Computing

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 & Lattice Simulations of Condensed Phases.

Number 37
May 1993

Contents

General News

STEERING COMMITTEE MEETING OF CCP5

A meeting of the steering committee of CCP5 will be held on 16th. September 1993 at the University of Keele. This is timed to coincide with the CCP5 annual meeting. It will be necessary to elect 3 new members to the executive committee at this meeting. N. Allan (Chemistry, Bristol), M. Rodger (Chemistry, Reading) and S. Price (Chemistry, University College London) will have completed three years. The other members of the executive committee are Dr. M. Allen (Dept. of Physics, Bristol), Dr. J. Goodfellow (Dept. of Crystallography, Birkbeck College London) and Dr. W. Mackrodt (ICI). The executive committee consists of the chairman, 6 other members and the two permanent Daresbury staff. The members serve on the committee for three years. The committee meets three times a year to deal with day-to-day business of CCP5. If you would like to nominate someone for the executive committee please return the slip below.

My nominations for executive committee:_____

are

_____

_____

Signed _____

FUTURE MEETINGS

A summary table is given below, further details may be found inside. CCP5 has been asked to publisise the molecular liquids meeting as it will be of interest to our readers but is not involved with its organisation.

TOPIC	DATES	LOCATION
LARGE SCALE MOLECULAR SIMULATION	SEPTEMBER 15-17 1993	UNIVERSITY OF KEELE
WORKSTATION CLUSTERS	JUNE 25 1993	DARESBURY LABORATORY
MOLECULAR LIQUIDS	SEPTEMBER 24-29 1993	UNIVERSITY OF KENT

CCP5 PROGRAM LIBRARY

Details are contained in this issue of accessing the CCP5 program library through E-mail automatically. Also details of accessing the Allen/Tildesley example programs at Cornell. A new improved version of MDCSPC4 is available incorporating modifications suggested

by Dr. U. Essmann, City University of New York. An updated version of SFMK has been supplied by the author A.P. Lyubartsev. New additions to the library from our readers are always welcome.

CRAY NEWS

CCP5 participants are reminded that CCP5 has an annual allocation of Cray time at Rutherford Laboratory. This 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.

INTEL NEWS

CCP5 also has an annual allocation of time on the Intel IPSC/860 at Daresbury. If any CCP5 member wishes to make use of some of this time please contact M. Leslie at Daresbury.

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

JANET: M.LESLIE@DARESBURY
INTERNET: M.LESLIE@daresbury.ac.uk
EARN/BITNET: M.LESLIE%daresbury.ac.uk@ukacrl

An appreciation of Igor Favorsky (1939-1990)

CCP5 wish to acknowledge the receipt of an account of the work of Igor Favorsky. We are grateful to Dr. P. N. Vorontsov-Velyaminov (St. Petersburg University) for sending

this to us. Igor Favorsky performed Ising model calculations with purely dipole-dipole interactions in the seventies and was the first in Russia to do so. Among other techniques, he developed the reciprocal space method to account for long-range dipole interactions. Systems studied included dysprosium ethyl sulphate for which his simulations managed to reproduce the experimentally derived critical point. In the eighties he studied quantum lattice systems such as the conventional quantum Heisenberg model, including materials such as $CuK_2Cl_4.2H_2O$. As with most Russian scientists during the period of soviet rule, he never attended any international conferences outside the Soviet Union. He died in 1990 at the comparitavely young age of 50.

A fuller account of his work with a list of publications may be obtained from the editor.

REQUEST FOR CONTRIBUTIONS

The deadline for contributions for the next 2 newsletters will be **15 June 1993** and **15 September 1993** Readers are reminded that contributions are always welcome. Contributions may be sent by Email in LaTeX; this makes the task of collating the newsletter simpler for the editor.

Contributors to the current issue

Our thanks go to:

M. P. Allen   Department of Physics
                    University of Bristol

M. Rodger   Department of Chemistry
                    University of Reading

N. L. Allan   School of Chemistry
                    University of Bristol

W. Smith   Daresbury Laboratory
T. Forester

R. Smith   Loughborough University of Technology

M. Mezei   Department of Physiology and Biophysics
                    Mount Sinai School of Medicine, CUNY,
                    New York, NY 10029, USA.

D. Fincham   Department of Physics
                    Keele University

K. Boryczko   Institute of Computer Science
M. Pogoda   AGH
J. Kitowski   Cracow
T. Malkiewicz   Poland
J. Mościński
M. Bubak
R. Slota
W. Alda
J. Baran
D. Nikolov

CCP5 ANNUAL MEETING

LARGE SCALE MOLECULAR SIMULATION

Keele University
15th - 17th September, 1993

The aim of this meeting is to report and discuss the simulation of large complex systems made possible by recent advances in high performance computing. The title is intentionally broad. Examples of problems and systems within the scope of the meeting are: polymers and biomolecules; structural organisation and self-assembly; micelles and surfactants; surface processes involved in STM; and many others.

The invited speakers are:

D.L. Beveridge,	Wesleyan University, Connecticut
S. Homans,	Dundee University
U. Landman,	Georgia Institue of Technology
B. Smit,	Shell Laboratories, Amsterdam
D.J. Tildesley,	Southampton University

Contributed papers are warmly welcomed, and there will be poster as well as oral sessions.

The conference will be held in the pleasant park-like surroundings of Keele University. It will begin with lunch on Wednesday September 15th and end with lunch on Friday September 17th. Accommodation will be available on campus. The cost of 40 pounds for non-residents includes registration, lunches on Wednesday, Thursday and Friday, and coffee and tea breaks. The fee of 120 pounds for residents includes in addition dinner, bed and breakfast for the nights of 15th and 16th September. Students can come at HALF PRICE. To book for the meeting please send the registration form below as soon as possible, and not later than 30th July, to

Dr. David Fincham
Department of Physics
Keele University
Staffordshire, ST5 5BG, U.K
Email: D.Fincham@UK.AC.KEELE
FAX: +44 - 782 - 711093

REGISTRATION FORM, "LARGE SCALE MOLECULAR SIMULATION"

Name:_____

Address:_____

_____

_____

_____

Email:_____

Please tick one:

Resident   £120   ☐

Student resident   £60   ☐

Non-resident   £40   ☐

Student non-resident £20   ☐

Students please enclose a supervisor's letter.

Special dietary requirement:_____

U.K participants should pay in advance: please enclose a cheque payable to "CCP5 Meeting".

Contributed paper: please give title and enclose abstract.

Title:_____

7

JOINT CCP1/CCP5/CCP9 WORKSHOP ON WORKSTATION CLUSTERS

Daresbury Laboratory
10.30am — 4.0pm, June 25, 1993

Current technology is enabling workstations to be coupled together on local area networks running at 100Mbit/sec, while emerging technologies promise in excess of 1Gbit/sec. With such network speeds it becomes possible to perform serious parallel calculations on workstation clusters. To discuss this prospect we have organised a 1 day workshop. The workshop will draw heavily on the experiences gained at Daresbury using Hewlett-Packard and IBM workstation clusters with a variety of different interconnects (Ethernet, FDDI, SOCC, UltraNet). The tentative program is as follows.

10.30	Introduction
	Technical Considerations
10.40	Communications, hardware and harnesses an overview
11.10	System administration and NQS
11.30	Coffee
	Vendor Update
11.45	Hewlett-Packard
12.15	IBM
12.45	Lunch
	Application Talks
2.00	Crystal Hartree Fock
2.30	Molecular quantum chemistry
3.00	Tea
3.15	Car Parrinello
3.45	Classical Simulation of Condensed Matter
4.15	Close

In addition to the workshop there will be an opportunity for a limited number of participants to attempt to mount their own codes on the workstation clusters at Daresbury. If you wish to take advantage of this please contact us as soon as possible.

Those interested in attending please contact one of the following;

Alistair Rendell	ph. (0925) 603553	email A.P.Rendell@daresbury.ac.uk
Paul Sherwood	ph. (0925) 603553	email P.Sherwood@daresbury.ac.uk
Vic Saunders	ph. (0925) 603204	email V.R.Saunders@daresbury.ac.uk

Alternatively please complete and return the following form by Friday 4th June 1993.

JOINT CCP1/CCP5/CCP9 WORKSHOP ON WORKSTATION CLUSTERS

Daresbury Laboratory
10.30am — 4.0pm, June 25, 1993

To: Dr A.P. Rendell, SERC Daresbury Laboratory, Warrington, WA4 4AD.

I wish to attend the workstation cluster workshop.

Name:

Address:

Phone:

Email:

RESEARCH CONFERENCE ON

MOLECULAR LIQUIDS:

Computer Simulations and Experiments

organized in association with the

European Molecular Liquids Group (EMLG)

University of Kent at Canterbury, United Kingdom, 24-29 September 1993

Chairperson   A. Geiger (Dortmund)
Vice-Chairperson: R.M. Lynden-Bell (Cambridge)
Local Organisation: J.C. Dore (Canterbury)

Scope of the Meeting

The interpretation of experimental data on molecular liquids very often suffers from the necessity to use oversimplified analytic models, which are not able to reproduce the details of the structure and dynamic in such systems. Recent developments in computational techniques and the continuous improvement of interaction potentials now allow the realistic simulation of molecular liquids. This opens the possibility to use simulations for the evaluation of experimental data. This largely increases the power of many experimental techniques.
The goals of the planned meeting are

- to discuss the present state of simulation techniques and their power to reproduce 'real' molecular liquids,

- to discuss the possibilities to extract data from simulations, which are directly comparable to various experimental results,

- to plan experiments, which are suitable for combination with simulations,

- to give recent examples of such efforts.

A list of scientists who have so far accepted to give a presentation or to act as session chairpersons is as follows:

S. Bratos	*Université P. et M. Curie, Paris, France*
M. Ferrario	*Università di Messina, Italy*
D. Frenkel	*FOM Institute for Atomic and Molecular Physics, Amsterdam, The Netherlands*
E. Guàrdia	*Universitat Polytècnica de Catalunya, Barcelona Spain*
B. Guillot	*Université P. et M. Curie, Paris, France*
W.G. Hoover	*University of California at Davis/Livermoore, USA*
G. Kneller	*Centre d'Etudes Nucléaires de Saclay, Gif-sur-Yvette, France*
P. Madden	*Oxford University, U.K.*
A. Maliniak	*Arrhenius Laboratory, Stockholm, Sweden*
G.W. Neilson	*University of Bristol, U.K.*
G. Palinkas	*Hungarian Academy of Sciences, Budapest, Hungary*
J.A. Padró	*Universitat de Barcelona, Spain*
H. Posch	*Universität Wien, Austria*
J.G. Powles	*University of Kent at Canterbury, U.K.*
J. Schnitker	*University of Michigan, Ann Arbor, USA*
W.A. Steele	*Pennsylvania State University, USA*
A.J. Stone	*University of Cambridge, U.K.*
S. Toxvaerd	*Ørsted Institute Copenhagen, Denmark*
R. Vallauri	*Università degli Studi di Trento, Povo, Italy*
P.-O. Westlund	*University of Umeå*
M.D. Zeidler	*RWTH Aachen, Germany*

A poster session will also be organized. A few contributed papers can be admitted for short oral presentation.

JOINT CCP3/CCP5 POSTDOCTORAL POSITION

'THE FIRST-PRINCIPLES SIMULATION OF SURFACE PROCESSES'

Cray Research Inc. have announced that they will provide funding for a three-year joint CCP3/CCP5 postdoctoral position on 'The First-Principles Simulation of Surface Processes'.

Major advances in high-performance computing are expected over the next three years, and teraflop speeds are likely to become available in this period. Techniques for performing accurate first-principles simulations of large systems are also evolving rapidly. The ambition of the project is to exploit these advances to study the atomic structure and dynamics of surfaces - a field of interest to both CCPs. It is planned that there will be an emphasis on the properties of the surfaces of oxide materials.

The post-doctoral position will be based at Daresbury Laboratory, which is a major centre of expertise both in the scientific application of parallel computing and in computational condensed-matter science. A start-date for the project has not yet been set, but informal expressions of interest in the position are invited now. The salary will be on the standard scale for SERC research establishments. Enquiries may be made either to Dr. Paul Durham (CCP3) or to Prof. Mike Gillan (CCP5) at the following addresses:

Dr. P. Durham
TCS Division
SERC Daresbury Laboratory
Warrington WA4 4AD

tel: 0925-603263
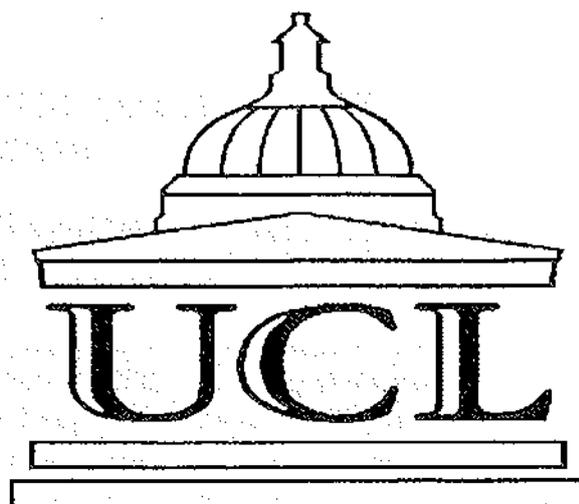fax: 0925-603634
e-mail: p.durham@uk.ac.daresbury

Prof. M. J. Gillan
Physics Dept.
Keele University
Keele, Staffordshire ST5 5BG

tel: 0782-583326
fax: 0782-711093
e-mail: pha71@uk.ac.keele.seq1

SERC EARMARKED STUDENTSHIP

Prediction of the Crystal Structures of Polar Molecules using Realistic Electrostatic Models

Recent advances in the theory of intermolecular forces now enable realistic models for the electrostatic interactions between molecules to be derived from *ab initio* wavefunctions. A crystal structure prediction code DMAREL is being developed which will enable these electrostatic models to be used to study the crystal packing of important polar molecules, such as nucleic acid bases, drugs and molecules with high non-linear optical coefficients. The SERC's support of this major project includes the award of an earmarked studentship for postgraduate research, leading to a Ph.D. degree.

Applications for this studentship are sought from final year undergraduates who expect to fulfil the normal SERC eligibility requirements. Some previous experience of computational chemistry would be an advantage.

