Daresbury Laboratory
INFORMATION QUARTERLY FOR COMPUTER SIMULATION OF CONDENSED PHASES
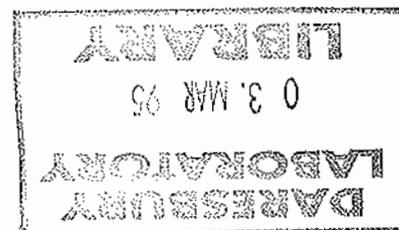
An informal Newsletter associated with Collaborative Computational Project No.5 on Molecular Dynamics, Monte Carlo & Lattice Simulations of Condensed Phases.

Number 43   February 1995

Contents

General News

Hardware failure

Due to a hardware failure, anonymous ftp and WWW access to the program library and newsletters was not available for an extended period during late December 1994. Please accept our apologies for any difficulties this may have caused.

UK Telephone numbers

All telephone numbers in the UK have changed; however the existing numbers will continue to work until April 1995. To make the change, insert an extra digit 1 after the international code (44) but before the local area code. The Daresbury telephone number is noted in full below.

FUTURE MEETINGS

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

TOPIC	DATES	LOCATION	ORGANISER
The Structure and Properties of Oxide Surfaces	5-6 April 1995	Daresbury	CCP3
Structure and Order in Liquids	22-27 September 1995	Blankenberge	European Science Foundation / European Molecular Liquids group
Simulation of Molecular Materials	6 September 1995	Sheffield	Royal Society of Chemistry

Full details of the ESF conference program may be obtained from

Dr. Josip Hendekovic,	Email	euresco@esf.c-strasbourg.fr
European Science Foundation,		
1 quai Lezay-Marnésia,	Tel.	+33 88 76 71 35
67080 Strasbourg Cedex,	Fax	+33 88 36 69 87
France		

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.

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 £200 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 at the address below.

CCP5 VISITORS PROGRAM

CCP5 organizes 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.

ELECTRONIC DISTRIBUTION OF CCP5 NEWSLETTERS AND WORLD WIDE WEB

All newsletters starting from issue 39 (October 1993) are now available on line, together with some articles from earlier newsletters. An index of recent newsletter articles can be found on the World Wide Web server; readers can access the individual articles by this means or by anonymous ftp. (Anonymous ftp will not access the index). The URL for the CCP5 home page is

http://www.dl.ac.uk/CCP/CCP5/main.html

HOW TO GET THIS NEWSLETTER BY FTP

1.	move to the desired directory on YOUR machine	
2.	type:	ftp ftp.dl.ac.uk
	or	ftp 148.79.80.10
3.	enter userid:	anonymous
4.	enter passwd:	*enter your name and site*
5.	change to ccp5.newsletters/43 directory:	cd ccp5.newsletters/43
6.	change to postscript or latex subdirectory	cd ps
	or	cd latex
7.	to get the required files from the directory :	
	postscript from ps directory	get nl.ps
	compressed postscript from ps directory	get nl.ps.gz
	latex from latex directory	get nl.tex
8.		quit

Below is an index of the information held.

History of the project.

Organisation of the project.

Current research interests .

A library of computer software maintained by the project.

An index of future meetings and workshops which CCP5 is involved in organising or has been asked to publicize.

A list of proposed visitors sponsored by CCP5 with itinerary.

An index of articles from recent issues of the newsletter.

A copy of recently published newsletters commencing with Issue 39 (October 1993).

Registration and de-registration details.

Other related information on the Web.

Job vacancies

Readers may now **register** by filling in an on-line WWW form. Existing readers may also notify registration changes in this way.

The section on other related information has been expanded, and I will add any further links notified to me.

In addition to notification of newsletters, we occasionally send other messages about meetings to the Email list. If you want us to send **notification of newsletters only**, let me know and I will place your Email address on a separate list. This will allow readers to restrict the amount of incoming Email if this will be a problem due to limited bandwidth or if readers are charged for incoming Email.

This newsletter is available by anonymous ftp either directly or by accessing the Daresbury World Wide Web server. The newsletter has been placed (in separate directories) both as postscript files and as the source latex files.

THE CCP5 PROGRAM LIBRARY

Copies of the newsletter no longer include a complete description of the program library. If readers wish to obtain a copy of the documentation it is available by anonymous ftp or through the World Wide Web page. The program library description is in ccp5.newsletters/library directory (postscript and ASCII text versions).

Users of fast Fourier transforms may like to note the following. Keith Refson from the Earth Sciences Department, Oxford, has been carrying out timing tests on a FORTRAN implementation of Clive Temperton's GPFA FFT algorithms (C. Temperton, Siam J. Sci. Stat. Comput 13(3), 676-686 (1992)) and has found very favourable performance compared with existing Fortran implementations.

REQUEST FOR CONTRIBUTIONS

Contributors to the current issue

Our thanks go to:

Ramzi Kutteh	Pacific Northwest Laboratory, Richland, WA 99352 USA
P. Lindan N. Harrison W. Smith T. Forester	DRAL Daresbury Laboratory Warrington WA4 4AD UK
Dr. D. Gay Dr. A. Rohl	The Royal Institution, London
Dr. M. Allen M. Warren	Department of Physics University of Bristol
Dr. M. Wilson	Lancaster University
Dr. A. Sauron	Sheffield Hallam University
Dr. K. Gubbins	Cornell University

The deadline for contributions for the next 2 newsletters will be **1 May 1995** and **1 August 1995** Readers are reminded that contributions are always welcome. This newsletter was delayed because the editor had insufficient material. Contributions may be sent by Email in LaTeX. WORD documents should preferably be sent in rtf format. We would be prepared to consider other formats on a trial basis.

Address

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MEETING AND WORKSHOP ANNOUNCEMENTS
THE STRUCTURE AND PROPERTIES OF OXIDE SURFACES

Daresbury Laboratory April 5-6, 1995

This workshop is being organised by CCP3, but is in the area of interest of CCP5. This informal workshop is concerned with recent progress in the theoretical and experimental description of oxide surfaces and interfaces. The topics which will be covered include:

- Recent progress in the first principles description of surface structure and spectroscopy

- Simulation of complex processes at surfaces; molecular adsorption and diffusion.

- Advances in experimental techniques; diffraction and real space imaging.

- The applicability of empirical models.

A registration form, schedule, and some general information are attached below.
Postscript versions of these forms are available on request or by;

1. anonymous ftp to "ftp.dl.ac.uk/ccp3"

2. The WWW page "http://www.dl.ac.uk/CCP/CCP3/main.html"

The registration fees can be paid at the registration desk or by (sterling) cheque payable to "Daresbury Laboratory".
Deadlines: The form must be returned (by post or EMAIL) by 13th March.

Schedule

Wednesday 5th April 1995

10	COFFEE		
10-30	Opening Remarks	N.Harrison	(Daresbury)
11	Exploring oxide surfaces with density functional theory	M Gillan	(Keele)
12	A comparison of different models in the study of chemisorption in infinite systems.	R.Dovesi	(Torino)
1 - 2	LUNCH		
2	Calculation of properties of an oxide/metal interface	M Finnis	(Stuttgart)
3	Ab initio, classical and analytic approaches to oxide surface structure	N Harrison	(Daresbury)
4	COFFEE		
4-30	Contributed talk The calculation of STM images as a tool for interpreting STM data and for understanding geochemical surface reactions at an atomic level.	U Becker	(Virginia)
5.00	Contributed talk.		
5.30	Poster session		
7.00	Discussion / Refreshments		
8.00	Conference Dinner		

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Thursday 6th April 1995:

Time	Title	Speaker	Affiliation
08.30	Simulation studies of the stability of oxide surfaces.	P. Lindan	(Daresbury)
09.30	Classical and quantum calculations of oxide surfaces	W Mackrodt	(St-Andrews)
10.30	COFFEE		
11	Oxygen vacancies on MgO (100) : electronic structure and reconstructions	C Noguera and E. Castanier	(Paris)
12	Contributed talk Modelling the surface structures of silicates and barium sulphates.	D. Gay and AL. Rohl	(Royal Institution)
12.30	Contributed talk Atomistic simulation of atomic force imaging of ionic systems	A. Shluger	(Royal Institution)
1-2	LUNCH		
2	Structure/property relations for TiO_2 surfaces	G Thornton	(Liverpool)
3	The surface structure of MgO revisited	K Refson	(Oxford)
4	General Discussion / Posters		
5	Farewell and Coffee.		

General Information

Attendance and Financial Arrangements

If you wish to attend, please complete and return the enclosed application form as soon as possible and no later than Monday 13 March 1995.

