

Daresbury Laboratory

# INFORMATION QUARTERLY FOR COMPUTER SIMULATION OF CONDENSED PHASES

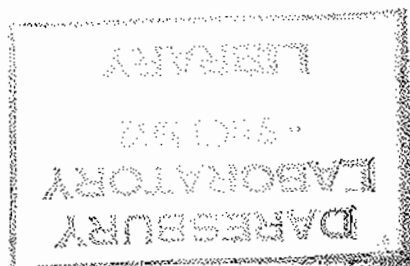
An informal Newsletter associated with Collaborative Computational Project No.5  
on Molecular Dynamics, Monte Carlo & Lattice Simulations of Condensed Phases.

Number 35

September 1992

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## General News

### FUTURE MEETINGS AND WORKSHOPS

A summary table is given below, further details may be found inside.

TOPIC	DATES	LOCATION
AQUEOUS SYSTEMS	READING UNIVERSITY	December 18 1992

### 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 are repeated from the last issue.

### CRAY NEWS

As most of our readers are aware, the Atlas Centre now has a Cray Y-MP81/8128 installed. It is currently available for trial use. There are 8 processors, 128Mwords of memory and 100Gbytes of disk storage. Each processor has about 1.4 times the peak performance of an X-MP processor.

CCP5 participants are reminded that CCP5 has an annual allocation of Cray time at Rutherford which will be transferred to the Y-MP. 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

The past year has been one of considerable activity for the Parallel Supercomputing Service at Daresbury. In the autumn of 1991 the SBCC established a Parallel Supercomputing Committee (chaired by Professor C.R.A.Catlow) to consider, under peer review, bids from HEI groups to use the Intel iPSC/860 system. In the initial review 26 substantial allocations were approved, together with a number of more modest pump priming awards. Recently the ABRC/SMC has funded, as part of the ABRC's renewed programme of investment in National High Performance Computing, an upgrade of the iPSC/860 to a 64-processor system, doubling the present machine cpu capacity. Accompanied by an increase in disc capacity of the Concurrent File System (to 12 GBytes), the upgrade is now complete and offers a resource capable of housing both resident SERC Board communities and new users from other Research Councils.

The Committee is scheduled to meet in November/December to consider allocations for the coming year, and it is important for both existing and new users that proposals should be submitted as soon as possible (definitely not later than 25 October). It remains our aim to provide a high level of scientific

support to users of the iPSC/860, should you apply for parallel supercomputer resources, a computational scientist at Daresbury will be nominated to give you as much help as possible with your project. If you would like any further information, please do not hesitate to contact Dr Yeung (tel. 0925-603178, Email address : h.k.f.yeung@uk.ac.daresbury), Dr Martyn Guest (tel. 0925-603247, Email address : m.f.guest@uk.ac.daresbury) or Dr Paul Durham.

## 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. Recent visits sponsored by CCP5 have been by Professor C. Zannoni and Professor V. S. Filinov. 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

## UPDATE TO MAILING LIST

It is some time since readers were asked to confirm their entry on our mailing list. Readers are asked to notify any changes by filling in the form in this issue and returning it to the address on the form. It is not necessary to complete the form if your address is correct.

## EMAIL distribution list

We also maintain an EMAIL distribution list to allow us to notify people about forthcoming conferences and workshops. A large number of the EMAIL addresses on this list are now incorrect due to changes in computers and networks. Please notify your correct EMAIL address if you do not receive EMAIL from us. A message was sent to all members on the list in September. UK universities are also gradually installing central mail servers and it is

preferable if your entry on our list is of the form Persons name@university rather than userid@address of computer as we then do not need to update our list if you move to a new machine. It would be helpful to us if you are registered with a mail server to let us know so that we can amend the mailing list. Notification of Email address changes may be made on the form provided in this issue or by Email to

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

## REQUEST FOR CONTRIBUTIONS

The deadline for contributions for the next newsletter will be 31 December 1992. Readers are reminded that contributions are always welcome. We do need more contributions for the next issue.

Contributors to the current issue.  
Our thanks go to:

C. E. Dean	Daresbury Laboratory
M. Leslie	
S. E. Marshall	
W. Smith	
D. Fincham	Department of Physics Keele University
D. Tildesley	Department of Chemistry Southampton University
S. C. Parker	School of Chemistry University of Bath



**SERC DARESBUURY LABORATORY**  
**CCP5 REGISTRATION FORM**  
**COMPUTER SIMULATION OF CONDENSED PHASES**

In order to receive the CCP5 newsletter and information regarding activities of CCP5, it is necessary to register your name on the CCP5 mailing list. Please complete the section below.