Further details are available from Dr Sally Price, Department of Chemistry, University College London, 20 Gordon Street, London WC1H 0AJ.

The CCP5 Program Library

W. Smith

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.

Programs 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.

The programs from "Computer Simulation of Liquids" are also available. To access them use program-name F.01, for example.

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.

Availability of the Allen/Tildesley example programs at Cornell

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. This facility is no longer operational as advertised, due to software and hardware 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 quotes, note underscore character - not hyphen -).

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 EMAIL message to: statmech@cheme.tn.cornell.edu Commands are sent in the body of hte 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 a 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".

Steve Thompson, School of Chemical Engineering, Cornell University, Ithaca NY 14853 USA.

THE CCP5 PROGRAM LIBRARY.

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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,TB+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
NEMD       [MD,LJA,SLLOD,Macintosh]   D. J. Evans
NSCP3D     [UT, Hard sphere packing] M. Bargiel & J. Moscinski
PIMCLJ     [PIMC,LJA,MC,TH+RDF+QC] K. Singer & W. Smith
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SCN       [MC,LJA,RFD,TH]   N. Corbin
SMFK      [MC-SCF, Cylindrical Polyelec.] A.P. Lyubartsev
SLS_PRO   [MD,Proteins,LF,TH+RDF] 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
                    SLLOD   Thermostatted SLLOD equations


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
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Programs from the Book "Computer Simulation of Liquids"

Liquid Crystal Simulation

M. P. Allen

Introduction

CCP5 sponsors a collaboration in the area of liquid crystal simulation. This enables several UK research groups to get together from time to time, exchange recent results and, especially, concentrate on the major technical challenges to progress in modelling these phases. The most recent meeting was held in Bristol on Friday 26 March 1993. It was attended by: Mike Allen, Carl Mason, Mark Warren (Bristol, Physics), George Jackson, Dave Williamson, Alejandro Gil (Sheffield, Chemistry), Geoffrey Luckhurst, Doug Cleaver (Southampton, Chemistry), Andrew Masters (Manchester, Chemistry) and Mark Wilson (Lancaster, Physics/Materials). These groups currently use models at all levels of complexity, from lattice spins to fully-realistic atom-atom potentials, but most of the discussion related to hard nonspherical particles and to the Gay-Berne, soft attractive ellipsoidal potential. This article is an account of the discussions that took place at that meeting.

Hard particle simulation

George Jackson described a systematic programme of Monte Carlo simulations of hard spherocylinders and hard-sphere chains, in progress at Sheffield. Simulations of spherocylinders with $L/D = 3, 5$ (i.e. length-to-width $= 4, 6$) are initially intended to check earlier work by Stroobants, Frenkel and Veerman, as a reference system prior to studying the same system with added point dipoles. For both elongations, the isotropic phase pressure-density curves agree well with previous results, and also are well represented by Boublik's equation of state. Further work is necessary on the nematic, smectic and solid phases. There was some discussion of the value of constant-pressure simulations, especially near the phase transitions, and the need to adjust box dimensions independently for some of these phases. The next phase is to add a point dipole at the centre, both along the symmetry axis and in a transverse direction, and to put a dipole in an off-centre position giving a chiral molecule.

The group has studied the whole range of N-atom linear rigid chains of tangential hard spheres, from $N = 2$ to $N = 6$, by Monte Carlo, with simulations of $N = 7$ now in progress. These simulations are quite expensive, with a month of cpu time required per state point for the longer chains. Configuration evolution is sluggish, with the (very knobbly) molecules tending to get locked with each other. The group had greatly improved the situation by using reptation Monte Carlo moves, in which an atom is transferred from one end of the chain to the other. No nematic phase had been seen for $N \leq 6$; the equation of state for the isotropic phase is well represented by the BHS (bonded hard sphere) theory originally due to Wertheim.

Dave Williamson gave further details of the Sheffield simulations, and described the application of Onsager theory, based on the second virial coefficient with a Parsons-type resummation of higher virials, to these systems. There are significant differences between hard-sphere chains and spherocylinders of the same overall dimensions. In minimizing the free energy as a function of the orientational distribution function $f(\Omega)$, the group uses a tabulated function and a Monte Carlo simulated annealing approach, rather than the traditional method based on trial functions of specified form.

At Lancaster, Mark Wilson has been conducting molecular dynamics simulations of hard-sphere chains for some time. In these systems the degree of flexibility is adjustable, via a set of maximum and minimum constraints on interatomic distances. For a nearly-rigid model, molecular dynamics runs up to 20 times faster than a program written for an equivalent fully-rigid system. A constant-pressure ensemble is studied: standard constant-P Monte Carlo box scalings are carried out in between periods of normal dynamics. This assists equilibration. There was some early study of a 5-atom chain, but this did not yield any oriented fluid phases; subsequent work concentrated on the $N = 7$ case.

For the most rigid 7-atom chain molecule studied, isotropic, nematic and smectic phases have been observed. The isotropic phase equations of state agree well with the BHS form. On relaxing the molecular rigidity somewhat, the smectic phase is lost, the isotropic-nematic phase transition is pushed to higher density, but there are indications that the solid may also be destabilized, so the nematic range is extended. For the fully flexible chain (a model of the kind studied before by Rapaport) there is no liquid crystal. These systems can show long periods of quasi-stability in the order parameter, which can be misleading. There was some interest in the change of molecular shape with density. The flexible systems tend to contract (radius of gyration becomes smaller) on increasing the density. The semi-rigid systems become longer and thinner in the nematic phase as the order parameter goes up with density. Similar effects are seen in 'realistic' simulations and in experiment. Another interesting point is that, in the nematic phase, the average value of the order parameter $\langle P_4(\cos\theta)\rangle$ is always positive, and the distribution function $f(\cos\theta)$ is always peaked along the director, contrary to many Raman (and other optical) measurements.

At Bristol, hard ellipsoids of revolution are being studied in a variety of ways. Mike Allen described a new system of twisted periodic boundary conditions, which permits the simulation of a uniformly twisted nematic liquid crystal, with a prescribed helix pitch. This has already been used to calculate the Frank twist elastic constant in a direct way. Most recently, it has proved possible to calculate the helical twisting power β for a chiral dopant molecule dissolved in a nematic phase. This is the coefficient of proportionality between the concentration of right-handed (or left-handed) molecules (assumed dilute) and the wavenumber of the helical structure induced by these molecules. The relation may be manipulated to relate β to the chemical potential difference between mirror image forms of the molecule in the artificially twisted solvent. Preliminary results have been obtained for a particular choice of dopant molecule (an ellipsoidal dimer, in a scissors arrangement) and it is hoped to extend the method to treat more general cases.

Carl Mason described three further projects currently under way at Bristol. Firstly, extensive simulations of highly nonspherical ellipsoids have been carried out, to compare equations of state and phase transition points with the predictions of an Onsager/Parsons type of theory due to Evans and Samborski. Secondly, a detailed study of the $e = 3$ ellipsoid system is in progress. Some doubt has been shed on the stability of the nematic phase here; the original studies were by Frenkel and Mulder, but more recent work of the Orsay group suggests that, as the system size increases, the phase is squeezed out between isotropic liquid and solid. This is being checked in some detail. To date, spontaneous formation of nematic (at a density in the middle of Frenkel and Mulder's range) from isotropic has been seen for $N = 108$, 256 and 512, using Monte Carlo and molecular dynamics. MD is significantly more cost effective: the nematic forms within days rather than weeks of running. More work is needed before any firm conclusions can be reached:

22

formation of nematic from solid is being attempted, using constant-pressure MD, and free energy calculations are needed. Lastly, studies of the distribution of director orientations within the simulation box are being carried out for relatively small system sizes, but with very long runs (several million MC sweeps), for systems well within the nematic region. The aim is to start quantifying finite size effects, an area which has always been of concern (especially for the calculation of Frank elastic constants). Very preliminary results suggest that the effect may be significant, and that cubic boxes behave differently from truncated octahedral boxes. In the cubic case, the director prefers to align along the cube axes, with the body diagonal very disfavoured, while for TO boundaries alignment nearly (but not exactly) along the diagonal seems preferred. It should be possible to associated a free energy with this effect; more work using special windowing and non-Boltzmann sampling techniques is needed.

Gay-Berne potentials

Geoffrey Luckhurst described the work being undertaken at Southampton to develop a strategy for choosing the parameters of the Gay-Berne potential, based on a knowledge of the types of molecules we wish to model. It is necessary to choose a shape anisotropy parameter, which is relatively easy, a well-depth anisotropy, which is slightly more difficult, and a pair of exponents μ and ν which determine the way the well depth varies with changing orientation of the molecules and the vector between their centres. Different groups have tinkered with the values of these exponents, and the growing variety of different versions of the potential is unfortunate in some ways. The original fit was to a molecule of 4 fused Lennard-Jones spheres. Best fits to systems of 4–9 LJ atoms give varying choices of μ and ν. Such a fitting procedure, applied to realistic models of mesogens, can at least be used to choose the exponents in a rational way.

There was some discussion of the observation that in simulations of smectic B phases using the Gay-Berne potential, the director (and layer normal) invariably seemed to point along the body diagonal of the simulation box. A layer spacing less than the molecular length pointed to some interdigitation, and the possibility that translational constraints imposed by the periodic boundary conditions were having an effect on the overall orientation. For the smectic B, a rippling of the molecular layers had been observed, and the preferred position for each molecule seemed to be above the midpoint of a line between two molecules in the layer below, rather than above the centre of a triangle of molecules in the layer below.

Simulations using disk-like molecules, constructed in the Gay-Berne fashion, were also in progress. Here the face-to-face energy parameter was chosen to be five times the edge-to-edge value. A state point in the discotic-nematic region of the phase diagram was chosen by referring to the hard-ellipsoid results of Frenkel and Mulder. The Gay-Berne model also forms a columnar phase, in which the columns of disks are interdigitated and, probably as a consequence, are packed in a tetragonal or square arrangement at certain densities; on lowering the density the more common hexagonal structure is seen. Finally, lyotropic systems formed from disk-like micelles are under investigation, using a model in which the edge-to-edge attraction is larger than the face-to-face value. Here the disks form lamellae, which are stacked in a (possibly incommensurate) layered fashion.

Mark Warren described his initial progress on a project started last autumn at Bristol, using the Gay-Berne potential. A molecular dynamics program has been written, in which the director of the nematic phase is precisely constrained by Lagrange multipliers. An

initial application is to calculate the Frank elastic constants, where it is convenient to fix the director so that wavevectors consistent with the box axis vectors are also stationary in the director frame. A second application is to examine the distribution of the director within the simulation box (as discussed above) by directly integrating the constraint force with respect to orientation to find the associated free energy function. There are several more potential applications of the technique. The programs have been written in parallel form to run on the DAP at Bristol and the Intel at Daresbury, in collaboration with Bill Smith.

Doug Cleaver described a series of Monte Carlo simulations of the Gay-Berne system in the nematic phase, carried out with Andy Emerson, at Southampton. In this work, the director is constrained to lie within a cone of prescribed angle (typically 5 degrees) of the z axis, by rejecting Monte Carlo moves that would take it outside this range. The aim (just as at Bristol) is to facilitate the calculation of Frank elastic constants. Preliminary results had already been achieved for one state point, and they seemed to be of the expected magnitudes. There was some discussion of the equivalence, or non-equivalence, of applied orienting fields (which 'quench' the orientational fluctuations), Monte Carlo biasing functions, and windowing functions.

Other work

Mike Allen described a recent advance in our understanding of diffusional processes in the nematic phase, due to Tang and Evans (Oregon). By formulating the kinetic theory of hard nonspherical bodies in a way that accounted for the different directions of molecular motion, molecular symmetry axis and (for the nematic) the director, they had obtained excellent agreement with the diffusion coefficients of ellipsoids (parallel and perpendicular to the director), including the interesting dependence on density that had been observed on the high-density side of the isotropic-nematic transition. Moreover, the two-exponential decay of the velocity autocorrelation function was also reproduced with impressive accuracy, by a theory with no adjustable parameters, which simply required the collision rate and order parameter as input. Andrew Masters described his own kinetic theory (Boltzmann equation) analysis of ellipsoid diffusion coefficients (which should be essentially equivalent to that of Evans). An interesting feature of the simulation results was the accuracy with which the particular combination $\mathcal{R} \equiv (D_\parallel - D_\perp)/(D_\parallel + 2D_\perp)$ fitted the 'affine transformation' prediction of Hess, over a wide range of order parameter and molecular elongation. Hess' theory relates the ellipsoidal system to a perfectly aligned system of ellipsoids, and hence to hard spheres. For perfectly aligned ellipsoids the Boltzmann analysis can be taken through to a final form for $\mathcal{R}$ which looks much more complicated than the Hess expression, but which is numerically very close indeed over most of the range of elongations. For imperfectly aligned ellipsoids $\mathcal{R}$ must be obtained numerically, but again it is very close to the Hess prediction. The separate diffusion coefficients $D_\parallel/D_{\text{hardsphere}}$ and $D_\perp/D_{\text{hardsphere}}$, however, differ significantly from Hess' theory.

Geoffrey Luckhurst described simulations of rod-plate mixtures using a lattice system, using $\pm \varepsilon P_2(\cos \beta_{ij})$ interactions with a positive or negative sign to represent unfavourable or favourable terms. The aim here is to look for biaxial nematic phases for the mixture, which would be competing against the phase separation predicted by a theory of Dunmur's. The tricky problem of identifying elements of the ordering tensor, and averaging them in an appropriate manner to obtain uniaxial and biaxial order parameters, was discussed.

There was no time to discuss realistic liquid crystal simulations in detail, but Doug

24

Cleaver mentioned that a model of the cyanobiphenyls had been developed at Southampton, and was being used to simulate layers of these molecules on graphite for comparison with atomic force microscope experiments. Mark Wilson is developing a code to simulate a realistic model of a mesogen in a non-mesogenic solvent (e.g. carbon tetrachloride) to study the effects of varying concentration, and certain specific chiral interactions.

Conclusions

Recurring themes in the discussion were the need to conduct runs of the order of several millions of MC sweeps or MD timesteps, in order to properly equilibrate systems near phase transitions, and properly sample order parameter distributions. Also, the long-standing questions regarding system-size effects, and the influence of the box on orientational ordering, have come to the fore once more; some groups are seeking to quantify this and/or control the director more closely in simulations. This is particularly critical, in that it may affect directly some of the properties of most interest, namely the elastic constants. Finally, many groups are paying attention to the various ingredients of molecular interactions that may influence liquid crystal behaviour: shape and size, flexibility, long-range electrostatics, and the general shape and range of the attractive well.

