DARESBURY LABORATORY

INFORMATION QUARTERLY for COMPUTER SIMULATION OF CONDENSED PHASES

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

Number 34 March 1992

Contents

Editor: Dr. William Smith
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Science & Engineering Research Council,
Daresbury Laboratory, Daresbury,
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General News

FUTURE MEETINGS AND WORKSHOPS A summary table is given below, further details may be found inside.

TOPIC	DATES	LOCATION
STATISTICAL MECHANICS OF INDUSTRIALLY IMPORTANT MATERIALS AND PROCESSES	8-10 JULY 1992	UMIST
STATIC AND DYNAMIC STUDIES OF FINITE SYSTEMS	17 JULY 1992	UNIVERSITY OF SUSSEX
POLYMER MODELLING	2-4 SEPT 1992	UNIVERSITY OF READING

CCP5 PROGRAM LIBRARY Details are contained in this issue of accessing the CCP5 program library through E-mail automatically. Also a number of new programs have been added to the library.

CRAY TIME CCP5 participants are reminded that CCP5 has an annual allocation of Cray time at Rutherford (Cray XMP-48), which is available for the development of simulation programs which are of general use to the CCP5 community. Readers who wish to use some of this allocation should write to the CCP5 Secretary, Dr. M. Leslie, TCS Division, SERC Daresbury Laboratory, Daresbury, Warrington WA4 4AD.

CCP5 FUNDS FOR COLLABORATIONS CCP5 can make available funds of up to £300 per annum for groups of two or more UK researchers wishing to undertake a collaborative project within the scientific area covered by CCP5. The funds are intended to cover travel and subsistence costs. Researchers who wish to apply for funds are requested to submit a brief proposal (about 1/2 a page) describing the intended work to Dr. M. Leslie, SERC Daresbury Laboratory, Daresbury, Warrington, Cheshire. Alternatively reply by Email to M.LESLIE@UK.AC.DARESBURY

CCP5 VISITORS PROGRAM CCP5 organises a visitors program which funds the visit to the UK of overseas collaborators. We would normally expect a visitor to visit three sites in the UK and give a lecture at each site. These lectures would be open to all members of CCP5 as well as members of the host university. The visit would normally last between one or two weeks. CCP5 would pay for the cost of travel to the UK and within the UK between universities. CCP5 would expect some contribution towards accommodation expenses at the host university to be met by the university. We will also consider longer collaborations or visits just one place if this can be justified by the nature of the work to be done. If you have an overseas collaborator who you would like to invite under this program, please make a request to Dr. M. Leslie, SERC Daresbury Laboratory, Daresbury, Warrington, Cheshire. UK Alternatively reply by Email to M.LESLIE@UK.AC.DARESBURY

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UMIST

Statistical Mechanics

& Thermodynamics Group

Faraday Division
ROYAL
SOCIETY OF
CHEMISTRY

Statistical Mechanics of Industrially Important Materials and Processes

8-10 July 1992
The Manchester Conference Centre

First announcement and call for contributions

The aim of this meeting is to focus attention on selected areas in which the techniques of statistical mechanics are being applied to study materials and processes of direct industrial relevance. These areas are polymer blends, cohesion and adsorption, and the rheology of powders and colloids.

Speakers invited include K.Binder (Mainz), Sir S.F.Edwards (Cambridge), R.Koningsveld (Geleen), A.Lips (Unilever), L.Leibler (Paris), and L.Woodcock (Bradford). In addition there will be some short contributed talks and also a poster session. Facilities will be available for the posters to be displayed for the whole duration of the meeting.

The meeting, which is being jointly sponsored by the **Macro Group UK** and the **SERC CCP5**, is being held over one and a half days at the new purpose-built Conference Centre at UMIST. The location is close to the city centre and is well served by air, rail and road links.

Organising Committee: Dr. J.H.R.Clarke (Chairman), Dr. R.F.T.Stepto, Dr. M.Cates, Dr. M Rodger

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Please return this reply slip as soon as possible (and not later than 28th February 1992) to
Dr. R.F.T. Stepto
Polymer Science and Technology Group
Manchester Materials Science Centre
University of Manchester and UMIST
MANCHESTER M1 7HS Tel. 061 200 3574 fax 061 200 3586

Please send further information and application forms concerning the conference on the **Statistical Mechanics of Industrially Important Materials and Processes.**

Name ....

Address ....

....

Tel./ fax / email ....

I would like to present a paper/poster: yes/no (*delete as appropriate*)
and the tentative title is ....

signed .... date.......................................

Static and Dynamic Studies of Finite Systems

A joint meeting between the Collaborative Computational Project Groups CCP5 and CCP6 is to be held at Sussex University on Friday **17th July 1992**. It is anticipated that the meeting will take the form of a workshop, with the following speakers being invited to stimulate discussion through reviews of current techniques for studying clusters.

- Prof. R. J. LeRoy (Waterloo):- Computer simulation of the structural and spectroscopic properties of atomic and molecular clusters.
- Dr. A. J. Stace (Sussex):- Experimental studies of dynamic processes in atomic and molecular clusters.
- Dr. P. A. Madden (Oxford):- Computational techniques for studying metal clusters.
- Prof. H. Haberland (Freiberg):- Experimental studies of metal clusters.

The meeting will start at 10.30am in the School of Chemistry and Molecular Sciences, Sussex University. There is no registration fee and refreshments and lunch will be provided for those participants invited to join the workshop.

All those wishing to attend the workshop should register with Dr. A. J. Stace, School of Chemistry and Molecular Sciences, University of Sussex, Falmer, Brighton BN1 9QJ by the 1st of July.

POLYMER MODELLING

An International Conference Organised By

POLYGEN / MOLECULAR SIMULATIONS

in association with

The Collaborative Computational Project No. 5 and Silicon Graphics

to be held at

Polymer Science Centre, University of Reading, U.K.

on

2nd - 4th September 1992

This conference is open to all scientists in academia and industry who are interested in modelling polymers. Scientific topics have been chosen which span the wide range of length-scales and time-scales present in polymer systems, from picosecond studies of atomistic models, through course-grain Monte-Carlo methods, to quantitative structure property relationships. Applications for which new modelling methods are being developed, such as free energy calculations and polymers at interfaces, and the structural analysis of amorphous and liquid crystalline polymers through a combination of modelling and diffraction experiments, will all be addressed. The invited speakers include:

Prof W A Goddard III, California Institute of Technology

Dr D N Theodorou, University of California
Prof A J Hopfinger, University of Illinois
Dr A H Windle, University of Cambridge
Dr G R Mitchell, University of Reading

Dr B Smit, Shell Research
Dr K Kremer, KFA Jülich
Prof K Binder, Universität Mainz
Dr J H R Clarke, UMIST

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The CCP5 Program Library

W. Smith

October 25, 1991

News

We have received a number of programs in the last year. Particularly welcome are the programs for parallel computers.

- MDCSPC2P - by W. Smith. A molecular dynamics program for simulating ionic systems with Born-Huggins-Mayer potentials. This is a parallel FORTRAN 77 program designed primarily for the Intel iPSC machines. It can however be adapted easily to serial machines. It can simulate constant volume or constant pressure ensembles, the latter by either Parrinello-Rahman, or Brown-Clark constant pressure algorithms. The parallel algorithm is the replicated data algorithm due to Smith.
- SLS_PRO - by A. Raine. A molecular dynamics program for simulating protein residues *in vacuo*. This is a parallel OCCAM program designed specifically for transputer based machines. The program uses the SLS-GO systolic loop parallel algorithm of Raine, Fincham and Smith.
- SOTON_PAR - by M.R.S. Pinches. This is a directory of FORTRAN parallel programs for simulating Lennard-Jones atomic systems using the parallel link-cells algorithms. The programs were written primarily for the Intel iPSC machines. 2- and 3- dimensional programs are available, both comprised of a master program, which resides on the host and a worker program, which resides on the network of nodes.
- SFMK - by A.P. Lyubartsev. A FORTRAN program for Monte-Carlo - Self-Consistent Field simulation of the cylindical polyelectrolyte. Written and tested on an IBM PC/AT-286.

All of these programs are available through the CCP5 Program Library in the usual ways (see below.)

Our thanks go to everyone who has contributed the above programs.

CCP5 Program Library Conditions of Distribution

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..Please supply a magnetic tape to receive the copies. Industrial and commercial applicants should enclose a £100 handling charge. No magnetic tape need be sent in this case. Listings of programs are available if required. Please note that use of inappropriate packing for magnetic tapes (e.g. padded bags) may result in them being 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.

All applicants will be required to sign an agreement not to exploit the programs for commercial purposes e.g. for resale or distribution as part or whole of a commercial product.

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

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

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

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

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

M.P.Allen

CCP5 Program Library E-Mail Service

From January 1 1991 it will be possible for CCP5 members to get copies of CCP5 programs through E-mail *automatically*. To do so they should send an E-mail message to **info-server@uk.ac.daresbury**. The contents of the e-mail message should be as follows (Note: the use of upper and lower case is significant - this is a unix system!):

```
request sources
topic index CCP/ccp5
topic CCP/ccp5/program-name
```

Where program-name is the name of the desired source code. A mail server will automatically process this message and return a copy of the source code to your e-mail address. Please note the following however:

The program source will be returned to you in uue format, which is a form of encoding most suitable for mail messages. It can easily be decoded on any unix system using the uudecode command. (Check your local unix *man* file for details). Also, to speed the transfer, the source will be split into files of 1200 records each, so expect two or three such files for the average CCP5 program. Once again, uudecode will help you to sort things out.

Readers who do not have unix facilities should include the following lines at the start of the above message:

```
line-limit: nnnnn
coding: off
```

Where nnnnn is the number of records in the source (in most cases 6000 should be enough). The program will be sent in plain FORTRAN as a single file. It may take a while to arrive, but be patient! Also beware in case your system mailer cannot handle messages of this size.

Readers must realise that the terms of use and distrubution of the CCP5 programs that have applied hitherto will be maintained. Users should not redistribute or sell the programs, nor is any liability accepted for their use, either by SERC or the program authors. It is a requirement on the user that the programs be fully tested for their intended purpose. Any bugs found should be reported to the librarian, for the benefit of other users.

Lastly readers should realise that this means of transfer does not include any program documentation. So if you are unable to make sense of the programs, write for the documentation!

We are grateful to Mr. P. Griffiths of Daresbury's ITS Division for implementing this facility.

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
MDCSPC2P	[PRMD,BHM,LF,TH+STF+RDF+VACF+MSD]	W. Smith
MDCSPC4B	[PRMD,BHM+FC,G5+G4,TH+STF+RDF]	W. Smith
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
MD3DLJ_C	[MD,LJA/MIX,LF/LC,TH+MSD+RDF]	M. Bargiel, W. Dzwinel, J. Kitowski and J. Moscinski
MDMANY	[MD,LJS+FC,LF+QF,TH]	D. Fincham & W. Smith
MDMIXT	[MD,LJS/MIX,LF+QF,TH]	W. Smith
MDMPOL	[MD,LJS+FC/MIX,LF+QF,TH]	W. Smith & D. Fincham
MDNACL	[MD,BHM,LF,TH+MSD+RDF]	W. Smith
MDPOLY	[MD,LJS,G5+Q4,TH+MSD+QC]	S.M. Thompson
MDMULP	[MD,LJS+PD+PQ/MIX,LF+QF,TH]	W. Smith
MDSGWP	[MD,LJA/SGWP,LF,TH+VACF+RDF+QC]	W. Smith & K. Singer
MDTETRA	[MD,LJT,G5+Q4,TH+MSD+QC]	S.M. Thompson
MDZOID	[MD,GAU,LF+QF,TH+MSD+RDF+VACF]	W. Smith
NAMELIST	[UT, Namelist emulation]	K. Refson
NSCP3D	[UT, Hard sphere packing]	M. Bargiel & J. Moscinski
PIMCLJ	[PIMC,LJA,MC,TH+RDF+QC]	K. Singer & W. Smith
SCN	[MC,LJA,RFD,TH]	N. Corbin

SFMK	[MC-SCF,Cylindrical Polyelec.]	A.P. Lyubartsev
SLS_PRO	[MD,Proteins,LF,TH+STR]	A. Raine
SOTON_PAR	[MD,LJA,LC,TH]	M.R.S. Pinches
SURF	[MD,BHM/TF/2D,LF,TH+RDF]	D.M. Heyes
SYMLAT	[LS,PIL,EM+SYM,TH+STR]	Harwell
TEQUILA	[GP]	A. Wilton and F. Mueller-Plathe
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
	PRMD	Parrinello-Rahman MD
	LS	Lattice simulations
	SD	Stochastic dynamics
	DA	Data analysis
	UT	Utility package
	PIMC	Path Integral Monte Carlo
	GP	Graphics program
System models:	LJA	Lennard-Jones atoms
	LJD	Lennard-Jones diatomic molecules
	LJL	Lennard-Jones linear molecules
	LJT	Lennard-Jones tetrahedral molecules
	LJS	Lennard-Jones site molecules
	RPE	Restricted primitive electrolyte
	BHM	Born-Huggins-Meyer ionics
	SGWP	Spherical gaussian wavepackets
	TF	Tosi-Fumi ionics
	VS	Variable site-site model
	BA	Bond angle model
	PD	Point dipole model
	PQ	Point quadrupole model
	MIX	Mixtures of molecules
	GAU	Gaussian molecule model
	FC	Fractional charge model
	PIL	Perfect ionic lattice model
	DIL	Defective ionic lattice model
	3B	3-body force model
	2D	Two dimensional simulation
	SF	Shifted force potential
	FC	Fractional charge model
	AQ	Aqueous solutions
Algorithm:	G5	Gear 5th order predictor-corrector

	Q4	Quaternion plus 4th. order Gear P-C.
	LF	Leapfrog (Verlet)
	QF	Fincham Quaternion algorithm
	QS	Sonnenschein Quaternion algorithm
	LC	Link-cells MD algorithm
	CP	Constant pressure
	CT	Constant temperature
	TA	Toxvaerd MD algorithm
	CA	Constraint algorithm
	EM	Energy minimisation
	SYM	Symmetry adapted algorithm
	RFD	Rossky-Friedman-Doll algorithm
Properties:	TH	Thermodynamic properties.
	MSD	Mean-square-displacement
	RDF	Radial distribution function
	STF	Structure factor
	VACF	Velocity autocorrelation function
	QC	Quantum corrections
	STR	Lattice stresses

Programs from the Book "Computer Simulation of Liquids"

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

Availability of the Allen/Tildesley example programs

Steve Thompson,
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Ithaca NY 14853

October 8, 1991

Appendix F of the book "Computer Simulation of Liquids" by M.P.Allen and D.J. Tildesley describes a method whereby the example programs may be obtained from the statistical mechanics group FTP facility at Cornell. As a number of people have recently discovered, this facility is no longer operational as advertised, due to hardware and software changes. However, the programs are still available. To obtain them, please follow the procedure outlined here. The description below is taken from the HELP file that is distributed by the file server; to obtain the Allen/Tildesley example programs, simply use "ALLEN_TILDESLEY" as the package name (without the double quotes).

Please note that the internet address for cheme.tn.cornell.edu has changed to 128.84.243.48 (from 128.84.253.7 as previously listed). This address may change in the future as the local network is reconfigured. If you use a name server, you should be immune to these changes.

Other packages will become available as time allows; notice will appear in this newsletter.

STATMECH is a file distribution service for the Statistical Mechanics community that uses electronic mail facilities to deliver files. To communicate with STATMECH, send an E-mail message to:

statmech@cheme.tn.cornell.edu

Commands are sent in the body of the message you send to STATMECH (not in the subject line). Several commands may be sent at one time; just put one command per line.

STATMECH Commands:

SENDME package	Sends all parts of the specified package.
SENDME package.n	Sends part 'n' of the specified package.
LIST [pattern]	Gives brief description of all packages matching "pattern". If pattern is omitted, a description of all packages is sent.
HELP	Sends this help file.

For each request you make, a transaction log is returned to you indicating the status of the request. The status report will indicate whether the request was successfully completed, and when the file was or will be sent. Large files are sent only during off-peak hours.

Problems, questions, and comments about STATMECH service on this system should be directed to "statmech-mgr@cheme.tn.cornell.edu".

Molecular dynamics simulation of plastic deformation of 2-D solid *

(MD hydrodynamics at 1 K)

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November 21, 1991

Abstract

The purpose of presented computer experiments is the study of phenomena resembling plastic deformation of materials. The simulation has been conceived as a qualitative observation of processes and as a test of possibility of obtaining effects analogous to macroscopic ones. The system has been composed of three elements: unmovable obstacle forming a slit, piston, and plastic material. Although number of moving particles in the model is very small impressive images of plastic deformation has been obtained.

1 Introduction

Recently molecular dynamics *(MD)* [1]–[2] is being used for simulation of macroscopic phenomena e.g. fluid flows [3]–[5]. The purpose of presented computer experiments is the examination of phenomena resembling plastic deformation of materials. The simulation has been conceived as a qualitative observations of processes and so a very simple system was applied: monoatomic molecules, 6/12 Lennard-Jones interactions and regular initial structure. The other goal was to test the possibility of obtaining effects analogous to macroscopic ones but achieved on a very small sample. We were also looking for the microscopic parameters range in which these phenomena may be observed. We have already tried this, more or less succesfully, with microscale hydrodynamics [6]–[7].

2 Model

In all simulations the system has been composed of three elements:

- unmovable obstacle forming a slit,
- piston,
- plastic medium.

The obstacle is built up of extremely heavy ($10^{10} m_{Ar}$, m_{Ar} – mass of Argon) particles and this makes them actually unmovable although they interact with the rest of the system and are considered in the Newtonian equations of motion.

The piston also consists of such heavy particles and could behave just like the obstacle, but externally applied velocity moves it continuosly along the x–axis, and moving piston simply pushes the plastic medium. It should be stressed that piston movement is not affected by any means by the dynamics of the system.

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*Poster presented at the Summer School of the NATO Advanced Study Institute "*Microscopic Simulation of Complex Hydrodynamic Phenomena*", Alghero, Italy, July 15–26, 1991.

Consequently its velocity can not be too high to avoid unpredictable and unrealistic effects. Natural consequence of the low velocity of the piston is that simulation runs have to last about $10^5 \div 10^6$ timesteps and this fact does not depend on the size of the sample.

Plastic medium is somehow artificial. We have started with the mass, density and potentials of liquid Argon, but after preliminary runs we were forced to enlarge ϵ parameter in L-J potential about five times to get stronger bindings between particles and to let them behave more like a solid. All particles in plastic medium are identical, and different colours in the figures (see below) are introduced only to enable observation of separate layers movement.

3 Software and hardware environment

As a simulation program subsquent C–language and Fortran two-dimensional versions of our earlier *basic* code for *MD* simulation of particles with Lennard-Jones potentials have been applied [9]. We have also used EDSIMP v3.0 [8] program for the system initial structure editing, results visualisation and preparation of figures. Runs have been performed on PC/AT 486 25MHz, and on plug-in board with i860, 40 MHz processor.

4 Simulation runs and results

Large number of runs have had to be performed to choose instructive images. In all runs plastic medium remained the same, and the shape and width of the slit as well as the piston velocity have been varying. In this paper we present three runs with the same initial conditions, the same geometry and differing only in the velocity of the piston. Number of moving particles in the presented system is small – equal to 784. In all simulations the timestep was set to $10^{-14}s$. To make the system behave like a solid rather then like a liquid we have been obliged to "freeze" it by scaling temperature to 1K every several timesteps of simulation.

Presented runs have been performed for three piston velocities: 20×10^{-4}, 4×10^{-4}, $1 \times 10^{-4} \AA/timestep$; the snapshots of particle distributions are presented in Figures 1, 2, 3, respectively. It can be seen that the "nose" of the extracted medium keeps its shape well. However, with the fast piston movement medium compresses significantly before the slit and then pours out like a liquid and presses the forehead (see the zig-zag deformation of the central blue layer in the Figure 1). For runs with slower piston movement such deformations do not occure. To complete these runs we needed 75000, 375000 and 700000 steps.

Images in Figure 4 show particles momenta in a relatively small time interval for the run with piston velocity $v = 1 \times 10^{-4} \AA/timestep$. Every arrow represents a mean momentum of several particles (≈ 10). Two items should be mentioned: the first is strongly coupled collective behavior of particles (seen in top and bottom images), and the second is a complex wave movement which leads to chaotic motion between more ordered stages (middle image).