FEE:

The conference fee is 70 pounds for academics and 100 pounds for industrial participants. Lunches and refreshments will be provided, as will a Conference dinner which will be held on Wednesday 5 April at the Laboratory. Please indicate on the attached form if you wish to attend the dinner. Cheques (remitted in pounds sterling) should be made payable to "Daresbury Laboratory".

Accommodation

Accommodation is at the Lord Daresbury Hotel at a cost of 69.00 per night including VAT. Accommodation is available for the nights of Tuesday 4 April and Wednesday 5 April. Further nights may be available on request. Any changes to accommodation must be made well in advance of the meeting by post, fax or e-mail.

Travel

Participants must find their own funds for travel.

Bursaries

A limited number of bursaries are available. Please contact Dr N M Harrison at the postal address below or e-mail n.m.harrison@dl.ac.uk

Registration Form

DRAL

Daresbury Laboratory

CCP3 MEETING ON OXIDE SURFACES

5 - 6 April 1995

APPLICATION FORM

SURNAME: (Prof , Dr , Mr , Mrs , Ms *) .... Male/Female*
(BLOCK letters please)
FIRST NAME(S) ....

MAILING ADDRESS of Home Institute or Place of Work: ....

....

....

....

....

Tel ....Fax ....

Electronic Mail Address ....

D L Staff please state division ....

1. ACCOMMODATION: Please note delegates should settle their bill directly with the Hotel.

1.1. I will require accommodation as follows:

The Lord Daresbury Hotel

Single accommodation: £69.00 including VAT (B & B) Tue 4 April YES/NO*

Single accommodation: £69.00 including VAT (B & B) Wed 5 April YES/NO*

If any further accommodation is required please specify:

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1.2. Other Hotels: If all our accommodation has been allocated would you like a list of local hotels where you could make your own arrangements? YES/NO*

2. SPECIAL REQUIREMENTS: Please specify any special requirements such as diet, disability etc...

3. POSTER SESSION

I/we wish to present a poster YES/NO*
Note: No   poster   bookings   will   be   accepted   without   full   information   below.
Lead Author: ....

Affiliation: ....

Co-Author(s): ....

Affiliation(s): ....

Title: ....

....

....

To avoid duplicated poster bookings, has one of your co-authors already applied to exhibit this poster? YES/NO*

4. TRAVEL ARRANGEMENTS

Car: I will arrive by car: YES/NO*   My registration No. is
           Please send a map: YES/NO*   ....
Please return this form to arrive no later than 13 March at:

SAS Conference Office
DRAL Daresbury Laboratory
Warrington WA4 4AD
or e-mail conference@dl.ac.uk
* Please delete where inapplicable

Office Facilities

There will be an information desk at the meeting where participants will be able to make transport arrangements. There will be NO banking or currency exchange facilities. Postal arrangements will be limited to a mail delivery and pick-up service. There will be a restricted photocopying facility.

Postal address: c/o   DRAL Daresbury Laboratory, Warrington WA4 4AD, England
Telephone: Warrington (01925) 603235
Fax: 01925 603195

For further information please contact

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    WA4 4AD
    United Kingdom
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RESEARCH CONFERENCE ON

MOLECULAR LIQUIDS:

Structure and Order in Liquids

A European Research Conference run by the European Science Foundation in association with the European Molecular Liquids Group.

Blankenberge, Belgium, 22-27 September 1995

Chairman:	R.M.Lynden-Bell	(Cambridge)
Vice-Chairman:	G.Palinkas	(Budapest)

This meeting is the second Euroconference on Molecular Liquids held in association with the European Molecular Liquids Group. Although liquids are disordered on the large scale there is considerable order at the molecular scale. At this meeting there will be discussion of recent experimental and simulation results on local order in liquids and solutions. Both freezing into an ordered crystalline phase and glass formation are affected by the degree of local order and there will be sessions on these topics. The aim of the meeting will be to give a clear picture of the current state of theory and experiment and to highlight areas of future research. Participants are encouraged to contribute to the discussion and poster sessions.

Preliminary Programme

Order in Liquids

D.Frenkel	(Amsterdam):	Local order and molecular shape.
I.Cabaço	(Lisboa):	Neutron studies of benzene and perfluorobenzene.
MA.Ricci	(Roma):	The structure of water above its boiling point.
H.Versmold	(Aachen):	Investigation of local structure in fluids by light scattering.

Solvation

ADJ Haymet	(Sydney):	Calculating the dissociation of water.
E. Guardia	(Barcelona):	Computer Simulation of Ions in Solution.
H.Wengärtner	(Karlsruhe):	Liquid-liquid phase separation and criticality in electrolytes.
P.M.Rodger	(Reading):	Solvent induced structure of the solvation shell.

Freezing and Melting

D.Oxtoby	(Chicago):	Density functional theory of crystallization dynamics.
P.Madden	(Oxford):	Nucleation in hard sphere liquids.
C.Körber	(München):	Freezing of aqueous solutions - the advancing solid-liquid interface.
J-P. Hansen	(Lyon):	Studies of a sol-gel system.

Glass formation

L.Sjögren	(Göteborg):	Mode Coupling theory of glass formation.
D.Kivelson	(Los Angeles):	Supercooled liquids and glasses: A thermodynamic theory?
R.Vallauri	(Firenze):	Dynamics of supercooled liquids and glasses though normal modes.

SIMULATION OF MOLECULAR MATERIALS

Royal Society of Chemistry Autumn Meeting,
Sheffield,
6 September 1995.

Invited Speakers are:

Julian Clarke   (Manchester)
Alejandro Gil   (Sheffield)
Mike Klein   (Pennsylvania)
Neal Skipper   (University College, London)
Dominic Tildesley   (Southampton)

There is space for short contributions.

George JACKSON   Tel: (0114) 282 4781
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Sheffield S3 7HF   E-Mail: G.Jackson@sheffield.ac.uk
United Kingdom

Post Doctoral Position

Static and Dynamic Properties of Water

Florence, Italy

A post-doc position is available under a contract with EEC for the study of static and dynamical properties of water. This is for one year to be spent in Florence for doing computer simulation on model systems. Another part of the project includes neutron scattering measurements mainly performed at RAL (supervision Alan Soper and Javier Bermejo). Salary will be in accordance with experience. For further information please contact

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Post Doctoral Position

Molecular Simulation of Zeolites

Paris, France

A postdoctoral position is available at the European Centre for Computational Science and Technology in Paris to study adsorption in zeolites. The research will involve the application of novel molecular simulation methods (grand canonical Monte Carlo and grand canonical molecular dynamics of molecules in zeolite frameworks) to gas adsorption. Close contact will be maintained with related work at the Daresbury Laboratory employing ab initio methods and with scientists at Unilever Research. The position (which will be based in Paris) is available now for one year initially.

Please send email/fax/letters of application/CV to

Prof. Nick QUIRKE
Deputy Director
European Centre for Computational Science and Technology
BIOSYM Technologies Sarl
Parc Club Orsay Universit'e   Tel   : 33-1-69 41 99 08
20 rue Jean Rostand   Fax   : 33-1-69 41 99 09
91893 Orsay Cedex, France   email   nick@biosym.fr

The European Centre

The European Centre for Computational Science and Technology is Biosym's European research centre. It is located in new accommodation in Orsay (south of Paris) adjoining the university campus, in the midst of one of the largest concentrations of academic and government research facilities in the world. The centre has very strong links with local and international research groups including the CEA in Saclay, the Université de Paris, the Institut Français du Pétrole as well as groups in other European countries. Our staff hold professorial positions at major European and North American universities.

The centre has excellent computing facilities including powerful workstations It has the full range of BIOSYM modelling software in both release and prerelease forms as well as state of the art in-house research codes not available elsewhere. As well as a general expertise in modelling software and applications methodologies the centre has special expertise in the adsorption, transport and characterisation of porous media (zeolites, carbons...), organic films and interfaces; oil field chemistry, catalysis and materials science as well as the prediction of phase equilibria.

A Simpler and More Efficient Formulation of The Cell Multipole Method

Ramzi Kutteh

High Performance Computing Group
Molecular Science Research Center
Pacific Northwest Laboratory
Richland, WA 99352

I examine the particular forms of the potential multipole expansion and multipole moments used in the cell multipole method (CMM) of Ding et $al.$ [1]. I show that alternative definitions of the moments corresponding to a common alternative form of the multipole expansion, may be more advantageous to use in CMM than the moment definitions adopted by Ding et $al.$ [1]. Specifically, the shifting expressions for the new quadrupole and higher order moments are easier to derive, more simple and symmetric (i.e., easier to code), and more computationally efficient than the shifting expressions for the previously adopted moments.

I demonstrate here that an alternative form of the potential multipole expansion, with corresponding multipole moment definitions, may be more advantageous for use in the cell multipole method (CMM) of Ding et $al.$ [1] than the particular form adopted by the authors.

