(-\alpha^2 r_{jm}^2)\right] \qquad (5)$$

The equation of motion for the box will require the calculation of $\frac{\partial U}{\partial h_{\alpha\beta}}$.

The real space term U_R gives

$$\frac{\partial U_R}{\partial h_{\alpha\beta}} = \frac{1}{2} \sum_{j,m} \frac{\partial U_R}{\partial r_{jm}} \frac{r_{jm\alpha} r_{jm\delta}}{r_{jm}} h^{-1}_{\beta\delta}$$

or

$$\frac{\partial U_R}{\partial h_{\alpha\beta}} = -\frac{1}{2} \sum_{j,m} q_j q_m \left[\frac{\operatorname{erfc}(\alpha r_{jm})}{r_{jm}} + \frac{2\alpha}{\sqrt{\pi}} \exp(-\alpha^2 r_{jm}^2)\right] \frac{r_{jm\alpha} r_{jm\delta}}{r_{jm}^2} h^{-1}_{\beta\delta} \qquad (6)$$

The Fourier space term U_F gives

$$\frac{\partial U_F}{\partial h_{\alpha\beta}} = \frac{\partial U_F}{\partial k^2}\frac{\partial k^2}{\partial h_{\alpha\beta}} + \frac{\partial U_F}{\partial \Omega}\frac{\partial \Omega}{\partial h_{\alpha\beta}}$$

or

$$\frac{\partial U_F}{\partial h_{\alpha\beta}} = \frac{4\pi}{\Omega}\sum_k A_k \sum_{j,m} Q_{jm}\left(1 + \frac{k^2}{4\alpha^2}\right)\frac{k_\alpha k_\delta}{k^2} h^{-1}_{\beta\delta} - \frac{2\pi}{\Omega}\sum_k A_k \sum_{j,m} Q_{jm}\, h^{-1}_{\beta\alpha} \qquad (7)$$

where the term Q_{jm} is independent of $h_{\alpha\beta}$ and $\frac{\partial k^2}{\partial h_{\alpha\beta}} = -2\, k_\alpha\, k_\delta\, h^{-1}_{\beta\delta}$

Putting (6) and (7) into (3), we have

$$W \underline{\underline{h}}'' = (\underline{\underline{\pi}} - p\underline{\underline{I}})\,\Omega\, \underline{\underline{h}}'^{-1}$$

with

$$\Omega\,\underline{\underline{\pi}} = \sum_j m_j \underline{v}_j \underline{v}_j + \frac{1}{2}\sum_{j,m} q_j q_m \left[\frac{\mathrm{erfc}(\alpha r_{jm})}{r_{jm}} + \frac{2\alpha}{\sqrt{\pi}}\exp(-\alpha^2 r_{jm}^2)\right]\frac{\underline{r}_{jm}\underline{r}_{jm}}{r_{jm}^2}$$

$$- \frac{4\pi}{\Omega}\sum_k A_k \sum_{j,m} Q_{jm}\left(1 + \frac{k^2}{4\alpha^2}\right)\frac{\underline{k}\,\underline{k}}{k^2} + \frac{2\pi}{\Omega}\sum_k A_k \sum_{j,m} Q_{jm} \qquad (8)$$

$\underline{\underline{\pi}}$ should be interpreted as the stress tensor since it is expected that the simulation cell is driven by the imbalance between internal and externally applied stresses.

4. Stress tensor calculation

In this section, I will show that equation (8) above is indeed the stress tensor for the Coulombic interaction. I will consider first the derivation for the diagonal stress components. The pressure is given by

$$p = kT\,\frac{\partial \log Z}{\partial V} \qquad (9)$$

where Z is the configuration integral (partition function)

$$Z = \int \exp(-\beta U)\, d\underline{r}^N$$

Using the scaling $\underline{r} = \Omega^{1/3}\,\underline{s}$, Smith [3] was able to calculate the pressure for the Coulombic system. Diagonal stress components also can be calculated with the same technique but with different scaling function. Using

$$r_\alpha = h_\alpha s_\alpha \quad ; \quad \alpha = x,y,z$$

where h_α is the cell size, the volume of the cell is then

$$\Omega = h_x h_y h_z$$

Keeping two dimensions of the cell constant and varying the third will allow us to calculate the pressure along that direction. For example

$$p_{xx} = kT \left.\frac{\partial \log Z}{\partial V}\right|_{h_y, h_z = \text{constant}}$$