5 Conclusions

Using a very simple system and a very small sample we have obtained quite impressive images of extraction, flow and deformation of plastic material. The pictures are similar to real life observations or to results obtained with direct numerical solutions of the Navier–Stokes equations. We treat it as a preliminary study of subsequent, maybe more realistic simulations, aimed at the establishing of relationships between microscopic parameters of the mediun and its macroscopic behavior in the plastic deformation process. We intend to perform simulations for larger samples, vary the piston velocity in a wider range – especially for lower velocities, and study carefully the wave propagation throug the medium.

6 Acknowledgements

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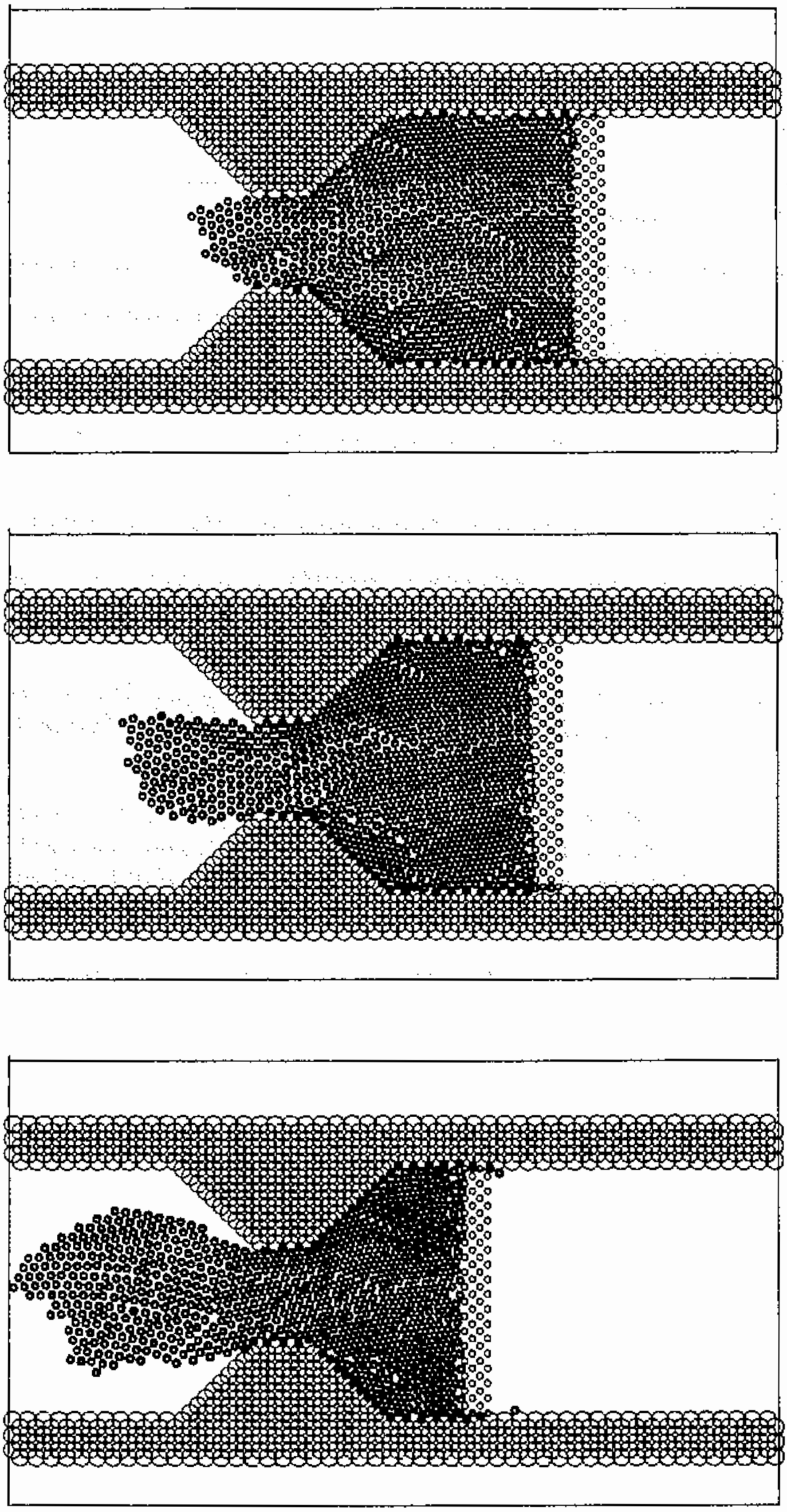

Fig. 1. Change of the form of the plastic material in the pressing out process; piston velocity $v = 20 \times 10^{-4} \mathring{A}/step$;
upper figure - step 30000, middle - 37500, bottom - 50000.

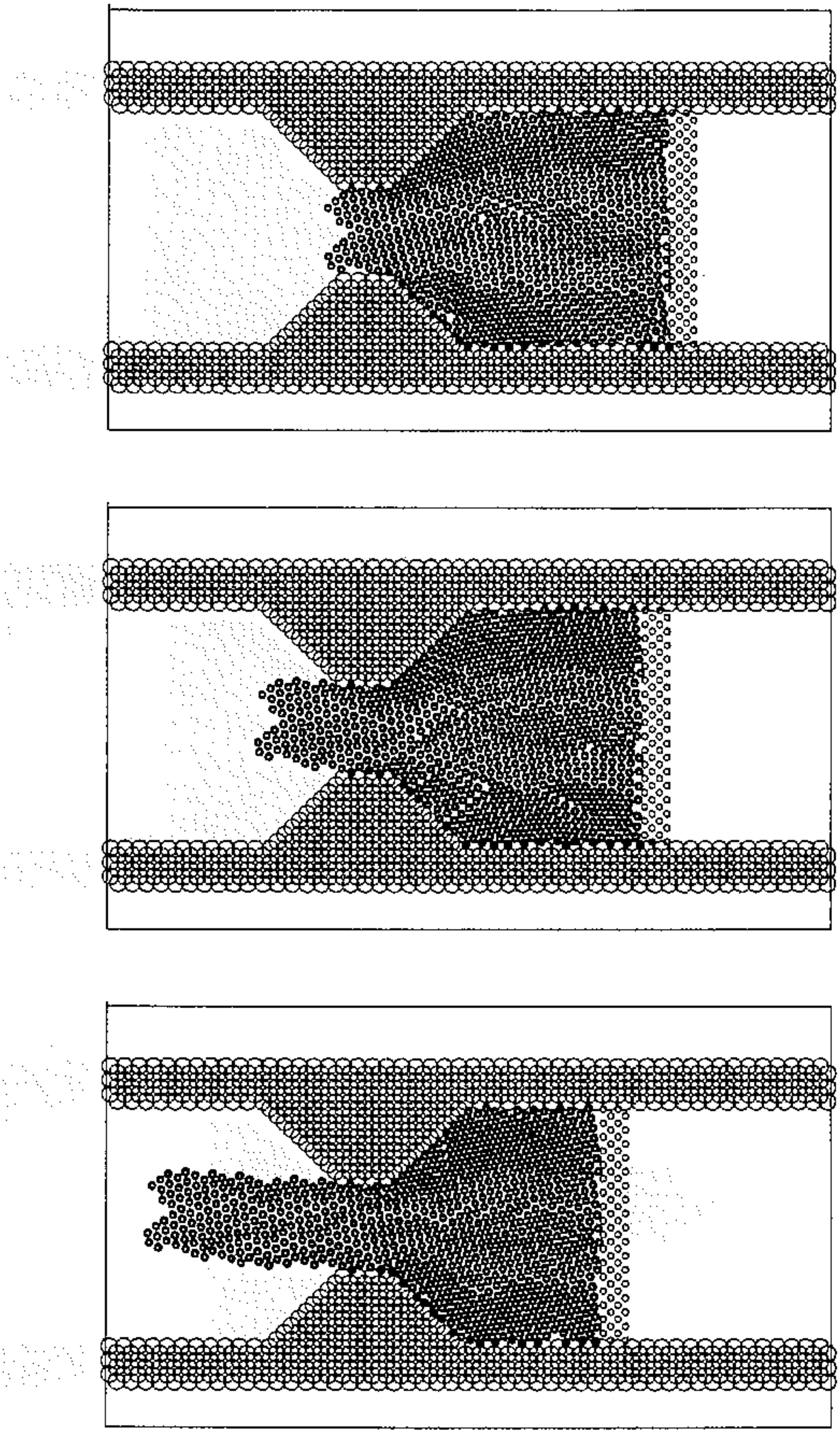

Fig. 2. Change of the form of the plastic material in the pressing out process; piston velocity $v = 4 \times 10^{-4} \mathring{A}/step$;
upper figure - step 125000, middle - 150000, bottom - 187500.

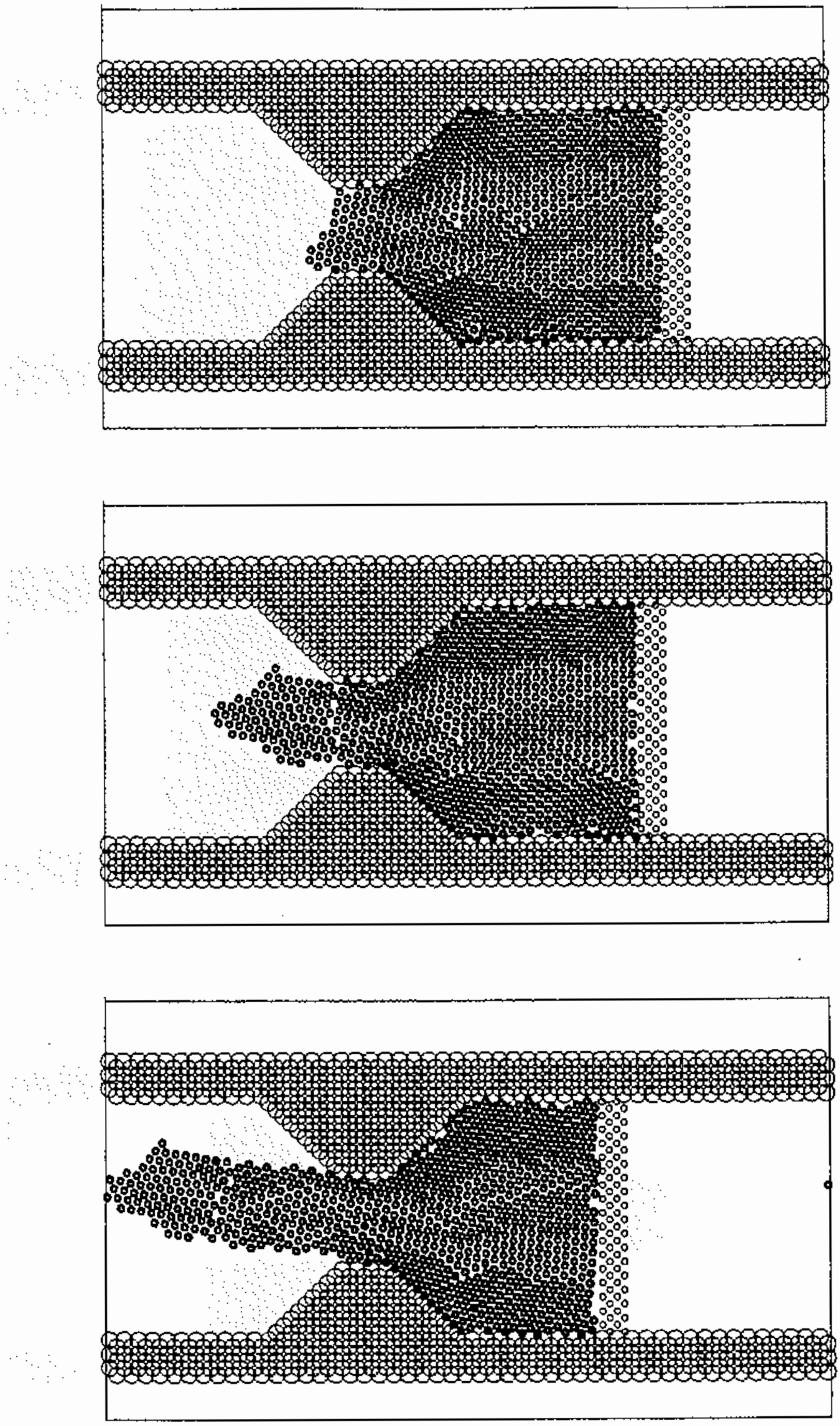

Fig. 3. Change of the form of the plastic material in the pressing out process; piston velocity $v = 1 \times 10^{-4} \mathring{A}/step$; upper figure - step 500000, middle - 600000, bottom -750000.

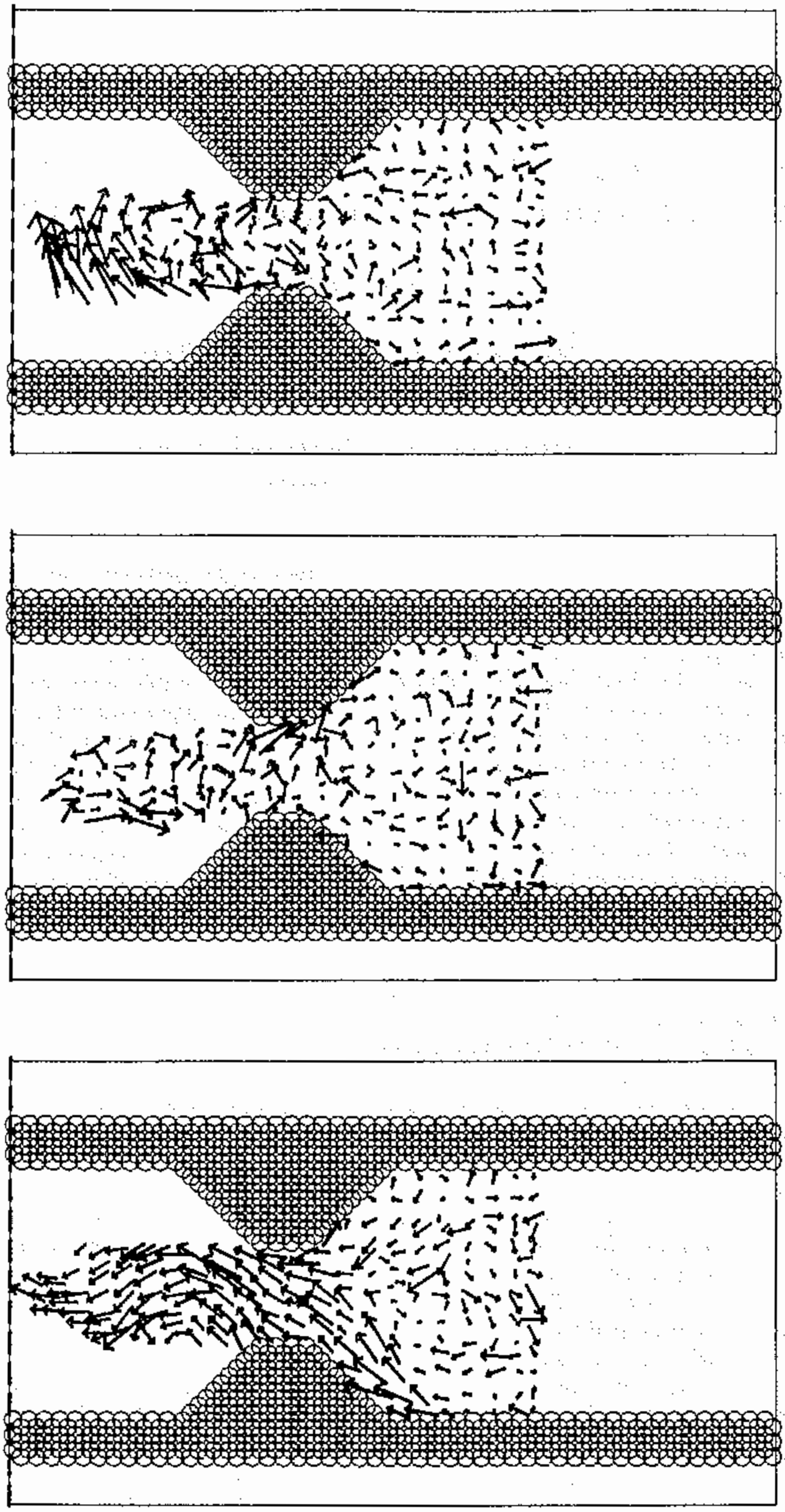

Fig. 4. Velocities in the pressing out process;
piston velocity $v = 1 \times 10^{-4} \mathring{A}/step$;
upper figure - step 710000, middle - 720000, bottom -730000.

A Parallel Implementation of a Molecular Dynamics Algorithm using the PCP Programming Paradigm and its Application to Orthogonal Metal Cutting *

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Abstract

The molecular dynamics (MD) method has proved to be one of the most important tools in theoretical condensed matter physics. The basic input is a description of the interatomic interactions. The method has been traditionally used to extend our knowledge concerning these interatomic forces and to explore equilibrium phase diagrams. More recent applications have focussed on providing details beyond the current resolution of experiment. Here, we apply the method to the single point diamond turning of simple metals. Because the simulation time-step must be a small fraction (typically 1/50) of the interatomic vibrational period ($\tau_E \approx 10^{-12}$sec), the CPU time required to simulate the chip formation process is enormous. For this reason, we are exploring the utility of massively parallel computers, such as the BBN TC2000, to perform MD simulations. We divide the large MD simulation cell into many small sub-cells. Atoms in a given subcell interact only with atoms in neighboring sub-cells. We parallelize over these sub-cells. The performance of the code running on 64 processors on the TC2000 is comparable with a vectorized version running on a single Cray X/MP processor. However, with 96 processors, we estimate our parallel efficiency to be about 60% (75% for the force routine). This performance, though seemingly good, is limited by inherently serial sections in the code (primarily the application of complex boundary conditions). In order to fully exploit the $10^3 - 10^4$ processors expected in the next generation parallel supercomputer, we will need to eliminate these serial sections. Our code uses the interleaved shared memory to store atomic positions and forces. We estimate the shared-memory overhead to be about 50%. In our future work, we plan to explore a larger domain decomposition scheme that assigns many subcells to a single domain. Each processor is assigned a domain and the storage for that domain is private to the processor. This scheme will win when the amount of inter-domain communication is small.

Keywords: Molecular Dynamics, Single Point Diamond Turning, Orthogonal Metal Cutting, BBN TC2000, Cray X/MP, shared memory, private memory, parallel efficiency.

1 Introduction

State of the art single point diamond turning (SPDT) machines, such as the large optics diamond turning machine (LODTM) operated by the Precision Engineering Program (PEP) at LLNL, routinely achieve mirror quality finishes without additional polishing! In SPDT, a tool with a very sharp diamond tip (tip radius $\leq$ 100nm) is used to scrape a small amount of material off a surface in a controlled manner. Typical depths of cut are ≤ 1 μm and can be as small as a few nanometers. A cutting speed of ~ 1 m/s is normally used, while speeds of several hundred meters per second are used for special applications. At these depths of cut and cutting speeds, the entire chip formation process occurs on time scales less than 1 μsec. The work material moves 1 μm in 1 μsec at a cutting speed of 1 m/s. Also, the total number of atoms di-

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rectly participating in the deformation is at most 10^9. These observations suggest that a molecular dynamics model, which explicitly takes into account atomic motion, may yield new and useful information about the cutting process.

During metal cutting, there is very little flow of material orthogonal to the cutting direction and most of the relevant physics is contained in a two dimensional model. For this reason, we have begun our molecular dynamics study of metal cutting by performing two dimensional simulations containing at most 10^6 atoms. We consider tip radii ≤ 20 nm and cutting speeds of 10–100 m/s. Even at these relatively fast speeds, millions of time-steps are required to simulate the chip formation processes and a single calculation runs for several hundred CPU hours. Fully three dimensional calculations are beyond our present capabilities and await the next generation teraflops machine. We anticipate that this machine will contain $\sim 10^4$ very fast processors ($\sim$ 100 megaflops) and we are designing our algorithms to be scalable to this processor count.