CMM consists of an upward pass followed by a downward pass. In the upward pass, the multipole moments of the cells are first computed at the finest level of refinement. I refer to this computation as step (I). The definitions used to compute the moments correspond to the following form of multipole expansion of the potential of a collection of charges inside a cell A (this expansion is obtainable from a Taylor or equivalently a binomial expansion of the Coulomb potential):

$$V(\mathbf{r}) = \frac{Z}{R} + \frac{\sum_\alpha \mu_\alpha R_\alpha}{R^3} + \frac{\sum_{\alpha,\beta} Q_{\alpha\beta} R_\alpha R_\beta}{R^5} + \frac{\sum_{\alpha,\beta,\gamma} O_{\alpha\beta\gamma} R_\alpha R_\beta R_\gamma}{R^7} + \cdots , \tag{1}$$

where $Z = \sum_i q_i$ is the monopole moment, $\mu_\alpha = \sum_i q_i \bar{r}_{i\alpha}$ is the dipole moment, and

$$
\begin{aligned}
Q_{\alpha\beta} &= \frac{1}{2} \sum_i q_i [3\bar{r}_{i\alpha}\bar{r}_{i\beta} - \delta_{\alpha\beta}\bar{r}_i^2] \\
O_{\alpha\beta\gamma} &= \frac{1}{2} \sum_i q_i [5\bar{r}_{i\alpha}\bar{r}_{i\beta}\bar{r}_{i\gamma} - (\bar{r}_{i\alpha}\delta_{\beta\gamma} + \bar{r}_{i\beta}\delta_{\alpha\gamma} + \bar{r}_{i\gamma}\delta_{\alpha\beta})\bar{r}_i^2]
\end{aligned}
\tag{2}
$$

are the quadrupole and octopole moments, respectively. In the above equations $\mathbf{R} = \mathbf{r} - \mathbf{r}_A$, where $\mathbf{r}_A$ is the position of the center of cell A; q_i is the charge of particle i, and $\bar{r}_{i\alpha}$ is the α component of the position vector of particle i with respect to the center of cell A. I refer to the definition of the quadrupole and all higher moments as in Eq (2), as definition (A). At coarser levels, the multipole moments of every parent cell at level $(l-1)$ are computed by shifting and adding the multipole moments of its eight children cells at level l. I refer to this computation as step (II). For example, the shifting expression for the quadrupole moment with definition (A) is

$$
\begin{aligned}
Q_{\alpha\beta}^{(l-1)} &= \sum_{k=1}^{8} [Q_{\alpha\beta}^{(l)}]_k + \frac{3}{2}\sum_{k=1}^{8} \{[\mu_\alpha^{(l)}]_k [C_\beta]_k + [\mu_\beta^{(l)}]_k [C_\alpha]_k\} - \sum_{k=1}^{8} [\mu^{(l)}]_k \cdot [C]_k \delta_{\alpha\beta} \\
&\quad + \frac{1}{2}\sum_{k=1}^{8} [Z^{(l)}]_k \{3[C_\alpha]_k [C_\beta]_k - [C^2]_k \delta_{\alpha\beta}\} ,
\end{aligned}
\tag{3}
$$

and for the octopole moment with definition (A)

$$
\begin{aligned}
O^{(l-1)}_{\alpha\beta\gamma} &= \sum_{k=1}^{8}[O^{(l)}_{\alpha\beta\gamma}]_k + \sum_{k=1}^{8}\{[Q^{(l)}_{\alpha\beta}]_k[C_\gamma]_k + [Q^{(l)}_{\alpha\gamma}]_k[C_\beta]_k + [Q^{(l)}_{\beta\gamma}]_k[C_\alpha]_k\} \\
&+ \sum_{k=1}^{8}\{[Q'^{(l)}_{\alpha\beta}]_k[C_\gamma]_k + [Q'^{(l)}_{\alpha\gamma}]_k[C_\beta]_k + [Q'^{(l)}_{\beta\gamma}]_k[C_\alpha]_k\} \\
&- \sum_{k=1}^{8}\{[Q'^{(l)}_{\alpha}]_k \cdot [C]_k\delta_{\beta\gamma} + [Q'^{(l)}_{\beta}]_k \cdot [C]_k\delta_{\alpha\gamma} + [Q'^{(l)}_{\gamma}]_k \cdot [C]_k\delta_{\alpha\beta}\} \\
&+ \frac{1}{2}\sum_{k=1}^{8}\{5([\mu^{(l)}_{\alpha}]_k[C_\beta]_k[C_\gamma]_k + [\mu^{(l)}_{\beta}]_k[C_\alpha]_k[C_\gamma]_k + [\mu^{(l)}_{\gamma}]_k[C_\alpha]_k[C_\beta]_k) \\
&\quad - ([\mu^{(l)}_{\alpha}]_k\delta_{\beta\gamma} + [\mu^{(l)}_{\beta}]_k\delta_{\alpha\gamma} + [\mu^{(l)}_{\gamma}]_k\delta_{\alpha\beta})[C^2]_k\} \\
&- \sum_{k=1}^{8}[\mu^{(l)}]_k \cdot [C]_k\{[C_\alpha]_k\delta_{\beta\gamma} + [C_\beta]_k\delta_{\alpha\gamma} + [C_\gamma]_k\delta_{\alpha\beta}\} \\
&+ \frac{1}{2}\sum_{k=1}^{8}[Z^{(l)}]_k\{5[C_\alpha]_k[C_\beta]_k[C_\gamma]_k - ([C_\alpha]_k\delta_{\beta\gamma} + [C_\beta]_k\delta_{\alpha\gamma} + [C_\gamma]_k\delta_{\alpha\beta})[C^2]_k\} \, ,
\end{aligned}
$$

(4)

where $[C]_k$ is the vector from the center of a parent cell to the center of its kth child cell, and $Q'_{\alpha\beta}$ is defined in Eq (6). In the downward pass, the Taylor coefficients of the cells are first computed at the coarsest level (level 2 for vacuum boundary conditions) by Taylor expanding Eq (1). I refer to this computation as step (III). At finer levels, the Taylor coefficients of every child cell are the sum of two contributions. The first contribution is the sum of the Taylor coefficients from the cell's interaction list. I refer to this computation as step (IV). The second contribution comes from shifting the Taylor coefficients of the parent cell. I refer to this computation as step (V).

An alternative common form of the potential multipole expansion [2, 3] is obtained by rewriting Eq (1) in the form

$$
\begin{aligned}
V(\mathbf{r}) &= \frac{Z}{R} + \frac{\sum_\alpha \mu_\alpha R_\alpha}{R^3} + \frac{1}{2}\frac{\sum_{\alpha,\beta} Q'_{\alpha\beta}[3R_\alpha R_\beta - \delta_{\alpha\beta}R^2]}{R^5} \\
&+ \frac{1}{2}\frac{\sum_{\alpha,\beta,\gamma} O'_{\alpha\beta\gamma}[5R_\alpha R_\beta R_\gamma - (R_\alpha\delta_{\beta\gamma} + R_\beta\delta_{\alpha\gamma} + R_\gamma\delta_{\alpha\beta})R^2]}{R^7} + \cdots ,
\end{aligned}
$$

(5)

where the quadrupole and octopole moments are now given by

$$
Q'_{\alpha\beta} = \sum_i q_i \bar{r}_{i\alpha} \bar{r}_{i\beta} \, , \qquad O'_{\alpha\beta\gamma} = \sum_i q_i \bar{r}_{i\alpha} \bar{r}_{i\beta} \bar{r}_{i\gamma} \, ,
$$

(6)

respectively. I refer to the definition of the quadrupole and all higher moments as in Eq (6), as definition (B). In the following, I show that the multipole expansion in Eq (5), with definition (B) of the moments, may be more advantageous for use in CMM than the expansion in Eq (1), with definition (A) of the moments.