Title: \_\_\_\_\_ Initials: \_\_\_\_\_ Surname: \_\_\_\_\_

Job Title: \_\_\_\_\_

Department: \_\_\_\_\_

Organization: \_\_\_\_\_

Street: \_\_\_\_\_

Town: \_\_\_\_\_ County/State: \_\_\_\_\_

Zip/Postcode: \_\_\_\_\_ Country: \_\_\_\_\_

Electronic Mail Address \_\_\_\_\_

**IMPORTANT NOTICE**

Under the terms of the UK's DATA PROTECTION ACT 1984, we are obliged to notify you that you are on our regular mailing lists and that your name and address are held on our computer. The Act requires your consent to your name and address being so held. Our receipt of this completed form will indicate your acceptance.

Signature: \_\_\_\_\_

Please return this form to:-

W. Smith, TCS Division, SERC Daresbury Laboratory, Warrington WA4 4AD, U.K.

Please complete section below to enable us to ammend our records.

New application

Change of title or name

Change of Address

Change of EMAIL Address



## Advertisement for PDRA

Applications are invited from computational physicists and chemists with an interest in molecular simulation, for a postdoctoral Research Associate position in macromolecular simulations with the aid of parallel computers. The position is tenable for two years and will be based at Daresbury Laboratory in the Theory and Computational Science Division.

The position is funded by an SERC grant to CCP5, the Collaborative Computational Project for the Simulation of Condensed Phases. The aim of the project is threefold:

1. To develop macromolecular simulation programs for parallel computers.
2. To study techniques for incorporating long range forces.
3. To study the dynamics of macromolecules in solution.

The project will be supervised by Drs. W. Smith and D. Fincham. Informal enquiries may be made to Dr. Smith (Tel: 0925 603257; E-mail: W.Smith@uk.ac.daresbury).

Daresbury Laboratory is a leading centre in the application of parallel computing to scientific research, the major facility being a 64-processor Intel iPSC/860 supercomputer. The Associate will be expected to collaborate with several university groups in the U.K.

The starting salary will be in the JRA/SRA range (11,234-16,420 pounds sterling) and will depend on qualifications and experience etc.

Closing date: 15 October 1992.

## Workshop on aqueous systems: preliminary announcement

A CCP5 workshop to discuss the behaviour of aqueous systems will be held at the Reading University Chemistry Department on December 18, 1992. The meeting will be held on an informal basis and no registration will be needed. There will be four 1 hour talks and plenty of time for discussion. Speakers will include A. Soper, A.J. Stone and A. Wallqvist. Further inquiries may be addressed to

Dr P.M. Rodger  
Chem. Dept.,  
Reading Uni,  
Whiteknights,  
Reading, RG6 2AD

E-mail scsroder @ uk.ac.rdg.am.cms



# POLYMERS in MOTION

16th December 1992

Organised by the Institute of Physics as part of the  
**CONDENSED MATTER AND MATERIALS CONFERENCE**

15th - 17th December 1992

The second one-day symposium on the general field of Polymer Dynamics entitled "Polymers in Motion" follows the successful 1990 meeting in Cambridge. This time it takes place within the large CMMP '92 conference in Sheffield, allowing participants to make use of adjoining symposia, industrial exhibitions and plenary events. Topics to be covered include:

- Dynamics of Polymer-like Fluids (Surfactants, Colloidal Assemblies)
- NMR Techniques
- Molecular Rheology
- Dynamics at Surfaces and Interfaces
- Dynamics of Segregation
- Polymeric Liquid Crystals

Confirmed speakers to date include:

M. Brereton (Leeds)

D. Durand (Le Mans and CNRS)

G. Odell (Bristol).

M. Cates (Cambridge),

M. Mackley (Cambridge),

Further contributions to both oral and poster sessions are invited.

To submit a title or request registration details please send to:

CMMP '92  
Meetings and Conferences Department  
The Institute of Physics  
47 Belgrave Square  
London SW1X 8QX

For further information on the symposium please enquire from:

Dr. Tom McLeish  
Department of Physics  
University of Sheffield  
Housfield Road  
Sheffield S10 2UN

## 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 *uu* 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 distribution 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 the message you send to STATMECH (not in the subject line). Several commands may be sent at one time; just put one command per line.