Consider only the virial term (the kinetic term is simply NkT or $\Sigma\, mv^2$)

$$\Omega p_{xx} = - < \frac{\partial U}{\partial h_x} > h_x \qquad (10)$$

Inserting the expression to the Ewald sum (4), we have

$$\Omega p_{xx} = \frac{1}{2} \sum_{j,m} q_j q_m \left[\frac{\operatorname{erfc}(\alpha r_{jm})}{r_{jm}} + \frac{2\alpha}{\sqrt{\pi}} \exp(-\alpha^2 r_{jm}^2) \right] \frac{r_{jmx}^2}{r_{jm}^2}$$

$$- \frac{4\pi}{\Omega} \Sigma A_k \sum_{j,m} Q_{jm} \left(1 + \frac{k^2}{4\alpha^2}\right) \frac{k_x^2}{k^2} + \frac{2\pi}{\Omega} \Sigma A_k \sum_{j,m} Q_{jm}$$

Similarly, p_{yy} and p_{zz} can be calculated. Since the term for p_{xx} contains $r_{jmx} \cdot r_{jmx}$ and $k_x \cdot k_x$, it is reasonable to expect the term p_{xy} to contain $r_{jmx} \cdot r_{jmy}$ and $k_x \cdot k_y$. So we have

$$\Omega \underline{p} = \frac{1}{2} \sum_{j,m} q_j q_m \left[\frac{\operatorname{erfc}(\alpha r_{jm})}{r_{jm}} + \frac{2\alpha}{\sqrt{\pi}} \exp(-\alpha^2 r_{jm}^2) \right] \frac{\underline{r}_{jm} \underline{r}_{jm}}{r_{jm}^2}$$

$$- \frac{4\pi}{\Omega} \Sigma A_k \sum_{j,m} Q_{jm} \left(1 + \frac{k^2}{4\alpha^2}\right) \frac{\underline{k}\,\underline{k}}{k^2} + \frac{2\pi}{\Omega} \Sigma A_k \sum_{j,m} Q_{jm}$$

which agrees with the virial term of equation (8). So far as the diagonal elements are concerned, the $\underline{\pi}$ matrix (equation 8) is indeed the stress tensor for the Coulombic interaction.

When the off diagonal elements are considered, equation (9) can be written as

$$\Omega \underline{p} = \frac{\partial F}{\partial \underline{\underline{\varepsilon}}}$$

where F is the free energy (kT logZ) and $\underline{\underline{\varepsilon}}$ is the strain tensor. Using the scaling function $\underline{r} = \underline{\underline{h}}\ \underline{s}$ we have, after a long calculation (detail not given here),

$$\Omega \underline{p} = - < \frac{\partial U}{\partial \underline{\underline{h}}} > \underline{\underline{h}}'$$

which is a generalized form of (10).

5. Summary

Equations of motion for Coulombic interaction are derived using the Parrinello-Rahman method. These equations are useful for molecular dynamics simulation at constant stress.

I would like to thank Dr. W. Smith for his communication. I have greatly benefited from discussions with J. Lutsko.

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PROPOSAL OF A VECTORIZED MD ALGORITHM FOR A VERY LARGE NUMBER OF PARTICLES[1]

Jacek Mościński and Jacek Kitowski

Institute of Computer Science, AGH, 30-059 Cracow, Poland

INTRODUCTION

Recently we have presented the vectorized algorithm for a MD simulation of a very large number of particles interacting by short-ranged forces and confined in a long cylinder with periodic boundary conditions along the cylinder axis only [1]. The approach is suitable for fluids of uniform density. The algorithm is based on vectorized sorting of particles (which is fast, and according to Sullivan et al. [2] takes less than 10 % of CPU time per MD timestep) along the axis of the cylinder and gathering the values of the other two coordinates due to indices of the sorted list. Introduced in addition to the classical cutoff distance the integer cutoff number and a proper organization of data structures result in the fully vectorized force loop. In this note we present an idea of extending that approach to the 3D bulk system with classical periodic boundary conditions and of a very large (of order 10^4 to 10^5) number of particles. We hope to get some response (criticism would be specially welcome) from the Newsletter readers and maybe someone would like to try to

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[1] Talk presented at the "CCP5 Discussion Meeting - Parallel Computers and Molecular Simulation", University of Keele, UK, 6-7 April, 1988.

implement the scheme (and perform timings) on a vector machine which is unfortunately not available for us at present.

For simplicity in some parts of the text we limit our discussion to the 2D case because we believe that the implementation in the 3D model is based on the obvious extension.