The quadrupole and all higher order moments in definition (B) have simpler forms than the quadrupole and all higher order moments in definition (A) (compare Eq (2) with Eq (6)). More explicitly, the moments in Eq (6) do not require the computation of atomic distances. The optimum

number κ of particles per cell at the finest level depends on the nature of the system, its size, the order of approximation, and the number of levels. For example, for five levels of refinement, the finest level has 32768 cells. Typically, I have found κ for this case will range in value from 10 to 100. Adopting definition (B) for the moments, instead of definition (A), results for this case in a savings of $\kappa \times 32768$ or on average ≈ 2 million atomic distance computations, leading to a more computationally efficient step (I). The expansion in Eq (5) has a more complex functional form (i.e., dependence on $\mathbf{R}$) than the expansion in Eq (1). Hence the Taylor coefficients obtained by Taylor expanding Eq (5) also have more complex forms than the coefficients obtained by Taylor expanding Eq (1). However, in contrast to the difference between Eq (2) and Eq (6) noted above, the Taylor coefficients obtained from Eq (1) and Eq (5) *both* require cell-cell distance computations (i.e., from R). This means that no additional quantities (such as cell-cell distances) are required to compute the extra terms in the Taylor coefficients introduced by adopting definition (B) of the moments. Therefore using definition (B) for the moments, instead of definition (A), leads to a negligible computational overhead in step (III). Step (IV) involves the computation of the Taylor coefficients of 189 cells for every cell, starting at level 3 and down to the finest level. For example, for five levels of refinement and taking the interaction list of any cell to be 189 cells (this number is actually smaller for non-interior cells), levels 3, 4, and 5 require the computation of ≈ 7 million cell-cell distances, *regardless* of which definition of the moments is adopted. As for step (III), the additional cost of incorporating the extra terms in the Taylor expansions is small, since cell-cell distances are already available.

In step (V), the shifting expressions for the Taylor coefficients are independent of the forms of the coefficients. Hence, even though the Taylor coefficients obtained by Taylor expanding Eq (5) (i.e., using definition (B) for the moments) are more complex than the coefficients obtained by expanding Eq (1) (i.e., using definition (A) for the moments), the Taylor shifting expressions are identical in both cases. This is the key difference between the Taylor shifting expressions and the moment shifting expressions which is exploited below. With regard to steps (I), (III), (IV), and (V), using definition (B) of the moments instead of definition (A) will most likely result in a speed-up, although in some cases there may be no advantage in selecting one definition over the other.

However, in step (II) there are two clear advantages to favoring definition (B) for the quadrupole and higher moments, over definition (A). First, the shifting expressions for the moments with definition (B) are easier to derive than the shifting expressions for the moments with definition (A). They are also simpler, and more symmetric (i.e., easier to code) than the shifting expressions with definition (A). They parallel in simplicity and symmetry the Taylor shifting expressions in step (V). For example, the shifting expression for the quadrupole moment with definition (B) is

$$Q_{\alpha\beta}^{\prime(l-1)} = \sum_{k=1}^{8}[Q_{\alpha\beta}^{\prime(l)}]_k + \sum_{k=1}^{8}\{[\mu_\alpha^{(l)}]_k[C_\beta]_k + [\mu_\beta^{(l)}]_k[C_\alpha]_k\} + \sum_{k=1}^{8}[Z^{(l)}]_k[C_\alpha]_k[C_\beta]_k , \qquad (7)$$

and for the octopole moment with definition (B)

$$
\begin{aligned}
O_{\alpha\beta\gamma}^{\prime(l-1)} &= \sum_{k=1}^{8}[O_{\alpha\beta\gamma}^{\prime(l)}]_k + \sum_{k=1}^{8}\{[Q_{\alpha\beta}^{\prime(l)}]_k[C_\gamma]_k + [Q_{\alpha\gamma}^{\prime(l)}]_k[C_\beta]_k + [Q_{\beta\gamma}^{\prime(l)}]_k[C_\alpha]_k\} \\
&+ \sum_{k=1}^{8}\{[\mu_\alpha^{(l)}]_k[C_\beta]_k[C_\gamma]_k + [\mu_\beta^{(l)}]_k[C_\alpha]_k[C_\gamma]_k + [\mu_\gamma^{(l)}]_k[C_\alpha]_k[C_\beta]_k\} \\
&+ \sum_{k=1}^{8}[Z^{(l)}]_k[C_\alpha]_k[C_\beta]_k[C_\gamma]_k .
\end{aligned}
\qquad (8)
$$

Eqs (7) and (8) are clearly more compact expressions than Eqs (3) and (4), respectively. The relative ease in deriving and coding the shifting expressions for moments with definition (B) becomes more significant when higher order moments are needed. Shifting expressions for octopole (see Eq (4)) and higher moments (e.g., hexadecapoles,...) with definition (A), are increasingly tedious to derive and code. Second, the shifting expressions for the moments with definition (B) contain fewer terms (i.e., operations) than the shifting expressions for the moments with definition (A) (compare Eqs (7) and (8) with Eqs (3) and (4), respectively). Again, Eqs (7) and (8) do not require child-parent distance computations. They are much cheaper to compute than the shifting expressions with definition (A). Again, the relative gain in efficiency increases with increasing order of moments used. The gain in efficiency in step (II), resulting from the use of definition (B) for the moments, will result in substantial speed-up. Overall then, adopting definition (B) for the moments (with expansion in Eq (5)) in CMM is more beneficial than using definition (A) (with expansion in Eq (1)).

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And the rest is chemistry...

Philip Lindan and Nic Harrison.

Using ab initio calculations to understand how surfaces relax, reconstruct and react chemically with water, ammonia or other molecules demands serious computer power. For oxides the task is especially difficult, and the work we are undertaking on TiO_2 surfaces would be impossible without machines like the new CRAY T3D at Edinburgh . Using such massively parallel machines means that another exciting push forward for first-principles simulations is underway in the UK.

This article was first published in a new Daresbury newsletter on high performance computing "HPC Profile".

In just ten years, quantum mechanical calculations of the energetics of condensed matter, based on the use of density-functional theory, pseudopotentials and a plane-wave basis set, have risen from relative obscurity to dominance in ab initio structural calculations [1]. Leaps in both algorithmic techniques and computer technology produced this explosive growth in the power of the method. In 1985 the key features which were to prove so successful were drawn together by Car and Parrinello [2]: the most important of these was that finding the self-consistent electronic ground state could be tackled through global minimisation rather than matrix diagonalisation. The crucial feature of this "Car-Parrinello" approach is the improved scaling with system size, meaning simply that more atoms can be studied for the same computer cost. However, for moderate system sizes (e.g. 20-100 silicon atoms) on conventional supercomputers this cost is still considerable, while for large systems it becomes prohibitive.

Naturally, then, there exists a strong desire to exploit the enormous potential of parallel computing technology which has been rapidly maturing over the same period. The focus of efforts within the UK has been the "Grand Challenge" project devoted to ab initio simulation on parallel computers, conceived to exploit the newest and best high-performance computer technology to do great science. The UK Car-Parrinello (UKCP) consortium of which our work is a part is a bigger and more ambitious outgrowth of the original project. Judged by any standards these efforts have been and continue to be remarkably successful scientifically, largely because they bring exceptional computer resources to bear on otherwise intractable problems.

The 320-processor, 64 MB-per-node CRAY T3D is comfortably the most powerful machine currently available to the UK's academics, even though the theoretical 40 GFlop rating has not been approached in practice. The UKCP community is already exploring the capabilities of the new machine, benefiting from the several years of intensive code development and experience with parallel calculations using the CETEP [3] code. The reality is that calculations which were at the limit of previous resources' capabilities are almost routine on the T3D, indicating that new horizons are within reach.

We believe that understanding chemical processes at the surfaces of oxide materials via first-principles simulation lies within these new horizons. Our project, funded by CRAY research and jointly managed by CCP3 and CCP5 at Daresbury, targets molecular processes at TiO_2 surfaces. To place this in a broader context, three other TiO_2 ventures are underway at Daresbury: one is using fluid dynamics to model gas-phase production of the material, funded by Tioxide Ltd.; a ROPA award from the OST is supporting classical modelling of the morphology and growth of TiO_2 crystals; and a Europe-wide HCM collaboration applying crystal Hartree-Fock methods to oxides incorporates work on TiO_2 surface properties. A clue as to why so much interest is being

aroused comes from the diverse uses of TiO_2, which include those as a catalyst, a paint pigment and a gas sensor, all of which depend crucially on its surface chemistry. The amount of hard information to hand is surprisingly limited though, since experiments must overcome problems inherent in the study of oxides. To take an example, STM imaging runs into trouble due to surface charging. However, as previous first-principles work has shown [4], a vital, fundamental contribution to understanding can be gained from simulation. Add to these facts the nature of TiO_2 - semi-ionic in character, with anomalously large, anisotropic dielectric constants and unusual vibrational properties - and a pleasant cocktail of incentive, challenge and possible reward is formed.

Our initial goal is to unravel the question of whether or not some of the surface orientations of TiO_2 are more stable in a reconstructed state. An illustration of this appears in "HPC-Profile". While careful experimental work has shown that such reconstructions may occur [5], atomic-level interpretation of the results is difficult and sample condition hard to control. For us, even this relatively modest aim will involve dealing with a large system, and additionally the combination of transition-metal and oxygen ions results (through the difficult pseudopotentials) in very demanding calculations - a characteristic of Car-Parrinello studies of oxides [4]. Once we move onto more complex studies such as water absorption and dissociation, or the reaction of SO_2 at TiO_2 surfaces, the technical demands become enormous. It is no exaggeration to say that the T3D is at present the only resource for the job, and it offers an opportunity for this project, and others like it, to impact decisively upon problems at the very forefront of surface science research.