2 Molecular Dynamics Model of Orthogonal Metal Cutting

Molecular dynamics modeling is very simple in principle. Given the positions of all of the atoms, calculate the force on each atom due to its neighbors and advance the positions with a finite difference integration scheme. Both predictor-corrector and central difference are commonly used. In our simulations, we employ an embedded atom method (EAM) to express the forces between the atoms in a simple metal[1]. The total potential energy is written as:

$$\Phi_{total} = \frac{1}{2}\sum_{i,j}\phi(r_{ij}) + \sum_{i}F(\rho_i) \qquad (1)$$

with

$$\rho_i = \sum_{j \neq i} f(r_{ij}). \qquad (2)$$

The first term is the usual two body interaction energy and the second term is the energy required to embed the atoms into the local electronic charge density (ρ_i). The Newtonian equations of motion for the embedded atom method are

$$\begin{aligned} m\frac{d^2x_k}{dt^2} &= -\sum_{j\neq k}(\phi'(r_{kj}) + (F'(\rho_k) + \\ & \qquad F'(\rho_j))f'(r_{kj}))\frac{x_k - x_j}{r_{kj}}. \qquad (3) \end{aligned}$$

These equations are inherently nonlocal—they depend on both the embedding densities ρ_k and ρ_j. They must be solved in a two step manner. The embedding density at all atomic sites is evaluated first, then the forces may be calculated. Precise details concerning the potential functions employed here may be found in the recent paper by Holian et. al[2]. The equations are integrated by approximating the time derivative by a central difference:

$$\frac{d^2x}{dt^2} \approx \frac{x(t+\Delta t) - 2x(t) + x(t-\Delta t)}{\Delta t^2} \qquad (4)$$

with a time-step (Δt) of about 1/50 of the vibrational period (τ_E).

The vibration period in simple metals is about 10^{-12} seconds. In covalently bonded materials, such as Silicate glasses, the vibrations are much faster and $\tau_E \sim 10^{-13}$ seconds. Thus, the time-step in our calculation is at most $\Delta t \sim 10^{-14}$ seconds. The clock time for our best currently available processors is $\sim 10^{-8}$ seconds. We expect no more than one order of magnitude improvement in the near future. The best parallelism we can reasonably expect is one processor per atom or one MD time-step per clock. In this one dimensional world of non-interacting atoms, we require one second of CPU time to simulate one micro-second (10^{-6}) of real time. However, life is three dimensional and the computational complexity of the time-step itself costs us about one order of magnitude. The atom interacts with at least 10 of its neighboring atoms, the nature of this interaction is complex and requires many clocks to fetch the positions from neighboring processors. These three effects cost us an additional three orders of magnitude. We might still expect to obtain one time-step per clock if we had available $10^3 - 10^4$ processors per atom and the simulation of a macroscopic piece of material ($\sim 10^9$ atoms in one grain in a metal) would require a truly massively parallel machine containing $> 10^{12}$ processors. Even so, this machine will take months of dedicated CPU time to simulate one second of real time. The current generation CM2 Connection Machine has $\sim 10^3$ floating point parallelism. The simulation of 1 μsec with 10^9 atoms will take the CM2 $\sim$ 100 years of dedicated CPU time to perform. Another direction, that could revolutionize the performance of MD codes, is implicit algorithms that increase the time-step by many orders of magnitude. However, the equations are stiff and we see little hope in this direction.

In our simulations of metal cutting, we have used up to 10^6 atoms in two dimensions (10^9 are required in three dimensions). We perform the calculation on the TC2000 with $\sim 10^4$ atoms per processor and expect

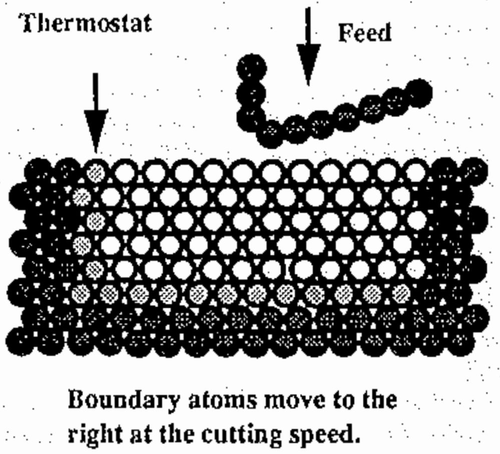

Figure 1: The geometry of our steady-state variable-particle molecular dynamics model of orthogonal metal cutting in two dimensions.

at least 10^8 seconds (3 years) of CPU time to simulate 1 μsec! By performing the calculation for several hundred hours, we have simulated times as long as 10 ns. This is the time scale for chip formation at cutting speeds of $\sim$ 100 m/s. We need at least two more orders of magnitude in performance to simulate chip formation at cutting speeds of 1 m/s and four orders of magnitude beyond that for the three dimensional simulation of 1 μsec with 10^9 atoms, using several hundred CPU hours.

We define the computational complexity of an MD simulation to be the number of atoms times the number of MD time-steps. In this regard, the calculations presented here (10^5 atoms $\times 10^6$ time-steps) represent some of the largest MD simulations ever performed. Naturally, our measure must be multiplied by a measure of the complexity of the interatomic force calculation. We have considered nearest neighbor models in which the number of neighbors in 2D is $\sim$ 6 and the number of neighbors in 3D is $\sim$ 18. Materials, such as Silicate glass, require a significantly more complex $(10-100$ fold) description of the interatomic forces.

The cartoon in Figure 1 illustrates the geometry of our steady state MD model of the orthogonal cutting process. The MD simulation cell is a fixed "window" in the reference frame of the tool. All of the motion is constrained to two dimensions. The boundary atoms are used to impose the cutting speed—they move to the right at the cutting speed. One of our future goals is to couple this boundary region with a continuum mechanics simulation outside the MD cell. The boundary will dynamically relax, so that both stress and strain are continuous across the interface. Far from the tool tip, we expect the continuum mechanics solution to be more than adequate for both elastic and plastic deformation. In order to produce a steady state flow in our MD model, new atoms are continuously inserted from the left, while atoms that leave the top or the right hand side of the cell are *thrown away*. Next to the boundary, we place a region of thermostat atoms. A time dependent viscous damping is added to the equation of motion for these atoms[3, 4]:

$$m\frac{d^2x}{dt^2} = Force - \zeta m\frac{dx}{dt} \tag{5}$$

with

$$\frac{d\zeta}{dt} = \frac{1}{\tau^2}\left(\frac{T_{calc}}{T_{desired}} - 1\right). \tag{6}$$

The purpose of the thermostat atoms is to draw away heat produced by doing work at the tool tip. The remaining material atoms are free to dynamically respond. The tool atoms do not vibrate and are fed into the work material at 1/5 the cutting speed until the tip most atom reaches the desired depth of cut. The tool atoms interact with the material atoms via the purely repulsive WCA potential model[5].

One major failure of the embedded atom method is that it does not model the thermal conductivity of simple metals. The thermal conductivity of simple metals is primarily due to the "free–electrons." The EAM assumes that the electrons are always in thermal equilibrium and their contribution to the force on the atoms can be expressed within a local density approximation. The EAM includes only the "phonon" contribution, from the center of mass motion of the atoms, to the thermal conductivity. In order to model the thermal conductivity due to the electrons, we are introducing an additional viscous damping to the motion of the atoms. A local-temperature dependent random force is used to exchange energy between the electronic and atomic degrees of freedom. The rate of exchange is known from the value of the electron-phonon coupling. The local temperature is that of the electrons. We plan to simulate the flow of heat through the electron degrees of freedom by numerically solving the diffusion equation with the known thermal conductivity of the electron gas. We are also introducing heat flow into the tool in a similar manner—diamond has a very high thermal conductivity. Coupled particle and continuum simulations of this type are currently at the forefront of computational physics. Our

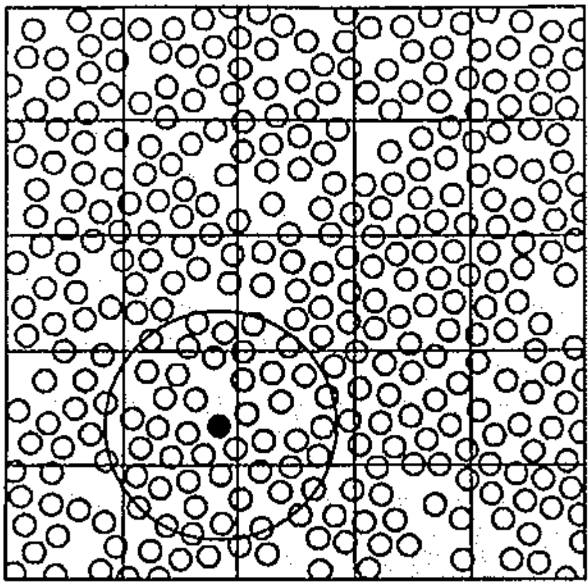

Figure 2: A typical MD simulation cell. The atom at the center of the circle interacts with all atoms inside the circle. In the linked-cell domain decomposition scheme, atoms in a given sub-cell interact with atoms in neighboring sub-cells only.

two dimensional results display considerable temperature gradients at 100 m/s and little or none at 10 m/s. Suggesting that, at the slower cutting speeds, the heat generated per unit time is small and the phonon mechanism has plenty of time to propagate the heat out of the system. This may be all that is required at 1 m/s.

Our molecular dynamics computer simulation code is written in the C programming language. C provides for complex data structures, pointer arithmetic, and dynamical allocation of memory. All of which we find indispensable for performing variable particle simulations. When storage for a new atom is needed, it is allocated from interleaved shared memory using the shmalloc function. When an atom is removed, its storage is given to a buffer which in turn is used when required for new atoms. The atoms are connected with a double linked-list. The structure for an atom contains (in addition to the atomic positions, forces and EAM density) a series of linked-list pointers to other atoms. Two of which (labeled NEXT and PREVIOUS) are used to traverse the list of atoms either forwards or backwards. Both are needed to "reconnect" the list when an atom is removed. New atoms are always added to the end of the list.

Table 1: The output from the UNIX profiler running on the Sun SparcStation-1 for the top few routines. The calculation simulated the motion of 32256 atoms.

%time	secs	#call	ms/call	name
76.8	76.53	22	3478.64	_force
6.1	82.62			mcount
1.9	84.53	118376	0.02	.rem
1.7	86.26	21208	0.08	__big_flt_times
1.6	87.82			.div
1.3	89.14	10066	0.13	_file_to_dec
1.0	90.13	338510	0.00	.umul
1.0	91.08	22	43.18	_bcs
0.8	91.85	22	35.00	_kinetic
0.6	92.46	2306	0.26	__doprnt
0.5	92.95	537344	0.00	.urem
0.4	93.37	1	420.00	_main

3 The Importance of the Force Calculation

The vast majority of the time, spent in any molecular dynamics simulation program, is spent calculating interatomic forces. To illustrate this, we show in Table 1 the output from the UNIX profiler on a serial version of our code. The example was run on a Sun SparcStation-1 which has a performance (~2 megaflops) comparable to a single node on the BBN TC2000. The profiler monitors library routines as well as those in the code. In this simulation, the force routine used 77 times more CPU time than the boundary conditions routine (the second most expensive routine in our code). Naturally, we place most of our effort into parallelizing the force calculation.

In order to understand how a parallel force routine is designed, it is instructive to review how forces are calculated in MD simulation codes. Figure 2 shows a typical simulation cell. The algorithm used to calculate the forces depends on the range of interaction between the atoms. In materials with long ranged Coulomb forces, such as Silicate glasses, every atom interacts with every other atom. In simple metals, such as Copper and Nickel, the interatomic forces are short ranged and every atom interacts with at most a few dozen of its nearest neighbors. Here, we focus on this latter case. Systolic loop algorithms used to parallelize the long range force calculation are a hot research topic, currently being pursued by David Fincham and coworkers[6].

There have been two algorithms developed to optimize the force calculation for short ranged forces. The CPU time, required to calculate the force, scales linearly with the system size for both algorithms. In the Verlet neighbor list method[7], a list of all neighbors within the cut-off range plus a skin depth is maintained for every atom in the simulation. When any atom moves a distance equal to the skin depth, the entire neighbor list must be rebuilt. There are two drawbacks to this method: it requires a storage location for each neighbor of every atom and the CPU time required to rebuild the neighbor list scales as the number of atoms squared. The second method, used to calculate forces, is based upon the concept of linked lists[8, 9]. The large simulation cell is divided into many small sub-cells, the size of which is determined by the interaction range. A linked list is evaluated for every sub-cell. This linked list contains one entry per sub-cell that points at the first atom in the sub-cell and one entry per atom that points at the next atom in the cell. The entry for the last atom in the sub-cell contains the null pointer. The CPU time required to generate the linked list scales linearly with the number of atoms in the simulation and the memory overhead is quite small—one pointer per atom. Because the linked list method examines all atoms in the neighboring sub-cells (the force is evaluated only for those within the cut-off), the method runs slower than the neighbor list method for small system sizes on serial machines. The cross over is $\sim 10^2 - 10^3$ atoms. The neighbor list method performs well on vector supercomputers and we find it useful to retain some of its spirit in our code. The best algorithm for parallel machines with vector processors is a hybrid algorithm in which mini-lists are created on the fly from the linked-cell lists. The mini-list contains the addresses of all the atoms in a given sub-cell and all of the atoms they interact with. This allows our code to perform well in serial mode on vector supercomputers such as the Cray X/MP.

4 A Parallelization Strategy for the BBN TC2000

Our current development machine is the BBN TC2000, operated by the Massively Parallel Computing Initiative (MPCI) at LLNL. The MPCI TC2000 consists of 126 fast RISC microprocessors (Motorola 88100). Each processor is located on a separate board, along with 16 megabytes of local memory. The nodes are interconnected by a scalable "butterfly" switch. At boot time, some of each processor's local memory (6 megabytes) is allocated to an interleaved shared memory pool. It takes about four times longer to access this shared memory through the switch than to access private memory, local to the processor's board. Thus, an efficient computer code must use private memory for its computationally intensive tasks.

The development system on the MPCI TC2000 is aimed at a multi-user and multi-tasking environment. A small number of nodes (8) are dedicated to a public cluster. These run the familiar UNIX operating system and perform the editing, compiling and job control that defines the user's interface to the machine. The remaining nodes (118) are assigned to a gang scheduled cluster. This is the cluster where parallel programs are executed. The gang schedular assures that each user's task is run is a timely and fair-share manner. The parallel programming tools on the machine consist of BBN's extensions to FORTRAN, the Parallel C Preprocessor (PCP)[10, 11] and its extension to FORTRAN (PFP), an implementation of message passing (LMPS) based upon the Argonne message passing system[12], and various utilities to monitor an executing program. We have chosen the C programming language for our variable particle molecular dynamics primarily because, as yet, the FORTRAN programming language does not support the constructs required for an efficient implementation. In this report, we explore the utility of interleaved shared memory and the PCP paradigm for the implementation of molecular dynamics algorithms. Message passing schemes for molecular dynamics are concurrently being explored on the TC2000 at LLNL by Tony DeGroot.

PCP provides an extension of the single-program-multiple-date (SPMD) programming model in the familiar C programming language. Each processor executes the same code and flow control is placed into the hands of the programmer. PCP introduces the concept of a "team" of processors. A team may split into sub-teams in order to divide up work. Each team has one master processor. We find the master block (a section that only the master enters) most useful in performing serial work on shared memory—work that all processors must know about before the calculation can proceed. Flow synchronization is obtained through the **barrier** statement. Every processor reaching a **barrier** waits until all members of its team (including the master) reach that **barrier**. A fast waiting algorithm has been implemented for PCP runtime support. Additional flow control for critical sections is accomplished with locks. A critical section is a region of the code in which many processors access the same resource and, to allow them to do so, would corrupt the results. Accumulating partial sums into a shared sum is a commonly encountered example. PCP provides the **lock(&lock_variable)** and **unlock(&lock_variable)** functions to isolate critical sections. The lock variable is stored in shared memory. The first processor entering the critical section sets the lock variable to **locked** and proceeds with the calculation. Meanwhile, the remaining processors test the lock variable to see whether it is locked. When the first processor finishes the calculation, it sets the lock variable to **unlocked**. The next processor to find it unlocked immediately locks it and proceeds with the calculation.

Parallelism is accomplished with the **forall** loop. The for loop in C is similar to the **do** loop in FORTRAN. The **forall** loop divides the indices of a **for** loop evenly amongst the available processors. Each processor does the work for the value of the index it knows about. Possibly one of the most useful aspects of PCP is the transparent access to both shared and private memory. Declarations are made with the private and **shared** storage class modifiers and dynamical memory allocation is made using the **prmalloc** and **shmalloc** functions.

To see how these constructs are used in an MD code, it is useful to examine the MD algorithm in more detail. The MD algorithm has many features in common with most computer simulation algorithms:

1. Initialization
   - (a) read input file
   - (b) initialize positions and velocities
   - (c) bcs–apply boundary conditions
2. Main Simulation Loop
   - (a) **celler**–generate linked-cell lists
   - (b) **force**–calculate interatomic forces
   - (c) **advance**–obtain new positions using central difference
   - (d) **kinetic**–calculate kinetic energy
   - (e) **output**–accumulation and output
   - (f) **bcs**–apply boundary conditions
   - (g) finish?–otherwise loop again
3. clean up and close files

The initialization block represents a small amount of work that is performed only once. We place a master block around this section and concentrate on the main simulation loop. The bulk of the work is performed in the **force** routine and we discuss that first.

Our **force** routine consists of three pieces (the calculation of the EAM density, the interatomic forces and the tool atom forces) as shown in the following code fragment:

```
for( i = 0; i < nx; i++ ){
for( j = 0; j < ny; j++ ){
for( k = 0; k < nz; k++ ){
    a_ptr = cell[i][j][k].start_ptr;
    while( a_ptr != NULL )
    {
        eam_density_work;
        a_ptr = a_ptr- >next;
    }
}}}

for( i = 0; i < nx; i++ ){
for( j = 0; j < ny; j++ ){
for( k = 0; k < nz; k++ ){
    a_ptr = cell[i][j][k].start_ptr;
    while( a_ptr != NULL )
    {
        atomic_force_work;
        a_ptr = a_ptr- >next;
    }
}}}

t_ptr = first_tool_atom;
while( t_ptr != NULL )
{
    tool_force_work;
    t_ptr = t_ptr->next;
}
```

As described by Rapaport[13], the use of linked-cell lists introduces a "natural" domain decomposition parallelism into the MD algorithm. We simply convert the three for loops into a single **forall**. As each processor encounters the loop, it does all of the work for the sub-cell it is assigned to. Care is taken to assure that each processor has private copies of all parameters in the force calculation. The positions of the two interacting atoms are copied into private memory while the total force on each atom is accumulated into shared memory. In that each sub-cell contains ~ 10 atoms, the number of atoms in the simulation must be $>> 10^3$ to provide sufficient parallelism for our present machine (~ 100 processors). We typically run the simulation with $\geq 10^5$ atoms. The serial version of our code takes advantage of the fact that forces are equal

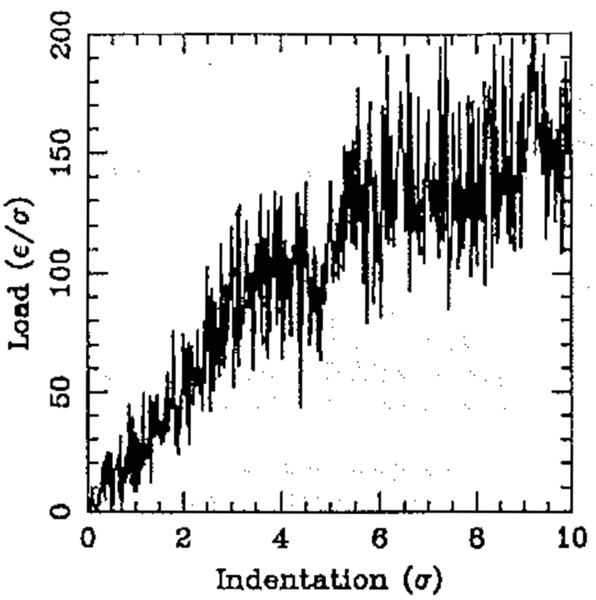

Figure 3: The instantaneous force (load) on the tool as a function of indentation for a 2D EAM simulation containing 43440 atoms in 160 layers and a tip radius ~ 5nm.

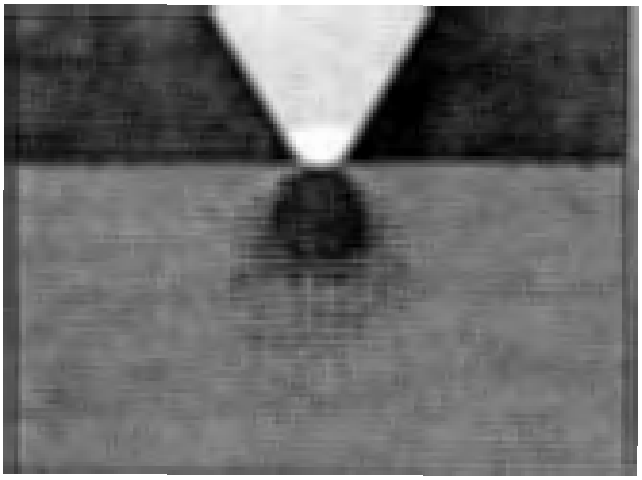

Figure 4: The calculated shearing stress field for an elastic indentation of 3 layers in the system containing 43440 atoms in 160 layers in 2D. Each atom is shaded by the local expectation value of the shearing stress.

and opposite—the pair interaction is only calculated once. This imposes the placement of locks at each pair calculation and the resulting speed-up does not exceed 6–7. By performing twice the work, we eliminate this "race" condition and have achieved speed-ups ~ 75 on 96 processors.