CCP5 Workshop on aqueous systems

M. Rodger

The overseas visitor to the workshop was Dr A. Wallqvist, who gave a talk on simulation studies of the structure of water solutions. This included a discussion of the strengths and weaknesses of existing water potentials, and then considered the effect on water structure of adding hydrophobic molecules such as methane, or hydrophillic molecules such as methanol. There were also three UK speakers: Dr A.J. Stone, who gave a very enlightening talk on the state of the art for accurate ab initio potentials for water, and how well these reproduce 2-body properties; Dr D.N.J. White, who presented his work on polypeptides interacting with an ice surface, and the degree to which binding is specific to one of the growth faces of ice; and Dr A.K. Soper, who addressed experimental neutron scattering techniques, and the possibilities they have for elucidating solvation structure, including recent developments towards measuring orientational correlations directly. More than 40 people attended the workshop.

Dr Wallqvist also gave a seminar at Birkbeck College. This dealt with the subject of protein folding, using a new and simple model that Dr Wallqvist has developed. This model mimics solvent effects by using Lennard-Jones interactions between hydrophobic groups, but repulsive interactions between hydrophillic groups, and manages to reproduce qualitatively much of the behaviour observed in protein folding.

CCP5 WORKSHOP - THE MODELLING OF SURFACES
Bristol University, April 1st 1993

This took the form of seven invited talks. All speakers gave excellent presentations, and a wide range of subject areas were covered. Striking features of all of the talks were the degree of contact with experiment and also the increasing rôle of *ab initio* methods, via density functional or Hartree-Fock methodologies.

Professor M. Gillan (Keele) and Dr. W.C. Mackrodt (ICI Chemicals and Polymers) discussed aspects of the surface chemistry of oxides. Mackrodt ("Aspects of oxide surfaces and surface calculations") concentrated on aspects of surface relaxation, including the good agreement between ionic model simulations based on electron gas potentials and new SCF Hartree-Fock results obtained using the CRYSTAL code. Gillan ("Oxide catalysis from first principles") reported impressive LDA results for systems such as Al_2O_3, where again the new quantum mechanical results appear to bear out those from earlier classical simulations.

On a different theme, Professor M. Klein (Pennsylvania) described recent molecular dynamics simulations of self-assembled monolayers. Systems studied included alkylthiolates on gold surfaces, long chain alkanes, and also water absorbed on SAMS with different chain terminal groups. Dr. K. Rogers (Strathclyde) addressed the important area of crystal morphology ("The absolute polarity and polar morphology of crystalline urea"), where simulations, incorporating calculated SCF charge densities and a suitable force-field, predict a polar morphology for urea that is in good agreement with that of crystals prepared from the vapour phase, and allow an absolute assignment of the polar forms as {1 1 1}.

Two talks concentrated on molecular dynamics of metallic systems. With the help of a excellent video animation, Sutton (Oxford - "Mechanical and electrical properties of nanometre metallic contacts") described the results of simulations of a tip-substrate configuration, similar to those in AFM and STM. Lynden-Bell (Cambridge - "The effects of temperature on metal surfaces") reported work on the dynamical properties of metal surfaces and surface disorder at high temperatures, and the calculation of surface free energies.

Finally Dr. A. Rohl (Royal Institution) outlined his new code (MARVIN) for the simulation of surface structures of inorganic systems, using the ionic model (incorporating the shell model) and incorporating two, three and four body potentials. Further details can be obtained from andrew@uk.ac.ri.ricx.

Neil Allan

Report on Computer Simulation and

Atomistic modelling of Materials

R. Smith

Introduction

This meeting, organised by the atomic collisions in solids group of the IOP, was attended by 37 participants from various academic backgrounds and industry. An abstract booklet is appended which includes a list of all the invited and contributed talks.

The theme of the meeting was to be both educational and state of the art. The day's programme included discussion of ab-initio potential calculations, semi-empirical potential development, Monte-Carlo and molecular dynamics (MD) simulations and their application to a number of interesting chemical and physical phenomena including novel ionic materials and scanning tunnelling microscopy. The attached abstracts give more detail of the individual lecture content.

An important message which the meeting communicated (besides the rapid development of parallel computing) was the importance of visual representation. All the lectures were elucidated by the use of graphics visualisation packages and during the meeting three MD video presentations were also given. Video presentations are becoming a popular source of disseminating material and the dynamic visualisation of a number of processes revealed features which would have been more difficult to understand and explain without them. The videos showed the process of adhesion and wear of STM tips on a metal substrate, the process of sputtering, implantation and the formation of surface waves by C_{60} molecules on graphite. A final video depicted the process of radiation damage formation in metals by energetic collision cascades.

The general feeling of participants at the end of the meeting was that it had been a useful exercise and one that might well be worth repeating in about 18 months or 2 years time.

Fundamentals and Overview

M. J. Gillan

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The talk will give a brief survey of the main techniques that are currently important in the simulation of materials. There will be an emphasis on new developments that will lead to progress in the next few years. Particular attention will be given firstly to ab-initio methods of various kinds and semiempirical quantum methods, and secondly to the exploitation of rapidly growing parallel processing power.

Ab-Initio Calculation of Solid State Properties

R. Jones

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A discussion is given of the problems involved in constructing and carrying out first principles local density functional pseudopotential calculations of the structural and electronic properties using *real space* basis functions. The particular method used at Exeter will be briefly discussed and illustrated with several examples. The most important conclusions are that it is now possible to relax clusters as large as 100 atoms within a few days using a small workstation and these calculations lead to a wealth of data on the structural, electronic and dynamic properties of a wide variety of defects in solids and which is of considerable value to experimental groups. The problems involved in extending the method to deal with diffusion barriers and gradient corrections are also described.

29

Computer Modelling of Ceramics and Catalysis

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In recent years computational methods have developed into a major technique for studying the structures, properties and reactivities of materials.

Both simulation and electronic structure techniques may now be used routinely to model the structures (at the atomic) level of crystalline and amorphous solids and of surfaces and defects. The current status of the field will be reviewed by reference to two important classes of material: first *ceramics* (including nuclear ceramics and high T_c superconductors), where we shall concentrate on the use of modelling methods in elucidating the crucial effects of defects and impurities: second. *heterogeneous catalyst* (including the fascinating. microporous zeolitic materials) where modelling methods are being used increasingly as an adjunct to experiment to predict the structural properties of catalytic materials and the sorption. diffusion and reaction of molecules on their surfaces and within their pores.

Defects in Metals

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Recent progress in two areas of defect modeling in metals will be described. In one. the core structure and mobility of dislocations in twin boundaries in the h.c.p. metals has been considered. and a wide variety of properties has been found. In the other. displacement cascades produced by energetic primary recoils have been simulated for energies up to 10keV. By modelling pure metals and alloys. considerable insight has been gained into the mechanisms and efficiency of defect production in cascades.

The advantages and limitations of atomic-scale computer simulation will be discussed in relation to both these topics.

Adhesion, Lubrication and Wear

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When two surfaces come into contact they touch only at the asperities of the surfaces, unless the surfaces are atomically flat. In this talk I shall discuss adhesion and frictional sliding of a metallic tip on a metallic substrate. The approach is to use molecular dynamics to model a tip of nanometre dimensions and a substrate. The effect of a layer of impurities on the force of adhesion (the force required to pull the tip off the substrate), and the mechanism of lubrication, will be shown in video recordings of animations of the simulations. A simple "liquid drop" model was suggested by these simulations to explain the reduction in the force of adhesion by a layer of impurities. Without a layer of impurities frictional sliding is accompanied by junction growth.

Molecular Dynamics Simulations of Surface Chemical Reactions

B.J. Garrison

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University Park, PA. 16802

Applications of the use of molecular dynamics simulations for surface chemical reactions (i.e. making and breaking of bonds) will be given. Examples include keV particle bombardment of solids, F atom etching of Si, and growth of diamond films. The many-body potentials used in such simulations will also be discussed.

The Simulation of Energetic Particle Collisions with Solids - a Visual Representation

R. Webb[1], R. Smith[2], E. Dawnkaski[3], B. Garrison[3] & N. Winograd[3]

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3. *Department of Chemistry, Pennsylvania State University,*
   University Park, Pa 16802, USA

A set of animated sequences of various ion and cluster impacts on different material substrates are shown. The ion/target combinations used for these are: 25keV Ar impact on Rh{100}, 500eV B on Si{110} and C_{60} on graphite {0001}. Molecular Dynamics simulations using many body potentials are used throughout the calculations. Different aspects of both the collision process and the simulation technique are demonstrated.

1. The difference between individual ion impacts, in which a high sputtering event is contrasted with a low sputtering event.

2. The propagation of energy in a collision cascade, in which it is observed that the high energy portion of the cascade propagates outwards while the inner portion loses energy.

3. The number of collisions in a cascade which are non-binary in nature is shown to be significant and a number of five body interactions are found for quite energetic interactions.

4. Implantation from the view point of the ion, in which two particles are followed, one channelling and one dechannelling. The dechannelling event leads to a focused collision sequence which is shown.

5. The impact of a large cluster impact in which a large acoustic wave is seen to spread across the surface and evidence of a hypersonic energy transport mechanism prior to this.

Computer Modelling of Phase Transformations in Solids

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Recent developments will be described in modelling the following types of phase transformations in solids.

1. Discontinuous precipitation in austenitic steels.
2. Continuous precipitation.
3. Grain boundary precipitation in Al alloys and steels.
4. Combined grain boundary segregation and precipitation in Al alloys.

A brief review will be given of microcrystallisation modelling in steels and superalloys.

Empirical Potential Functions for Covalent Materials and Metals

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Empirical potentials based on 2-body and 3-body terms can give an accurate fit to lattice energy, lattice distance, phonon frequencies, elastic constants and vacancy formation energy. They have been shown to give a good picture of small cluster structures and stabilities and are now being used to study surfaces. Systems studied so far are C. Si. Ge. Sn. Al. the alkali metals, Cu. Ag. Au. Fe. Unlike many other potentials the functions used can represent any cubic structure, and lower symmetry structures. A potential optimised to the properties of one phase, gives sensible energies and lattice distances for other solid phases.

Metastability in Synthetic Phases of Silicon

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It is possible to synthesize superdense Si by pressure treatment. The resulting phase, known as BC8, is semimetallic and very long lived. We have performed calculations on this phase to calculate its internal distortions under pressure and its relative stability with respect to diamond. This work has been done using both empirical and ab initio methods, which agree well with one another. These calculations show that BC8 is primarily a covalently bonded material. A further phase, ST12, has been investigated and compared to BC8. Simple free energy calculations suggest that ST12 will be stable with respect to BC8 at higher temperatures.

Surface Topology of Coatings formed by Unbalanced Magnetron Sputtering

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The technique of unbalanced magnetron sputtering can be used to deposit coatings of a wide range of metals, alloys and ceramics, including highly supersaturated solid solutions and glassy metals. Under appropriate conditions, the surface topography of the coating is virtually identical to that of the substrate, reproducing sub-micron surface features in coatings more than 1mm thick. Examples of such coatings will be shown and suggestions for modelling the coating growth process will be discussed.

Monte-Carlo Simulation of Ge Epitaxial Deposition on the 2 × ? - Reconstructed Si{001} Surface

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The surface processes involved in thin film heteroepitaxial growth have been investigated intensively in recent years because of the technological importance of this growth technique. particularly in fabricating photonic devices such as Ge/Si superlattices. Accuracy in controlling film thickness has reached the monolayer level. Of particular interest theoretically are details of the initial stages of growth in which Ge adatoms are deposited onto a Si substrate and adatoms migrate on the surface.

A fast computational procedure has been developed which allows the simulation of heteroepitaxial growth. based on the Metropolis energy minimisation algorithm and Tersoff empirical many-body potentials for the atomic interactions. Periodic boundary conditions are imposed on the system in two directions. while in the vertical direction, the growth direction. the surface is kept free.

We have mapped out the potential-energy surface seen by a single Ge adatom for the following two cases:

1. Si{001} 2 × 1 reconstructed surface both with and without surface atom relaxation.

2. Si{001} 2 × 1 reconstructed surface with one Ge adatom already present.

    The difference between the potential-energy maps are discussed. The deposition of Ge adatoms over the flat (2 × 1) reconstructed Si{001} surface also have been studied. Results will be presented illustrating details of growth processes.

Computer Simulations of Irradiation Damage Cascades at Harwell

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Some 400 irradiation damage cascades have been simulated in metals (Cu and Fe) with knock-on energies ranging from 60eV to 10keV and temperatures up to 900K. The effect of small pre-existing features on the evolution of the cascades has also been investigated. The cascade simulations have been made using the MOLDY computer code with three fast PC's, a workstation and a Cray 2 supercomputer and have involved blocks of up to 1/4 million atoms. The main purpose of this work is to determine the amount of displacement damage that is likely to be produced by a given spectrum of neutron energies. This has been shown to be significantly less than had been previously expected because of the extensive recombination of point defects that occurs during the evolution and cooling down of the cascades.

DL_POLY : Progress report

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May 4, 1993

DL_POLY Progress report

In issue 35 (September 92) of this publication the inauguration of work on a package DL_POLY was announced. The purpose of this package is to apply parallel molecular dynamics methods devised by participants in the CCP5 (the Collaborative Computational Project for the computer simulation of condensed phases) project into a sophisticated package capable of accurate modeling of complex systems. It is hoped that the final product will be a world-beating package available *free* to academic groups. The target machines for the package is the Intel iPSC/860 parallel computer and workstations. We emphasis that DL_POLY is designed as a *package* not as a program. It thus highly modular in nature and relatively easy to taylor to modelling specific systems.

DL_POLY is being developed at Daresbury Laboratory under the auspices of CCP5 and the Advanced Research Computing Group (ARCG) at Daresbury Laboratory. The package is the property of the United Kingdom Science and Engineering Research Council (SERC).

The special emphasis of the package is on macromolecules but the package is designed to be flexible enough to incorporate a wide range of systems including ionic melts, liquid mixtures, polymers, crystals etc.