#### STATMECH commands:

SENDME package	Sends all parts of the specified package.
SENDME package.n	Sends part n of the specified package.
LIST [pattern]	Gives 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.

ADMIXT [MD,LJA/MIX,LF,TH+MSD+RDF] W. Smith  
 CARLOS [MC,VS+Aquo,TH] B. Jonsson & S. Romano  
 CARLAN [DA,CARLOS structure analysis] B. Jonsson  
 & S. Romano  
 CASCADE [LS,DIL,EM,TH+STR] M. Leslie & W. Smith  
 CURDEN [DA,Current Density Correlations] W. Smith  
 DENCOR [DA,Density Correlations] W. Smith  
 HLJ1 [MD,LJA,LF,TH+MSD+RDF] D.M. Heyes  
 HLJ2 [MD,LJA,LF,TH+MSD+RDF+VACF] D.M. Heyes  
 HLJ3 [MD,LJA,LF/LC,TH+MSD+RDF] D.M. Heyes  
 HLJ4 [MD,LJA,LF/CP+CT,TH+MSD+RDF] D.M. Heyes  
 HLJ5 [MD,LJA/SF,LF,TH+MSD+RDF] D.M. Heyes  
 HLJ6 [MD,LJA,TA,TH+MSD+RDF] D.M. Heyes  
 HMDIAT [MD,LJD,G5+Q4,TH+MSD+QC] S.M. Thompson  
 HSTOCH [MD/SD,VS+BA,LF+CA,TH] W.F. van Gunsteren  
 & D.M. Heyes  
 MCN [MC,LJA,TH] N. Corbin  
 MCLSU [MC,LJA,TH] C.P. Williams & S. Gupta  
 MCMOLDYN [MD/MC,LJS+FC+AQ,LF+QF/G5+QS,TH+RDF] A. Laaksonen  
 MCRPM [MC,RPE,TH+RDF] D.M. Heyes  
 MDATOM [MD,LJA,G5,TH+RDF+MSD+QC] S.M. Thompson  
 MDATOM [MD,LJA,LF,TH+MSD+RDF] D. Fincham  
 MDCSPC2P [PRMD,BHM,LF,TH+STF+RDF+VACF+MSD] W. Smith  
 MDCSPC4B [PRMD,BHM+FC,G5+G4,TH+STF+RDF] W. Smith  
 MDDIAT [MD,LJD,LF+CA,TH+MSD] D. Fincham  
 MDDIATQ [MD,LJD+PQ,LF+CA,TH+MSD] D. Fincham  
 MDIONS [MD,BHM,LF,TH+MSD+RDF+STF] D. Fincham  
 & N. Anastasiou  
 MDLIN [MD,LJL,G5+Q4,TH+MSD+QC] S.M. Thompson  
 MDLINQ [MD,LJL+PQ,G5+Q4,TH+MSD+QC] S.M. Thompson  
 MD3DLJ\_C [MD,LJA/MIX,LF/LC,TH+MSD+RDF] M. Bargiel,  
 W. Dzwinel, J. Kitowski and J. Moscinski  
 MDMANY [MD,LJS+FC,LF+QF,TH] D. Fincham & W. Smith  
 MDMIXT [MD,LJS/MIX,LF+QF,TH] W. Smith  
 MDMPOL [MD,LJS+FC/MIX,LF+QF,TH] W. Smith & D. Fincham  
 MDNACL [MD,BHM,LF,TH+MSD+RDF] W. Smith  
 MDPOLY [MD,LJS,G5+Q4,TH+MSD+QC] S.M. Thompson  
 MDMULP [MD,LJS+PD+PQ/MIX,LF+QF,TH] W. Smith  
 MDSGWP [MD,LJA/SGWP,LF,TH+VACF+RDF+QC] W. Smith  
 & K. Singer  
 MDTETRA [MD,LJT,G5+Q4,TH+MSD+QC] S.M. Thompson  
 MDZOID [MD,GAU,LF+QF,TH+MSD+RDF+VACF] W. Smith  
 NAMELIST [UT, Namelist emulation] K. Refson  
 NSCP3D [UT, Hard sphere packing] M. Bargiel & J. Moscinski  
 PIMCLJ [PIMC,LJA,MC,TH+RDF+QC] K. Singer & W. Smith  
 SCN [MC,LJA,RFD,TH] N. Corbin