The while loop used for the tool force calculation is characteristic of linked-list data structures. The bulk of the work throughout the rest of the program consists of loops of this type. PCP does not provide a construct for parallelizing this loop, even though all of the work for each atom pointer is intrinsically parallel! This is because the addressing in memory is random and there is no *a priori* way to divide the work. We convert this while loop into a forall loop by defining an array of "first atom pointers." These are generated once per time-step at the end of the boundary conditions routine (assuring load balancing). The length of the array is equal to the number of processors executing the program (obtained from the PCP read only variable _NPROCS). The work is divided evenly amongst the processors as follows:

```
forall( int i = 0; i < _NPROCS; i += 1 )
{
     a_ptr = first_tool_atom[i];
     n_ptr = first_tool_atom[i+1];

     while( a_ptr != n_ptr )
     {
          tool_force_work;
          a_ptr = a_ptr->next;
     }
}
```

The linked-cell list generating routine (celler) presents a special problem in that all of the work is in critical sections. However, by introducing a separate lock variable for each sub-cell, most of the race condition is eliminated. The boundary conditions routine (bcs) performs the work of creating and removing atoms and generating the overall linked-list data structures. This work is inherently serial and, as we shall see, limits the performance of our code for large processor counts. In a constant particle number simulation, however, this work need be performed only once.

5 Test Problem Results

As described above, we are applying the molecular dynamics method to orthogonal metal cutting. This is a dynamic tribological problem in which two interacting surfaces are in relative motion. In our case, the diamond surface is significantly harder than the metal surface and we model it as infinitely hard, choosing to concentrate on the elastic and plastic deformation of the work material. Before studying the more gen-

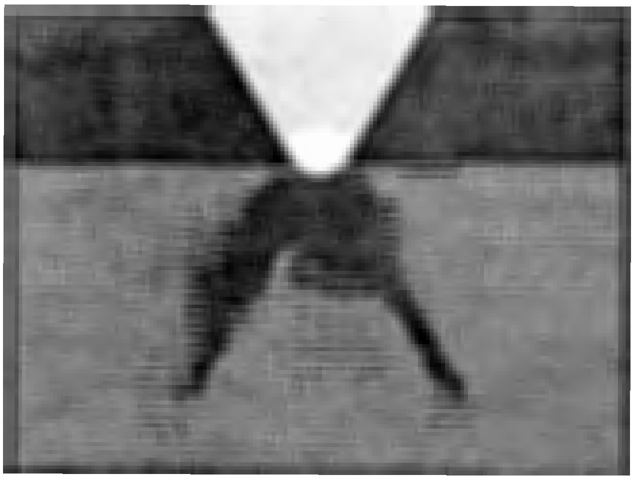

Figure 5: The calculated shearing stress field for a plastic indentation of 6 layers in the system containing 43440 atoms in 160 layers in 2D. Each atom is shaded by the local expectation value of the shearing stress.

eral problem of sliding surfaces, we have found it instructive to first study the indentation of a stationary surface.

A vast amount of information is known concerning the indentation of metal surfaces[14]—this is the experimental method of measuring "surface hardness." The results presented here are for a two dimensional simulation of an embedded-atom material. We are currently extending the work to three dimensions. The work material contains 43440 atoms in 160 layers initially on a triangular lattice. The tool tip radius is ~ 5 nm. We perform the calculation in an iso-thermal and quasi-static manner: all of the material atoms are coupled to a thermostat at room temperature and the indentation rate (1 layer per 1000 Einstein vibrational periods) is constant and slow enough to allow all of the material atoms and dislocations to relax to equilibrium. Faster rates do not allow this and results obtained at faster rates do not represent the experimentally measured properties. Our calculation ran for 1.5×10^6 MD time-steps. Shown, in Figure 3, is the resulting load on the tool as a function of indentation (1 layer $\approx 1\sigma$). Between 0 and 3 layers, all of the deformation is elastic and the load rises linearly with indentation. At 3.5 layers, the material yields by creating a dislocation that propagates down one side. The load relaxes slightly, until at 4.5 layers, stress begins to build on the other side. At 5.5 layers, that side yields as well. Further indentation produces further plastic work of the material. Figures 4 and 5 display our calculation of the shearing (deviatoric) stress field at 3 and 6 layers, respectively. Stress is an inherently macroscopic concept and, to make connection with the microscopic MD model, we must perform an ensemble average over a finite region of space. In our calculation, we stop the tool at the desired indentation and average the microscopic stress tensor within each subcell for 5,000 MD time-steps. The figures are generated by shading the atoms with the local expectation value of the shearing stress. The circular pattern in Figure 4 is the well-known Hertzian elastic stress field.

Figure 6: A snapshot from our molecular dynamics simulation of the orthogonal cutting of an EAM material in two dimensions containing ~ 100000 atoms in 200 layers. The simulation is performed at room temperature and the depth of cut is 32 layers (~ 8 nm). The atoms are shaded by the local expectation value of the shearing stress and the material flows from the left to the right at 100 m/s past the stationary tool.

Our simulation has many features in common with experiment[15, 16]. Micro-indentation experiments, however, are performed at a constant load. When a critical load is achieved, the tool suddenly jumps forward. This corresponds to the initial yield as shown in Figure 3 and the jump is clear across to the next build up of stress. The micro-hardness (load divided by the area of contact), calculated from our simulation, is $H \sim 3Y$, where Y is the ultimate yield strength of the material. This is 10 – 100 times larger than expected for a macroscopic hardness. However, recent experiments on this microscopic length scale, observe a dramatic increase in hardness[16]. We conclude that when the deformation occurs on a length scale much smaller than the material grain size, the work required to plastically deform the surface is the work of "creating" dislocations in addition to the work required to

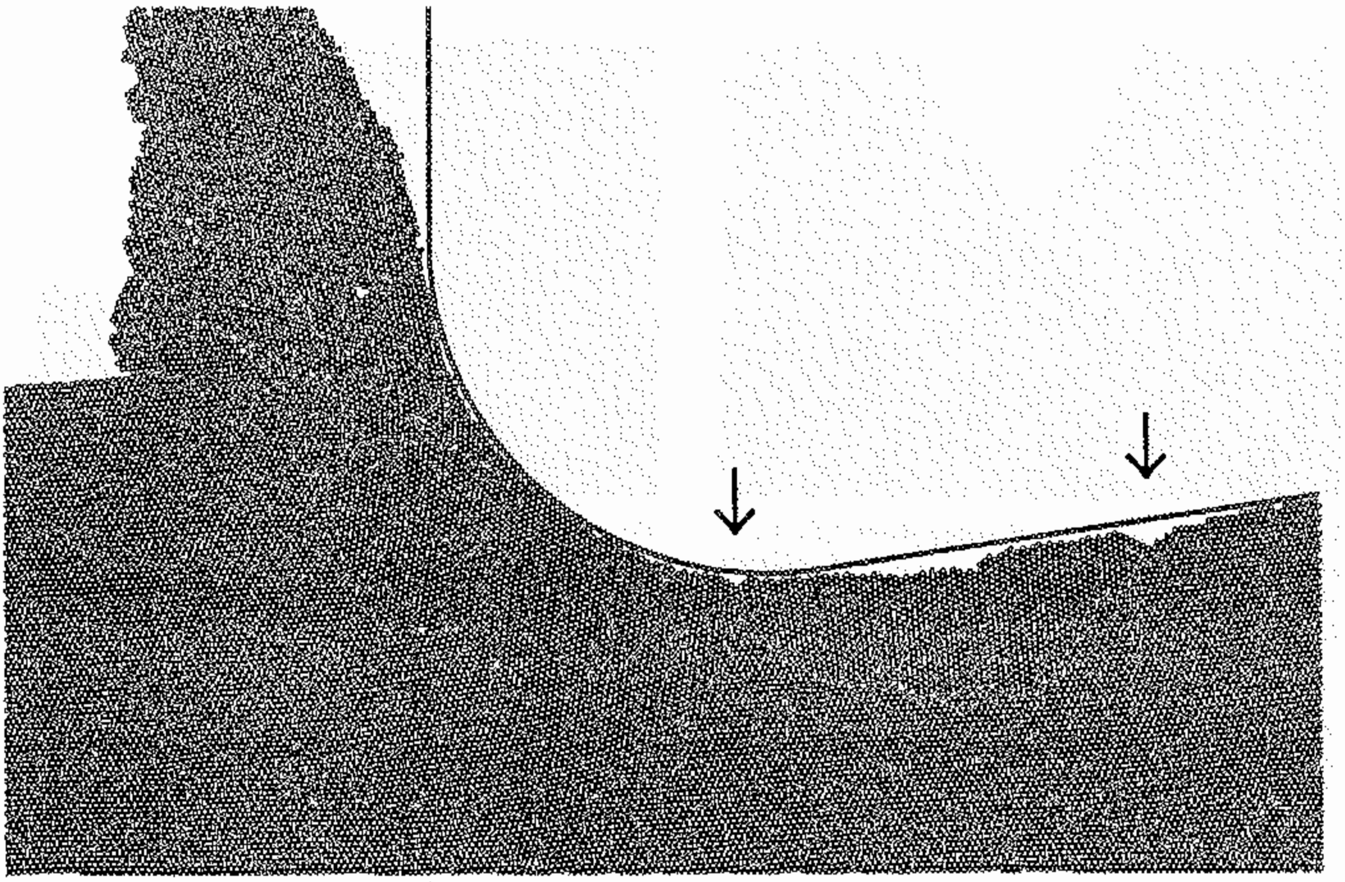

Figure 7: A close up of the region near the tool tip for the snapshot shown in the previous figure. The figure displays ~ 10000 atoms. The primary slip band takes the form of a grain boundary and, as indicated by the arrows, a small grain is formed on the fatigued surface. The simulation is forming localized bands of intense shear as found in ultra-high-speed machining.

move them. Another interesting result from our simulation, is that when the tool is removed, the dislocations anneal out—they propagate back to the surface leaving no sub-surface damage behind! The time scale for this dislocation motion is nanoseconds and simulations of shorter times will not observe effects of this type.

Of far more technological significance is our MD simulation of metal cutting—two interacting surfaces in relative motion. Shown in Figure 6 is a snapshot from our orthogonal cutting simulation containing ~ 100000 atoms in 200 laters in 2D, a tip radius of 20 nm, a depth of cut of 8 nm, at room temperature, and at a cutting speed of 100 m/s. This speed is about two orders of magnitude faster than the speed we would like to run the code at (~ 1 m/s). Shading is used again to represent shearing stress and many active shear bands are clearly evident. The primary shearing of material occurs along a curve that runs from in front of the chip, underneath the tool and onto the clearance face. This curve is a grain boundary interface and is observable in Figure 7. Figure 7 shows a close up of the region near the tool tip. Underneath the clearance face is a small grain on the surface that has been generated by the primary shear band. This structure is strongly reminiscent of the mechanism by which wear particles are believed to be generated on fatigued surfaces[17, 18].

The ultimate success of any computer simulation model is determined by how well it reproduces experimental measurements and its ability to help interpret and extend our description of reality and the application of this description to useful technology. In Figure 8, we show a comparison of our simulations with the recent measurements of Moriwaki and Okuda[19]. Our results are preliminary. However, we find a rather interesting result—the specific energy (the work performed by the tool per unit volume of material re-

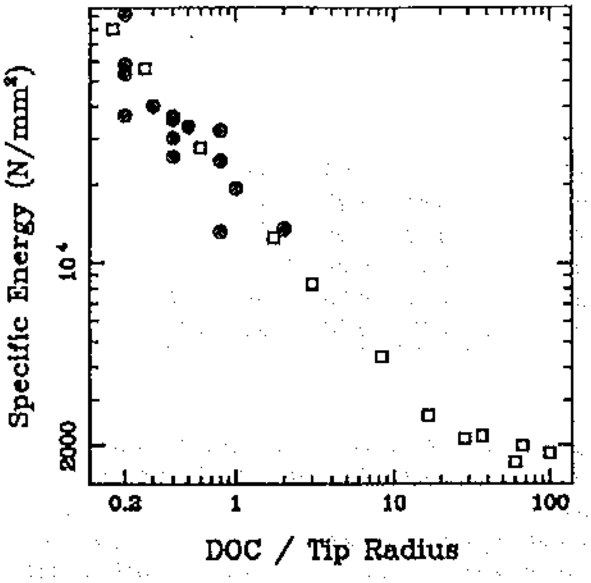

Figure 8: The specific energy (work per unit volume of material removed) plotted versus the depth of cut normalized by the tool tip radius. The open squares are the experimental measurements of Moriwaki and Okuda for the micro-machining of Copper at 23 m/s. The solid circles are the molecular dynamics results. The simulations were performed for tool tip radii 1.25nm, 2.5nm, 5.0nm, and 20.0nm at cutting speeds of 10 and 100 m/s.

moved), when plotted versus the depth of cut divided by the tool tip radius, falls onto a universal curve! There are two distinct regions of this curve. For depths of cut much greater than the tip radius ($d \geq 1\ \mu$m), we find $E \sim (d/r)^t$, with $t \approx -0.2$. For small depths of cut, $t \approx -0.8$. These two regions occur because of differences in the mechanism of plastic deformation. At large scales, the deformation occurs along grain boundaries, with little or no deformation within the grain. The exponent of $t \approx -0.2$ is well-known for macroscopic metal cutting[20]. At smaller scales, all of the deformation occurs within a grain (grain sizes are typically $\sim 1\ \mu$m). The work performed by the tool is the work required to break and reform every bond in the path of the tool. We are pleased that the simulation agrees with experiment over the two orders of magnitude for which we have done the calculation. Complete reports of both our indentation simulations and orthogonal metal cutting simulations in two dimensions are currently being prepared for submission to the *Journal of Applied Physics*. A preliminary report of the indentation simulation was presented at the MRS Symposium on Atomic Scale Calculations of Structure in Materials[21] and a preliminary report of the orthogonal metal cutting simulations was presented at the 1990 Annual Meeting of the American Society of Precision Engineers[22].

Table 2: A comparison of single processor performance on the BBN TC2000 and the Sun SparcStation-1 simulating the motion of 32256 atoms in three dimensions.

	TC2000(sh)	TC2000(pr)	Sparc-1
Total(sec)	551.17	284.89	144.61
celler	1.50	0.80	0.40
force	540.32	278.44	138.19
adv+io	4.23	2.43	1.25
kinetic	2.64	1.49	2.01
bcs	2.49	1.74	2.76

6 Performance Results

Our parallel molecular dynamics algorithm has been implemented on the BBN TC2000 using the PCP programming paradigm and has been used to generate the results described above. In this section, we present performance results for the code running on the TC2000 with up to 100 processors and compare to the performance of the Cray X/MP and a commonly available desktop scientific workstation, the Sun SparcStation-1. The performance of the RISC based Sparc CPU ($\sim$ 2 megaflops) is comparable to the RISC based Motorola 88100 ($\sim 3-4$ megaflops) and we use the Sparc-1 as our base unit of performance. The current memory configuration (6 megabytes of interleaved shared memory per node) of the TC2000 at Livermore allows us to fit up to $\sim 5 \times 10^6$ atoms in core ($\sim$ 100 bytes per atom). Simulating the motion of 5,366,592 atoms on 108 processors, our code performs one 3D time-step in 20 minutes of CPU time and one 2D time-step in 4 minutes of CPU time. The factor of 5 difference in performance is due to the additional degree of freedom per atom and a factor of 3 increase in the number of interacting neighbors in 3D over 2D. Timing comparisons with fewer processors are prohibitively expensive for this large system size. Our present simulation code is fully three dimensional and the bulk of our future calculations will be with this code. Thus, we present here, timing comparisons for 3D EAM molecular dynamics simulations containing 4032, 32256 and 258048

Table 3: CPU times to simulate one molecular dynamics time-step of a 3D EAM material containing 4032 atoms on the BBN TC2000 with 1 – 96 processors.

processors	1	2	4	8	12	16	24	32	48	64	96
Total(sec)	68.73	34.75	17.69	9.20	6.18	4.77	3.39	2.65	2.03	1.62	1.56
celler	0.19	0.09	0.05	0.03	0.02	0.02	0.01	0.01	0.01	0.01	0.01
force	67.31	33.90	17.14	8.70	5.85	4.43	3.05	2.33	1.68	1.31	1.21
adv+io	0.56	0.31	0.17	0.11	0.06	0.08	0.09	0.07	0.09	0.06	0.09
kinetic	0.34	0.18	0.10	0.05	0.04	0.04	0.03	0.03	0.04	0.04	0.05
bcs	0.33	0.27	0.24	0.21	0.21	0.20	0.21	0.20	0.20	0.20	0.21

atoms. All of our calculations are performed with 64 bit floating point precision. The benchmark calculations were performed on a quiet system—no other jobs in the gang scheduled cluster.

Shown in Table 2 are timings for the code executing on a single processor for the Sparc-1, the TC2000 using only node private memory, and the TC2000 using interleaved shared memory for the ATOM and CELL structures. In both cases, the processor has a private copy of all parameters (other than atomic positions) that define the calculation. The serial code running on the Sparc-1 assumes forces are equal and opposite and hence performs about half the operations of the parallel code to achieve the same *useful work* (a molecular dynamics time-step). The shared memory overhead is about a factor of two and appears to be uniform throughout the code. As described above, the basic loop in our code is:

```
a_ptr = first_atom_ptr[i];
n_ptr = first_atom_ptr[i+1];
while( a_ptr != n_ptr )
{
      x_p = a_ptr->x;
      more_work;
      a_ptr = a_ptr->next;
}
```

The pointer variables (`a_ptr`, `n_ptr`) are private to the processor, while the starting pointers (`first_atom_ptr`) are shared. The private floating point variable `x_p` is used to copy the positions of the atoms into local private memory for the calculation. The additional work (especially for the force routine) should far exceed the overhead for this copy. Atoms travel from sub-cell to sub-cell and, to perform variable particle simulations, we dynamically create and remove atoms from anywhere in the list. Thus, the storage for the ATOM structure is equally likely to be in any node's memory. If we were to determine *a priori* which atoms are in which processor's local memory, we should expect to obtain a considerable speed-up. A larger domain decomposition scheme, that assigns a set of atoms to each node, achieves the desired mapping. However, interdomain interactions and diffusion complicate the program structure and effect load balancing. Nevertheless, this may be the only solution and we will pursue it in our future work. Considering the factor of two in operations performed, the TC2000 using private memory is comparable to the Sparc-1. We had expected the TC2000 to be ~ 1.5 times faster. The difference is most likely due to the PCP constructs used to obtain parallelism, none of which exist in the serial code. The celler routine is an extreme example in which the PCP code locks every inner loop.

The Cray X/MP vector supercomputer, operated by the Open Computing Facility (OCF) at LLNL, is representative of the class of computer currently used to run large scale scientific codes. The clock speed of the X/MP (9.5 ns) is about 5 times the clock speed of the Motorola 88100 and Sparc-1 *killer microprocessors* (50 ns) and this would be all of the performance gain we would find on the Cray if we do not take advantage of the vector capabilities. Furthermore, we anticipate that future generation *killer micros* will have vector subsystems. As described above, our force routine generates "mini-lists" from the linked-cell lists. The GATHER/SCATTER scheme, as described by Fincham and Ralston[23], is used to vectorize the force calculation. We obtain a speed-up of 12.5 over the Sparc-1 for a single node on the 4 processor X/MP. A detailed analysis of the force routine reveals that ~ 50% of the time is spent in the scatter section, in which no useful work is performed! We have devised a memory intensive scheme to vectorize the scatter section. However, it is prohibitively memory expensive

Table 4: CPU times to simulate one molecular dynamics time-step of a 3D EAM material containing 32256 atoms on the BBN TC2000 with $1 - 96$ processors.

processors	1	2	4	8	12	16	24	32	48	64	96
Total(sec)	551.17	276.70	140.26	71.31	48.64	36.94	25.78	20.26	14.66	11.89	9.35
celler	1.50	0.75	0.38	0.19	0.13	0.10	0.08	0.06	0.05	0.05	0.05
force	540.32	270.50	136.30	68.56	46.26	34.73	23.72	18.22	12.71	9.96	7.73
adv+io	4.22	2.12	1.10	0.57	0.40	0.34	0.29	0.30	0.26	0.25	0.25
kinetic	2.63	1.32	0.66	0.34	0.23	0.17	0.12	0.10	0.08	0.07	0.07
bcs	2.49	2.01	1.82	1.65	1.61	1.59	1.57	1.58	1.56	1.55	1.55

Table 5: CPU times to simulate one molecular dynamics time-step of a 3D EAM material containing 258048 atoms on the BBN TC2000 with $1 - 96$ processors.

processors	1	2	4	8	12	16	24	32	48	64	96
Total(sec)	4424.29	2221.09	1125.90	572.42	388.40	295.71	206.30	160.01	116.37	93.56	72.48
celler	11.94	5.97	3.03	1.54	1.07	0.81	0.59	0.48	0.39	0.36	0.35
force	4340.05	2172.74	1094.79	550.70	369.38	278.38	190.04	144.32	101.14	78.76	57.82
adv+io	31.71	15.96	8.38	4.33	3.10	2.48	2.17	2.01	1.86	1.67	1.68
kinetic	20.72	10.40	5.21	2.65	1.79	1.35	0.92	0.70	0.50	0.40	0.31
bcs	19.88	16.01	14.49	13.20	13.06	12.69	12.57	12.50	12.47	12.36	12.32

when the motion of more than a few hundred atoms is simulated.