Currently DL_POLY has the following features :

The parallel strategy is that of *Replicated data*. The integration algorithms include; Verlet leapfrog (NVE); Nose - Hoover with Verlet (NVT); Evans thermostat with Verlet leapfrog (NVT); multiple timestep; and Shake. All common periodic boundary conditions are available including: none, cubic, rectangular; parellelpiped; truncated octahedral; and rhombic dodecahedral.

The default force field is that of GROMOS but all common force fields for macromolecules (e.g. AMBER, Universal force field) will be accommodated. At present the force field contains terms for: all common short-range atom-atom potentials; the Coulombic potential; a truncated coulombic potential (non-periodic systems); valence angle potentials; dihedral angle potentials; and improper dihedral angle potentials. In periodic systems the Coulombic potential is handled by the Ewald sum for point charges.

It is anticipated that a first general release of the package will be available in time for the CCP5 annual general meeting in september 1993. At present work is being carried out to thoroughly test and refine the existing package before the first public release.

The case for keeping simulated clusters spherical.

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Several molecular modeling packages offer the option to solvate a molecule with a layer of solvent (usually water) of a certain thickness. The user then can run molecular dynamics on this cluster with the expectation that the a large portion of the solvent effect has been included into the system relatively economically. What has been left apparently unnoticed (with apologies to those by whom it has not) was that the surface tension of the cluster would introduce a bias toward more spherical shapes, therby introducing variations into the water layer thickness and possibly distorting the conformation of the solute. Clearly, neither of these effects are desirable.

To get an idea of the significance of this effect, I set up a simple model examining the deformation of a spherical droplet into an ellipsoidal one. The input of the model is

1. V_o, the volume of a solvent molecule in the bulk (30 Å^3 for water);

2. α, a contraction factor ($\alpha \leq 1$) so that the volume of a molecule on the surface is αV_o;

3. N, the number of molecules in the droplet;

4. σ, the surface tension of the solvent (72 dyne/cm = 0.104 kcal/mol Å^2 at room temperature for water).

The work of deforming a sphere into an ellipsoid will be obtained from the change in the surface area.

The number of solvent molecules on the surface, N_s, is estimated as

$$N_s = S/[r_s^2 \ 1.5^{1.5}] \tag{1}$$

where r_s is the radius of the solvent molecule on the surface, by assuming that the surface S is covered with close-packed hexagons with inscribed sphere radius r_s. For waters in the bulk, r_s is estimated (assuming FCC close packing) as

$$r_s = (V_o/2)^{1/3} / 2^{1/2} . \tag{2}$$

Extending this estimate for solvents on the surface,

$$r_s = (\alpha V_o/2)^{1/3} / 2^{1/2} . \tag{3}$$

The total volume to the droplet is

$$V = N_s \alpha V_o + (N-N_s)*V_o = [N + N_s*(\alpha-1)]V_o \tag{4}$$

The volume of an ellipsoid of revolution is given as

$$V = 4\pi a^2 b/3 \tag{5}$$

where a,b are the lengths of the axes and its surface is

$$S = 2\pi ab[b/a+(a/c)\ln((b+c)/a)], \tag{6}$$

with

$$c = (b^2-a^2)^{1/2} . \tag{7}$$

Defining r=b/a, this can be rewritten as

$$V = 4\pi a^3 r/3 \tag{8}$$

$$S = 2\pi a^2 r[r+\ln(r+(r^2-1)^{1/2})/(r^2-1)^{1/2}) \tag{9}$$

Substituting (1) and (3) into (4) eliminates N_s and r_s substituting (8) into (9) eliminates a, leaving us with a system of two equations involving S and V:

$$V = \{N +(\alpha-1)*S/[(\alpha V_o/2)^{2/3}/2 * 1.5^{1.5}]\}V_o \tag{10}$$

$$S = 2\pi(4\pi/3)^{-2/3} V^{2/3} r^{1/3} [r+\ln(r+(r^2-1)^{1/2})/(r^2-1)^{1/2}) \tag{11}$$

For $\alpha=1$, V becomes independent of S and thus the system is easily solvable analytically, and for $\alpha<1$ the $\alpha=1$ solution serves as the starting point of an iteration.

Tables 1 and 2 give the calculated surface free energies in kcal/mol using various α and r values for two droplets containing 1000 and 5000 waters, respectively, resulting in droplets of radius 19 Å and 33 Å, respectively. The surface free energies were obtained by multiplying the surface value (in $Å^2$) by the surface tension, σ. Clearly, the effect is significant.

Table 1.
Estimated surface free energies of an ellipsoidal droplet of
1000 waters.

Axis ratio	Contraction factor	Surface free energy	Excess over spherical
1	1	485.0	0.0
1.05	1	501.2	16.2
1.1	1	517.6	32.7
1	.95	471.3	0.0
1.05	.95	486.6	15.3
1.1	.95	502.0	30.8
1	.9	457.2	0.0
1.05	.9	471.6	14.4
1.1	.9	486.1	28.9
1	.85	442.8	0.0
1.05	.85	456.3	13.5
1.1	.85	469.8	27.0

Table 2.

Estimated surface free energies of an ellipsoidal droplet
of 5000 waters.

Axis ratio	Contraction factor	Surface free energy	Excess over spherical
1	1	1418.0	0.0
1.05	1	1465.5	47.5
1.1	1	1513.5	95.5
1	.95	1394.4	0.0
1.05	.95	1440.3	45.9
1.1	.95	1486.7	92.2
1	.9	1369.8	0.0
1.05	.9	1414.0	44.2
1.1	.9	1458.6	88.8
1	.85	1343.9	0.0
1.05	.85	1386.3	42.4
1.1	.85	1429.2	85.3

A language for molecular dynamics

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Introduction

Most programs for molecular dynamics developed in the academic environment, such as those in the CCP5 library, are comparatively simple, since they are generally written to simulate a particular system or a restricted class of systems, e.g molecular liquids, ionic solids. Setting up a simulation job is usually a matter of editing an input file which specifies such things as the parameters of the interaction potential, and control variables such as number of steps in the run and frequency of r.d.f calculation.

Commercially-produced software capable of performing simulations has been available for some time in the bio-molecular field and is becoming available in the materials modelling area. Such programs are more complex as they need to be able to handle almost any system the user may be interested in, and typically they are driven by an interactive front end running on a workstation. The program is controlled by menu selection and graphical model building. Such sophisticated software can be very useful in some academic research, but is unsuitable for the researcher who wants to extend the use of simulation into new areas or develop new techniques, since the source code is necessarily complex and hard to modify, and in any event not normally accessible by users.

A third method of "driving" a simulation program, intermediate between the "parameter file" and "graphical user interface" is the use of a command language. The purpose of this article is to describe the command language Dynamo on which I now base all my simulation programs, and to commend this approach as being extremely suitable for the development of programs in the academic research environment. The language interpreter is written in Fortran and forms part of my programs Moliq-Dynamo (molecular _liquids) and Shell-Dynamo (ionic_materials with shell-model option) which are being included in the CCP5 program library.

Advantages

The use of a command language has numerous advantages over the "parameter file" approach for academically-developed programs.

(a) *Ease of development*. Programs are normally developed in stages: typically one gets the basic algorithm going for a simple system; then it is extended to more complex systems; and then various options and analysis features are added. If a parameter file is being used, more and more parameters need to be added as the program evolves, so

the format of the file is continually changing. Old files then cease to work, and to recreate the original, simple, test runs may involve extensive editing of what is, by now, quite a complex file. Using a command language one develops the program by adding new commands; but the old command files still work, and can be rerun to test that no errors have been introduced. The use of a command language encourages a modular and incremental approach to program development which minimises errors and speeds progress.

(b) *Ease and flexibility of use.* Editing a parameter file to set up a particular simulation can be a tedious and error-prone task, particularly if it involves remembering the values and purposes of a large number of control switches. Use of a command language is much easier since commands can have meaningful names and only the commands and parameters actually required need to be specified. More importantly, the use of a command language can give great flexibility in the simulation protocol adopted. Most simulation programs controlled by parameter files have only one option: perform N steps of equilibration followed by M steps of measurement. Using the Dynamo language the user has complete freedom to change algorithms or parameters at any stage of the simulation, switch on or off any analysis, restart averaging or print selected outputs. Within one execution of the program it is quite possible to simulate several state points, change a mixture composition, or even simulate completely different systems.

An illustration

The general form of a command in Dynamo is very simple: it consists of a command name, followed by none or more sub-commands, followed by none or more string parameters, followed by none or more numerical parameters. Commands and sub-commands may be abbreviated to four characters, and are case-insensitive.

I will illustrate Dynamo by describing a file of commands which repeats one of the early simualations of Verlet, using Moliq-Dynamo (see Figure 1).

The command MOLECULE introduces the definition of a molecule type and gives it a name. The molecule definition is terminated by the ENDMOLECULE command. In this case it is necessary to specify only one interaction site using the LJSITE command. It is possible to have multiple interaction sites, massless sites and masses without interactions. The BOUNDARY PSC command specifies the boundary as periodic-simple-cubic: this is actually the default and this command could have been omitted, but other options are available. The NUMBER command is used to specify the number of each type of molecule included in the simulation. The command STATE is used to specify the desired state point, here with subcommands TEMPER (required temperature in K) and MOLARV (molar volume in cm^3). Other subcommands enable a density rather than volume to be specified, and in addition a pressure for controlled pressure simulations.

The VALUE command is used to specify various numerical parameters: here the timestep and cutoffs for the interaction and the neighbour list. All quantities have defaults: for example the default value for the interaction cutoff is half the box length. FILLBOX sets up the intial lattice, and SETVELS sets the intial velocities, according to the required temperature. NEIGHBOUR APLIST sets the neighbour search algorithm, in this case an all-pairs neighbour list; the usual options are available such as LINK (link-cells) and LCLIST (neighbour list created by link-cell search).

The command OUTPUT THERMO gives an interval in steps between output of thermodynamic quantities, and like many commands it controls what happens during subsequent RUNMD commands. RUNMD is the only command which actually performs a simulation, and has a sub-command which specifies the type of dynamics to be used. EQUIL (equilibration dynamics) involves temperature windowing in combination with a Berendsen heat-bath. Other options include LEAP (standard energy-conserving leapfrog) and TPBATH (Berendsen temperature and pressure control) among others.

After equilibration in the example a restart file (coordinates and velocities) is written using the command SAVE RESTART. The converse operation is LOAD RESTART. If SAVE CONTINUE and LOAD CONTINUE are used instead the file contains in addition all accumulators so that a run can be continued exactly from the point at which it was terminated.

The command ZERO is particularly important in Dynamo. Any type of measurement may be used in conjunction with any type of dynamics, and thermodynamic quantities are always calculated and incrementally averaged. ZERO resets to zero all the accumulators, of correlation functions as well as of thermodynamic quantities, and so restarts all averaging and analysis. The commands RDF, ACF and MSD switch on radial distribution function, time auto-correlation function and mean square displacement analyses for the next RUNMD call. They have a few sub-commands and numerical parameters which it is not necessary to describe here. OUTPUT CORREL will print out all non-zero correlation functions.

Other features

The Dynamo language has too many features to be described fully here, and there are necessarily differences between Moliq-Dynamo and Shell-Dynamo because of the different forms for the interactions. A few points are worth noting.

Commands are read from standard input so the Dynamo programs can be run interactively, which is useful during testing. A command OBEY enables a file of commands to be read and obeyed. It is useful to establish a library of such files describing various model systems. There is also a looping feature in the language. An ECHO command enables the output file to be annotated freely. Numerical parameters are read using Fortran list-directed reads. This enables built-in facilities for such reads to be

used: for example, values may be ommitted and will then take their default values.

Conclusion

I hope this article has given a flavour of the Dynamo language and convinced you that it can make life easier for the simulator. The structure of the Dynamo programs is very modular and well-documented. If you are planning to develop a new simulation program one of them might be a good starting point. I would be happy to assist with advice. Let me know how you get on!

Figure

Command file for an argon simulation

```
MOLECULE Argon
!              x   y   z   sig    eps    q   m
LJSITE Arg 0.0 0.0 0.0 0.3405 119.8 0.0 40
ENDMOLECULE
BOUNDARY PSC
NUMBER Argon 864
! State point corresponds to T*=1.036 and rho*=0.65
STATE TEMPER 124.11
STATE MOLARV 36.58
VALUE DT 0.025
VALUE CUTOFF 0.86
VALUE OUTERC 0.96
FILLBOX FCC
SETVELS
NEIGHBOUR APLIST
OUTPUT THERMO 50
! Equilibration
RUNMD EQUIL 250
FIXCM
SAVE RESTART argon.864
! restart averaging: switch on correlation functions
! then run for 10 ps using leapfrog dynamics
ZERO
RDF LIMITS 0.2 1.0 0.02
RDF CC 20
ACF VELOCS 1 50
MSD 4 50
RUNMD LEAP 400
OUTPUT CORREL
```

Molecular dynamics and communication experiments on iPSC/860 computer

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Abstract

In this paper we present timings of a parallel, short-range Lennard-Jones molecular dynamics algorithm and results of communication tests obtained on iPSC/860 in Daresbury. They are compared with results from homogeneous networks of workstations under PVM control.

1 General introduction

For many years our group is in good scientific contacts with the Authorities of the CCP5 Project. These result in participation in meetings, exchange of information, publications of results in CCP5 Newsletter and simulation programs in CCP5 Program Library.