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	Rosky-Friedman-Doll algorithm	

Properties:

TH	Thermodynamic properties.
MSD	Mean-square-displacement
RDF	Radial distribution function
STF	Structure factor
VACF	Velocity autocorrelation function
QC	Quantum corrections
STR	Lattice stresses

## Programs from the Book "Computer Simulation of Liquids"

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

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## DL\_POLY: A Macromolecular Simulation Package

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W. Smith                      Daresbury Laboratory  
C. Dean  
D. Fincham                    Keele University and Daresbury Laboratory  
D. Tildesley                   University of Southampton

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The Collaborative Computational Project CCP5, dealing with computer simulation of molecular systems, has recently been awarded a grant by the Computational Science Initiative for postdoctoral assistance to develop a *Macromolecular Simulation Package* on the Daresbury Laboratory Intel iPSC/860 parallel computer. The project is expected to become fully active in late 1992, though much preliminary work has already been done.

The purpose of this package, named DL\_POLY, will be to apply the parallel molecular dynamics methods devised by participants in the CCP5 project [1-8] in a sophisticated package capable of accurate dynamical modelling of complex systems, with a special emphasis on macromolecules, but with capabilities in most other areas of molecular simulation. It is hoped that the wide range of expertise available through CCP5 will permit the development of a world-beating package that will be *free* to academic groups. The open nature of the project is intended to encourage wider utilisation of the best techniques of simulation, provide proven and adaptable source code essential to the new projects and reduce the dependency of the community on commercial 'black box' codes, which are incompatible with free academic exchange.

The initial objective is the development of a *Replicated Data* (RD) [1] program which will

be suitable for both the Intel iPSC/860 and serial workstations. The program will incorporate traditional simulation models, including atomic and molecular ions, rigid and flexible (macro-)molecules, multicomponent systems and a variety of ensembles and boundary conditions. Bond forces (including valence and dihedral angles) will also be incorporated. Nonbonded forces will be handled by the Replicated Data method. The long ranged forces will optionally be handled via direct summation or the Ewald method [4,7].

In the longer term, domain decomposition algorithms (i.e. Link Cells) will be incorporated, based on existing parallel methods [6,8]. The *Fast Multipole Method* (FMM) [10] will be developed for long range forces, with the PPPM [9] method as an option for periodic systems.

It is intended that the code development take place in conjunction with a study of polymeric species in solution.

In the initial phases the project will be assisted by the Parallel Applications Team at Daresbury.

## References

- [1] W. Smith, *Comp. Phys. Comm.* (1991) **62** 229.
- [2] D. Fincham, *Molecular Simulation* (1987) **1** 1.
- [3] A.C. Raine, D. Fincham and W. Smith, *Comp. Phys. Comm.* (1989) **55** 13.
- [4] W. Smith, *Comp. Phys. Comm.* (1992) **67** 392
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## CASCADE and THBREL - Implementation on the INTEL iPSC/860

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### Introduction

CASCADE and THBREL are energy minimization programs in the CCP5 program library dealing with ionic crystals defects. The energy is minimised using a modified Newton-Raphson technique.

### The programs

In both programs a second derivative matrix and gradient vector are calculated, the matrix is inverted and a step direction calculated from the product of the inverse second derivative matrix with the gradient vector. A step is then taken in this direction. This is only carried out once, as subsequent steps use a matrix update algorithm which involves only calculating the gradient vector and matrix vector multiplications. The time consuming parts of the codes are the calculation of the gradient vector and updating the second derivative matrix inverse using matrix vector multiplication.

The codes have been parallelised using the portable harness FORTNET and has run on INTEL, MEIKO(I860) and MEIKO(T800). To parallelize the gradient calculation step the existing vector code is used. This sets up a list of pairs and then calculates the interactions between them. The pairs list is set up on all nodes but the interaction calculation is only carried out on one node controlled by a master process using a global counter. A global sum is then carried out to give the gradient vector. The global counter is stored in FORTNET. On the INTEL the master process is interrupt-driven and runs on one of the nodes that performs floating point arithmetic. On the MEIKO the master process currently runs on a node which performs no other floating point arithmetic. The three-body part of the gradient calculation can be divided into sections which do the same amount of work. This part is therefore be parallelised more easily by sharing the work equally over all the nodes.