ALGORITHM

The goal is to process the forces routine with a large degree of vectorization, and in order to accomplish this we have to devise a strategy for structuring the data. A 3D structure suitable for vector processing is correctly visualized as consisting of a collection of adjacent pencils of memory cells with suitable boundary conditions. In order to get this structure, first - one has to divide a computational box into strips of width $\geq$ cutoff radius RCUT and to sort particles into suitable strips (Fig. 1a), and second - to perform sorting of the particles within the strips along Z axis into ascending sequence of Z values and to gather X and Y coordinates due to Z indices (Fig 1b).

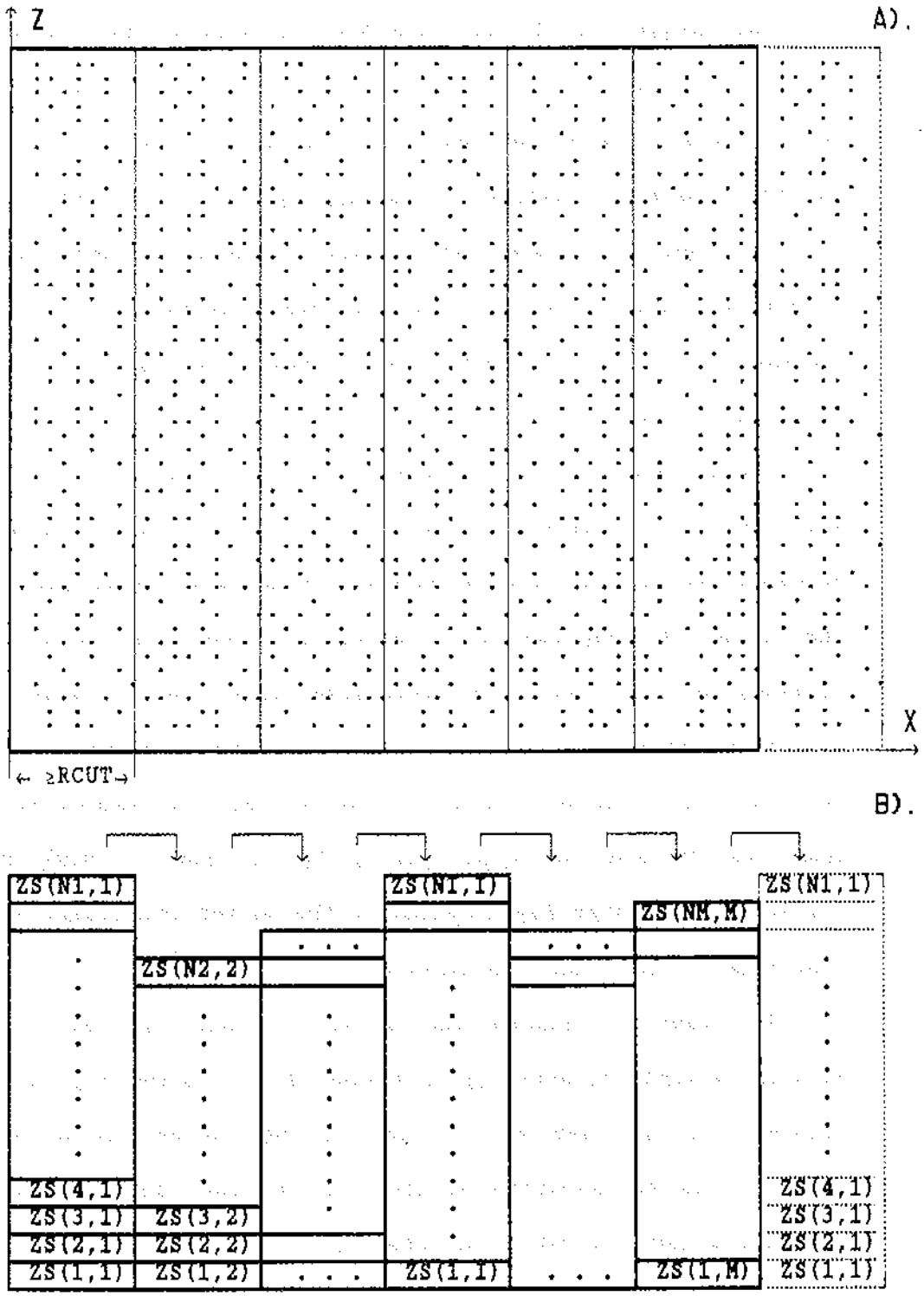


Fig. 1. The "linked-strip" method (NI-number of particles in the I-th strip). The arrows between the adjacent strips show the way of handling the boundary conditions in X direction.