In December'92 in kind agreement with the Steering Committee of CCP5 and much help from Dr. William Smith two of us (Mr. Mr. K. Boryczko and M. Pogoda) had opportunity to visit Daresbury Laboratory and obtained permission for using iPSC/860. At this point we would like to express our appreciation to the Steering Committee of CCP5 and especially to Bill Smith for his efforts making the visit possible and profitable.
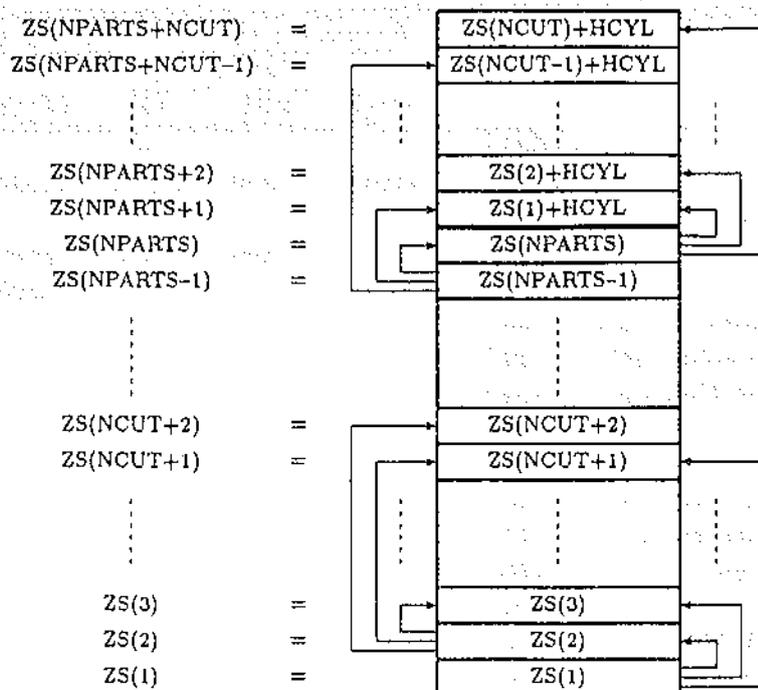
One of the fields of interest in our Institute is parallel and distributed computing with Molecular Dynamics (MD) and Lattice Gas Algorithms (LGA). For this purpose we use a network of transputers ($16 \times T800$) under Helios and *ParaSoft* Express as well as clusters of workstations (SUN SPARC, IBM RS/6000, HP 9000, of total number about 25). The clusters operate under control of different programming environments, as for example: PVM, Network Linda, *ParaSoft* Express and p4. The problems cover molecular simulation approach to fluid flow modelling, developing and shedding of turbulence, flow in porous media, thermal instabilities and others (e.g.[1]-[10]).

Metacomputing, one of the most exiting problems in computational science at present, empowers users by providing transparent access to a variety of computer services. Our approach to this field is large-scale MD simulation on a network of different computers, including CONVEX 3210 as a processing node [11].

In this paper we present timings for a parallel, short-range Lennard-Jones molecular dynamics algorithm and results of communication tests obtained on iPSC/860 in Daresbury. They are compared with results for homogeneous clusters of workstations using public domain PVM from Oak Ridge Lab.

2 Simulation algorithm

For the study presented in this paper we adopted one of our short-range 6/12 Lennard-Jones (L-J) algorithms, developed originally in ETA Fortran 77 for ETA 10-P supercomputer and modified then for other vector machines [1, 2].

ZS(NPARTS+NCUT)	=	ZS(NCUT)+HCYL
ZS(NPARTS+NCUT-1)	=	ZS(NCUT-1)+HCYL
ZS(NPARTS+2)	=	ZS(2)+HCYL
ZS(NPARTS+1)	=	ZS(1)+HCYL
ZS(NPARTS)	=	ZS(NPARTS)
ZS(NPARTS-1)	=	ZS(NPARTS-1)
ZS(NCUT+2)	=	ZS(NCUT+2)
ZS(NCUT+1)	=	ZS(NCUT+1)
ZS(3)	=	ZS(3)
ZS(2)	=	ZS(2)
ZS(1)	=	ZS(1)

$$ZS(1) \leq ZS(2) \leq \ldots \leq ZS(NPARTS) \leq \ldots \leq ZS(NPARTS+NCUT)$$

Figure 1: Data structure and scheme of distances calculations for the *pipe method*.

The computational box is a long cylinder, so it could be used for studies of fluid and mixtures in microcapillaries. The algorithm is called *Pipe Method* (MP) and it is briefly described below (see Fig.1).

Periodic boundary conditions (*pbc*) are introduced along the cylinder axis only (in z-direction). Since in fluid of uniform density the number of neighbours interacting with a given molecule is nearly constant – on a base of the cutoff radius, R_C, the integer cutoff number $NCUT$ is introduced, where $NCUT$ is a number of neighbours interacting potentially with a given particle and $NPARTS$ is the number of particles in the computational box. Particles in the cylinder are sorted due to their Z coordinates (forming ZS vector) and the index vector is set up to returning to original particles indices. X and Y particle coordinates are gathered due to the index vector, which results in XS and YS vector determination. For forces calculation the computational cylinder is stepwise shifted in respect to its copy to subsequent neighbouring particles from 1 to $NCUT$. In this way the forces calculations are fully vectorized.

In Table 1 the execution *cpu* time (per timestep and particle) for MP method on different super-computers is presented together with timings for other algorithms using the cubic computational box: a family of *Stick Methods*, MS; *Bulk Shift Method*, BS; *Vector Link-Cell Method*, VLC; coded in Fortran 77 (except ETA 10-P for which ETA Fortran was applied) and previously published in [7]. Their essential feature are original geometric partitions of the computational box instead of applications of nearest neighbours arrays.

Computer	MP	MS methods				VLC	LC
		MSB	ESL	LD	LD/20		
DSI-020	8600.[1]	–	–	–	–	99000.	22000.
AT-386	2800.[1]	46100.	49300.	33200.	32800.	35500.	8900.
MicroVAX 3400[A]	2200.[1]	–	–	–	–	–	–
T800	1300.[1]	–	20100.	18000.	17800.	–	3500.
AT-486	630.[1]	–	–	–	8200.	–	1500.
SUN SPARCstation SLC	700.[1]	–	–	–	–	–	1500.
SUN SPARCstation IPC	540.[1]	–	–	–	–	–	1100.
SUN SPARCstation 1+[A]	490.[1]	–	–	–	–	–	–
NeXT[A]	470.[1]	–	–	–	–	–	–
OPUS	–	–	–	–	–	–	1000.
SUN SPARCserver 470	250.[1]	–	–	–	–	–	–
SUN SPARCstation 2	230.[1]	–	–	–	–	–	–
SGI IRIS Indigo	200.[1]	–	–	–	–	–	–
i860	190.[1]	–	–	–	–	–	420.
IBM RS/6000-320	140.[1]	–	–	–	–	–	530.
IBM RS/6000-540	88.[1]	–	–	–	–	–	–
HP Apollo 9000/720	79.[1]	–	–	–	–	–	–
CONVEX C120	180.	–	–	–	–	–	–
CONVEX C3210	64.	–	–	–	–	–	–
IBM 3090-150/VF	–	550.	–	–	~300.	430.	–
IBM ES/9000-720/VF	51.	–	–	–	–	–	–
IBM ES/9000-900/VF	37.(?)	–	–	–	–	–	–
ETA 10-P	16.	310.	320.	290.	160.	630.	–
CRAY Y-MP4E/232	9.	–	–	–	–	–	–

Table 1: Execution time for the *pipe method*.

The timing procedure considers the time-loop only (with forces evaluation, motion and total values computing); this part of the program consumes more than 95% cpu time of the program.

The execution time is compared with that obtained on sequential machines, for which the original vector algorithms were slighty modified (which is mentioned by ([1]) and ([2])), to get higher performance (reorganization of "if" block to avoid forces calculations unless distance or particles is equal to or less than the cutoff radius of the potential, R_C). In addition, timings for sequential Link-Cell Method, LC, are also shown. The simulated medium is Argon at $86.5K$ or $116K$ with the reduced density, $\rho^* = \rho\sigma^3$ (σ is L-J parameter), equal to 0.76 for MP or 0.72 for the rest of methods, and $R_C = 2.5\,\sigma$. For sequential computing the algorithms were coded in Fortran 77 and C. In Table 1 ([A]) indicates calculations on a remote machine via Internet.

3 Parallel approach

For parallel computing domain decomposition is proposed. The cylindical computational box is divided along z direction into loosely coupled domains allocated on different processing nodes [8, 10] (see Fig.2). The following elements are decomposed and calculated independently in the domain: interparticle interactions, interactions between the particles and the wall of the computational box, solution of the Newtonian equations of motion, physical quantities and sorting. Number of

particles in every node, *NpartsK*, is equal, thus the overall number of particles in simulation is *Nparts= K×NpartsK*, where *K* is a number of nodes taken for simulation. The communication is needed only for particles moving from one domain to another (if determined by the motion equations), for interparticle forces calculations at the boundaries of the domains and for sending partial global results from each domain to form characteristics of the whole box.
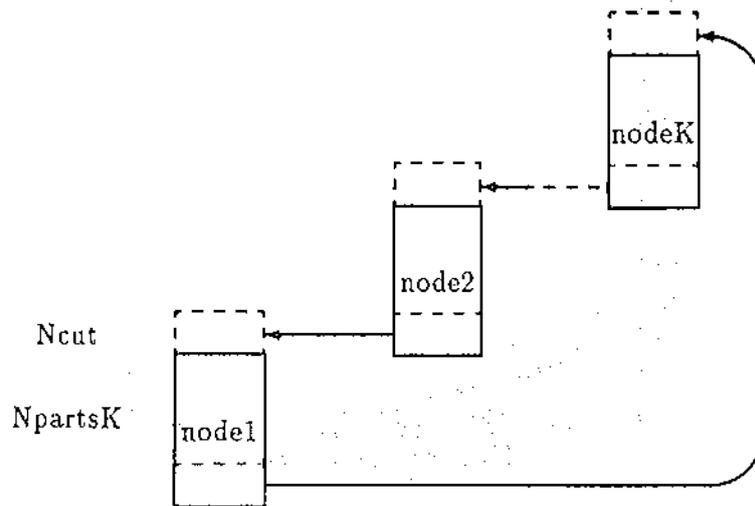

Figure 2: Sending particles positions.

For the forces calculations at the boundaries the first *Ncut* particles positions from the "upper" domain are sent to the "lower" one, increasing its number of particles by *Ncut*, to direct forces calculations, which are in turn sent back as reaction forces to the "upper" domain.

In Fig. 3 execution time (per timestep and particle) of the parallel *pipe method* as a function of number of iPSC/860 processing nodes is presented for two optimization options. Total number of particles for 64 nodes was *Nparts=* 2048256, giving $\tau = 2.3\mu s$ (for -Knoiece option). For the largest experiment with 64 nodes, *Nparts=* 4096512 and $\tau = 1.27\mu s$.

It is worth to mention that in early stage of program development in Cracow for iPSC/860, using Intel iPSC simulator for SUN workstations was very useful.

For distributed computing with PVM (v2.4) on a homogeneous network of computers the measure of the algorithm performance is the execution *wall-clock* time obtained with function gettimeofday(). During the experiments, the networks were almost perfectly isolated from external load. The results are shown in Figs.4 and 5 for the networks of SUN SPARC SLC and SUN SPARCstation2.

Results show high level of performance and parallel efficiency of iPSC/860 for numerically intensive computing.
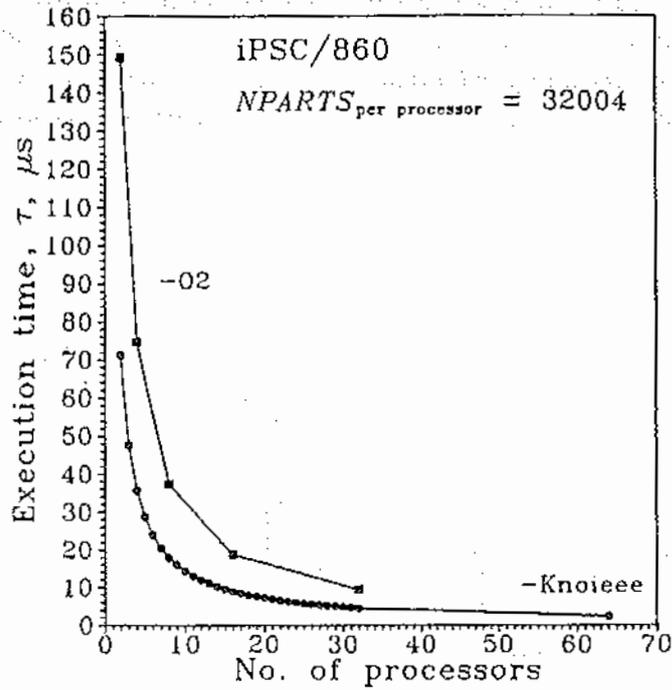
Figure 3: Execution time (per timestep and particle) on iPSC/860 for two optimization options.
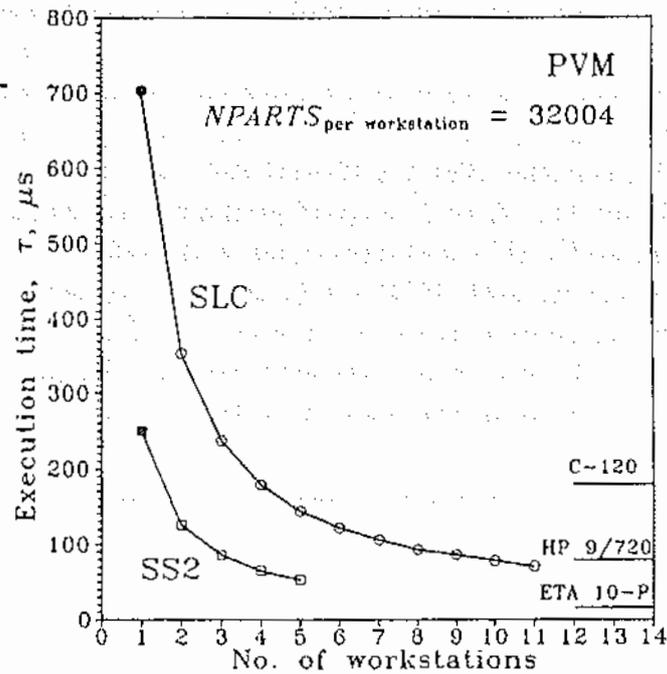

Figure 4: Execution time (per timestep and particle) on two clusters of workstations: SUN SPARC SLC and SUN SPARCstation2.
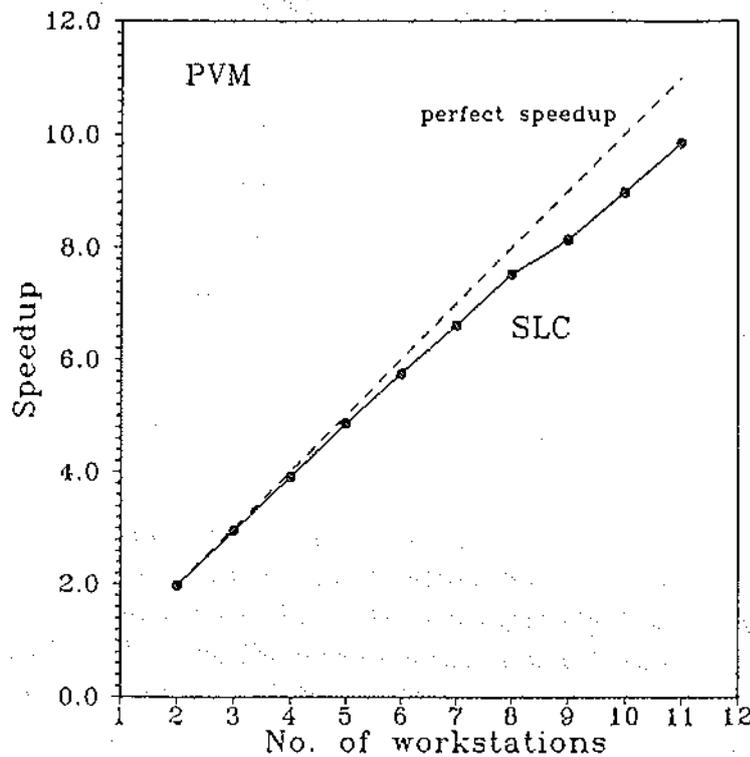
Figure 5: Speedup for the distributed *pipe method* on SUN SPARC SLC cluster.