The partially vectorized Cray version performs half the operations per time-step as does the parallel version and contains none of the parallel overhead. Given the timings in Table 2, we require a speed-up of at least 48 on the TC2000 to obtain comparable performance with the Cray—the same number of MD time-steps in the same wall clock time. Shown in Table 3, 4, and 5 are timings for 3D EAM simulations with 4032, 32256, and 258048 atoms, respectively. The timings were obtained with the `get64bitclock()` function and were performed on a quiet system—no other jobs in the gang scheduled cluster. Several observations may be made:

1. With small processor counts, the force calculation is by far the dominant part of the calculation.

2. We begin to exhaust the available parallelism for the small system with large processor counts.

3. The boundary conditions routine has not been parallelized and is becoming comparable to the force routine for large processor counts. We must eliminate this serial section if we are to ever take advantage of the $10^3 - 10^4$ processors expected in the next generation parallel supercomputer.

4. The force routine achieves only 75% efficiency with 100 processors. In order to achieve 75% efficiency with 1000 processors, we must obtain 97.5% efficiency with 100 processors.

5. The timings scale better than expected with system size! The linked-cell algorithm is expected to scale linearly with the number of atoms. The time required with 258048 atoms is actually less than the expected 64 fold increase from that with 4032 atoms. This is undoubtedly due to the many-fold increase in available parallelism.

6. We achieve a speed-up of 48 with $\sim$ 64 processors. This is the performance required to do the same *useful work* as the partially vectorized Cray code. It must be re-iterated that this is for a full production MD code!

Figure 9 is a plot of the parallel efficiency of the various routines in our MD code simulating the motion of 32256 atoms. The parallel efficiency is defined to be the time to execute on one processor divided by the time to execute on n processors divided by the number

neering Program (PEP) at LLNL. His continuing encouragement is gratefully acknowledged. The computational aspects of the MD model presented here have been discussed with Bill Hoover. The graphics rendering was made possible with the help of Mike Allison. His rendering routines are available on the MPCI TC2000. The calculations presented here would not have been possible without the generous support of the Massively Parallel Computing Initiative at LLNL.

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Very efficient Molecular Dynamics Codes for Multi-million Particle Systems

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Timing results for two O(N) MD programs for the simulation of large 3-D short-range interaction systems are given. The programs are based on two recently published codes [1,2] and they have been developed and optimized for the Hitac M-series serial computers (M-280,M-680, M-880). The first program called MDSP1H corresponds to the scalar pyramid described in paper [1] and it does not use any nearest-neighbour (NN) list, while the second one called HISPNL [2] uses a NN list. Consequently the first one requires less computer memory (memory for this program does not depend on the choice of cut-off radius R_c) but is about 2.5 times slower than the HISPNL program. Both programs are truly order of N programs and their cpu time for the calculation of forces t_n (per time step and per particle) is strictly proportional to the average number of NN contained in the R_c sphere ($n_{av} = 4\pi R_c^3 \rho/3$, where ρ is the number density). This cpu time contributes to 90-95% of cpu time for the entire simulation and can be simply expressed as:

a) MDSP1H program,

$$t_n = n_{av} \times T^*_{int} \qquad (1)$$

b) HISPNL program,

$$t_n = n_{av} \times (T_{int} + T_{ass}/\mathrm{NTUPDA}) \qquad (2)$$

where T_{int} and T_{ass} are the cpu times per single interaction (i.e. per a single local neighbour) that are needed for the calculation of interactions (distances, forces, potentials, virial ...) and assignment of NN, respectively. NTUPDA is the frequency of the NN list updating (typically 10 to 20) and T^*_{int} in eq. (1) combines both T_{int} and T_{ass} (these times cannot be separated in that code). The tests have been performed for n_{av} from 33.5 which corresponds to R_c equals a half side of a cube containing N=64 particles (R_c=H(64)) up to n_{av}=113 (R_c=H(216)) and over very large range of N (from N=64 to N=8788000) showing very stable values of T_{int} and T_{ass} cpu times. On the Hitac M-880 single processor serial computer with 64 bit word length these times are equal to:

$$T^*_{int} = 1.5\pm0.1\mu s \qquad (3a)$$

$$T_{int} = 0.56\pm0.03\mu s \qquad (3b)$$

$$T_{ass} = 0.9\pm0.1\mu s \qquad (3c)$$

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As an example in Table 1 are given the cpu times per time step and required memory (in brackets) for these programs on the M-880 computer for selected sizes of 3-D systems (for HISPNL, NTUPDA=20).

Table 1. Cpu time per time step (in seconds) and required central memory (in Mb; the values given in brackets) for the HISPNL/MDSP1H programs on the Hitac M-880 main frame.

code	system size N			
	128	1000	110592	1000000
SPNL	0.0027 -	0.020 -	2.4 (27)	19.3 (226)
SP	0.0065 -	0.050 -	6.2 (14)	50.3 (116)

Both programs can be easily adopted for the simulation of 2-D systems. An estimated cpu time for a 2-D version of the HISPNL program on the M-880 computer and for similar conditions to those quoted in ref. [3] is between 2 and 3 seconds per step for $N=10^6$ and therefore, almost two times less than for the LLC method on the Cyber 205 vector computer [3].

Presently, work on the vectorized MD code based on the method described in refs. [4,5], as well as on an MD code for the simulation of large multi-ionic systems with direct Ewald summation used for the coulombic forces, are in progress. Preliminary estimation of cpu times for these vectorized codes on the Hitac S-820 vector computer (single processor, 4 ns clock period) are as follows: 2-2.5 s per time step for $N=10^6$ (3-D, short-range interaction, $n_{av}=33.5$), 0.3 s per step for $N=10^6$ (2-D, short-range interaction, $n_{av}=5$) and order of 10 cpu second per time step for $N=10^6$ (3-D, multi-ionic systems). Therefore, an estimated cpu time for a 2-D simulation of 1000 time steps and $N=10^6$ is order of 5 cpu minutes on the S-820 supercomputer. More detailed data regarding the speed performance of these new vector programs will be published in the near future.

The M-880 is equipped with huge memory (up to 2Gb main memory plus 8 Gb fast extended memory with the speed transfer of 2.2 Gb/s) that makes it possible to simulate 3-D MD systems containing up to 90 millions of particles by the MDSP1H program and up to 45 millions by the HISPNL program. For 2-D systems these figures may be increased by factors of 1.5 (MDSP1H program) and 2 (HISPNL program), respectively. On the S-820 supercomputer it is possible - in terms of cpu time and memory requirements (up to 12.5 Gb combined memory) - to simulate the systems as large as $N \sim 10^8$ particles. In a 2-D case such a simulation would require order of 30 cpu seconds per time step.

It should be pointed out that those vector programs are very suitable for multiprocessor vector computers. Typically more than 85% of the total cpu time in these programs is consumed just for the calculation of mutual interactions between particles and this is performed over vectors of length N [4]. This part of the calculation can be simply (and arbitrary) divided into smaller parts (sub-tasks) that can be calculated independently, and therefore at the same time, on different processors.

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USSR

June 5, 1991

In December 1989 I received an invitation from Dr W Smith to visit the UK within the framework of the CCP5 project. This invitation was quite unexpected and I was very glad to accept it. A year and a half before, Professor J S Rowlinson had visited our Laboratory and we had had many interesting and stimulating discussions. I was acquainted, of course, with the work of some British research groups which were involved in computer simulation of physical chemical systems on the molecular level, and our Laboratory regularly received CCP5 Newsletters. With the help of FAX and TELEX the schedule of my two week journey was soon worked out. As I am involved in computer simulation of various aqueous systems, both biological and inorganic, I wanted to visit, besides Daresbury Laboratory, Birkbeck College in London, J S Rowlinson's laboratory in Oxford and a group involved in X-ray structural analysis of DNA and polynucleotides. Dr W Smith suggested I visit Professor W Fuller's group in Keele.

I had planned to arrive in London on the 7th of May 1990 but my entrance visa was not ready, so I arrived on the 12th. I spent two days, Monday and Tuesday, in very intensive and stimulating discussions with Julia Goodfellow and her colleagues. The work performed in J Goodfellow's group is very close to my interests. Being a crystallographer by education, I have been interested for a long time in the structure of water and aqueous solutions, hydrogen bond patterns in crystals and hydration of biopolymers. I discussed all these problems in Birkbeck. My one hour lecture was dedicated to computer simulation of the DNA hydration shell.

On Wednesday I walked to the Royal Institution. I plunged there into the atmosphere of mineralogy and inorganic chemistry. We discussed with Professor C R A Catlow and his students the problems of the structure and lattice dynamics of oxides and silicates, diffusion of adsorbed molecules in zeolites and other topics. I told Professor Catlow about our works (performed by M M Frank-Kamenetskii and myself) on the Monte Carlo simulation of the zeolite A - water system. The unique atmosphere of this Institution, where modern computers with excellent molecular graphics are surrounded by a XIX'th century interior and where the presence of M Faraday's spirit can still be felt, stimulated fruitful discussions.

My schedule in London was very tough, so I had very little time for sight-seeing and cultural programme. I spent four hours in the British Museum (one needs at least an order of magnitude more time to get even a superficial idea about what is exhibited there) and, due to the courtesy of Julia Goodfellow, saw Coriolanus at the Barbican. Perhaps it was not bad for the first visit to London. I spent a pleasant time in J Goodfellow's house and walked along London streets.

On Thursday at nine o'clock in the morning I was on the train to Oxford. Two hours later I was met by Professor J Rowlinson at the railway station. He took me to his laboratory, then I walked a little and we met near Exeter College where we had our lunch. Professor J Rowlinson showed me to the room for the guests of the College with a huge sitting room where I could give a reception for a least 20 guests (unfortunately I had not so many acquaintances in Oxford!) and a very cosy bedroom. At four o'clock I gave a lecture on the computer simulation of water in small pores of zeolite and carbon adsorbents. Some people from the Royal Institution were also present. After the seminar I had discussions with the researcheres at the laboratory and saw some experimental equipment. The Physical Chemistry Laboratory Headed by Professor J S Rowlinson is a modern, well-equipped Laboratory where experimental, theoretical and computational works are optimally combined. The main directions of the work of the Laboratory are very close to those of the Institute of Physical Chemistry where I work. It was very pleasant for me to hear Professor Rowlinson's high appreciation of experiments on adsorbtion performed at the Laboratory of Adsorbtion in our Institute.

At seven o'clock I was invited to dinner at the College. Some fellows of various specialities were present so there was very interesting general discussion.

Though I had read something about Oxford, reality surpassed all my expectations. The atmosphere in the city, in the College, and especially during the dinner was so unusual that I felt absolutely unprepared for it. I am very grateful to Professor J S Rowlinson that I have had the opportunity to spend some days in that wonderful place.

On Friday I went by car with some young colleagues from the laboratory to a meeting in Southampton. Talks on molecular dynamics simulation of monolayers, Langmuir-Blodget films, micelles and polymers performed in Oxford, Southampton, Manchester and, perhaps, other places were given there. After lunch an absorbing lecture covering all the mentioned subjects was delivered by M Klein. Unfortunately too little time was left for the discussion. After the meeting we returned to Oxford and I enjoyed the hospitality of Mrs and Professor Rowlinson.

On Saturday Mrs and Professor Rowlinson took me to Stratford-upon-Avon, this sacred place where the genius of world culture was born and died. We saw there a very original production of "Comedy of Errors".

On Sunday I crossed half of Britain and left the train in Warrington. I was met by Dr W Smith who brought me at first to the hostel and then to his home. How different British families are but all I met were extremely cordial and hospitable. After dinner I was taken to Chester a small town full with historical monuments, where one can feel breath of history.

Daresbury Laboratory is an ideal place for a scientist to work. I shall not describe it for it will be well-known to most of the readers. Surrounded by country and picturesque landscape it creates all the possibilities for creative work, for concentration of strength and mind. But I had no time for such concentration. Seminar on Monday, visit to Keele and seminar there on Tuesday, discussions, discussions, discussions. In my lecture at Daresbury I spoke about some approaches we used in our work on the simulation of aqueous systems: the F-structure concept, dynamical criteria of hydrogen bonding in simulated liquid and the application of Grivtsova-Grivtsov formula for estimation of the diffusion coefficient in capillars and porous media. In Keele I gave a talk on the structure of the DNA hydration shell. It was a somewhat different version of my talk in Birkbeck for the majority of the audience were crystallographers directly involved in the determination of the polynucleotide structure. Unfortunately Professor W Fuller was in Moscow at the time, but I had very interesting discussions with his colleagues. I had an opportunity to discuss some problems of the state of adsorbed molecules in zeolites as well.

A short excursion to the Daresbury Laboratory impressed me greatly. Such a variety of methods, approaches and subjects of investigation!

And I am again in the train, making its way to the North, to Glasgow. I saw tremendous landscapes through the window. I was met by Dr David White at the station. The third lecture on DNA hydration, the third version of it. I tried to make it more popular, for specialists in different fields were present. And then again to the South, back to Oxford.

Professor J Finney met me at the station at 5 pm on Friday. The atmosphere in Rutherford Laboratory is somewhat different from that in Daresbury. Perhaps it's because they are given counters of radiation there. Again such a variety of methods and objects. Most of all I was impressed by the determination of the structure of a rather complex sample using only powder neutron diffraction data. Work on the structure of the surface of liquid water, on biopolymers and many others were also very interesting. For me the day ended with a rabbit pie in the pub in the international company of J Finney and his colleagues. After this informal meeting scientists from the Lab returned to their working places and I went to bed in a small cosy hotel on the bank of the Thames. Next morning I was taken to Heathrow by car through Robin Hoodian forests. This was the end of my fascinating trip to Britain in the merry month of May.

I am very grateful to the CCP5 project and to Bill Smith who organised my unforgettable journey, to J Goodfellow, J S Rowlinson, D White, J Finney and all their colleagues for their hospitality and patience. I am also grateful to Dr K Heinzinger and to Max-Planck-Institut für Chemie in Mainz where I currently have the opportunity to work quietly. In the bustling life of Moscow I could not have found the time and inspiration to write this story.

An Appreciation of Allan Grivtsov (1937-1991)

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June 5, 1991

Allan Grivtsov died on the 12th January 1991. Born on April the 15th 1937 in Moscow, he was one of the pioneers and enthusiasts of molecular dynamics simulation. Allan was a student of the Chair of Biophysics headed by Professor L A Blumenfeld when the idea of molecular dynamics simulation came to him. At that time he did not know that this method had already been used by other scientists. He approached S E Shnol, lecturer in biochemistry, a very broad-minded scientist and a man of deep understanding of the problems of natural sciences (it was he who proposed to his student A M Zhabotinsky to study Belousov's reaction) for advice. S E Shnol said his brother, E E Shnol, a mathematician, got interested in the problem. The first of A Grivtsov's works on molecular dynamics simulation is an unpublished report (37 type-written pages), written by him in collaboration with E E Shnol in 1967. Its title was "On the numerical modelling of the molecular motion in a liquid". A Grivtsov started to propagandize the method. He spoke at various scientific conferences (some of his remarks were published in the discussion sections of the conferences' proceedings) trying to stimulate the interest of the specialists in various fields. After the discussion at the conference on the theory of adsorbtion he became a scientific worker of the Institute of Physical Chemistry. He performed, as far as I know, the first works on simulation of structuralisation of liquid near the solid wall and of adsorbtion. He was one of the first who used molecular dynamics simulation to study motions in a polymer chain. His candidate (Ph.D. equivalent) thesis, written in 1973 was entitled "Numerical experiments on modelling motions of the molecules". Soon, just after publication of Rahman and Stillinger's work he elaborated an original, very efficient algorithm for simulation of rigid multiatomic molecules and wrote a programme to simulate water.

A Grivtsov simulated dislocations in crystals, the deformation of a molecular crystal, dynamics of the polymer crystal, studied influence of impurity on the strength of a crystal and performed many other excellent pioneering works. He delivered lectures, organised seminars, workshops and schools. Due to this activity computer simulation became rather popular in the USSR. I would like to mention four workshops on the application of mathematical methods to study of polymers. At these workshops, which took place in Pushchino (a scientific centre to the South from Moscow), the efforts of mathematicians, theoreticians, molecular biologists and polymer scientists were united. For several years he headed a very prestigious seminar on the computer simulation of polymers and condensed matter at Moscow University. It is impossible to enumerate all the scientific events in organisation of which A Grivtsov took part.

A Grivtsov had many disciples. He taught them to be strict in formulation of the tasks and the methods chosen to fulfil them. He thought a lot about fundamental principles of computer simulation and his contribution to their development was invaluable.

His favourite creation was his group in the Institute of Physical Chemistry. By and by after hard efforts and struggle it turned into the Laboratory of Mathematical Modelling of the physico-chemical processes. He passed away when he was 53 years old.

A list of A Grivtsov's publications comprises more than 70 items. For the most part they are abstracts, short communications and preprints, almost all in Russian. This brilliant scientist knew foreign languages rather poorly. Best of all he could read and speak in Esperanto, but few scientists are fluent in this artificial language and there is practically no scientific literature in it. It is one of the reasons why he is not as well known in the world as he deserves to be. The main reason was his modesty and the difficulty of travelling abroad for a real scientist during the years when he was in his prime.

List of main publications of Allan Grivtsov

1. On the structuralization of liquid near the solid surface. Doklady Akademii Nauk SSSR v.190, N4, p.868, 1970
2. Numerical modelling of the deformation of the molecular crystal. Ibid., v.215, N1, p.148-151, 1974 (with V S Yushchenko and E D Shchukin)
3. Numerical modelling of the motion of a linear polymer chain. Ibid., v.220, N5, p.1096-1098,1975 (with N K Balabayev and E E Shnol)
4. On the analysis of the mechanism of the adsorbtional decrease of the strength. "Fizico-khimicheskaya mekhanika materialov" N1, p.31, 1976 (with V S Yush--chenko)
5. Stability and dynamics of a drop on the solid state surface. "Kolloidnyi Zhurnal",v.39, N2, p.335-338, 1977 (with V S Yushchenko and E D Shchukin)
6. Heterogeneous crystallization (Kinetics and computer simulation). A book. (with D Fedoseev and P Chuzhko) Moscow, Nauka, 1978 (A Grivtsov wrote a chapter about molecular dynamics simulation - one of the best manuals in the world)
7. Geometrical sense of the temperature of the ergodic system. Zhurn. Fizicheskoi Khimii, v.54, N1, p.250, 1980
8. Molecular dynamics study of the distribution of the kinetic energy in the polyethylene molecule. Vysokomoleculyarnye soyedineniya, v.23b, p.121-123, 1981 (with N K Balabayev)
9. Numerical modelling of rotational crystalline states of the n-parafin Doklady Akademii Nauk, v.227, N2, p.412-415, 1984 (with M A Mazo, N K Balabayev et al)
10. Diffusion of the molecules in narrow pores. Kolloidnyi Zhurnal, v.5, p969, 1982 (with L A Grivtsova, N V Churaev, L F Chuikova)
11. Numerical modelling of protein molecular dynamics. Molekulyarnaya Biologiya, v.17,N3,p.587-616,1983 (with G G Malenkov and L V Abaturov)

12. Mathematical modelling of the adsorbtional processes In: Adsorbtsiya i adsorbenty, Moscow, Nauka, 1987, p.81-87
13. Geometrical criterion of the hydrogen bond in computer simulated water. Zh.Strukturnoi Khimii, v.28, N2, p.81-85, 1987 (with G G Malenkov and M M Frank-Kamenetskii)
14. Molecular dynamics simulation of the vitrification of two-dimensional Lennard-Jones fluid. Rasplavy, v.1, N6, p.101-106, 1989 (with M I Kotelyansky and M A Mazo)

All these publications are in Russian. English translations of the most part of journals are available.