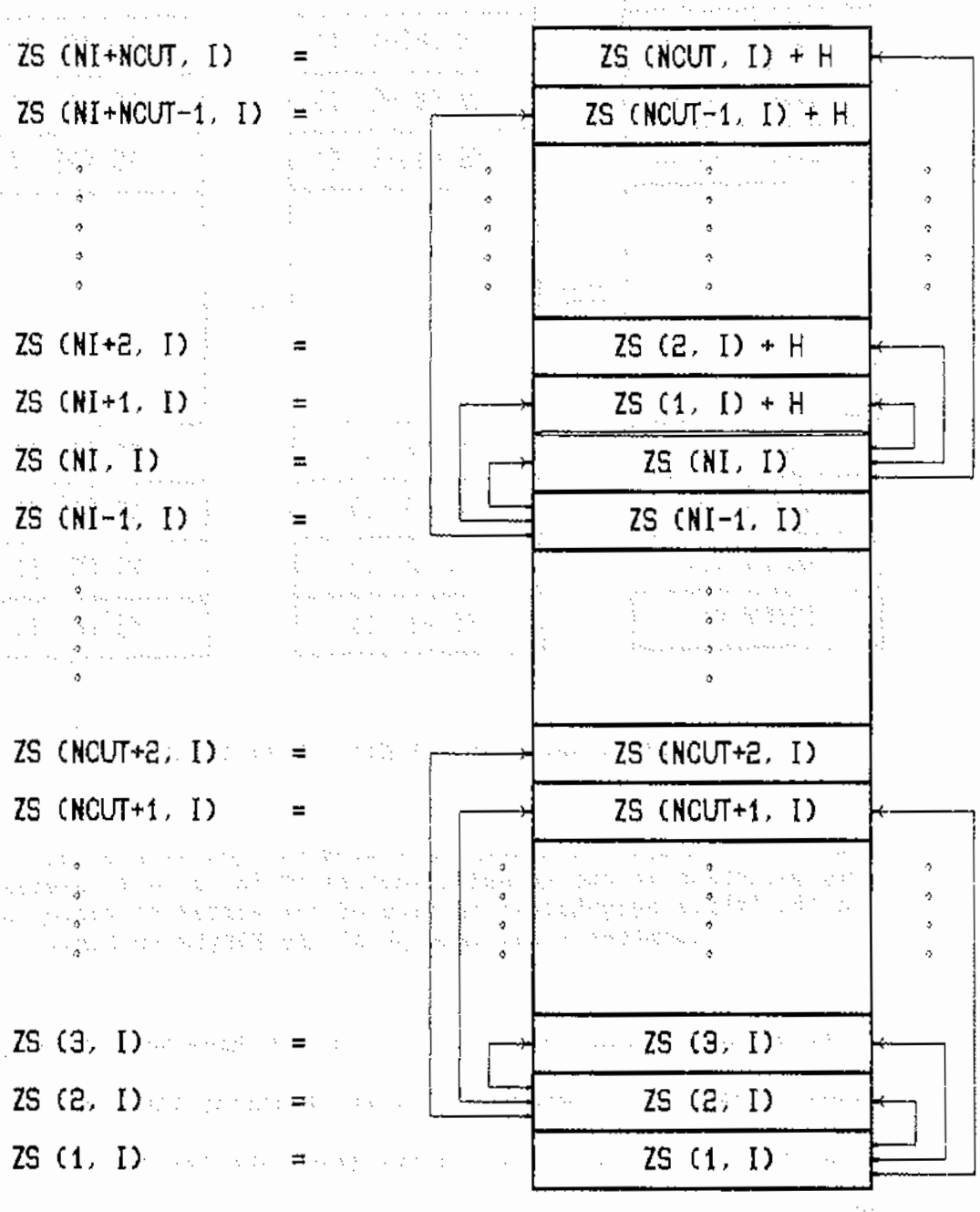
The integer cutoff distance NCUT is defined as a number of particles contained in a slice of the strip of a height equal to RCUT + DELTRC. The DELTRC represents an extra thickness introduced due to a stochastic nature of the mapping of RCUT to NCUT.