4 Tests of communication speed between nodes

It is well known that efficiency of parallel algorithms is much dependent on communication. This is why one of the first things we usually do when familiarizing with a new parallel machine is testing performance of inter-processor communication system. Obtaining a few basic parameters enables us to estimate in advance how would resulting performance of our simulation programs scale with number of processors used and with size of the simulated system. Such knowledge also helps in proper design of new parallel programs.

We have measured performance of synchronous message passing system on iPSC/860 (csend() / crecv() routines) in two cases:

    a) point-to-point communication between any two processors;

    b) systolic communication on a ring of processors.

In the first test called "PAIR" we measured how transmission time depends on message length. The simplest self-sinchronizing scheme was applied where a message sent by one processor is reflected back by its partner and mean of the two transmission times is taken. We got almost perfectly linear dependence as shown in Fig.6, except for very short messages. Effective bandwidth of point-to-point message transmission, as estimated by linear regression, turns out to be as much as 2.7 MBytes/sec with latency of about 0.065 msec for messages shorter than 100 Bytes and 0.17 msec for longer ones.
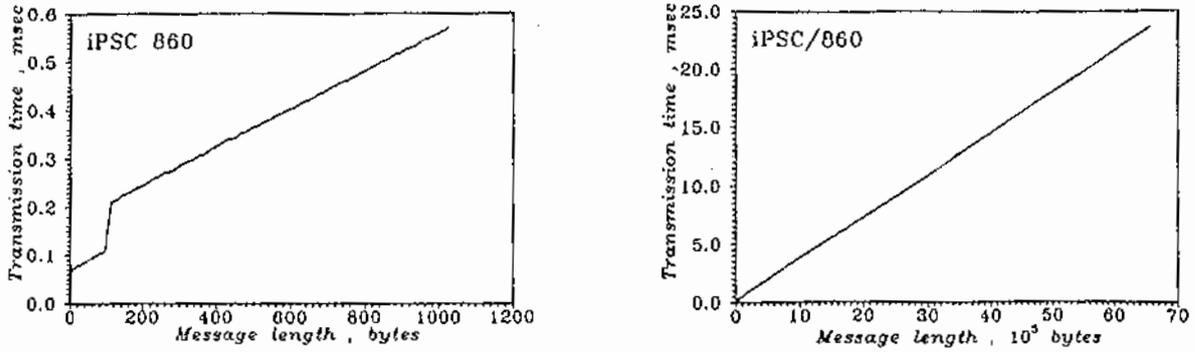
Figure 6: Results of the "PAIR" test on iPSC/860.

In the second test called "RING" we apply typical systolic communication scheme used in many simulation programs (also in our MP program). In this test each of processors forming a logical ring sends a message to its "right neighbour" and receives a message from its "left neighbour", all messages being of equal size. For this scheme to work efficiently, "send" operation has to be non-blocking (and csend actually is non-blocking). In addition, global synchronization of all processors forming the ring was necessary to be applied before start of timing procedure. Tests were made for "short" messages (1 kByte) and for "long" messages (1 MByte), with number of processors in ring varying from 2 to 32. Results presented in Fig 7 do not show any clear dependence of systolic transmission time on size of the ring, which prooves that all messages in a systolic pulse are transmitted fully in parallel. Effective systolic communication bandwidth appears to be about 1.1 MBytes/sec.

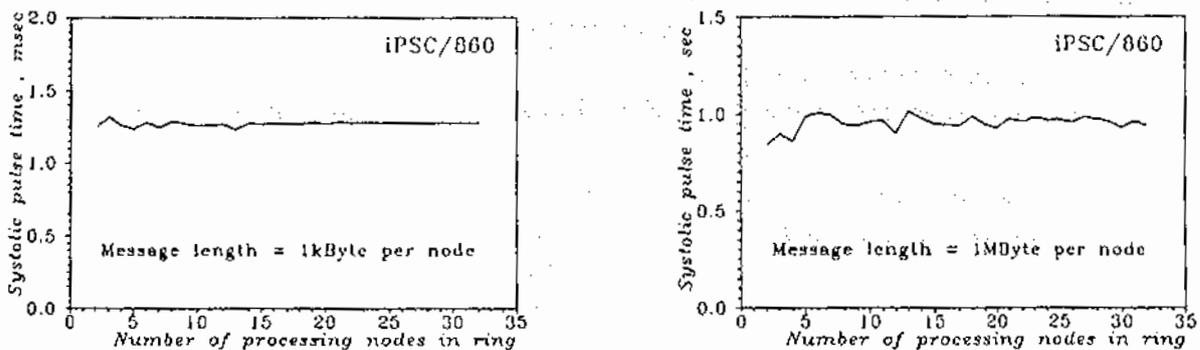In both tests timings were obtained by use of dclock() routine on i860 nodes.

Figure 6: Results of the "RING" test on iPSC/860.

We have made a preliminary theoretical analysis of efficiency of our MP algorithm using the above results and we found that this algorithm should keep near perfect speedup for much larger number of processors than it was tested on.

Acknowledgement

References

[1] J. Mościński, J. Kitowski, Z.A. Rycerz and P.W.M. Jacobs, "A vectorized algorithm on the ETA 10-P for molecular dynamics simulation of large number of particles confined in a long cylinder", *Comput. Phys. Commun.*, **54** (1989) 47.

[2] J. Mościński, M. Bargiel, J. Kitowski, Z. Skotniczny, Z.A. Rycerz and P.W.M. Jacobs, "Vectorized molecular dynamics algorithms for very large number of particles", *Proc. of 1989 International Conference on Supercomputing*, June 5-9, 1989, Crete, Greece (ACM Publications, Baltimore, USA).

[3] J. Tarbaj, M. Zimnoch, M. Bubak, J. Kitowski and J. Mościński, "Microscale hydrodynamics on microcomputers", *CCP5 Information Quarterly for Computer Simulation of Condensed Phases*, **33** (1991) 62-70 (informal Newsletter of Daresbury Laboratory, Warrington, England).

[4] W. Alda, M. Bubak, J. Kitowski and J. Mościński, "Molecular dynamics simulation of plastic deformation of 2-D Solid (MD hydrodynamics at 1K)", Poster at the Summer School of the NATO Advanced Study Institute *"Microscopic Simulation of Complex Hydrodynamic Phenomena"*, Alghero, July 15-26, 1991, also sl CCP5 Information Quarterly for Computer Simulation of Condensed Phases, **34** (1992) 16-22 (Informal Newsletter of Daresbury Laboratory, Warrington, England).

[5] W. Alda, M. Bubak, J. Kitowski, J. Mościński and D. Nikolov, "Case study of microscale hydrodynamics using molecular dynamics and lattice gas methods", *Proc. of Physics Computing'92*, Aug.24-28, 1992, Praha.

[6] M. Bubak, T. Malota, P. Szumlański, W. Alda, J. Kitowski and J. Mościński, "HPP lattice gas on computers and networked workstations", *Proc. of Physics Computing'92*, Aug.24-28, 1992, Praha.

[7] J. Kitowski and J. Mościński, "Microcomputers against Supercomputers ? – On the geometric partition of the computational box for vectorized MD algorithms", *Mol. Simul.*, **8** (1992) 305-319.

[8] K. Boryczko, M. Bubak, J. Kitowski, J. Mościński and M. Pogoda, "Molecular dynamics and lattice gas parallel algorithms for transputers and networked workstations", EUROMECH Coll.287, Sept. 21-25, 1992, Cagliari, Italy; also in preparation for publicaton in *Transport Theory and Statistical Physics*.

[9] W. Alda, W. Dzwinel, J. Kitowski and J. Mościński, "Penetration mechanics via molecular dynamics", Report AHPCRC, University of Minnesota, Minneapolis, in preparation.

[10] K. Boryczko, M. Pogoda, J. Kitowski and J. Mościński, "A Case Study of Distributed Molecular Dynamics on Transputers and Networked Workstations", in preparation for publication in *Mol. Simul.*

[11] J. Mościński, K. Boryczko, J. Kitowski, M. Pogoda, W. Alda, M. Bubak, W. Dzwinel and M. Noga, "Distributed molecular dynamics on a cluster of workstations and CONVEX supercomputer", 1993 Convex User Group Worldwide Conference, March 22-25, 1993, Richardson, U.S.A., to be presented.

Preliminary timings for FHP lattice gas program on iPSC/860

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Abstract

In the paper we present the preliminary timings for two approaches to decomposition of lattice gas simulation on INTEL iPSC/860.

1 Introduction

A considerable interest has been recently directed towards studying fluid dynamical phenomena via lattice gas automata (LGA) methods [1],[2] at a microscopic level. LGA consists in considering the fluid as an ensamble of particles of unit mass moving in discrete time steps with unit velocity on the nearest–neighbour bonds of a square (HPP model [3]) or a triangular (FHP model [4]) lattice. If several particles at one time reach the same site they are scattered with conserved both mass and momentum, so the LGA evolution consists of two phases: free particle streaming (propagation) and collisions.

Due to large lattices (10^8+ sites) involved into simulation (to avoid statistical noise) there is a need for parallel LGA algorithms and programs, and LGA inherent parallelism considerably facilites development of such programs.

In this paper we present preliminary results for two approaches to decomposition of FHP LGA simulation problem obtained on the INTEL iPSC/860 at Daresbury Laboratory.

2 Model and decomposition

The LGA model we have used is based on the FHP triangular lattice with the rest particle. Two-, three-, and four- particle collision rules are applied. There are also special sites on a lattice: reflectors, absorbers and injectors. At the reflector site particle changes its velocity to the opposite one, absorber sites remove all particles entering the site, and injectors generate particles in a given direction with a given intensity [5]-[6]. The evolution of the lattice consist of the following phases: absorption, collision, injection, and propagation.

Two algorithm has been tested: in the first one the averaging is only on the host processor (so the arrays with location of particles moving in all allowed directions should be send each averaging interval from nodes to host), and in the second this is accomplished on each node separately.

LGA parallel program was elaborated exploiting mainly geometric decomposition of the problem. The lattice is divided along $y-$ axis into several domains with equal number of lattice sites and each domain is assigned to a different node. Border rows of domains are copied between neighbourig nodes and after each timestep are transmitted between neighbours.

LGA simulation consists of two stages: evolution of lattice and calculation of averages of values on a grid superimposed on the lattice. Miltispin coding technique which enables to pack few velocities in a single computer word was applied, any binary digit denotes a particle or a hole.

3 Results

The dependence of execution time per timestep and lattice site on the number of iPSC/860 nodes is shown in Fig. 1. All measurements were done for simulation of 1000 steps of 960×960 lattice with two regions od different particle density.
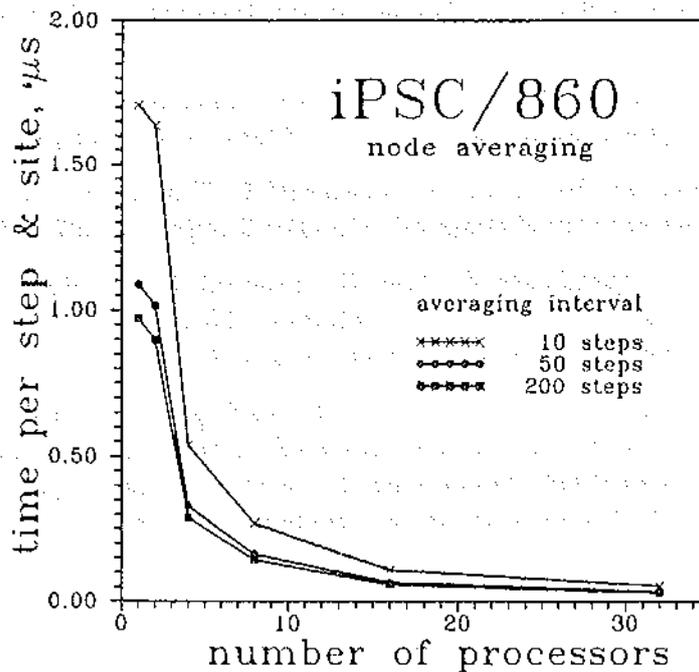
a)
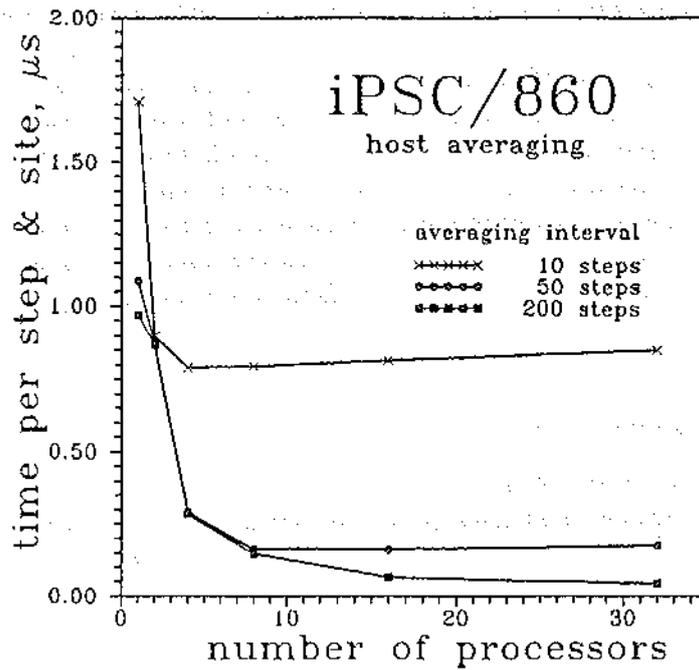
b)

Figure 1: Execution time per timestep and lattice site versus number of iPSC/860 nodes: a) averaging on host node, b) averaging on each node separately

It is apparent that averaging on each node separately is more efficient than averaging on master node. In the first case the efficiency is very close to 1.0 while in the second case efficiency strongly depends on frequency of average values calculation.