The matrix is distributed evenly over all the nodes. To do this the matrix is divided into sections consisting of a number of rows and all columns. Each section is calculated using the global counter method using all nodes storing the partial sums in a buffer. The buffer is then globally summed and copied to the elements of the distributed array on the nodes on which it is required.

A distributed matrix inverter has been written to carry out the matrix inversion. The input matrix is overwritten by the result and the work space required is of order  $N$  with only  $N^2/\text{numnodes}$  of words of storage per node for the matrix. (Numnodes = number of nodes). A 2048 x 2048 matrix takes

236 seconds to invert on 8 nodes corresponding to 73 Mflops. The BLAS library rank one operation routine DGER is called to perform most of the floating point arithmetic. It has a rated performance of 11.3 Mflops per node. 1 CRAY X-MP processor takes 150 seconds running at 206 Mflops using a different algorithm to perform the same calculation.

The final step in both calculations is the distributed matrix vector multiplication for which the gradient vector will be available on all nodes following the global sum.

### Timings

For "real" problems, CASCADE needs to be distributed over up to 8 iPSC/860 nodes. Timings for 1 (8) nodes on the ipsc/860, MEIKO(i860), MEIKO(t800) and CRAY X-MP for three problem sizes ( $N$  = number of variables) are (630 variables needs 16Mbytes for a single node calculation and could not be done on MEIKO)

MACHINE	N	INTEL I860	MEIKO I860	MEIKO T800	CRAY XMP
STEP					
Matrix	208	13.9 (3.4)	26.0 (10.0)	131.0 (55.0)	1.71
Calculation	410	34.3 (9.4)	65.0 (31.0)	320.0 (170.0)	4.24
	630	66.9 (19.4)	- (66.0)	- (372.0)	8.25
Matrix	208	1.8 (4.9)	17.0 (18.0)	105.0 (70.0)	0.28
Inversion	410	12.9 (13.6)	193.0 (58.0)	797.0 (290.0)	1.61
	630	45.3 (27.4)	- (150.0)	- (791.0)	5.88
Gradient	208	11.4 (2.0)	20.0 (4.0)	90.0 (21.0)	1.17
Calculation	410	27.5 (4.7)	48.0 (10.0)	216.0 (45.0)	2.81
(Per Cycle)	630	53.4 ( 8.9)	- (16.0)	- (83.0)	5.43
Iteration	208	122.6 (36.6)	238.0 (49.0)	923.0 (217.0)	12.24
Step	410	177.9 (47.3)	351.0 (64.0)	1339.0 (288.0)	17.41
	630	288.3 (59.9)	- (96.0)	- (439.0)	27.73
Total Time	208	436.1 (180.4)	685.0 (243.0)	3124.0 (979.0)	44.0
	410	709.1 (281.9)	1317.0 (438.0)	5898.0 (1872.0)	75.8
	630	1197.1 (441.1)	- (793.0)	- (3724.0)	133.0

The matrix calculation step runs 3.3 times faster on 8 nodes than on 1 node for the largest case; the timing ratio is getting worse for larger systems. This is because this step carries out  $O(N^2)$  communication. However the poor scalability is not important as this step is only carried out once and only represents 5% of the total time. The matrix inversion step scales very badly for matrices of this size. The communication is  $O(N)$  and the calculation is  $O(N^3)$  so the scalability improves rapidly with problem size. The poor scalability does not matter as the inversion is only done once and represents 10% of the total execution time. Larger systems will have better scalability for this step. The gradient calculation speedup on the INTEL is 5.8 for the largest system; this step improves its scalability with problem size. This step involves the bulk of

the execution time.

Comparing the INTEL and MEIKO, the MEIKO(I860) is about 2 times slower and the T800 is 10 times slower. For both machines the scalability on increasing the number of nodes is worse reflecting the slower communication.

## CCP5 Literature Survey 1991

W. Smith

August 5, 1992

We present in the following pages, the CCP5 Literature Survey for 1991. All the references included in this survey are selected from the INSPEC database and are reproduced with the permission of INSPEC, the Institution of Electrical Engineers. (The INSPEC Database covers all areas of physics, electronics and computing.) The printed survey has been retyped and proof read by our own staff, and INSPEC are not responsible for any errors that may result from this. We are grateful to Mr. Geoff Jones, Head of Selective Services at INSPEC for his advice and assistance.

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