In order to handle the periodic boundary conditions in Z direction (along a strip) the extended vectors of X, Y and Z coordinates of length NINCUT = NI + NCUT (see Fig.2) are set up for each strip:

XS(1,I;NINCUT), YS(1,I;NINCUT), ZS(1,I;NINCUT)

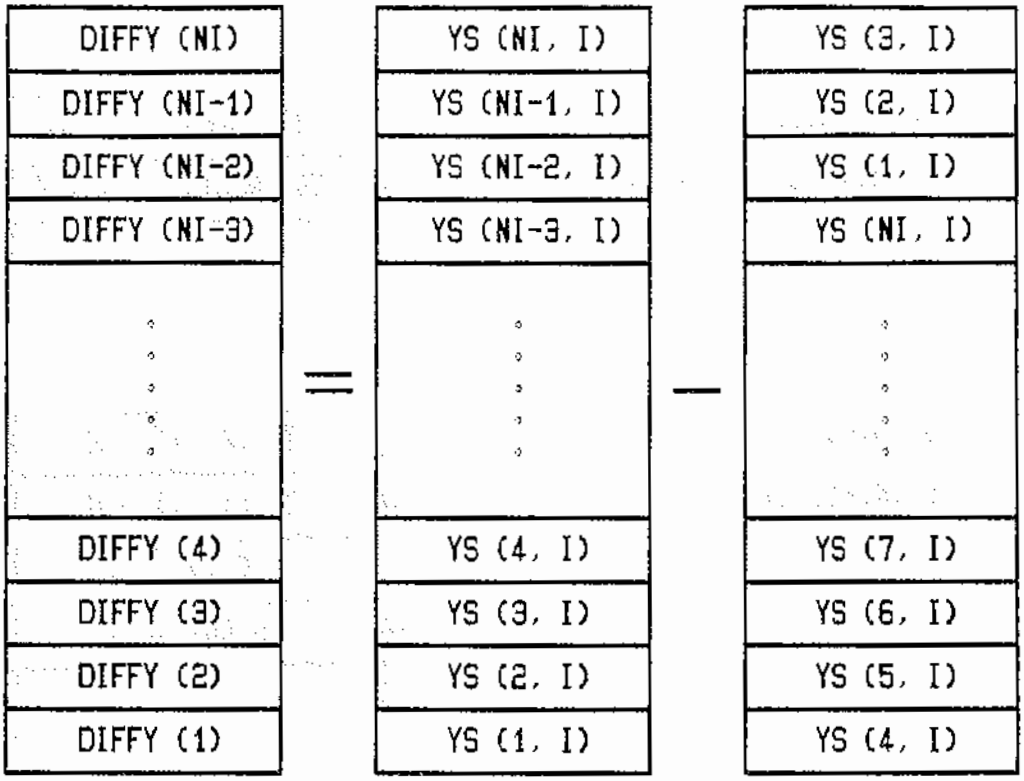
where NI is a number of particles in I-th strip. Using the extended vectors the forces between interacting particles within the strip are computed in a vectorized mode. Due to ascending ordering of the data the successive total vector differences throuhout the entire strip including periodic boundary conditions in Z direction can be formed by substracting the respective group from its forward neighbour simply by successive (NCUT times) off-setting the starting location of the sorted coordinate vectors (see Figs. 2 and 3 and the listing).

In order to handle the boundary conditions between the adjacent strips the strategy presented in Fig.1b and Fig. 4 can be adopted. In this way one can obtain the forces acting between particles in neighbouring strips. In 3D case, due to symmetry, each strip has its own 4 neighboring strips. The procedure seems to be also vectorizable. Due to the fact that the numbers of particles in the strips are a little bit different the vector alignment is necessary what is also related to the suitable choice of NCUT value.



$$ZS(1,I) \leq ZS(2,I) \leq \ldots \leq ZS(NI,I) \leq \ldots \leq ZS(NI+NCUT,I)$$

Fig. 2. An example of the data structure for the sorted extended vector ZS (of length equal to NI+NCUT) with the scheme of vectorized calculations of distances between particles lying within the I-th strip. H is the height of a computational box.




```
DIFFY(1;NI) = YS(1,I;NI) - YS(4,I;NI)
```

Fig. 3. An example of elementwise substraction within the I-th strip performed on the extended vectors YS for JJ = 4 (distances to the "third neighbours" in term of the sorted ZS vector are computed - see excerpt of the FORCES routine)

We do not discuss here the details of keeping the original indices of particles. Obviously, after obtaining the total forces acting on each particle the SCATTER procedure has to be used in order to return to original indices.