4 Concluding remarks

Obtained results are encouraging and indicate that it is reasonable to use averaging on nodes. Having in mind that the time per step and site was measured for constant number of lattice sites one can estimate that it shoud be possible to reach 10^8 sites updates per second on 16 nodes of iPSC/860.

Now we are developing parallel distributed FHP program with averaging on nodes. Two kind of particles will be introduced and collision rules will depend on *color* of colliding particles.

The purpose of our future investigation is twofold: the first one is the comparision of performance of LGA parallel program runing on networked workstations (under different software for distributed computing: PVM, p4, Linda, TOPSYS and PCN) and on massively parallel computers, and the second topic is study of convection, sedimentation, developing of turbulence, flows in porous media, shock waves propagation, and two component flows.

5 Acknowledgements

The authors are indebted to dr. W.Smith for arranging computer time on iPSC/860. M.Pogoda and K.Boryczko are acknowledge for running our programs during their visit at Daresbury Laboratory. We also thank dr. J.Kitowski and W.Alda for helpful questions and suggestions.

References

[1] Doolen, G.D., ed., "Lattice gas methods for partial differential equations", *Addison-Wesley, Reading, MA*, 1990.

[2] Mareschal, M., and Holian, B.L., eds., "Microscopic simulations of complex hydrodynamic phenomena", *NATO ASI Series, Series B: Physics VOL.292, Plenum Press, New York and London*, 1992.

[3] Hardy, J., de Pazzis, O., and Pomeau, Y., "Molecular dynamics of a classical lattice gas: Tronsport properties and time correlation functions", *Physical Review* **A13** (19760, 1949–1961.

[4] Frisch, U., d'Humières, D., Hasslacher, B., Lallemand, P., Pomeau, Y., and Rivet, J-P, "Lattice gas hydrodynamics in two and three dimensions", *Complex Systems*, 1 (1987) 649-707.

[5] Bubak, M., Molata, T., Szumlański, P., Alda, W., Kitowski, J., and Mościński, J., "HPP lattice gas on transputers and networked workstations", abstract: *Computers in Physics*, 6 (1992) 314; to be published in: *Proc. Physics Computing'92*, Praha, August 24–28, 1992.

[6] Boryczko, K., Bubak, M., Kitowski, J., Mościński, J., and Pogoda, M., "Molecular dynamics and lattice gas parallel algorithms for transputers and networked workstations", presented at EUROMECH 287 *Discrete models in fluid dynamics: theory, simulation and experiment*, Cagliari (Italy), 22–25 September 1992, in preparation for: *Transport Theory and Statistical Physics*.

Utilities for data edition and results visualization in molecular simulation

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Abstract

In this paper utility programs for microcomputers and workstations: MSGRAPH, sEDS, xEDS, DEMSI and VSPR, are presented. They use computer graphics in order to simplify input data editing and results visualization in molecular dynamics and lattice gas automata simulations.

1 Introduction

Molecular simulation (molecular dynamics [1, 2] – *MD*, Monte Carlo [3] – *MC*, and recently lattice gas automata [4] – *LGA*) is a very useful tool for studies of the structure and dynamic properties of the solid state and phases boundaries as well as complex fluid flows at microscopic level.

The initial nonuniform distribution of separate species in the molecular simulation computational box and the initial state of a lattice may be very difficult to be supplied into the simulation program using ordinary text editors, especially for large number of particles. Much more reasonably is to do it in a graphical way.

Molecular simulations produce enormous amount of information, so methods and utility programs are indispensable to extract essential features of the process. Quantities calculated in molecular simulation include usually thermodynamical, microstructure and transport coefficients. These integral quantities describe strictly the system under consideration, but more cognition may be gathered by qualitative analysis of molecules positions and momenta at successive time steps. Such an enrichement can be acquired using the computer graphics [5].

In the paper we describe graphical tools which simplify input data edition and result visualisation for *MD* and *MC* (*MSGRAPH* or *sEDS and xEDS*) and *LGA* (*DEMSI* and *VSPR*) simulations. The programs are designed to work in an interactive mode and almost all of their options are accessible through easy-to-understand menus.

2 MSGRAPH

MSGRAPH is a program designed to perform graphical presentation of results obtained in 2-D and 3-D *MD* or *MC* computer simulation using programs written in Fortran or C.

It runs in the following three stages:

- conversion of simulation results into a compressed file,

- setting of the form of graphical presentation,

- displaying of molecule positions or trajectories and optionally, creating files for subsequent printing or plotting.

The molecules coordinates are given in the floating-point form which is very inconvenient for storing and using in graphics program. So, *MSGRAPH* in the first stage converts molecules coordinates to integer form and generates a file (the so called "compressed file") for the current and subsequent presentation runs. The

a)

Please, choose what and how would you like to see -

1.Presentation of: T (
- **P**ositions of molecules
- **T**rajectories of molecules

2.Location and dimensions of computational box fragment for observation (in %):
- x: origin   0   length 100
- y: origin   0   length 100
- z: origin   0   length 70

3.History of: B
- **B**ox fragment
- Particles from box fragment, in **I**t
- Particles from box fragment, in **W**hole box

4.Scaling: F
- **P**roportional
- To **F**ull screen

5.Projection on: Y
- Plane **XY**
- Plane **YZ**
- Plane **ZX**

6.Range:
From timestep (>= 2000)   2000
To timestep   (<= 3000)   3000

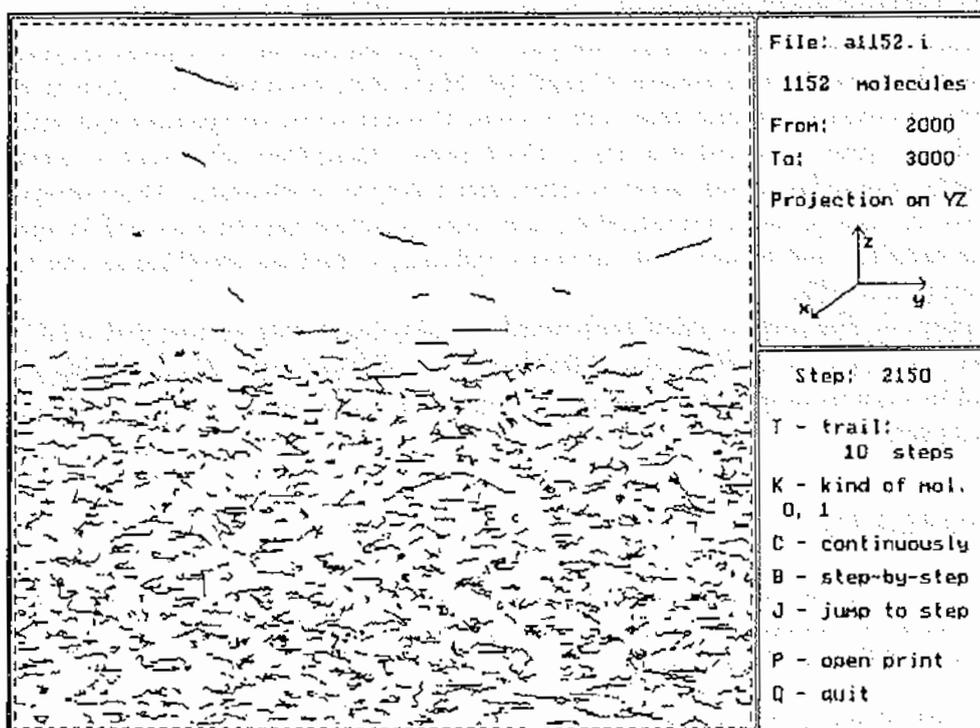**ESC** - quit to DOS **1,2,3,4,5,6** - to correct **Enter** - next Pg **E** - to end

b)

File: all52.i

1152 molecules

From: 2000
To: 3000

Projection on YZ

Step: 2150

T - trail:
        10 steps
K - kind of mol.
0, 1
C - continuously
B - step-by-step
J - jump to step

P - open print
Q - quit

Fig. 1. Program options (a) and typical example of output from MSGRAPH (b).

structure of the compressed file is almost the same as that of the rough file; only a scaling factor used to obtain integer position representation, the first and last simulation timestep numbers, and dimension of the model are added to it.

In the second stage the user chooses the mode of graphical presentation. The program enables to observe separate molecule positions in consecutive steps or continuous molecule trajectories in a given timestep interval. The positions (or trajectories) may be projected on one of the Cartesian coordinates planes. The user has possibility to follow the history of chosen molecules or the history of a fragment of the computational box. The molecules to be observed are chosen by defining a box fragment in which they were at the first recorded timestep of the simulation. Walls of the box fragment are parallel to those of the computational box. Molecules may be observed in the marked fragment or in the entire box. Scaling of molecule coordinates before the position or trajectory presentation may be accomplished in two ways. In the first one every coordinate is scaled-up independently to the full window dimension in a given direction, while in the second one molecule coordinates are transformed retaining the original coordinates proportions.

The third stage is the results presentation phase. A sample screen together with options to be settled are presented in Figure 1. To prepare hard copies of the displayed pictures of molecule positions and trajectories it is necessary to stop the presentation at the chosen timestep and then to start the creation of an intermediate file for the printer or plotter. Next, this intermediate file should be processed by the well known *GRAPHER* utilities [8]. This approach guarantees independence from printing and plotting devices.

MSGRAPH is written in the C language for IBM PC compatibilities according to the OLYMPUS conventions [6] and it uses graphics functions from the Turbo-C library [7]; recently the program was ported to SUN SPARCstations under OpenWindows software [10]. The program is suitable for a few thousand of particles and for a several hundred of registered simulation steps.

3   sEDS and xEDS

EDS is a software tool for graphical presentation of results from *MD* simulation and input data edition for it. It is prepared for two workstation platforms: SunView (*sEDS*) and X11 (*xEDS*). *sEDS* version is addressed for SUN stations while xEDS is more independent.

The program can display positions of the particles and their momenta at chosen timesteps of the simulation. Animation is possible, as far as the positions are concerned, with different lenght of traces, so one can better follow the trajectories. Using this program one can edit or create the input data. Line-drawing and area-filling options are added to make the editing easier.

The positions or momenta are read from a file and the current picture is drawn. All options are accessible through button-pressing or using other SunView gadgets [9]. The graphic library used is the standard SunView library called PixRect. xEDS system uses tools from X11R5 standard distribution. A hardcopy of the picture is created as a text file containing plotter-type commands (used by Plotcall system from Golden Software, Inc.)

The program is appropriate for 2-D *MD* simulations and is suitable for results presentation of non-equilibrium simulation for relatively large number of particles.

Editing the layout the user can place single particle or draw a line of particles. An area borded by particles can be filled up using the fill function.

With the output option the user chooses what should be displayed: positions, momenta or velocities. There is also scaling provided for better seeing if the density is too high and the particles can not be distinguished. Other choice items are: step to go, trajectory lenght for the animation and density histograms. Results can be presented step by step or animated. The user can choose which particles to be displayed with the toggle gadget called 'Drawing parts'. Simulation results should be organized in the same way as for *MSGRAPH*.

A sample of *sEDS* screen is shown in Figure 2.

4   DEMSI and VSPR

DEMSI is a graphic utility for editing initial state of lattice gas system and can be used for preparation input data for simulation using the following *LGA* models:
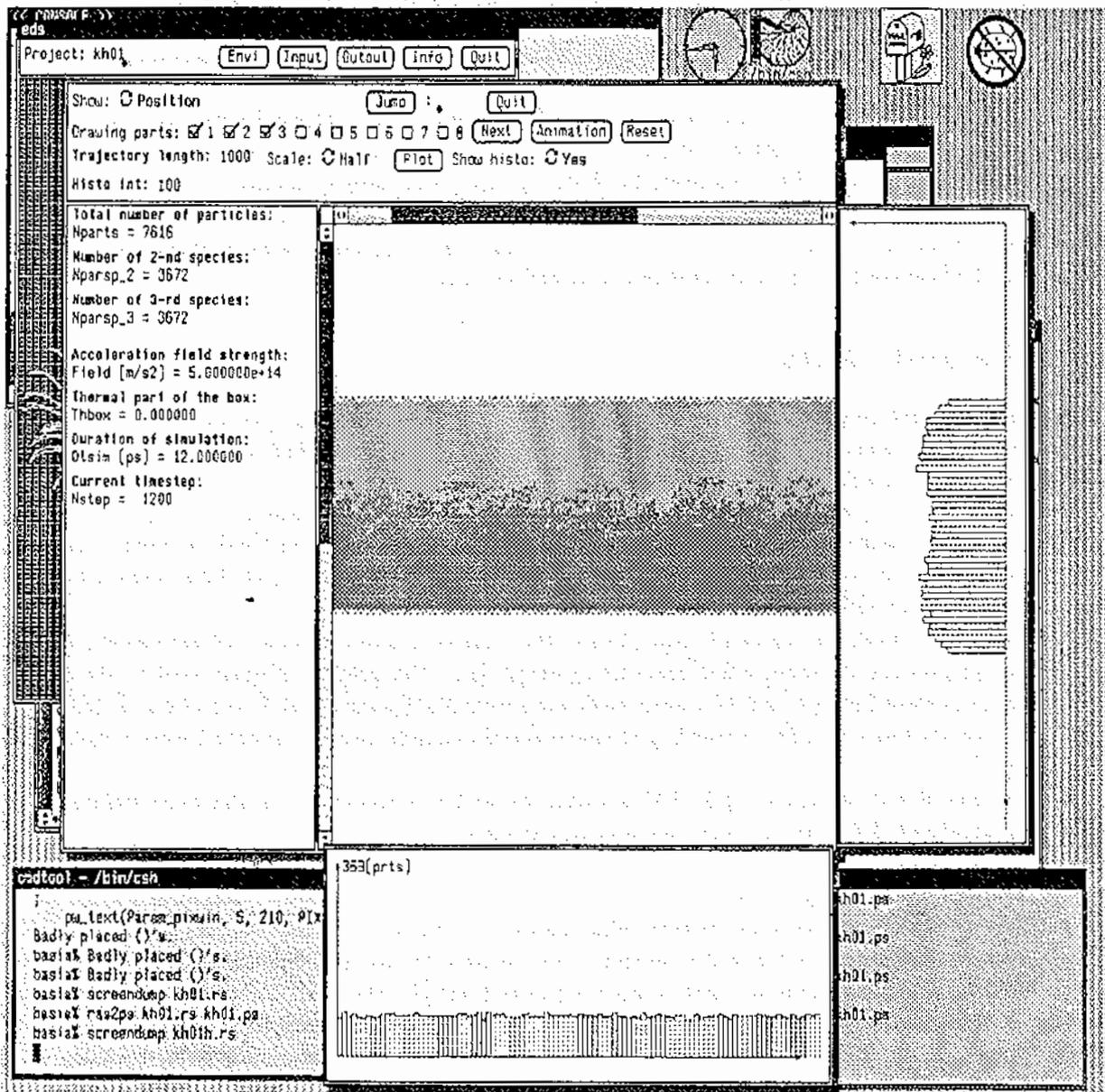
Fig. 2. Particle positions and density histograms in counterflow as presented by sEDS.