Below I give the full list of A Grivtsov's publications in English, including abstracts:

1. Mechanical behaviour of solid polymer - imitation by molecular dynamics method In: Molecular Mobility in Polymer Systems. P.336. Leipzig, 1981 (with N K Balabaev et al)
2. Molecular dynamics simulation of motion in solid polymers rotation phase of n-alkane. Polymer Bull. v.12, N4, p.303-309, 1984 (with M A Mazo, E F Oleynic et al)
3. Molecular dynamics simulation of the n-alkanes rotator phase In: Physical optics of dynamic phenomena and processes in macromolecular systems. p.413-425, Berlin, 1985 (with M A Mazo, E F Oleynic et al)
4. Molecular dynamics simulation of water: adsorbtion of water on -tridimite. J. Coll.I nterface Sci., v.126, N2, p.397-407, 1988 (with L T Zhuravlev, G A Gerasimova and L G Khazin)
5. Molecular dynamics simulation of liquids contacting the solid surfaces. Symposium on the structure of liquids and solutions August 24-27. Vesprem. Abstracts p.37-39, 1987
6. On the thermodynamically correct molecular dynamics simulation of water. International conference on solution chemistry. Jerusalem August p.102, 1989 (with M M Frank-Kamenetskii and D L Tytik)

Efficient calculation of the pressure in the canonical ensemble for inverse power central force models

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The pressure in the canonical ensemble is obtained as a function of the virial sum v[1]:

$$P = kT\ (N - v/3kT)/V \qquad (1)$$

with

$$v = \sum_{i<j}^{N} (\underline{r}_{ij} \cdot \underline{\nabla}_i e_{ij}) \qquad (2)$$

where k is the Boltzmann factor, T is the absolute temperature, N is the number of particles in the system, V is the volume, $\underline{r}_{ij}$ is the interparticle vector and e_{ij} is the energy of interaction between particles i and j. In general, calculation of the virial sum requires the calculation of the forces on the particles, a non-negligible amount of extra work (unless the force-biased displacement scheme[2] is used where the forces are also needed anyway) and is thus rarely done. However, if e_{ij} depends only on $|\underline{r}_{ij}|$ (i.e. there is only one interaction center per particle) and the interaction follows an inverse power law (or is a sum of inverse power terms) the contribution of particles i and j to the virial sum can be obtained with negligible extra work, since simple application of the chain rule shows that

$$(\underline{r}\cdot\underline{\nabla}\ (1/|\underline{r}|)^n) = -\ n/|\underline{r}|^n\ . \qquad (3)$$

Thus the calculation of the virial sum in this case require only the separate accumulation of the contributions to the total energy from the various distance powers during the simulation and their multiplication with the corresponding exponent n after the simulation.

Acknowledgements.

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1. Barker, J.A.; Henderson, D. Rev. Mod. Phys. **1976**, 48, 587.

2. Rao, M.; Pangali, C.; Berne, B.J. Mol. Phys. **1979**, 37, 1773.

Determining nearest image in non-orthogonal periodic systems.

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The simulation of crystalline systems where the crystal axes are non-orthogonal, raises the question of finding the nearest image of a particle. Smith has recently showed [1] that if a suitably chosen spherical cutoff is imposed on the interactions then the nearest image can be conveniently determined in the non-orthogonal system defined by the crystal axes and then simply transformed back to the orthogonal laboratory frame. The purpose of this note is to describe a relatively simple procedure to find the nearest image without the imposition of the spherical cutoff.

Assume that the columns of the matrix H contain the vectors spanning (in the orthogonal system) the unit cell corresponding to the nonorthogonal system. The coordinates of a point in the orthogonal system, $\underline{x}$, are given as

$$\underline{x} = H \, \underline{s} \qquad (1)$$

where $\underline{s}$ gives the fractional coordinates of the same point in the non-orthogonal system ($|s_k| \leq 1$ for points inside the cell). Assume that a particle is in the center of the cell that is also the center of the coordinate system. A point $\underline{s}$ is to be examined if it possesses an image that might be nearer to the center. The various images of $\underline{s}$ can be described as

$$\mathbf{H}\underline{s} + \sum_{k=1}^{d} c_k \underline{H}_k \tag{2}$$

where d is the dimension of the space (e.g. three for crystals) and c_k is either -1, 0 or 1. Thus the distance of an image described by $\underline{c}$ is

$$|H\underline{s} + \sum_{k=1}^{d} c_k \underline{H}_k|^2 =$$

$$|H\underline{s}|^2 + \sum_{k,l=1}^{d} c_k c_l (\underline{H}_k \cdot \underline{H}_l) + 2 \sum_{k=1}^{d} c_k (\underline{H}_k \cdot (H\underline{s})) = \tag{3}$$

$$|\underline{x}|^2 + \sum_{k,l=1}^{d} c_k c_l (\underline{H}_k \cdot \underline{H}_l) + 2 \sum_{k=1}^{d} c_k (\underline{s} \cdot \underline{H}^2_k) . \tag{4}$$

Here $\underline{H}^2_k$ stands for the k-th column of the square of the matrix H. As described in [1], simple translations along the non-orthogonal axes can ensure that the point $\underline{s}$ will be inside the unit cell and if its distance from the center (the first term in (3) and (4)) is less than the smallest half-width of the unit cell then it will be the nearest image. For larger distances, however, images outside the simulation cell may lie closer to the cell center. In this case, more work is needed to obtain the values of $\underline{c}$ that minimize (4).

The first term is independent of $\underline{c}$ and therefore will not affect the minimum. The second term depends only on $\underline{c}$ and the cell axes and therefore it can be calculated once at the beginning of the calculations for all 3^d possible $\underline{c}$. The last term contains d different coefficients that depend on $\underline{s}$ - these have to be calculated each time. The number of possibilites to be examined can be further reduced from 3^d to 2^d by recognizing that for each direction k, c_k can be only 0 or $-\mathrm{SIGN}(s_k)$ since $\underline{s}$ is already assumed to be translated inside the cell. We are thus left with comparing 2^d values of the type

$$S(\underline{c}) + (\underline{c}.\underline{B}) \tag{5}$$

where $B_k=2(\underline{s}.\underline{H}^2_k)$. As half of the c_k's to be considered is zero, (5) can be evaluated rather fast for the 2^d cases.

Once the value of c_k minimizing (4) is obtained, the nearest image can be simply obtained as

$$H\,\underline{s} + \underline{c}\,\underline{H}_k \;. \tag{6}$$

The second term can again be prepared at the beginning of the calculation for all 3^d possible $\underline{c}$.

Acknowledgement: Prof. K. Bencsath is thanked for a helpful conversation on the problem.

Reference:

1. W. Smith, Information Quartely for Computer Simulation of Condensed Matter, No 30, Apr. (1989).

Architecture and Algorithms in Condensed Phase Simulations

St Andrews 2 - 5 July 1990

A joint meeting of the Collaborative Computational Project 5 of the SERC and the Institute of Physics

The organizing committee wishes to thank the following companies for their generous sponsorship of the meeting.

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ABSTRACTS

A Survey of Molecular Dynamics and Monte Carlo Applications of the CM-2 Connection Machine Computer

by

Bruce M. Boghosian
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245 First Street
Cambridge MA. U.S.A.

This talk will survey the applications of the CM-2 Connection Machine Computer in the fields of molecular dynamics (MD) and Monte Carlo (MC) simulations. The survey will begin with fixed interaction topology MD codes, such as those used to study macromolecular dynamics and dislocation dynamics in crystalline lattices. Next, it will cover MD with general long-range forces, and describe an algorithm that maps this problem to the CM-2's hypercubic communications network in a way that makes full use of the network's maximum theoretical bandwidth. Next, it will describe "fluid" MD codes for the CM in which the forces are short range so that the full N-body problem is wasteful, but where the interaction topology is dynamic. Finally, Monte Carlo work on the CM will be discussed, including a Quantum Monte Carlo code for the study of the ground-state properties of the hydrogen molecule without making use of the Born-Oppenheimer approximation in the treatment of the nuclei.

Simulations of Disordering in Adsorbed Multilayers Using a DAP

by

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The distributed array computer (DAP) is well suited for simulations of a few layers of adsorbed molecules on the solid substrate. Each layer can be represented by either a DAP vector (64 molecules) or a DAP matrix (4096 molecules). In the low temperature solid phases where molecules retain their relative positions, there are no problems in evaluating forces and moving molecules in a standard molecular dynamics simulation. At higher temperatures the molecules begin to disorder and to move. This process starts at the surface and occurs layer by layer. In order to evaluate the forces efficiently, the molecules must be resorted into cells from time to time. Logical masks are useful for dealing with partially filled layers.

We have been particularly concerned with molecular motion. Use of logical masks in the smaller simulations allows us to track those molecules which do not change layers so that the intra-layer diffusion constants may be evaluated.

Results will be presented for simple multilayers, stepped surfaces and freezing together of two approaching surfaces.

Pearls and Perils of Parallel Processing

by

Allan R. Larrabee, Boeing Corporation.

Some characteristics of parallel code generation and factors which affect the programmer's acceptance of parallel programming tools are briefly discussed. Included are hardware considerations, language overlays, analysis tools, debug and correctness problems, standards and portability. Tools mentioned include STRAND, Linda, The Force, Schedule, GMAT, and KAP. The trade-off between time spent in code development (and "dusty deck" Fortran conversions) and the speedup that may be gained is considered from the parallel programmer's point of view as well as a comparison of the speedups due to hardware improvements, better algorithms, and parallelism. Some comparisons between the use of global memory versus local memory and between Fortran and the C language are made. Parallel processing via distributed hardwares communicating over networks is only briefly mentioned. Presented also are some predictions of the future developments that may and others that may not occur in this relatively new area of computer science.

Multicomputer Molecular Dynamics

by

David Fincham
University of Keele, Staffordshire, ST5 5BG, U.K.
and
SERC Daresbury Laboratory

This talk will first briefly review the well-established algorithms for multicomputer molecular dynamics, namely the circulating data, replicated data and spatial decomposition methods. Experience using Occam and Fortran on Transputers will be described. The incorporation of neighbour lists in the circulating data method will also be mentioned.

The problem of long-range forces will be studied. The effective-pair-potential approximations of Adams parallelise simply, but are not very efficient for ionic systems. Although a straight-forward implementation of the Ewald sum involves a communication overhead, this is the most practicable method for typical problems involving ionic materials. For large ionic systems the particle-particle/particle-mesh approach is used.

Three- and four-body forces can be implemented within the circulating data methods in a number of ways, and these will be analysed and compared. For polymers it is possible to ensure that such forces only involve pairs of groups. Otherwise the many-body list can be assigned to particular processors, or distributed over all processors. If it is necessary to locate interacting triples, as in a molecular fluid, this can be done by a triple circulation, or by construction from a pair list.

Finally the work of the Palermo group on dynamic load-balancing for inhomogeneous systems will be reviewed.

Supercomputers, Molecular Dynamics and Hydrodynamics

by

D.C. Rapaport, Physics Department,
Bar-Ilan University.

Algorithms designed for large-scale molecular dynamics simulation on vector and parallel computers are introduced, and the results obtained when these methods are applied to the modeling of fluid flow at the microscopic level are described. The molecular dynamics approach has been used to reproduce the familiar hydrodynamic effects of vortex formation in obstructed flow and convective roll development in a Rayleigh-B'enard cell; although the studies carried out so far involved between 20 and 270 thousand particles (depending on the problem), considerably larger systems will be needed for more detailed exploration in the future. In order to lay the foundation for work of this kind, feasibility studies addressing multi-million particle systems have been carried out on computers such as the Cray YMP and a 64-node Intel iPSC/2, using computational methods developed specifically for the vector and distributed processing environments.

Systolic Loop Methods for Molecular Dynamics Simulation Generalised for Macromolecules

by

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A generalisation of the efficient systolic loop methods of Raine, Fincham and Smith, for the molecular dynamics simulation of liquids is presented, which allows the simulation of complex macromolecules such as proteins. Simple rules for the division of the work are described which allow the three-and four-body interactions necessary to represent covalent bonds to be evaluated without departing from the original systolic loop scheme. Additionally, a method for parallelising the SHAKE algorithm for constraining bond- lengths is described. The implementation of a molecular dynamics program, which runs on a Meiko Computing Surface, and which uses these ideas is also described. Performance figures are given which demonstrate that the generalised molecular dynamics program retains the efficiency and scaling behaviour of the original method.

Biomolecular Energy Calculations using a Transputer array

by

Julia M. Goodfellow and D.M. Jones
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We have been using a Meiko Computing Surface and the Edinburgh Concurrent Supercomputer Centre to study the interactions of biomolecules. In our first application we have written and used a parallel versions of an energy minimization program used to analyse ligand protein interactions. Secondly, we have attempted a much harder project in which we are partially parallelising a Monte Carlo code which is used to calculate free energy differences on mutating one amino acid to another as in a protein engineering experiment. We are currently comparing this parallel code with results obtained from running several independent simulations with no communication between processors.

Refinement of Protein Structures Using Restrained Molecular Dynamics

by

Garry Taylor
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The use of 'simulated annealing' in the refinement of atomic structures of macromolecules from X-ray or two dimensional NMR data will be discussed. The method has been implemented in two computer packages: XPLOR, from Prof. Brunger at Yale, and GROMOS, from Prof. van Gunsteren at Groningen. The method has allowed convergence either more quickly, or from a cruder starting model, and is proving a useful tool particularly in molecular replacement studies, where the unknown crystal structure is structurally related to a known protein structure. Previous refinement procedures required iterative cycles of least squares refinement, with a relatively small radius of convergence, and periods of manual rebuilding of the model using computer graphics: this procedure would take several weeks. Although simulated annealing is more costly in computing requirements, access to fast processors has allowed reasonable run times. All the examples discussed in the talk were carried out on a Convex C210 processor at the Oxford Centre for Molecular Sciences, which was ideally suited for the large problems tackled using the method. The high memory bandwidth, fast scalar and vector processing allowed refinement of, in the largest case, foot and mouth disease virus with 8000 atoms and 135,000 x-ray observations in 8 days - a task which on a microvax II would have taken 1.5 years!

Vectorization of Algorithms for Monte Carlo Simulations in Lattice Models

by

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The study of phase transitions and critical phenomena in lattice models of condensed phases using Monte Carlo methods is computationally quite demanding. For systems with only near-neighbor interactions, the sampling of the lattice can be organized so that it is fully vectorizable. This is accomplished by subdividing the lattice into sublattices containing noninteracting sites each of which can then be treated as a single vector. For simple Ising-lattice gas models, multiple sites can be packed into each word and the combination of multisite coding and vectorization can increase the speed of the calculation by up to two orders of magnitude on the CYBER 205 (or ETA10) supercomputers. Some of the progress which has been made using this approach to study static and dynamic critical phenomena in systems with up to $2x10^7$ sites will be reviewed.

Parallelism in Computational Chemistry I. Hypercube-connected Multicomputers

by

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and
J.H.van Lenthe,
State University of Utrecht,
Transitorium III, Padualaan 8,
Utrecht-De Uithof,
The Netherlands,

An account is given of experience gained in implementing computational chemistry application software, including quantum chemistry and macromolecular refinement codes, on distributed memory parallel processors. In quantum chemistry we consider the coarse-grained implementation of Gaussian integral and derivative integral evaluation, the direct-SCF computation of an uncorrelated wavefunction, the 4-index transformation of two-electron integrals and the direct-CI calculation of correlated wavefunctions. In the refinement of macromolecular conformations, we describe domain decomposition techniques used in implementing general purpose molecular mechanics, molecular dynamics and free energy perturbation calculations.

Attention is focussed on performance figures obtained on the Intel iPSC/2 and iPSC/860 hypercubes. The present performance is compared with that obtained on a Convex C- 220 minisupercomputer, and from this data we deduce the cost effectiveness of parallel processors in the field of computational chemistry.

Simulation of Brownian Dynamics: A Problem Apparently Difficult to Parallelise

by

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We consider a system of N particles interacting with a pair potential $\phi(r)$ in periodic boundary conditions with a simple cubic cell of side L. The particles have hard cores of radius a and execute Brownian motion in a suspending fluid of viscosity η. The fluid obeys periodic boundary conditions and a stick boundary condition on the surfaces of the spheres. The stochastic equations of motion are solved with a first order solver and includes a random force term chosen with covariance matrix proportional to the mobility matrix $\mu(r_j r_k)$. If the net force and torque on particle j are F_j and T_j, then these are related to the velocity V_j and angular velocity Ω_j by the relation

$$\begin{bmatrix} V_j \\ \Omega_j \end{bmatrix} = \sum_{k=1}^{N} \mu(r_j, r_k) \begin{bmatrix} F_k \\ T_k \end{bmatrix}$$

Problems which arise are:
(i)how to interpret periodic boundary conditions for hydrodynamics;
(ii)how to approximate the mobility matrix in periodic boundary conditions;
(iii)how to ensure that the approximate mobility matrix used is positive definite;
(iv)how to implement a simulation in a reasonable time;
(v)development of parallel algorithms to implement Brownian dynamics.

(i)We describe the physical basis of self-consistent interpretation of periodic boundary conditions and how to extract quantities like zero frequency viscosity from them.

(ii)In free boundary conditions, two approaches to approximating the mobility matrix have been used:
(a)To expand $\mu(r_j r_k)$ in powers of $[a/r_{j,k}]$.
(b)To expand $\mu(r_j r_k)$ using a spherical harmonic expansion to a finite value ℓ_{max} of the angular momentum index ℓ. These are briefly described, with extensions to periodic boundary conditions.

(iii)We first derive an inverse friction matrix T which connects expansion coefficients for fluid velocity at a particle surface to expansion coefficients for the induced force density on the particle surfaces. We prove that this when this T matrix is calculated using a finite spherical harmonic expansion with $1 \leq \ell \leq \ell_{max}$, the T matrix is positive definite for all values of $\ell_{max} \geq 1$. We then construct μ as a partial inverse of this T and prove that these approximate mobility matrices are positive definite for all ℓ_{max}. The construction and proof are valid in both free and periodic hydrodynamic boundary conditions. Further, in free boundary conditions, explicit calculation shows that for $\ell_{max}=1$, the spherical harmonic expansion is not equal to the inverse power expansion to any particular power of $[a/|r_{j,k}|]$.

(iv)We note that serial computation times for the elements of the spherical harmonic expansion of T are $O(N^2\kappa^3)$ in periodic boundary conditions, where κ is the magnitude of the largest wave vector used in the Fourier part of the Ewald form for the mobility matrix. Serial times for the inverse power series are $O(N^p)$ if terms up to $[a/|r_{j,k}|]^p$ are used. The Choleski decomposition of the T matrix, necessary to construct μ in the spherical harmonic expansion takes computation times which are $O(N^3)$, but with a much smaller constant than those in the computation of the elements of T. Whichever form of the mobility matrix is used in a Brownian Dynamics simulation, a further Choleski decomposition of μ is needed, and that takes computation times which are $O(N^3)$.

(v)The processes involved in calculating the original T matrix from which we derive μ and may be calculated on array computers with algorithms whose computation times are predominantly concerned with on chip computation rather than data transfer. However, the Choleski decompositions of T and μ are matrix manipulation procedures whose computation times appear to depend an massive data transfers, which may well take more time than the actual computation. Some of the problems of producing parallel algorithms for these processes are discussed.

Dedicated Parallel Computers for Molecular Dynamics Simulations

by

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Although supercomputers have opened ways to perform large-scale computer experiments, only a small group of physicists and chemists use them as a standard facility due to their costs and availability.

As a low-cost alternative, special purpose computers have proven to be very efficient: supercomputing power at minicomputer costs. For example, The Delft Molecular Dynamics Processor (1982) has a speed comparable to the CRAY-1 for molecular dynamics (MD) calculations, yet it's costs were only 100 kf. It's parallel and pipelined architecture is partly hard-wired (force calculation pipe) and the algorithm is micro- coded. Other new parallel MD machines have been developed and built at IBM (San Jose) using a Fortran optimized basic instruction set for MD calculations (Spark), and at AT&T Bel laboratories (Murray Hill) optimized for three-body-interactions MD calculations (ATOMS).