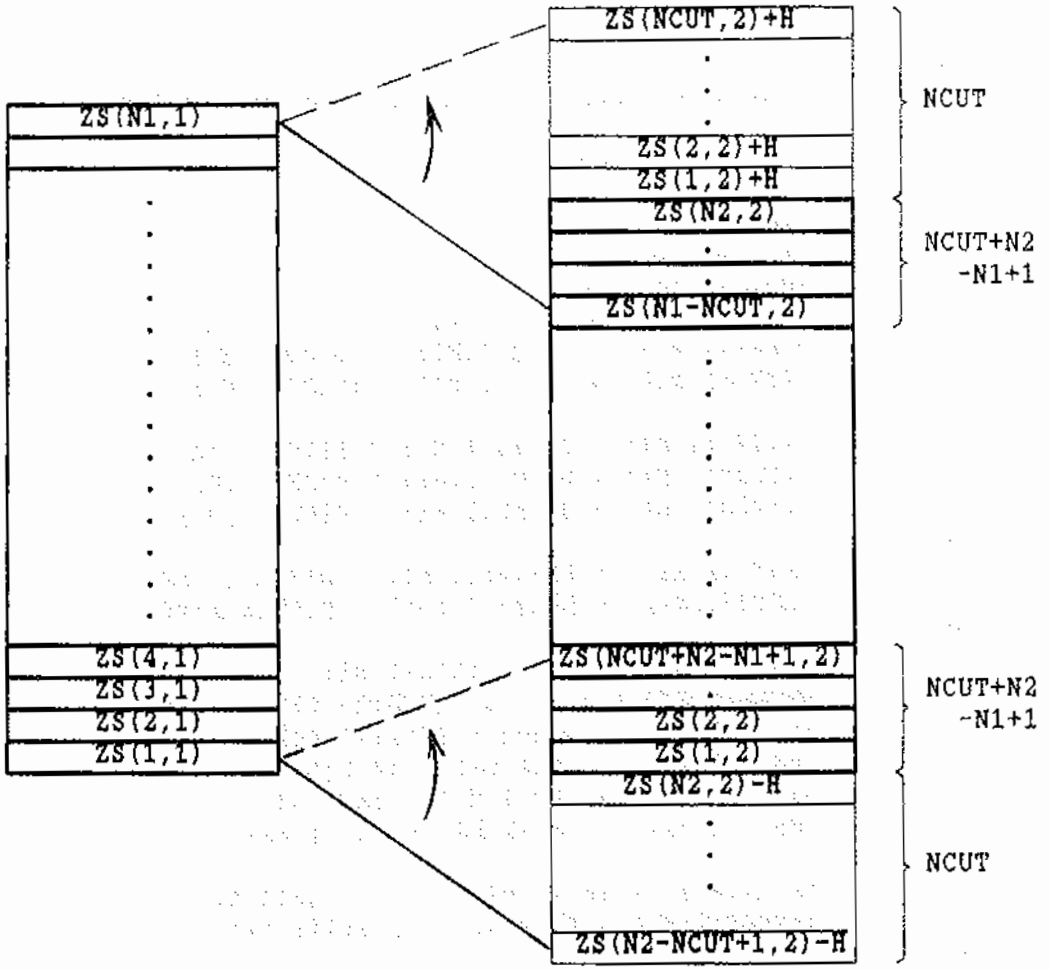


Fig.4. An example of the data structure for vectorized computing of the interactions between the particles in the adjacent strips.