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MARVIN: A new computer code for studying surfaces and interfaces

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1 Overview

Inorganic surfaces and their interaction with molecules play a significant role in a wide range of processes such as catalysis, crystal growth, corrosion and electrolysis. Only limited experimental information on the detailed structure of inorganic surfaces is available. Therefore, atomistic simulations can help us to understand the details of surface chemistry. It is this void that MARVIN'S PROGRAM (Minimisation And Relaxation of Vacancies and Interstitials for Neutral Surfaces, Program) or MARVIN is designed to fill.

To date, MARVIN has been applied to many types of surface simulation problems. A few of these problems include surface structure and crystal morphology, [1] the atomic force microscopy (AFM) imaging process, [2] and the structure of small clusters on surfaces [3].

MARVIN is not a program that uses new techniques, but a new program incorporating the ideas and formalisms of both MIDAS [4] and organic molecular mechanics modelling. The techniques used in MIDAS have been expanded to include more potential types and the concept of molecules and connectivity. These control the building of crystals and the specifying of potentials, the result of which is a more flexible program that allows not only the modelling of simple inorganic surfaces and their interfaces but also the surfaces of molecular and molecular ionic systems and the docking of molecules and ions.

2 Features

As in MIDAS, the foundation of MARVIN is a "full" 2-dimensional Ewald sum [5]. The short-range two-body interactions can be represented with the following functional forms: Lennard-Jones, Buckingham, Morse, harmonic, cubic spline, and coulomb-subtract. These can also be used in arbitrary combinations. The harmonic three-body bond bending and four-body torsion terms are also included for modelling silicates, molecular solids and organic molecules adsorbed on surfaces.

Currently, two different minimisers have been implemented in MARVIN, conjugate-gradient and BFGS [6]. The convergence properties of these minimisers is complementary. Conjugate-gradient works very well for large numbers of atoms and high gradients, while BFGS works better when the gradient is lower.

The program MARVIN was written in "C", to take advantage of three key features of the language. The first reason is that dynamic memory allocation routines are standardised in "C". This allows the program to allocate memory as it needs it and eliminates the need to recompile the program when the problem size increases. Also, "C" allows for data abstraction, for example structures and unions. This helps to create a cleaner program, with groupings of related parameters. The final reason, is the ease of writing an input parser that allows for a "user friendly" input file.
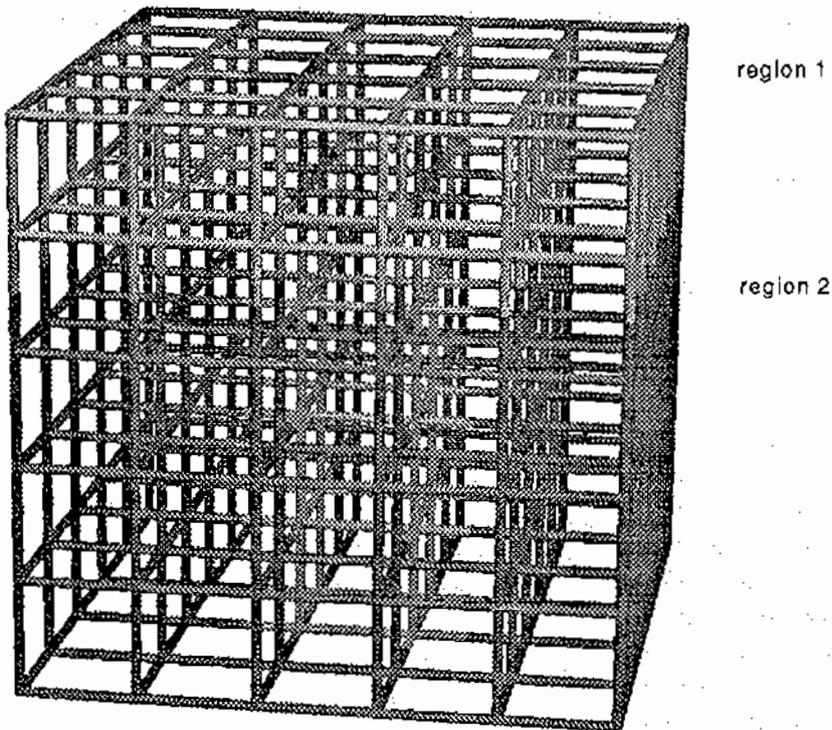
region 1

region 2

Figure 1: MgO (100) surface illustrating how MARVIN creates an infinite surface with semi-infinite depth. The centre contrasting atoms are the 2-dimensional unit cell. The top "light" region is region 1, and lattice repeats of region 1. The bottom "dark" region is region 2.

3   Methodology

Currently, MARVIN can perform energy minimisation of surfaces, interfaces and surfaces with molecules (small clusters, AFM tips) adsorbed near them. The program is limited to neutral defects because of the 2 dimensional periodicity. As mentioned earlier, the electrostatic contribution is computed with an Ewald sum. The short-range potentials are also computed with a lattice sum instead of using "minimum image".

The energy minimisation is performed for a 2 dimensional cell that is divided into two regions (see Figure 1). The two regions are called *region 1* and *region 2*. The atoms in region 1 are allowed to relax to minimise the total energy. While the region 2 atoms are fixed to reproduce the effect of the bulk crystal. The total energy is defined as the energy of region 1 embedded in a crystal composed of lattice repeats of itself and region 2.

Along with the total energy, MARVIN also calculates the surface energy, and the attachment energy before and after relaxation. The *surface energy* is the energy required to cleave the crystal. The *attachment energy* is the energy released when a "growth slice" is attached to the surface. The effects of relaxation on these quantities are significant and can be quite dramatic.
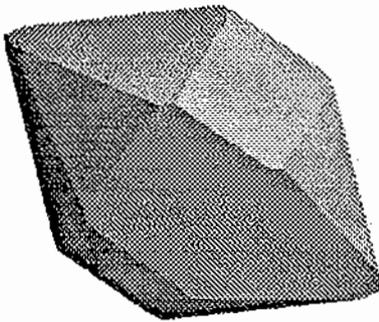
22

Figure 2: Growth morphology of α-quartz, based on relaxed attachment energies computed by MARVIN. This is very similar to geological samples of quartz.

4 Application: α-quartz

An example application of MARVIN is α-quartz. The surface of quartz has to be terminated with hydroxides to fill the bonds broken by cleaving the surface. The resulting *growth morphology* is shown in figure 2, resembles very closely the observed crystal. More details about these calculations will be published soon [7]. The equilibrium morphology for α-quartz system exhibits the systematic problem of equilibrium morphologies. This problem is the appearance of high index faces due to the large reduction of surface energy during the minimisation procedure. The result of this surface energy reduction is that the morphology becomes spherical. This problem has yet to be explained [8].

ACKNOWLEDGMENTS

5 Conditions for distribution

Presently, MARVIN is distributed free of charge as an executable only. The source code is available to groups that wish to establish a collaboration with the authors on specific projects requiring code development.

For information about the availability of the code and a rough draft of the manual please contact me at: "dgay@ricx.ri.ac.uk".

We have not had any trouble porting the code to any of the following workstations: IBM/ RS6000, SGI, HP, Sun Sparc, and DEC.

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Computer simulation of liquid crystals on the T3D

Mike Allen, Mark Warren (Bristol University)
Mark Wilson (Lancaster University)
Alain Sauron (Sheffield Hallam University)
Bill Smith (Daresbury Laboratory)

Over the last few years, CCP5 has supported a collaboration of U.K. simulation groups interested in the modelling of liquid crystals (M. P. Allen, Physics, Bristol University; C. M. Care, Physics, Sheffield Hallam University; D. J. Cleaver, Physics, Sheffield Hallam University; G. Jackson, Chemistry, Sheffield University; G. R. Luckhurst, Chemistry, Southampton University; A. J. Masters, Chemistry, Manchester University; M. Neal, Mathematics, Derby University; M. R. Wilson, Physics and Materials, Lancaster University). This has now evolved into a so-called 'Consortium' using the new Cray T3D parallel supercomputer at Edinburgh, within the EPSRC's High-Performance Computing Initiative.

Liquid crystals are important because of their technological properties; they also provide fascinating challenges in statistical mechanics. To understand them from the theoretical perspective, we frequently adopt very simple models of the constituent molecules. Representing the molecule as a hard, elongated, rigid body is a good starting point, as it includes the fundamental physics associated with packing effects in the liquid. Softening the repulsive potential, and adding simple attractive forces between the molecules, are the obvious next steps.