At Delft a new MD processor (2.5 Giga FLOPS), is now under construction, and will be a multi-purpose, C and FORTRAN programmable parallel computer. It's architecture, that will be discussed, is tailored to "local environment problems", such as found in MD calculations, and is based on the "linear processor array" concept.

GROMACS: A Hybrid Architecture for Molecular Dynamics

by

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Molecular Dynamics simulations of complex molecular systems as hydrated biological macromolecules involve a range of atomic interactions of varying complexity. Non- bonded interactions between atom pairs are relatively simple but involve 100-300 N interactions where N is the number of particles in the simulation. They also involve parameters depending on pairs of atom types. Bonded interactions include 3- and 4- body interactions, which are considerably more complex but involve only 1-2 N interactions. The updating of velocities and forces and further data analysis also is an order-N process, but one in which programmable flexibility is required.

The MD process can be functionally subdivided into three processes of different characteristics:

I.Neighbour searching: produces list pairs of particles within a prescribed range. Characteristics: low-accuracy integer operation based on particle coordinates.

II.Non-bonded interactions: produces forces on particles based on pair list. Functional form of forces must be flexible and includes parameters depending on particle types. Characteristics: 32 bit floating point operations, fixed algorithm if tabulated functions are used very high speed required.

III.Bonded interactions and update: produces bonded forces, updates velocities and coordinates, selected data analysis. Characteristics: flexibility required, variety of algorithms, operations based on particle number, dominantly floating point operations.

We are designing a special-purpose hybrid MD machine, called GROMACS (Groningen Machine for Chemical Simulation), which consists of three functional parts for the functional processes I, II, III, all communicating through standard transputer links. I is a special network of 200 T212/414 transputers; II is a pipelined unit based on floating point ALU's; III is a general purpose network with about 100 T800 transputers. GROMACS is designed to handle simulations according to the program package GROMOS.

This is a joint project of the Department of Computer Science (E.J. Dijkstra, H. Bekker, S. Achterop, W. Halang) and the Laboratory of Physical Chemistry (W.F. van Gunsteren, H.J.C. Berendsen) of the University of Groningen, supported by the Foundation for Applied Research (STW) of the Netherlands Research Organisation (NWO).

Classical & Quantum Simulations of Novel Condensed-Matter Systems

by

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We will describe some recent investigations of the statistical mechanics of novel materials systems using classical and quantum simulation methods. Examples may include studies of the phases of quasi two-dimensional physisorbed films on graphite, the structure and dynamics of solid membranes, the interpretation of puzzling images of the graphite surface using the Atomic Force Microscope (AFM), and the melting of the Abrikosov flux solid in high-Tc superconductors. For the rare-gas films, we will feature the microstructure of the incommensurate phases of classical krypton and quantum helium simulated by molecular dynamics and path integral Monte Carlo and show that the reentrant fluid is a domain-wall liquid with a hexagonal pattern for krypton and a striped pattern for helium. The solid membrane is a natural two-dimensional generalization of the linear polymer, and theory suggests that a compact structure occurs for this two- dimensional random surface moving in three dimensional space. We will describe molecular dynamics simulations of the self-avoiding "tethered" membranes and show that, in contrast to previous belief, this membrane does not crumple but remains in a "flat" state. Using the AFM to investigate the graphite surface structure, the experimental issue has been the large variety of measured images. A classic example is the puzzle that only "every-other-atom" may be seen. We have developed an empirical graphite potential and have calculated the image resulting from a graphite flake passing over the graphite surface at an arbitrary angle. Our generated images mimic the experimental pictures of many groups. Finally, we present Monte Carlo simulations of the intermediate flux state accessible in high-Tc superconductors where the Abrikosov flux lattice is melted over a significant portion of the (H,T) phase diagram and where an entangled flux liquid may exist.

Multiprocessor Chemistry

by

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Our experience will be described in using a four processor MIMD Silicon Graphics system on three types of problems of interest to chemists. First, a test of density functional quantum mechanics as run using a Fortran compiler which automatically partitions the job across processors. Second, the computation of molecular dynamics of chemical reactions in solution. Here the problem partitions naturally across processors, since ensemble averages of sets of independent trajectories are needed. Third, "presentation quality" molecular graphics for filming the molecular dynamics of chemical processes, in which an algorithm is implemented which dynamically repartitions the jobs among processors, automatically adjusting for frame to frame changes in the image as well as for the shifting demands of other job sharing the same processors. A stereo film will be shown illustrating the results of both multiprocessor dynamics and graphics.

Simulations in Non-Spacefilling Geometries: Molecular Dynamics of the Rhinovirus

by

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Virus particles have over a half million coat atoms and while that would seem to limit the applicability of computer simulations they also posses icosahedral symmetry. There are 60 asymmetric units of roughly triangular shape made up of 4 proteins that form the viral protein coat. Each of the asymmetric units contains over 7000 heavy atoms. Using the point group symmetry as a boundary condition, computer simulations of the minimum energy structure and equations of motion have been performed for an entire virion. In such a simulation cell linear momentum is no longer a constant of the equations of motion. Several other aspects of such non-spacefilling geometries such as the occurrence of antiperiodic boundaries will be discussed.

The cold virus is a member of the picornavirus family. This group of viruses consists of a spherical protein coat filled with RNA and solvent. The picornavirus assembly is roughly 300 Åin diameter. Antiviral compounds of the oxazole (isoxazole-heptane-phenoxy- oxazole) have been developed by the Sterling Winthrop Research Institute. These have been shown to have biological activity against the picornavirus family, of which cold viruses are members. Results will be presented for the dynamics of a single asymmetric unit with free boundaries and with icosahedral boundaries. The motions with and without an antiviral drug will be compared and contrasted. Particular mechanisms of drug action may be related to specific molecular details of the bound ligand.

CCP5 Workshop Report: Solid State Ionics, Daresbury Laboratory 7 November 1991

Compiled by W. Smith

10 November 1991

The meeting began with a talk by Dr. D.M. Heyes of Guildford University on the subject of computer simulation of barium sulphate (Barite). The work was the basis of a collaboration with M.P. Dexter (a summer student) and BP (Sunbury-on-Thames). Dr. Heyes described preliminary results of molecular dynamics computer simulations of crystalline barium sulphate at room temperature. Surprisingly little is known about the physical properties of this common material. Dr. Heyes began by describing how a suitable potential model was obtained, which was adequate for calculating the Madelung constant and the lattice parameters. He also described the work undertaken to implement a suitable MD program capable of handling the complexities of the unit cell and exploiting the Fincham implicit algorithm for the rotational motion of the sulphate ions with quaternions. Preliminary results were given, including internal energy, (for which exceptional agreement with experiment was obtained) and pair radial distribution functions. Dr. Heyes concluded with some practical queries, such as the verification of the rotational equations of motion, the thermostatting of the system and the significance of the Fourier contribution in the Ewald summation for calculating the electrostatic potential.

Mr. P.J.D. Lindan of the University of Keele presented the results of molecular dynamics calculations of the thermal conductivity of the ionic solids calcium fluoride and uranium dioxide. The work, which was a collaboration with Prof. M.J. Gillan at Keele, was motivated by the need to understand the anomalous temperature dependence of the thermal conductivity of uranium dioxide at high temperatures. The calculations, which were based on the Green-Kubo technique, yielded good agreement with experiment for calcium fluoride. For uranium dioxide, very close agreement was found for temperatures below 2000 K, but a large discrepancy existed above this. It was shown that the discrepancy arose from the effect of electronic excitations. Mr. Lindan went on to discuss two methods of performing molecular dynamics simulations using the shell model. The first was conjugate gradient minimisation of the shell configurational energy at each time step, and the second, the use of fictitious adiabatic dynamics to generate shell trajectories. Both these methods achieve the aim of keeping the system on the Born-Oppenheimer surface during the simulation.

Prof. N. Greaves of Daresbury Laboratory provided a summary of the current understanding of ionic transport in silicate glasses. This proved to be a multidisciplinary talk, with contributions from experimentalists, theorists and simulators. Experimentally ionic transport (of ions such as Cs^+, Rb^+ etc.) shows Arrhenius behaviour and there is a remarkable drop in conductivity in glasses where mixtures of ions are present. This is the so-called "mixed-alkali" effect. Prof. Greaves described the model currently used to explain these phenomena. In accordance with structural determinations (such as XAFS - X ray Absorption Fine Structure) the glass is described by a modified random network (MRN) in which the ions congregate and move in "channels" in the glass. The movement is via a hopping mechanism which involves the making and breaking of oxygen-metal bonds. The activation energy of the ion migration thus involves a binding energy contribution from the metal-oxygen bonds and a bond ordering energy arising from the redistribution of silicon-oxygen bonds as the ion migrates. A theory by S. Gurman was used to account for the bond ordering energy terms. Further insight into the phenomena of ion migration was provided by MD simulations by Vessal et al. which strongly endorsed the basic model. Finally, a simple Monte Carlo model incorporating a "memory effect" designed to mimic long lived distortion of the lattice by the migrating ions was shown to possess a pronounced "mixed alkali" effect, thus offering some clue as to the origin of the effect in glasses.

V. Nield of Oxford University described some neutron scattering studies of disorder in silver halides. Silver bromide possesses a rocksalt structure up to the melting point (701K), while silver iodide, which is in the β phase at NTP possesses a complex phase diagram, including an α phase (which is fast ion conducting) and a rocksalt low temperature phase. Both systems have been examined by neutron diffraction at the Institut Laue-Langevin. The reverse Monte Carlo (RMC) method of McGreevy has been used to determine the structure underlying the observed neurton diffraction. At 420K, the studied temperature, the location of the silver ions in crystalline silver iodide were found by RMC to be almost entirely in the tetrahedral sites. RMC starting structures in octahedral, tetrahedral trigonal and liquid like sites within the lattice of anions all gave the same result. The occupancy of the tetrahedral sites diminished as temperature increased. Work is continuing on the higher temperature data to see how much evidence there is for the order-disorder transition previously observed by Raman and Brillouin scattering. A bragg peak anomalously observed at 740 K may be related to this. The structure factor of silver bromide has been measured to within 0.25 K of the melting tempreature. There is considerable diffuse scattering even at room temperature and just below melting only two Bragg peaks are observed. Large anharmonic vibrations of silver ions arise in the $< 111 >$ direction, which lead to a few percent interstitials in the $(1/4, 1/4, 1/4)$ site near the melting point. The pre-melting disorder is thought to be a transition to a fast ion conducting phase which is interrupted by melting.

Dr. P. Madden of the University of Oxford continued the theme of silver halides in a talk on the mechanism of the $\alpha - \beta$ phase transition in silver iodide. The springboard for this study was the deceptively simple silver iodide potential of Vashista et al., which Tallon had shown to give a very accurate description of the phase diagram. Dr. Madden's MD simulations employed the same potential, but imposed rigid, cubic periodic boundaries on an 864 ion system in the α phase. Within the unit cell of this phase the silver ions can in principle reside on a variety of sublattices (six in all), all of which are comprised of tetrahedral sites. Formally, these sublattices are equivalent, but the occupation of any one has influence on the occupation of the others. Simulations show that at high temperature (900K) the probability of a silver ion being on any sublattice is equivalent. However at lower temperature (500K) it becomes apparent that the occupancy of the sublattices shows a distinct preference. Fluctuations from uniform occupancy of all sublattices are long lived. Furthermore, the simulations show that the diffusion of the silver ions at high temperature, becomes arrested at lower temperatures. (Note: the fixed cubic periodic boundary means that the iodine ions retain a body centred cubic lattice at all times.) Examination of the low temperature structure with computer graphics shows that only four of the six possible sublattices are occupied, but with a kind of partial ordering reminiscent of the β phase. It is Dr. Madden's conjecture that this ordering is a true precursor of the β phase, the transformation to which is thus signalled in the crystal structure from a remarkably long way away in the α phase.

Dr. W. Smith gave the first of two talks on sodium β"-alumina. This system has been studied intensively by molecular dynamics, in a collaboration with Prof. M.J. Gillan of Keele University. The material is a superionic conductor, particularly at high temperature, where the sodium ions are responsible for carrying the current. The crystal structure is hexagonal and complex, with the sodium ions confined to almost two-dimensional "conduction planes" between spinel blocks (aluminium oxide). The material is usually prepared in a nonstoichiometric condition, with vacancies in the conduction planes, a fact which is crucial to the conductivity. The high temperature simulations (500~1200 K) clearly showed the diffusion of sodium ions that enables the conductivity. At low temperature however (<500 K) the sodium vacancies become localised into an ordered structure called a vacancy superlattice, the structure of which is dependent on the vacancy concentration in the conduction planes. Concurrent with the formation of the vacancy superlattice is marked reduction in conductivity, leading to a non-Arrhenius temperature dependence. The activation energies calculated compared well with experimental determinations by Engstrom et al. The vacancy superlattice was first postulated by Boilot et al. from diffuse x-ray scattering experiments. A recently developed theory by Gillan, which owes much to the simulations, is able to account fully for the Boilot results. A detailed knowledge of the structure of the superlattice, including the precise structure of the vacancies themselves, proved to be crucial in accounting for the observed results.

Mr. T. Bush of the University of Kent at Canterbury (in collaboration with Dr. A. Chadwick) gave the second talk on Sodium β"-alumina. In this case the system was doped by neodymium ions in the conduction planes. (The facility with which the sodium content of the material may be exchanged for a variety of optically active ions suggests technological applications such as waveguide lasers and novel phosphors.) The important question to be addressed was the structure of the conduction planes, in particular the immediate environment of the neodymium ions. The methods used to resolve this question included experimental determinations (XAFS and x-ray powder diffraction on the Daresbury Synchrotron) and molecular dynamics simulation. Constant temperature and pressure molecular dynamics simulations have been performed on the Nd^{3+}/Na^{+} β"-alumina system at a series of temperatures and exchange concentrations, in an effort to characterise the ionic behavior of the system. Results of the simulations have been compared with the current experimental data, and conclusions can be drawn on the structural basis for the optical performance of Nd^{3+}/Na^{+} β"-alumina phases. Additionally, insight has been obtained into the marked variation of sodium diffusion coefficients at increasing levels of neodymium ion content.

The final speaker was Dr. X. Zhang of the Royal Institution (in collaboration with Prof. C.R.A. Catlow,) who described a molecular dynamics study of oxygen diffusion in the ceramic: $YBa_2Cu_3O_{6.91}$. The system was studied at high temperature (1400-1800 K) using Born model potentials. The diffusion of the oxygen at high temperature was found to occur mainly within the Cu(1)-O basal plane by a vacancy mechanism and the oxygen diffusion coefficient ($D=3.7\times10^{-4}\exp(-0.99eV/kT)\ cm^2s^{-1}$) was in good agreement with experimental results. A detailed examination of the diffusion mechanism was undertaken, with the assistance of molecular graphics techniques. The oxygen vacancies were found to migrate between the O(1),O(4) and O(5) sites, but not to O(2) and O(3) sites, while the jump paths for the diffusion were found to be O(1)-O(5), O(1)-O(4) and O(4)-O(5).

REPORT ON THE CCP5 WORKSHOP

"BEYOND THE PAIR POTENTIAL"

KEELE UNIVERSITY, 15-16 APRIL 1991

The subject of this meeting was the important advances in methods for calculating the energetics of condensed matter that have happened in the last few years. These advances recognise that for many (perhaps even most) materials, the energy cannot be adequately represented in terms of pair potentials, and that one needs an approach that derives the energy from the quantum mechanics of the electrons. The talks given at the meeting reflected the main strategies that are being pursued to achieve this aim. These include the first-principles approach based on density-functional theory and pseudopotentials, the Hartree-Fock method, and the more approximate but much simpler methods based on tight-binding theory or the CNDO approximation.

The meeting was organised because the subject was seen to be important and of general interest both within CCP5 and more widely. The enthusiastic response and the large participation fully confirmed this - there were 91 registered participants, many of them from overseas. A total of 16 papers and 8 posters were presented during the one-and-a-half days of the meeting. The set of abstracts of these papers and posters is produced below.

Mike Gillan

MODELLING 6-8 COORDINATED MG, CA AND O

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and

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Abstract

The programme CRYSTAL, developed by Causa et al. (1) allows us to calculate energies and electronic characteristics for crystal structures of modest complexity. The method used is the Periodic Boundary Hartree Fock Linear Combination of Atomic Orbitals. As with everything in life, this is a compromise: it is less computationally demanding than methods such as LAPW, but rather more so than electron gas calculations.

There are some attractions in a compromise at this level. It is in particular capable of examining the properties of crystal structures which are not experimentally accessible. This we felt might be a useful tool for the preparation of parameterized potential surfaces, which could be sampled systematically, rather than only at those points which could be made to exist. As we already had a project under way examining the distortion of MgO and CaO using CRYSTAL, we decided to extend this and to attempt to fit the surface generated by distorting the unit cell rhombohedrally from the B1 to the B2 structure. This fitting is of interest not only because of the geological significance of the system, but because it involves a continuous transition from six-fold to eight-fold coordination of both cation and anion.

The static electronic energy of MgO in 65 cells was determined, and that of CaO in 58. This allowed us to prepare energy surfaces for each. The fitting was done using a modification of the programme THBFIT by Leslie. Initially a simple pair potential was fitted. Work is in progress to improve upon this.

(1) Pisani, C.; Dovesi, R.; Roetti, C., Hartree-Fock Ab Initio Treatment of Crystalline Systems. Lecture Notes in Chemistry v 49 (1988) Springer, Heidelberg.
Dovesi, R.; Pisani, C.; Roetti, C.; Causa, M.; Saunders, V.R. CRYSTAL 88, Program No. 577, QCPE, Universit of Indiana, Bloomington, Indiana, U.S.A.

CALCULATION OF INTERIONIC POTENTIALS IN OXIDES

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and

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Abstract

We report progress in the calculation of interionic potentials in oxide materials using methods developed by Wood and Pyper (1986a,b). A particular problem in oxides is the energy required to create the ion in the crystalline environment. This, the rearrangement energy, may be written as

$$E_{\mathrm{Re}}\ (0^{2-}) - E_{\infty}\ (0^{-}) - E_{\infty}\ (e^{-})$$

This energy is highly sensitive to the details of the environmental potential since the oxide dianion is unstable in the gas phase.

When the ion wavefunctions have been calculated for the correct environment, the interionic potential may be obtained from

$$U(R) = < \Psi_{cr}(r_1, r_2, ..., r_n) \mid H \mid \Psi_{cr}\ (r_1, r_2, ..., r_n) >$$

where H is the standard crystal hamiltonian and $\mid \Psi_{cr}\ (r_1, r_2, ..., r_n) >$ the crystal wavefunction.

Results are presented for MgO and preliminary results are presented for UO_2.

- Wood CP and Pyper NC (1986a); Phil. Trans. Roy. Soc. **A320** 71.
- Pyper NC (1986b); Phil Trans. Roy. Soc. **A320** 108.

O-H VIBRATIONAL FREQUENCIES IN LIQUID WATER FROM COMBINED AB INITIO AND COMPUTER SIMULATION METHODS

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Abstract

The molecular-level structure and dynamics of **liquid water and ionic aqueous solutions** constitute a particular challenge to computational chemists and physicists. The difficulty lies in the accurate modelling of short- and long-range interactions of the polarizable water molecule and simultaneously incorporating this model in a statistical-mechanical description of liquids. We have been exploring a way to combine the techniques of **quantum chemistry and statistical-mechanical computer simulations** to study the internal O-H vibrations of water molecules in liquid water.

A number of system configurations were selected randomly from the atomic positions from a Monte Carlo simulation on bulk water (MCY potential, 300 K). For each configuration, ab initio calculations, of MP2 type (i.e. including electron correlation effects) were performed on a water pentamer supermolecule surrounded by point charges to mimick distant water neighbours out to 15 A. Intensity-weighted densities-of-states have been calculated and compared with experimental spectra. The results of this pilot-study are in quantitative agreement with the experimental band position and band width. It appears that the success of these computations relies on a model which incorporates (i) *ab initio* calculations with a large supermolecule, long-range electrostatic interactions and electron correlation effects, (ii) the determination of an anharmonic potential curve (force constants up to fourth order), and (iii) a quantum- mechanical treatment of the vibrational problem.