EXCERPT OF THE FORCES ROUTINE

The presented listing is an excerpt of the FORCES routine and shows calculations of forces between the NI interacting particles lying in the same strip I. For the chosen computational units EPS24 = 24 * EPS = 1, (EPS is the LJ parameter). Values of the potential energy are rescaled (with EPS4 = 4 * EPS) outside the presented loop. In the listing the FORTRAN 200 notation is used.

```
C
C  4.L-J FORCES BETWEEN NI PARTICLES CONFINED IN I-TH STRIP
C
      DO 1 JJ = 2, NCUT+1
C
         J2   = -JJ + 2
         J1   =  JJ - 1
         NPJ2 =  NI - JJ + 2
         DIFFZ(1;NI)  = ZS(1,I;NI) - ZS(JJ,I;NI)
         DIFFY(1;NI)  = YS(1,I;NI) - YS(JJ,I;NI)
         DIFFX(1;NI)  = XS(1,I;NI) - XS(JJ,I;NI)
C
         DIST2X(1;NI) = DIFFX(1;NI) * DIFFX(1;NI)
         DIST2Y(1;NI) = DIFFY(1;NI) * DIFFY(1;NI)
         DIST2Z(1;NI) = DIFFZ(1;NI) * DIFFZ(1;NI)
C
         DIST2(1;NI)  = DIST2Z(1;NI) + DIST2Y(1;NI)
         DIST2(1;NI)  = DIST2 (1;NI) + DIST2X(1;NI)
C
         DIST2(1;NI)  = 1. / DIST2(1;NI)
         WHERE(DIST2(1;NI) .LT. RRCUT2) DIST2(1;NI) = 0.
         SR   (1;NI)  = SIGMA * DIST2(1;NI)
         SR2  (1;NI)  = SR(1;NI) * SR(1;NI)
         SR3  (1;NI)  = SR2(1;NI) * SR(1;NI)
         SR6  (1;NI)  = SR3(1;NI) * SR3(1;NI)
C
         FI (1;NI)  = SR3(1;NI) - 2. * SR6(1;NI)
         DIFPOT(1;NI) = FI(1;NI) * DIST2(1;NI)
C
         FXI (1;NI) = DIFPOT(1;NI) * DIFFX(1;NI)
         FYI (1;NI) = DIFPOT(1;NI) * DIFFY(1;NI)
         FZI (1;NI) = DIFPOT(1;NI) * DIFFZ(1;NI)
         FZI    (J2;J1) = FZI(NPJ2;J1)
         FYI    (J2;J1) = FYI(NPJ2;J1)
         FXI    (J2;J1) = FXI(NPJ2;J1)
C  FORCES ON CURRENT PARTICLES
         FORCX(1,I;NI)  = FORCX(1,I;NI) - FXI(1;NI)
         FORCY(1,I;NI)  = FORCY(1,I;NI) - FYI(1;NI)
         FORCZ(1,I;NI)  = FORCZ(1,I;NI) - FZI(1;NI)
C  REACTION FORCES ON NEIGHBOURING PARTICLES
         FORCZ(1,I;NI)  = FORCZ(1,I;NI) + FZI(J2;NI)
         FORCY(1,I;NI)  = FORCY(1,I;NI) + FYI(J2;NI)
         FORCX(1,I;NI)  = FORCX(1,I;NI) + FXI(J2;NI)
C
         SR63 (1;NI)  = SR6(1;NI) - SR3(1;NI)
         EP             = EP + Q8SSUM(SR63(1;NI))
C
1     CONTINUE
```

ACKNOWLEGMENTS

We are grateful to Professor Jerzy Kapelewski for arranging a financial support of our activity under the project number CPBP 01.08 D 4.3. We wish to thank to Miss Monika Bargiel for many valuable discussions and suggestions.

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Correction to Cray-Vectorised Link Cell Code