One of the standard models of this kind, the 'Gay-Berne' model has been extensively studied in recent years. As well as the isotropic, or disordered liquid, it exhibits several liquid crystal phases, the simplest of which is the nematic: here the molecular orientations are preferentially aligned in space, but all other kinds of order are short-ranged. Various layered, smectic, phases are also seen. By applying suitable periodic boundary conditions, it is possible to twist the preferred direction (the 'director') into a helical structure, of the kind used in display devices. When such a twist is applied to a smectic phase, the director almost always finds it impossible to vary in a uniform fashion, because this would entail a substantial distortion energy for the layers; instead it forms domains of more-or-less uniform alignment, separated by grain boundaries at which a sudden jump in alignment occurs. These 'twist grain boundary phases' have become hot topics in theory and experiment over the last few years. To simulate them requires very large system sizes, both along the axis of twist (so that the twist period is not too short) and in the transverse directions (to allow the layers as much freedom as possible to choose an orientation subject to periodic boundary conditions).

We have recently developed an efficient code for running molecular dynamics of the Gay-Berne system on parallel computers. It is based on the CCP5 code for atomic fluids, MDMEGA It uses a domain decomposition technique with linked lists, and message-passing via PVM. This program has been benchmarked on a range of parallel computers including the new T3D at Edinburgh. It shows excellent speedup characteristics with increasing numbers of processors (see the figure) for system sizes of interest to us.

We have completed our preliminary simulations in which a twisted nematic liquid crystal system is cooled into the smectic region of the phase diagram, and the grain boundary formation is observed directly. We used 27000 Gay-Berne molecules, equilibrated for several tens of thousands of steps, and observed three smectic domains within the modified periodic boundaries. This is encouraging, but to increase our confidence that the domain orientation and thickness are not strongly influenced by the boundary conditions, we shall have to repeat the exercise with larger samples. As a separate exercise, we have quenched a 64000-particle isotropic system into the nematic phase, with the intention of examining the large-scale processes of defect annealing that accompany orientational

GBMEGA PROGRAM
- DOMAIN DECOMPOSITION APPROACH

approx. speed ups
relative to 1 processor

16384 molecules

2048 molecules

speed ups

processors
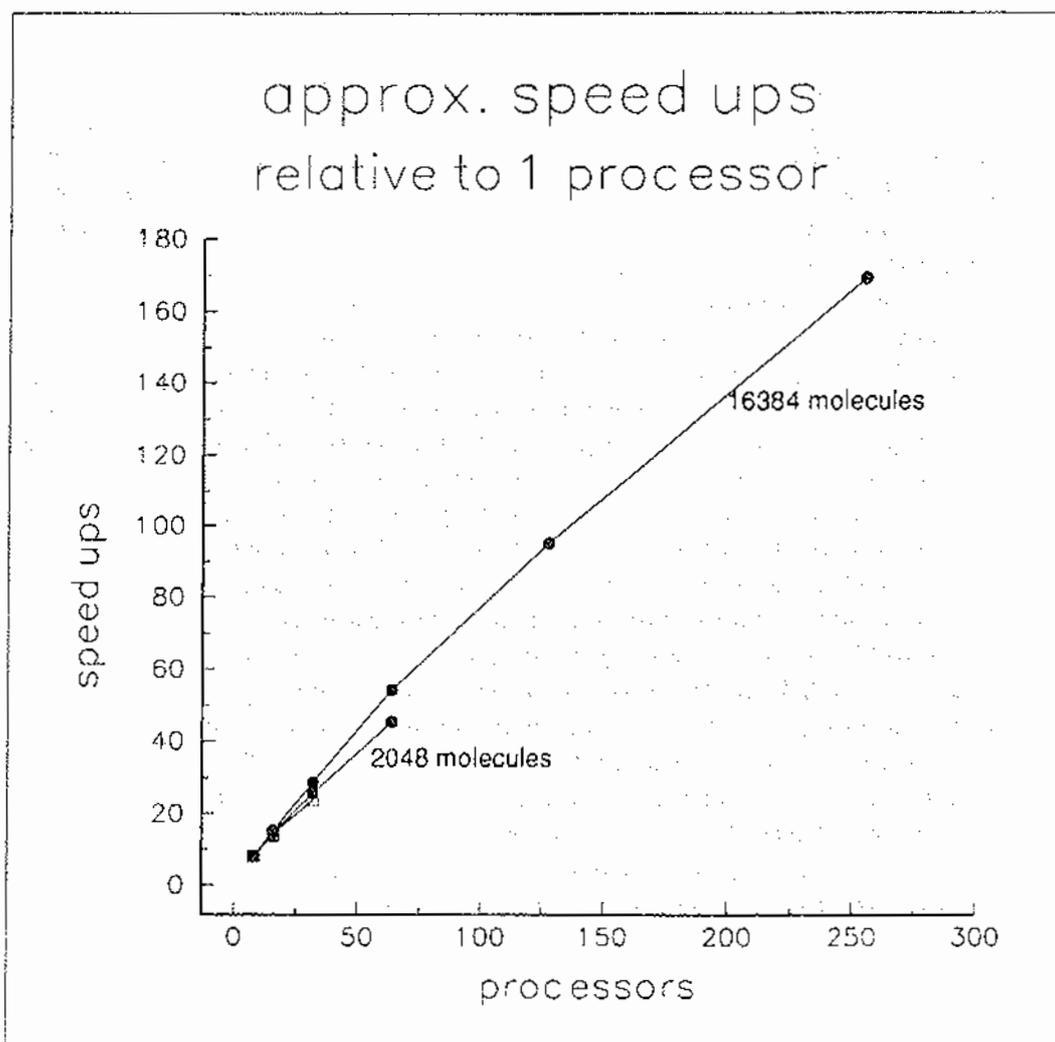
ordering. There is the prospect of extending this work to look at long-ranged director correlations in the equilibrated nematic sample, something that again requires large system sizes and reasonably long runs. Some colour pictures of configurations produced on the Edinburgh T3D may be seen on our WWW pages, starting at *http://www.phy.bris.ac.uk/ research/theory/simulation.html*.

Other members of the consortium are now actively looking at various extensions of the Gay-Berne potential which may produce liquid crystal phases with large-scale structural features of the kind that can only be investigated with powerful parallel computing facilities. At the same time, the Consortium has a code development programme, supported via the HPCI Centre at Southampton University, which should increase the range of models and simulation techniques that we can use on the T3D. We hope to produce reports on these activities in due course.

The DL_POLY Project

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Background

The DL_POLY project, one of the last to be funded by the former Science and Materials Computing Committee of the EPSRC, is now beginning to make a real impact on molecular dynamics simulation in the UK. The project was conceived as a flagship for CCP5, with the aim of developing a general purpose parallel simulation package to exploit the new generation of distributed memory parallel computers that were appearing with great promise in the early 1990s.

Work began on DL_POLY in 1992 at Daresbury Laboratory, where the Intel iPSC/860 computer was readily available as a development platform. The SMCC stepped in later that year and sponsored a PDRA to complete its development. This permitted two years of intensive effort, resulting in the first public release of DL_POLY (Version 1.1) which is described below. At the time of the SMCC award little was known about the procurement which later became the T3D supercomputer at Edinburgh. The appearance of that machine, which is ideally suited to the programming strategy of DL_POLY, encouraged the SMCC to support the project for a further two years. We are already well on the way to producing an enhanced version of the original code, as we describe below.

DL_POLY Version 1.1

As mentioned above DL_POLY is a parallel Molecular Dynamics simulation package capable of simulating a wide range of molecular and atomistic systems. Version 1.1 was made generally available in October 1994 and currently there are over 40 registered users world wide. The code was based on the Intel iPSC/860 architecture, which is a distributed memory machine with an underlying hypercube communications network. This communication network permits highly efficient global summation algorithms and this encouraged the adoption of a *Replicated Data* strategy for the parallelisation of the molecular dynamics. This strategy, we anticipated, would be reasonably efficient up to perhaps 100 nodes (we had 64) provided the simulated system was significantly large ($\sim$2000 atoms or more). However hardware developments have overtaken us here and we have since found the method to be highly efficient on 256 nodes of the T3D (see performance graph). Added to this, the RD strategy is very easy to scale down to a single processor, and in fact most of our users run the code on single processor machines and have found the adaptation straightforward. We hope that the temptation to upgrade to a multiprocessor will be overwhelming, since it can be accomplished trivially easily - the same data files can be used!