HPP – simple square lattice,

FHP6 – hexagonal lattice,

FHP7 – hexagonal lattice with the rest of particles,

FHPBR6 – hexagonal lattice with two kinds of particles,

FHPBR7 – hexagonal lattice with two kinds of particles and the rest of particles.

Using this program one can place on the lattice:

- *regions* of lattice sites occupied with a given particle densities,

- *reflectors* – lattice sites where the particle changes its velocity to the opposite one,

- *injectors* – lattice sites where the particles are generated with a given intensity in a given direction,

- *absorbers* – sites where particles are removed from the system.

Options provided in *DEMSI* and sample initial state of a lattice are shown in Figure 3.

The obtained layout of a lattice is written on *LayFile* and can be used for subsequent modifications or generating *ResFile* for *LGA* simulation program. *ResFile* file consists of direction arrays of particle at each lattice site in the first simulation step and positions of reflectors, injectors and absorbers. At present *DEMSI* enables to create lattices up to 10^8 sites.

VSPR is a program for presentation of results obtained in *LGA* simulation using above mentioned models.

Usually the simulation are realized on a very large lattices and hydrodynamical quantities (e.g. fluid velocities) are calculated by taking local spatial averages so that one gridpoint corresponds to many *LGA* sites. The averaged numbers of particles moving in a given directions are written on *AvgFile* file which together with *LayFile* file is the input to *VSPR*. Program enables to observe evolution of particle density and local velocities in consecutive simulation steps (see Figure 4.).

Velocity vectors may be shown as:

- scaled to the theoretical maximum,

- scaled to the maximal value in a current timestep,

- not scaled.

The same ways of scaling may be applied to density field, and in this case it is also possible to choose the mode of presentation:

- dotted rectangles,

- color rectangles,

- grayscale rectangles.

All files generated by *DEMSI* and produced in *LGA* simulations are written in a standard, machine-independent format. Both *DEMSI* and *VSPR* are written in C language in object-oriented fashion. Two version are available: for microcomputers under Turbo C as well as NDP C and for SUN SPARC workstations using graphic functions from OpenWindows environment [10].

5 Acknowledgements
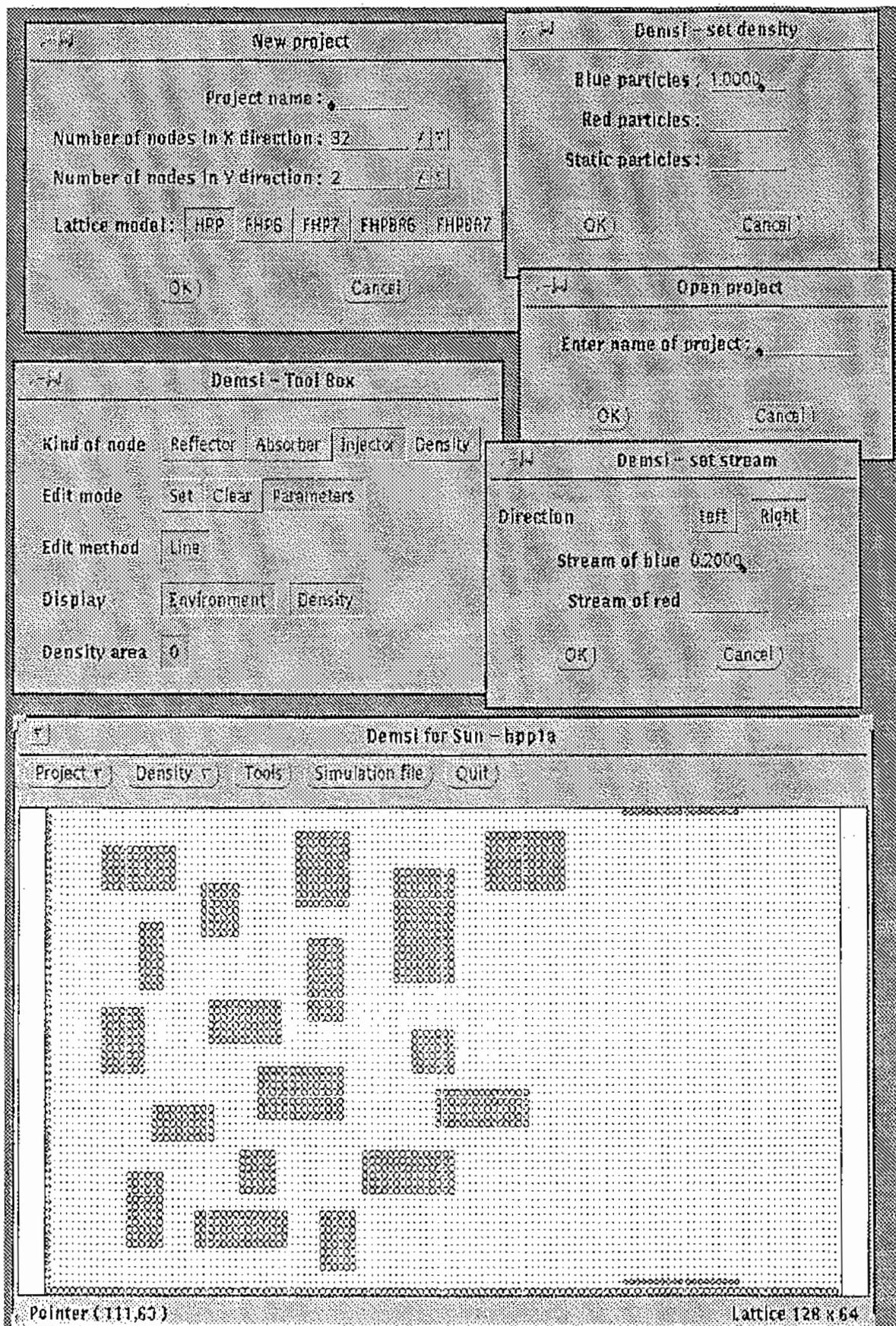
Fig. 3. Sample initial state of lattice prepared using DEMSI.
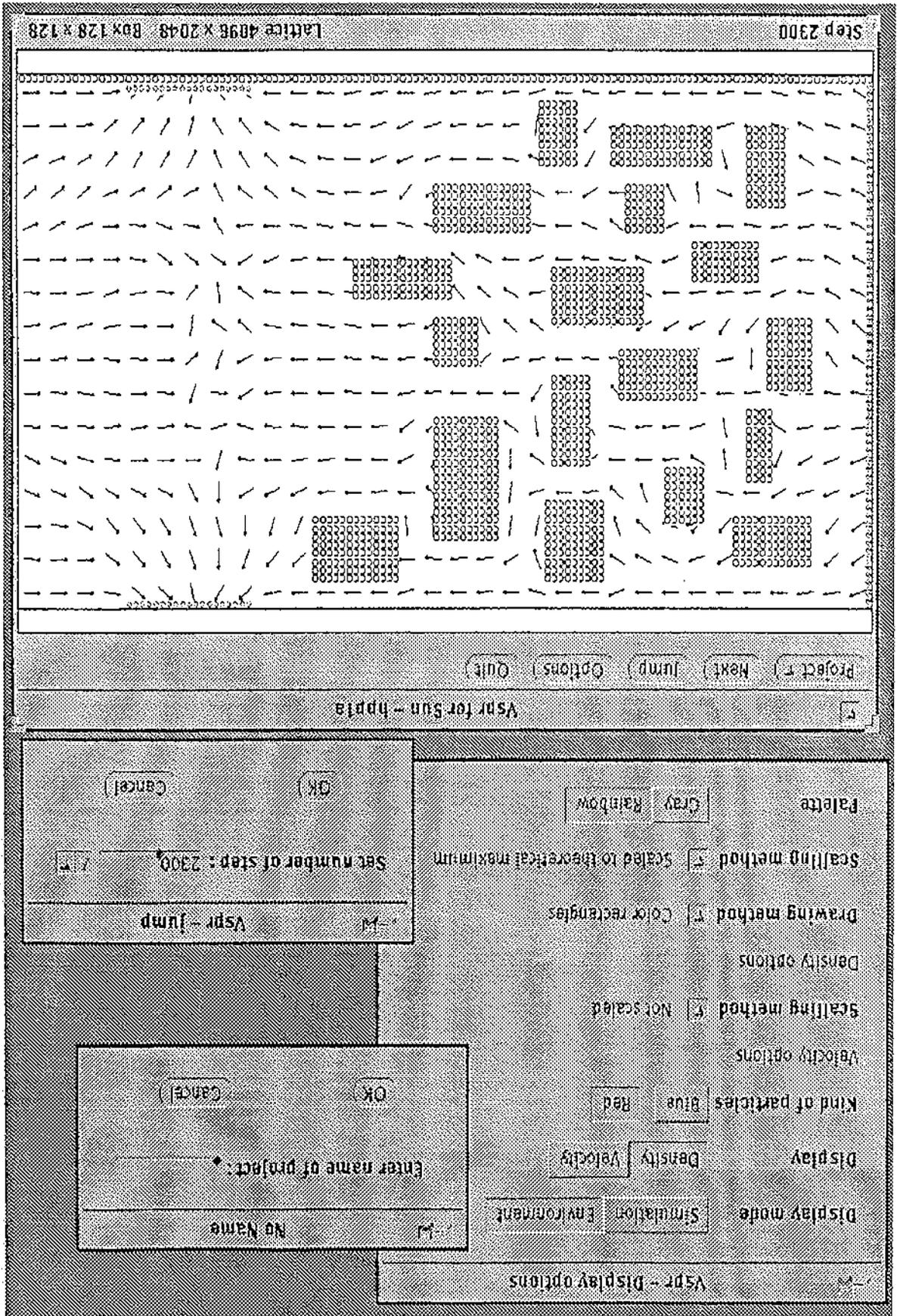
References

[1] Allen, M.P., Tildesley, D.J., "Computer simulation of liquids", *Claredon Press*, Oxford, 1989.

[2] Abraham, F. F., "Computational statistical mechanics. Methodology, applications and supercomputing", *Advances in Physics*, **35** (1986) 1-111.

[3] Binder, K., (Ed.), "Application of the Monte Carlo method in statistical physics", *Springer-Verlag*, Berlin, 1984.

[4] Frisch, U., d'Humières, D., Hasslacher, B., Lallemand, P., Pomeau, Y., and Rivet, J.P., "Lattice gas hydrodynamics in two and three dimensions", *Complex Systems*, **1** (1987) 649-707.

[5] Rogers, D. F., Earnshaw, R. A., "Techniques for Computer Graphics", *Springer-Verlag New York Inc.*, 1987.

[6] Hughes, M. H., Roberts, K.V., " OLYMPUS conventions, *Comput. Phys. Commun.*, 29 (1983) 15-43.

[7] "Turbo C Users Guide Version 2.0", *Borland International*, 1988.

[8] "GRAPHER", *Golden Softare, Inc.*, Colorado, 1987.

[9] "SunView", *Sun Microsystems Inc.*, 1989.

[10] "OpenWindows Version 2 User's Guide", *Sun Microsystems Inc.*, 1990;
"OpenWindows Version 2 Release Notes", *Sun Microsystems Inc.*, 1990

J.H. van Vliet, and G. ten Brinke, *Monte Carlo Simulation and Mean Field Analysis of Two-dimensional Random Copolymer/Homopolymer Blends*; Macromolecules 22, 4627 - 4631 (1989).

J.H. van Vliet, and G. ten Brinke, *Monte Carlo Simulations of Ultrathin Polymer Blend Films: Influence of Interaction Strength on Segregation and Shape of Coils*; Macromolecules 23, 2797 - 2801 (1990).

J.H. van Vliet, and G. ten Brinke, *Orientation and Shape of Flexible Polymers in a Slit*; J. Chem. Phys. 93, 1436 - 1441 (1990).

J.H. van Vliet, and G. ten Brinke, *Intrinsic Viscosity of Flexible Polymers in Unbounded and Bounded Newtonian Shear Flow*; Macromolecules 24, 5351 - 5356 (1991).

J.H. van Vliet, *Monte Carlo Simulations of Confined Polymer Systems*; Doctorate Thesis, University of Groningen, Groningen, The Netherlands, 137 pages, December (1991).

J.H. van Vliet, and G. ten Brinke, *Intrinsic Viscosity of Flexible Polymers in Couette and Poiseuille Flows*; Macromolecules 25, 3695 - 3701 (1992).

J.H. van Vliet, M.C. Luyten, and G. ten Brinke, *Scaling Behavior of Dilute Polymer Solutions Confined between Parallel Plates*; Macromolecules, 25, 3802 - 3806 (1992).