SIMULATIONS OF METALLIC SURFACES

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Abstract

Sutton and Chen(1) have recently suggested a relatively simple many-body potential for metals of the form:

$$V_i = \varepsilon \left(\frac{1}{2} \sum_{j=i} (a_f/r_{ij})^n - C \sqrt{\sum_{j=i} (a_f/r_{ij})^m} \right)$$

where V_i is the potential energy of atom i, a_f is the f.c.c. lattice parameter and ε an energy parameter. Note that the attractive part of the potential is a many-body term - the energy of an atom cannot be computed as a sum of separate pair interactions. The character of the potential may be changed by altering the values of m and n (from which C is also determined) and thus different f.c.c. metals may be accounted for.

An important aspect of the potential of Sutton and Chen is that despite being more complex than a pair potential it does not require orders of magnitude more computer time to use. A metal- atom molecular-dynamics program only runs twice as slowly, at most, than a similar Lennard-Jones program. Methods such as the Car-Parrinello technique require very large computing resources for even a moderate number of atoms.

Metal surfaces are known to undergo a surface relaxation in which the top few layers of atoms are contracted towards the bulk. This behaviour is to be contrasted with that of molecular crystals where outward relaxation occurs. Extrapolating this behaviour to a stepped metal surface leads to the conclusion that the rather exposed step atoms should be even more contracted toward their neighbours than surface terrace atoms. Energy minimisation calculations based on the Sutton-Chen potential show that this is indeed the case. The closest interatomic distances observed are those between step atoms and their neighbours directly below them. It is the many body term in the potential that is responsible for this behaviour. A simple pair potential would give an outward relaxation.

The molecular-dynamics technique is being used to investigate the way in which the surface of a metal starts to disorder as the temperature is raised. Results will be presented for flat (100) and (111) surfaces and also various stepped surfaces. Results for Rh, Pt and Ir - which are modelled with different indices m and n - will be compared.

(1) Sutton, A.P. and Chen, J., 1990, *Phil. Mag. Lett.*, 61, 139.

CHEMOS : SELF CONSISTENT MOLECULAR DYNAMICS OF COMPLEX SYSTEMS

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Abstract

Most theoretical physicists yearn for "first principles", for the words "a priori" represent a virtue, even if (like most virtues) it is claimed more often than found. Theoretical chemists and biologists, not to mention those in technology, are aware that there are many important problems for which the most basic methods are not yet helpful. It is this type of problem which I shall address; perhaps the title of my talk should have been "the niche for semi-empirical methods". Such methods, when used properly, can have several advantages: they are simple enough for many useful calculations to be done on a PC; they exploit well-known and widely-studied methods; they are self-consistent in the usual sense. The key to their extended value is the way they can be embodied in molecular dynamics, unlike static approaches, does not need to be told an answer in advance; indeed, one example showed behaviour of biological molecules which appears to be a new form of transmitter/receptor interaction.

The basic ideas of the method are simple. An initial geometry is selected and a reasonable (but incomplete) iteration to self consistency achieved. Analytical forces are found for that geometry, and molecular dynamics started. At each time step, a chosen number of iterations to self-consistency (typically 12) are carried out, and the process continues. External fields and force fields can be applied, and there are other options relating to finding saddle points or handling especially light ions. Damped dynamics can be used to optimise geometries. Clearly the strategy can be extended to methods which are closer to first principles, though it often suffices to give good qualitative and sensible quantitative predictions. This is so for the three examples of applications I shall discuss:

(1) Does the Scanning Tunnelling Microscope really measure geometries of molecules? Here the results offer an explanation of why CO absorbed on metals is not seen in the STM: the tip causes reorientation, and the predicted image (tunnel current versus probe position) does not have the structure anticipated.

(2) Should breathers be seen in polyacetylene? This is an example where simple interatomic potentials do not work (the bonding pattern changes dynamically) and where the behaviour after excitation to an electronic excited state has interesting subsequent dynamics.

(3) The neurotransmitter serotonin (which controls your sleep and sex life) acts by interaction selectively with receptors. The selectivity is partly by shape (the jig-saw picture) and partly by a molecular event (probably electron or proton transfer) at the receptor. We

have looked at the interactions with model receptors, and find a novel catalysed proton transfer. This may be characteristic of a range of biological processes, and it illustrates how self-consistent molecular dynamics can point to phenomena not easily recognised in other ways.

AB INITIO MD OF LIQUID AND AMORPHOUS SILICON

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Abstract

An extensive ab initio molecular dynamics (AIMD) study of liquid and amorphous silicon will be presented. In this scheme the interatomic potential is explicitly derived from the electronic ground-state treated with accurate density functional techniques. The present AIMD results show important differences when compared to results based on empirical potentials. These differences will be discussed in detail.

The AIMD provides an excellent description of the local order in the liquid. Analysis of the valence electronic charge density shows persistence of some covalent bonds in the melt. These bonds give rise in several system time correlation functions to well identifiable features associated with stretching vibrations. In the liquid the covalent bonds are continuously forming and breaking in response to atomic motion. On average the majority of bonds are broken leading to a fast diffusion and to the metallic behaviour of the melt.

The model amorphous sample was obtained by simulated quench from the melt. A cooling rate of 10^{14} K/s was sufficient to recover a tetrahedral network starting from the metallic liquid having average coordination larger than 6. Dramatic changes in physical properties are observed upon cooling. In particular a gap forms in the electronic spectrum indicating a metal to semiconductor transition. The as-quenched structure has average coordination very close to 4, but contains several coordination defects as well as a large fraction of distorted bonds. Subsequent annealing reduces the amount of strain and the number of defects present in the system. The average structural, dynamical and electronic properties of the model sample are in impressive agreement with the available experimental data. A detailed analysis of the structural relaxation processes accompanying annealing will be presented and compared with recent experiments.

* Work done at the International School for Advanced Studies, Trieste, Italy in collaboration with Profs. R. Car and M. Parrinello.

THE INTERACTION OF A POINT CHARGE WITH AN ALUMINIUM (111) SURFACE

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Abstract

The self consistent response of an Al(111) surface to the external potential of a negative electronic charge is calculated, as a function of the position of the external charge. The metal atoms are represented by norm-conserving pseudopotentials on a periodically repeated slab of three atomic planes separated by five atomic layers of vacuum, with twelve atoms per unit cell. Comparison of the energy is made with two classical models: (a) the classical continuum model (CCM) of a metal, in which a surface is characterised by the position of the image plane, and (b) a discrete classical model (DCM), in which the atoms are treated as polarisable point charges. The CCM gives an accurate description of the interaction energy when the charge is more than about 2.5 Angstrom from the surface atomic layer. At closer approach a strong corrugation appears in the interaction energy, which becomes lower over atom sites than hollow sites.

The image plane position with the CCM, fitted to the self-consistent calculations, is situated 0.15 Angstrom outside the geometrical surface (jellium edge). Separate calculations with an external charge of half an electron show the significance of non-linear response; with this weaker external charge, the effective image plane is 0.29 Angstrom outside the geometrical surface and the non-linear effect on the energy is relatively small. The interaction energy even at small distances is well described by the DCM, which correctly predicts the site dependence of the image interaction.

AB INITIO CALCULATION OF DEFECT ENERGETICS IN ALUMINIUM

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Abstract

A detailed study of the energetics and electronic structure of the vacancy, the interstitial hydrogen, and substitutional hydrogen in bulk aluminium is presented. The calculations are based on the supercell approach, with the bare Coulomb potential for hydrogen and a BHS ab initio pseudopotential for aluminium in the Kleinman-Bylander representation, the energy functional minimisation being performed with the conjugate gradients technique. Some special features which optimise the computational strategy for the high density free-electron-like metal environment will be discussed. The physical quantities studied are the vacancy formation energy, migration energy and volume of formation, the hydrogen relative energies at different interstitial sites, the diffusional hydrogen migration and vacancy-binding energies, and the hydrogen heat of solution. Preliminary results will be given for the aluminium self- interstitial. The host lattice full relaxation is found to be determinant for the impurity energy profiles, and the highly localised screening-charge distributions deviate significantly from the predictions of the spherically averaged jellium models. Results compare well with experiment and with some precedent theoretical work, supporting the adequacy of the present technique for the study of large metal defective systems energetics.

ON THE POSSIBILITY OF OBTAINING AN EFFECTIVE PAIRWISE ADDITIVE INTERMOLECULAR POTENTIAL VIA AN AB INITIO ROUTE BY FITTING TO A COOPERATIVE MODEL OF CONDENSED PHASE CONFIGURATIONS

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Abstract

The paper demonstrates the feasibility of obtaining an effective pairwise additive intermolecular potential for liquid water at room temperature by fitting a pairwise additive function to the cooperatively calculated energies and virial sums of simulated liquid water configurations. The procedure requires iterative refinement of the fit. The importance of trying different functional forms has been demonstrated as well as the importance of including the virial sum into the fitting process. The cooperative energies and virial sums were calculated with the Campbell-Mezei model (derived from ab initio dimer energies) that includes a dipole polarisation term(1,2).

The technique is not tied to any particular cooperative model and thus could be used in conjunction with any of the explicit cooperative techniques mentioned in the announcement.

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AB INITIO EMBEDDED-CLUSTER TECHNIQUES

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Abstract

A variety of computational schemes are becoming available which allow the electronic structure of clusters embedded in a crystalline environment to be investigated by using ab-initio quantum-mechanical techniques. They can have important applications in catalytic studies, and in the characterisation of local defects in solids. Different approaches adopt different models for describing the two subsystems (the cluster and the outer medium), and for taking into account their mutual short- and long-range interactions. After briefly reviewing existing proposals, a specific embedding scheme is considered (C. Pisani, R. Dovesi, R. Nada and L. Kantorovich, J. Phys. Chem. 92, 7448 (1990)) that embodies in a self-consistent procedure the effects on the cluster solution of orthogonality constraints and of Coulomb and exchange fields generated by the crystal-line environment. The problem is treated at an ab-initio Hartree-Fock level of approximation; the solution for the perfect host crystal is obtained by means of the CRYSTAL program (R. Dovesi, C. Pisani, C. Roetti, M. Causa and V.R. Saunders, QCPE Program No 577, 1989). Examples are provided concerning defects in covalent, ionic and molecular crystals in order to illustrate the different types of correction to the crystal solution, and to evidentiate capabilities and shortcomings of the method. The possible influence of long-range polarisation of the outer medium on the electronic structure in the cluster region and on defect formation energy is considered.

RESTRICTED-BONDING PAIR POTENTIAL FOR SILICON

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Abstract

Numerous recent attempts have been made to derive empirical potentials for use in simulations. Various attempts have been made based on many-body forces, embedded atom approaches and expansion in cluster terms. The main feature underlying all these approaches has been their lack of transferability between coordinations *without reparameterisation*. This failure is put into sharp focus by the relative ease with which silicon can be treated by psuedopotential electronic structure calculation.

Here, we present an empirical treatment of silicon simply in terms of restricted bonding pair potentials. We show that this level of approximation allows a simple qualitative description of the main features of silicon polytypes, point defects, surfaces and clusters and exhibits a degree of transferability without reparameterisation hitherto unrealised by empirical models.

Configurations found by empirical methods are viewed not as an end in themselves, but as a method of generating plausible geometries for investigation by *ab initio* methods and a guide to the type of interaction suitable for Monte Carlo simulations.

DENSITY DEPENDENT POTENTIALS FOR SIMULATIONS OF SIMPLE METALS

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Abstract

The total energies for simple metals have been calculated in terms of a density dependent pair potential and an explicitly density dependent term (the volume potential). The potentials are based on a first-principles nonlocal pseudopotential theory with a correction term in the volume potential to allow for the effects of the density dependence of terms beyond second order in perturbation theory, adjusted to give the observed equilibrium density. Simple analytic forms have been obtained for the pair and volume potentials. The constant volume forms of the pair potentials are known to be superior to those of the effective medium theory (EMT) in dealing with eg phonons and electron transport and it is likely that they should be more reliable than EMT when generalised to handle inhomogeneous systems.

DEFORMATION DIPOLE POLARISABLE ION POTENTIALS FOR MOLTEN SALTS

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Abstract

We have simulated the structure of molten CsCl using a 'deformation dipole' polarisable ion potential, where ions have both point charges and dipoles. The magnitude of a dipole is determined by the local electric field and the repulsive interaction between neighbours. This produces significantly better agreement with experimental results than rigid ion or shell model simulations, can run much faster than a shell model simulation and parameters are simpler to derive.

AB INITIO LDF CLUSTER CALCULATIONS OF DEFECTS IN SOLIDS

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Abstract

LDF calculations are intrinsically more efficient than Hartree- Fock ones and are capable of yielding accurate structural information on solids. For real-space basis functions, cluster methods are superior to supercell ones. Here we describe a fast LDF procedure useful for clusters as large as 100 atoms. We apply the method to various defects in solids. Since defect structures cannot usually be experimentally resolved, it is essential to compute other measurable quantities. These include local vibrational modes and hyperfine parameters. Several applications of calculating the former are described.

THE K.P METHOD IN TOTAL ENERGY CALCULATIONS

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Abstract

Calculation of the total energy of a metallic system requires a large number of k-points and is consequently very time consuming. We describe the k.p method which allows the rapid evaluation of very accurate data at a large number of k-points from exact data at very few k-points. The result is a reduction in computational times over traditional methods of up to several orders of magnitude.

We demonstrate the method in operation for a diverse range of aluminium structures. We carefully analyse all those errors present, those due to the k.p method and those due to the use of a finite number of k-points. We demonstrate that for these structures, the extra error introduced by the k.p method is negligible.

PERIODIC AND CLUSTER HARTREE-FOCK CALCULATIONS IN SILICATE SYSTEMS

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Abstract

Hartree Fock methods can play a major role in the study of the properties of both perfect and defective inorganic materials. The range and limitations of the techniques will be discussed with special reference to three recent studies:

- Electronic structure studies of 4 and 6 coordinate silicate minerals.
- Investigation of the activation of methanol in zeolite ZSM- 5.
- Derivations of interatomic potentials for Al_2O_3.

SIMULATIONS OF AMORPHOUS SILICON

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Abstract

We have used the Stillinger-Weber potential with two- and three- body components in standard molecular dynamics to study amorphous silicon. We start with the basic amorphous model of Wooton, Winer and Weaire composed of 216 atoms and put together blocks of such atoms to create a structure of more than 100,000 atoms. This structure is then heated rapidly to remove periodicity, followed by rapid cooling to zero temperature. The calculated structure factors agree extremely well with experimental measurements on amorphous silicon.

ANGULARLY DEPENDENT MANY BODY POTENTIALS WITHIN TB HUCKEL THEORY

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Abstract

Recently a new angularly-dependent many-body potential for the bond order has been derived within TB Huckel theory by doing perturbation theory about the bond. This provides explicit analytic expressions for the dependence of the σ, π, or δ bond orders on the local atomic environment. Applications to transition metals and semi-conductors will be discussed.

MOLECULAR MODELLING OF AROMATIC POLYESTERS

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Abstract

An important characteristic of a polymer chain is its conformation, as it is directly related to the structure of both crystalline and amorphous states, thus determining mechanical properties, optical properties (non-linear optical materials), electrically conducting properties and the stiffness of polymer chains (liquid crystalline polymers, LCP's). Chain conformation is mainly determined by the rotational degees of freedom. An approach finally leading to the capability of molecular design, therefore involves the determination of the corresponding rotational energy profiles.

Both the lack and difficulty of obtaining the necessary and accurate experimental data urge for a theoretical approach. The purpose of this paper is essentially to discuss the merits of various theoretical methods. An integrated approach employing ab-initio, semi-empirical (AM1) and force field (CVFF) methods to study torsional barriers in conjugated aromatic molecular systems is presented. It is the first time that such an attempt including full geometry optimisation up to the ab-initio level is reported. First, we have focussed on monomer-like units of polyparahydroxybenzoic acid (PHBA) and polyethylene terephthalate (PET). Coupling between the torsional motions was studied with the

semi-empirical AM1 method as well as with the Consistent Valence Force Field. Molecular Dynamics simulations were carried out on single chains; the relation between MD results and chain flexibility is discussed as well as the consequences of the uncertainty in barrier heights for the MD results and the calculated persistence length.

Large differences between results obtained by the different levels of calculation were obtained. This as well as the lack of sufficient and accurate experimental data hampers progress in modelling the properties of the conjugated aromatic molecules investigated here.

In a second step we searched for a calculational method that would predict the rotational barriers correctly. Results of the semi-empirical AM1 and MNDO-PM3 calculations were compared with experimental gas-phase structural data. Benzaldehyde was also subjected to a large variety of ab-initio basis sets, up to the correlated level. Being computationally very demanding, we could not find the ab-initio results to lead to the correct potentials, even when performed at the highest level reported here. However, by introducing one pragmatic scaling factor, it was found that the AM1 method reproduced the experimental results within 15%, which is a very important and practical result for the modelling of (conjugated) polymers.

The third step in the process, currently in progress, is the development of a force field based on the correct, i.e. involving the scaled AM1 data, potentials. This will subsequently enable us to perform the necessary Monte Carlo and Molecular Dynamics calculations which will now, in principle, lead us to the correct energetics and dynamics of the system under investigation.

COMPUTER SIMULATION OF THE GLASS TRANSITION

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Abstract

We have carried out computer simulations in a model of a transition-metal-boride glass ($N_{80}B_{20}$) with the aim of observing and understanding the glass transition. Various quantities such as the specific heat and the mean-square atomic displacement show physically significant changes in behaviour near the transition. This behaviour is examined and analysed.

TOTAL ENERGY PSEUDOPOTENTIAL CALCULATIONS ON PARALLEL COMPUTERS

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Abstract

The Car-Parrinello scheme(1) has made it possible to perform ab initio molecular dynamics simulations. Using the capabilities of conventional supercomputers, simulations can be performed for unit cells containing up to 100 atoms and for simulation times of the order of picoseconds. These numbers will appear relatively small to those who are accustomed to performing simulations using empirical potentials. There is no obvious way of significantly increasing either the number of atoms in the unit cell or the length of the simulations on a single processor computer without a fundamental change in computer technology. However, both of these quantities can be significantly increased by using the larger number of processing units available in parallel machines. The recent availability of low cost, high speed processors such as the Intel i860 makes such a course particularly attractive at the present time. In the present talk I shall discuss the use of parallel computers for total energy pseudopotential calculations and describe the prospects for performing large ab-initio simulations on such machines in the future.

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AB INITIO MOLECULAR DYNAMICS : A CLASSICAL TOOL TO STUDY QUANTUM EFFECTS

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Abstract

The talk will give a brief introduction to the principles of *ab initio* molecular dynamics. Recent progress in the technique will be reviewed. with emphasis on new directions, such as the calculation of free energies.

RMC OR 'WHEN DO YOU NEED A POTENTIAL'

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Abstract

It is rare that computer simulations of disordered systems based on an empirical potential, however complex produce structures that agree with the available diffraction data within its known errors. It is generally very difficult to modify potentials to improve the level of agreement, so while such simulations may give a good understanding of the *type* of structure in the system they are unsuitable for investigating structural *details*. Ab initio simulations are usually too small to give information on anything other than short range order.

Reverse Monte Carlo (RMC) simulation is a method of structural modelling that uses experimental diffraction data 'in place' of a potential. It is applicable to many different types of system and data. I will describe the algorithm briefly and then illustrate its use in studies of both simple and complex systems (e.g. expanded Caesium and fast ion conducting glasses) where potentials are difficult to develop. In particular I will stress the *detailed* information that is contained in diffraction data and the ways in which this might be used to provide information on potentials.

SIMULATION OF NON-ADIABATIC PROCESSES

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Abstract

Considerable experience has now been gained in generating accurate adiabatic energy surfaces for molecules and solids by ab initio and semi-empirical techniques. However, many questions in the theory of chemical reactions and defect processes involve non-adiabatic phenomena, where the Born-Oppenheimer approximation fails. We describe how approximate information about such processes can be obtained and give an example of such a calculation involving the F-centre in alkali halides.

The CCP5 Literature Survey 1990

W. Smith

October 22, 1991

In the following pages we present the CCP5 Literature Survey for 1990.

This year, by way of a bonus, we have a supplement to the usual INSPEC survey in the form of a directory of papers published in the journal Molecular Simulation, provided to us by the editor in chief N. Quirke, to whom we offer our thanks.

All the references included in the main list are selected from the INSPEC database and are reproduced with the permission of INSPEC, the Institution of Electrical Engineers. The INSPEC database covers all areas of physics, electronics and computing. It follows from the above paragraph that INSPEC is not responsible for missing references, nor for any typographical errors, which may have resulted from our retyping of the computer printout. We are grateful to Mr. Geoff Jones, Head of Selective Services at INSPEC for his advice and assistance.

Finally, we thank Mrs. C.M. Smith for proof reading the pages presented here and Miss A.P. Haskayne of the Daresbury Reprographic Service for typing it all.

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