D.M. Heyes,
Royal Holloway and Bedford New College,
Egham,
Surrey TW20 0EX

July 4, 1988

In a recent issue of the CCP5 Newsletter a partially vectorised CRAY-1 Link Cell, LC, code was described [1]. Unfortunately, a logical error was present, showing up if any of the LC are empty. This was introduced by me and discovered by Mike Finnis at Harwell. Many apologies! A corrected version is given below. For the LJ density 0.85, T=1.5, N=864 and NLCX=4 the time per step is 0.21 sec on the CRAY-1S at ULCC (as opposed to 0.92 sec taking all interactions).

```
C       CALCULATE LINK CELL INDICES
        DO 110 L=1,NCELLS
110     LTOP(L)=0
        DO 1654 I=1,N
        IX=INT(FNLX*RX(I)/S)
        IY=INT(FNLX*RY(I)/S)
        IZ=INT(FNLX*RZ(I)/S)
        ICELL=1+IX+NLX*(IY+NLX*IZ)
        J=LTOP(ICELL)
        LTOP(ICELL)=I
        LINK(I)=J
1654    CONTINUE
C
C       SET CONTROL VARIABLES FOR LOOP OVER CELLS
        IX=1
        IY=1
        IZ=1
C
C       PRIMARY LOOP OVER ALL CELLS
        DO 5001 IC=1,NCELLS
        I=LTOP(IC)
C
C       BYPASS CELL IF EMPTY
        IF (I.EQ.0) GOTO 4999 !! NEW LINE !!
        M=0
99      M=M+1
        JADDR(M)=I
```

```
      RXX(M)=RX(I)
      RYY(M)=RY(I)
      RZZ(M)=RZ(I)
      I=LINK(I)
      IF (I.GT.0) GOTO 99
      MSTART=M
C
C     SECONDARY LOOP OVER NEIGHBOURING CELLS
      DO 4001 KC=2,14
      SX=0.0
      SY=0.0
      SZ=0.0
      JX=IX+NIX(KC)
      JY=IY+NIY(KC)
      JZ=IZ+NIZ(KC)
C
C     MINIMUM IMAGE CONVENTION
      IF((IX.EQ.NLX).AND.(JX.GT.IX))THEN
      JX=1
      SX=S
      ELSEIF((IX.EQ.1).AND.(JX.LT.IX))THEN
      JX=NLX
      SX=-S
      ENDIF
      IF((IY.EQ.NLX).AND.(JY.GT.IY))THEN
      JY=1
      SY=S
      ELSEIF((IY.EQ.1).AND.(JY.LT.IY))THEN
      JY=NLX
      SY=-S
      ENDIF
      IF((IZ.EQ.NLX).AND.(JZ.GT.IZ))THEN
      JZ=1
      SZ=S
      ELSEIF((IZ.EQ.1).AND.(JZ.LT.IZ))THEN
      JZ=NLX
      SZ=-S
      ENDIF
C
C     INDEX OF NEIGHBOURING CELL
      JC=JX+NLX*((JY-1)+NLX*(JZ-1))
      J=LTOP(JC)
C
C     BYPASS CELL IF EMPTY
      IF (J.EQ.0) GOTO 4001
```

```
199     M=M+1
        JADDR(M)=J
        RXX(M)=RX(J)+SX
        RYY(M)=RY(J)+SY
        RZZ(M)=RZ(J)+SZ
        J=LINK(J)
        IF (J.GT.0) GOTO 199
4001    CONTINUE
C       WE HAVE NOW FINISHED FINDING ALL NEIGH. PARTICLES OF BOX IC.
        MAX=M
        IF (MAX.GT.NVECT) STOP
        MSTART1=MSTART
        IF (MAX.EQ.MSTART) MSTART1=MSTART-1
        IF (MSTART1.LE.0) GOTO 2749 !! CHANGED LINE !!
C
C       NOW DO THE PARTICLE-PARTICLE INTERACTIONS
        DO 6001 IM=1,MSTART1
        RXI=RXX(IM)
        RYI=RYY(IM)
        RZI=RZZ(IM)
        MM=0
        DO 6002 M=IM+1,MAX
        X=RXI-RXX(M)
        Y=RYI-RYY(M)
        Z=RZI-RZZ(M)
        RR=X*X+Y*Y+Z*Z
        RRI=1.0/RR
        RRI=CVMGP(RRI,0.0,CU2-RR)
        MM=MM+1
        R6I=RRI*RRI*RRI
        R12I=R6I*R6I
        FF=24.0*(R12I+R12I-R6I)*RRI
        FXI(MM)=X*FF
        FYI(MM)=Y*FF
        FZI(MM)=Z*FF
6002    CONTINUE
        MMAX=MM
        I=JADDR(IM)
        FX(I)=FX(I)+SSUM(MMAX,FXI,1)
        FY(I)=FY(I)+SSUM(MMAX,FYI,1)
        FZ(I)=FZ(I)+SSUM(MMAX,FZI,1)
        DO 3422 KK=1,MMAX
        J=JADDR(IM+KK)
        FX(J)=FX(J)-FXI(KK)
        FY(J)=FY(J)-FYI(KK)
```

```
      FZ(J)=FZ(J)-FZI(KK)
3422  CONTINUE
6001  CONTINUE
2749  CONTINUE !! NEW LINE !!
4999  CONTINUE !! NEW LINE !!
C
C     PRIMARY CELL INDEX CONTROL SECTION
      IX=IX+1
      IF(IX.GT.NLX)THEN
      IX=1
      IY=IY+1
      IF(IY.GT.NLX)THEN
      IY=1
      IZ=IZ+1
      ENDIF
      ENDIF
5001  CONTINUE
```

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CCP5 Literature Survey 1987

W. Smith

June 15, 1988

Here, somewhat later than in previous years (for which we apologise), we present the annual literature survey of publications relevant to the activities of CCP5. The survey covers the year 1987 and was compiled with the help of the University of London Computing Centre INSPEC service. We thank Dr. J. Altmann of U.L.C.C. for helping to make this survey possible. We also thank Mrs. Anne Ireland for typing and sorting the references and Mrs C.M. Smith for assistance with proof reading. Your editor reserves responsibility for any remaining errors.

As is now the custom, we invite additions and corrections from our readers, which we shall publish in our next issue. We hope that you find the survey presented here useful.

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