The range of systems DL_POLY can simulate is large. We are adding new features all the time. However, Version 1.1 is static and has the following capabilities

- all common periodic boundary conditions (including non-periodic)

- all common short-ranged pair potentials (Lennard-Jones, Born-Huggins-Meyer etc).

- atomic partial charges handled by the Ewald sum, direct summation or a distant dependent dielectric.

- rigid bond constraints (the SHAKE algorithm)

- extensible bonds

- three body and four body potentials (i.e. valence angle and dihedral angle potentials)

- external fields

- microcanonical and canonical ensembles.

Typical systems that can be simulated using version 1.1 are

- Simple atomic systems and mixtures e.g. Ne, Ar, Kr, etc.

- Simple unpolarisable point ions e.g. NaCl, KCl, MgO, etc.

- Rigid molecules with partial charges e.g. H_2O, CCl_4, SF_6 etc.

- Polymers with partial charges and a mixture of extensible and rigid bonds e.g. $C_nH_{(2n+2)}$, proteins etc.

- Macromolecules, Zeolites, and biological systems.

- Mixtures of all the above

Readers interested in finding out more about DL_POLY are invited to access the World Wide Webb page for the package as described in the following section.

In Version 1.1 there are no facilities for rigid body dynamics, beyond using simple bond constraints. This deficiency will be dealt with in later releases. The other point worth mentioning is that DL_POLY does support a multiple timestep algorithm, an essential for large scale simulations.

Obtaining the Source Code

To obtain a copy of DL_POLY it is first necessary to obtain a licence from Daresbury Laboratory. A copy of the licence form may be obtained in two ways: either by selecting the licence button on the World Wide Web page

```
http://www.dl.ac.uk/TCSC/Software/DL_POLY/main.html
```

and downloading and printing the file; or by using ftp to copy the postscript file from the CCP5 Program Library at Daresbury Laboratory in the following manner:

```
-> move to the desired directory on YOUR machine,
-> type: ftp 148.79.80.10 or ftp ftp.dl.ac.uk
-> enter userid: anonymous
-> enter passwd: (use your name and site)
-> change to the CCP5 directory: cd ccp5
-> change to the DL_POLY directory: cd DL_POLY
-> type: binary (for postscript files)
-> type: get LICENCE.ps.Z
-> type: quit
```

The licence file will need to be uncompressed (using the unix uncompress command) before printing.

Once you have obtained the licence form you must sign it and return it to: Dr W. Smith or Dr. T.R. Forester, by post, at the following address.

```
DL_POLY Program Library
Theory and Computational Science
EPSRC Daresbury Laboratory
Daresbury
Warrington WA4 4AD
England
```

When the signed licence has been received DL_POLY source code will be sent by ftp. To enable this we will require a *guest id and password on your machine*. Please note we will not create accounts on any of our machines for this purpose.

These restrictions do not apply to the DL_POLY documentation. The DL_POLY Manual will be freely available via World Wide Web or ftp, in the same manner as the licence form. The DL_POLY Reference Manual will be available by the above ftp procedure only.
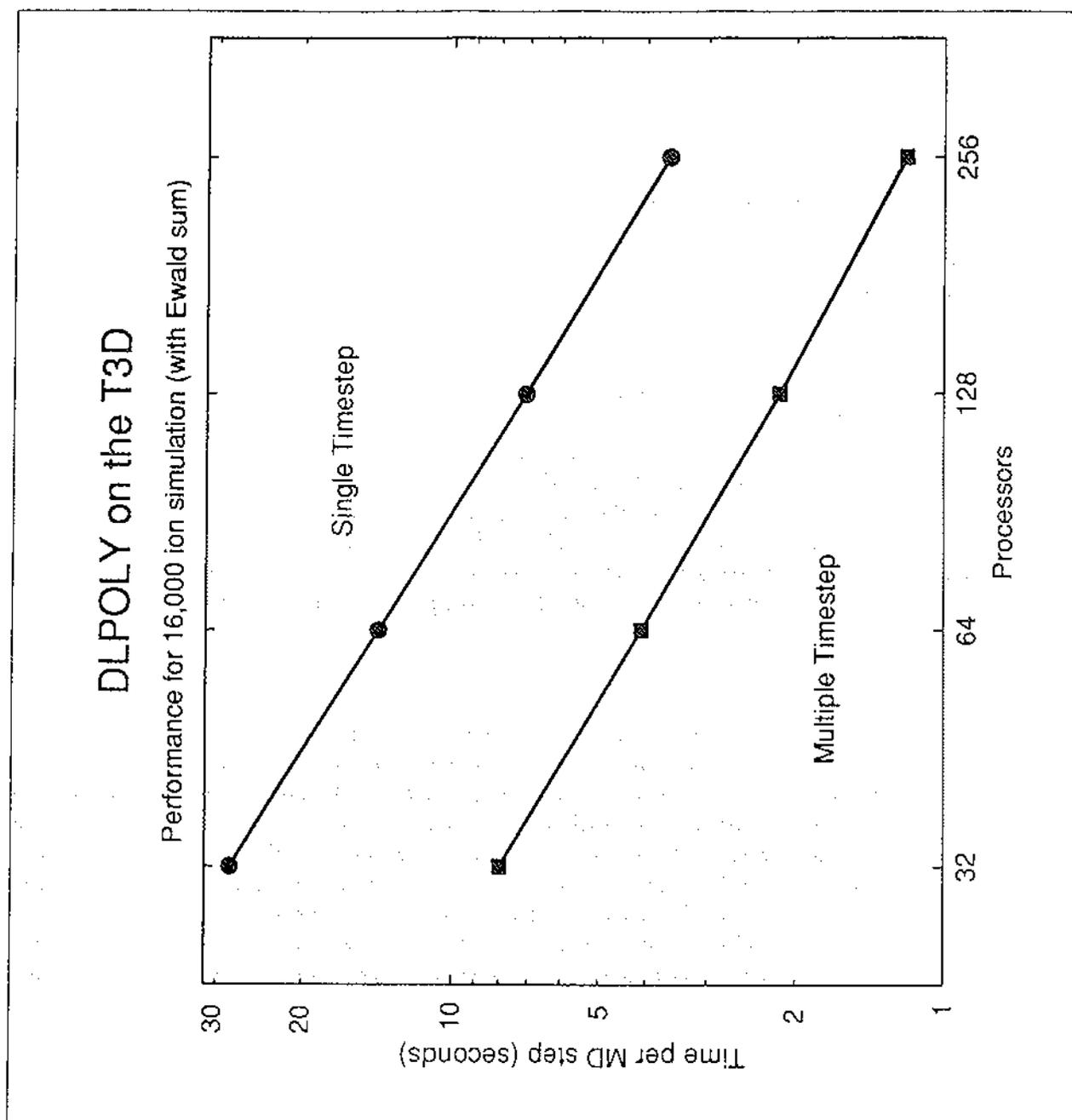
Please note that Daresbury Laboratory is the sole centre for the distribution of DL_POLY and copies obtained from elsewhere will be regarded as illegal and will not be supported.

DL_POLY and the Cray T3D

Over the past few months most of our work on the DL_POLY project has focussed on a version for the Edinburgh Cray-T3D. The adaptation of the code for the T3D was greatly accelerated by the assistance of the Edinburgh Parallel Computing Centre, in the person of Alan Simpson. In the event, the practice we had adopted in DL_POLY, of localising the communications inside a handful of short and easily identified routines, greatly aided the process. A full SHMEM version has been implemented and for suitably large systems (i.e. those with approx 15,000 atoms or more) the scaling performance up to the full capacity of the machine (256 processors) is very encouraging. With 256 processors a parallel efficiency of approximately 85% was obtained for a 16,000 atom case that included an Ewald sum converged to 6 significant figures. Higher efficiencies were obtained with smaller number of processors (*viz.* 128 or 64). The program runs at approximately 10-15 MFlops per processor, giving a performance of between 2-3 GFlops on 256 processors allowing a turn around of approximately 1.2 seconds per MD time-step for the 16000 ion Ewald sum simulation.

It is a very fortunate accident history that the Cray T3D became available just as the first version of DL_POLY was reaching fruition. As a result, the code became the natural choice for simulators seeking T3D time. The T3D code is an integral part of the "Long time-scale Molecular Dynamics" group of the Materials Consortium. (We should point out however, that for operational reasons this version of the code is currently available to *Consortium members only*. With this code good progress is being made on a number of key scientific projects including:

1. the capture and transport of potassium by the naturally occurring antibiotic valinomycin at a model membrane / water interface (Tim Forester, Daresbury);

2. diffusion of hydrocarbons in Zeolites (Paul Barram, Bath);

3. diffusion of alkali ions in silicate glasses (the "mixed alkali" effect) (Bill Smith, Daresbury); and

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DLPOLY on the T3D

Performance for 16,000 ion simulation (with Ewald sum)

Single Timestep

Multiple Timestep

Time per MD step (seconds)

30 20 10 5 2 1

32 64 128 256

Processors

4. amorphous polyelectrolyte systems (Rob Bell, Royal Institution).

These projects are at different stages, though a great deal has been done on the valinomycin and glass projects, about which we hope to report in later newsletters.

In addition to these projects, others are waiting to commence which will also require DL_POLY as a simulation platform, these include;

1. the phase diagram for clathrate hydrates (Mark Rodger, Reading);

2. the study of defects in ceramic materials (Donnell MacDonaill, Dublin);

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3. the structure and thermodynamics of oxide crystallites (Bill Mackrodt, St-Andrews); and

4. adsorption on surfaces (D.J. Tildesley, Southampton)

With the excellent projects currently running and those waiting in the wings, it is apparent that DL_POLY is set to become a major code in UK simulations. An outcome we hope fully justifies the resources made available to it. This is clearly an exciting era for large scale molecular dynamics simulation.

Fourth Liblice Conference on the Statistical Mechanics of Liquids

June 6-10, 1994, Lake Milovy, Czech Republic

Keith E. Gubbins Cornell University Ithaca, New York 14853

Organizers: Ivo Nezbeda (email: ivonez@earn.cvut.cz; tel:42-2-24311498; fax:42-2-342073), E. Hála Lab. of Thermodynamics, Inst. Chem. Process Fundamentals, Acad.Sci., Rozvojová 135, 165-02 Prague 6-Suchdol, Czech Republic; and Keith Gubbins (email: keg@cheme.cornell.edu; tel:1-607-255-4385; fax:1-607-255-9166), School of Chemical Engineering, Cornell University, Ithaca, New York 14853, U.S.A.

These conferences are held every 4 years, and cover both fundamental and applied aspects of theory and molecular simulation of liquids. They are organized by Ivo Nezbeda with help from some of his colleagues in the Czech Academy of Sciences, together with an international program committee. The first such conference was held in Liblice castle (hence the conference name), and the next two were held in another castle, Bechyne, used by the Academy. This fourth meeting departed from tradition in being held at a resort in the Czech-Moravian Highlands. Over 100 scientists attended, of whom over 90% were from overseas countries.

The conference followed its usual format, with an opening lecture on the Monday evening by a well-known specialist (John Valleau of Toronto University), followed by four morning, three evening and poster sessions. Afternoons were free for relaxation, discussions or excursions. A workshop sponsored by CECAM, "Novel Trends in the Simulation of Complex Liquids", and chaired by Daan Frenkel (FOM Amsterdam) formed an integral part of the conference, and occupied the first two sessions. A panel discussion towards the end of the meeting on "Perspectives for CECAM Initiatives on Simulation on Complex Fluids" was aimed at identifying topics for future CECAM workshops. Among the ideas put forward were several concerned with improved intermolecular potentials for both small molecules (particularly water) and macromolecules, and with the effects of confinement on fluid and material properties. Other sessions were concerned with theory of liquids, inhomogeneous fluids, polar and ionic fluids, associating fluids, and chain molecule fluids.

The oral papers presented are listed below. Please note that only the speaker is listed. Others may have been involved in the work. In addition to the oral papers listed below there were 78 poster papers.

The next conference, Liblice 5, is expected to take place in June 1998.

OPENING

J. Valleau	(Toronto):	Teaching an old dog new tricks: Some recent (and useful) Monte Carlo stunts

CECAM WORKSHOP:

NOVEL TRENDS IN THE SIMULATION OF COMPLEX LIQUIDS

Chairmen: D. Frenkel (Amsterdam) and D. Henderson (Mexico City)

A. Panagiotopoulos	(Ithaca):	Monte Carlo simulations of phase coexistence

D. Kofke	(Buffalo):	Phase coexistence properties by molecular simulation: Gibbs-Duhem integration
W.R. Smith	(Guelph):	Chemical and phase equilbria from a new reaction ensemble
J. Fischer	(Bochum):	MD study of evaporation from a free surface
B. Smit	(Amsterdam):	Simulation of complex fluids: Recent progress
E. de Miguel	(Sevilla):	Simulation of liquid crystals: An attempt to go beyond hard-core models
J.W. Perram	(Odense):	The object-oriented development vof a parallel application in polymer dynamics
B. Mulder	(Amsterdam):	Flexible formalism for persistent chains
P.T. Cummings	(Oak Ridge):	Molecular simulation of phase equilibria in electrolyte systems
I. Snook	(Melbourne):	Million atom simulations and application to surfaces and colloids
W.A. Steele	(University Park):	Simulation of fluids confined in pores of complex shape
R. Holyst	(Warsaw):	Edge dislocations in thin films and near surfaces
E. Piotrovskaya	(St. Petersburg):	Computer simulation of two-phase coexistence of the LJ fluid in narrow pores
J. Talbot	(West Lafayette):	Properties of a hard ellipsoidal fluid confined in a slit pore

THEORY

Chairman: J. Fischer (Bochum)

Y. Rosenfeld	(Beer-Sheva):	The "ideal" liquid: Definition, properties, and applications
J.K. Percus	(New York):	Structure of entropy functionals
P.A. Monson	(Amherst):	A theory of solid solutions
D. Evans	(Canberra):	Relations between phase space stability and thermophysical properties
S. Labík	(Prague):	A new geometrically-based integral equation hierarchy for hard sphere fluids

INHOMOGENEOUS FLUIDS

Chairman: W.A. Steele (University Park)

M.L. Rosinberg	(Paris):	Perturbation density functional theory for inhomogeneous polyatomic fluids
S. Sokolowski	(Lublin):	The effect of pore closure on capillary condensation using density functionals
G. Stell	(Stony Brook):	Quenched-annealed systems
E. Glandt	(Philadelphia):	Molecular fluids in random media

K.E. Gubbins	(Ithaca):	Molecular simulation of simple fluids and water in well-characterized pores
L. Blum	(Rio Pedras):	Structured charged interfaces: Theory and experiment
A.D.J. Haymet	(Sydney):	Water and electrolytes near charged interfaces
G.M. Torrie	(Kingston):	Recent results for wholly molecular theories of electrical double layers

POLAR AND IONIC FLUIDS

Chairman: J.W. Perram (Odense)

G. Patey	(Vancouver):	From dipolar fluids to ferroelectric liquid crystals
M. van Leeuwen	(Amsterdam):	Polar fluid mixtures
P. Kusalik	(Halifax):	The dielectric constant and the distribution of the total dipole moment in polar fluids
H. Nishimura	(Tokyo):	The HNC equation approach to polar liquids

ASSOCIATING FLUIDS

Chairman: K.E. Gubbins (Ithaca)

M. Mezei	(New York):	Issues in modeling liquid water
P.G. Debenedetti	(Princeton):	Supercooled and glassy water: Theory, simulations, and experiments
E.S. Yakub	(Odessa):	Statistical thermodynamics of fluids with saturative attractive forces
M.F. Holovko	(Lwow):	Integral equation theory for the effects of association in ionic fluids
L. Blum	(Rio Pedras):	The solution of the OZ equation for anisotropic sticky spheres: Towards a model of water

PANEL DISCUSSION:

PERSPECTIVES FOR CECAM INITIATIVES ON SIMULATION ON COMPLEX FLUIDS

Moderator: N. Quirke (Orsay)
    Speakers:
    P.T. Cummings (Oak Ridge)
    D. Frenkel (Amsterdam)
    K.E. Gubbins (Ithaca)
    J.W. Perram (Odense)

NORMAL AND CHAIN-MOLECULE FLUIDS

Chairmen: W.R. Smith (Guelph), E. Glandt (Philadelphia)

M.S. Wertheim	(Haughton):	Fluids of hard convex molecules
D. Henderson	(Mexico City):	Bridge functions and correlation functions for hard spheres using inhomogeneous integral equations
T. Boublík	(Prague):	Hard body fluids: The 3rd virial coefficient and equations of state
R. Lustig	(Aachen):	Simulating equations of state
B. Borstnik	(Ljubljana):	Approaching the Baxter's sticky limit by molecular dynamics simulations
J. Vrabec	(Bochum):	Vapor-liquid phase equilibria of mixtures from the NpT + test particle method
F. del Rio	(Mexico City):	Theory and simulation of square-well mixtures
C. Hall	(Raleigh):	Generalized Flory dimer theory for hard chain molecules
Y.C. Chiew	(Piscataway):	Equation of state for chain molecules: Monte Carlo and perturbation theory results
M. Banaszak	(Annendale):	Equation of state for Lennard-Jones chains