Computing

LENDING COPY

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 41 May 1994

Contents

Editor: Dr. M. Leslie

DRAL Daresbury Laboratory
Daresbury, Warrington WA4 4AD UK

General News

Last Paper Copy

This is the last paper copy of this newsletter which will be distributed by ordinary post to all of our readers. (See Below).

Change of Address

Following government reorganisation of science in the UK, the functions of the Science and Engineering Research Council (SERC) have been split between a number of new bodies. Daresbury Laboratory has merged with the Rutherford Appleton Laboratory in Oxfordshire; the name of the combined laboratories will be abbreviated DRAL. Please note our new address.

FUTURE MEETINGS

A summary table is given below, further details may be found inside. CCP5 has been asked to publicize the University of Minnesota Supercomputer Institute meeting but is not involved with its organisation.

TOPIC	DATES	LOCATION
How to derive the interatomic potentials needed for simulation studies	4-5 July 1994	Oxford
Cellular Automata and their applications to Molecular Fluids	18-20 July 1994	Manchester
CCP5 ANNUAL MEETING:- ORDER IN LIQUIDS	5-7 September 1994	Sheffield
HIGH PERFORMANCE COMPUTING: A NEW ERA	7 July 1994	London
International Symposium on Computational Molecular Dynamics	24-26 October 1994	Minneapolis

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.

The 256-node Cray T3D parallel supercomputer for use in "Grand Challenge" scientific applications has been installed at the Edinburgh Parallel Computing Centre. Each node is a DEC Alpha RISC processor with 64 MB of memory and 150 Mflops peak performance. The current date for general user service is 1 July. Readers may access information about the hardware by anonymous ftp to ftp.cray.com, or by WWW. (Transfer the file product-info/mpp/T3D_overview.ps) Initially communication will be by PVM. CRAY are also providing a version of high performance Fortran called CRAFT. Information about this may be found by anonymous ftp to the above address, file product-info/mpp/program_model.ps. CCP5 submitted two applications from consortia of people for early user access to the T3D, both have been given allocations of time.

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.

EMAIL MAILING LIST AND RE-REGISTRATION OF READERS

The editor wishes to thank all of our readers who responded to the request in the last newsletter for up-to-date Email addresses, and also to those readers who were asked to re-register and have done so. Welcome also to new readers of these pages. It is important to get the Email list up to date as paper distribution of newsletters will be limited (See Below) and if you are not on the Email list we will not be able to notify you about new newsletters. A small number of readers have sent in Email addresses on paper to which I am unable to send messages. If you did not receive Email notification of this newsletter please send your Email address. Readers from the UK and Europe who have not responded to a request to re-register are not being sent this newsletter but will be sent a final letter. Readers from elsewhere in the world may not yet have had time to respond and this newsletter will be sent with an additional request to re-register.

PROPOSED ELECTRONIC DISTRIBUTION OF CCP5 NEWSLETTERS

The last newsletter outlined proposals for distribution of newsletters by Email. Comments were invited from our readers and an abstract of these is given below. In general comments have been overwhelmingly favourable to this method of distribution.

> Distribution of the entire newsletter directly by Email was suggested by a number of readers. We were also cautioned against doing this by a reader who distributes another newsletter in this way, and found that this caused problems for people with limited email bandwidth. We therefore intend to continue with the existing method of broadcasting a message to the Email list when a new newsletter is ready on the ftp server, with an index of articles.

Use of a searchable method was suggested for electronic distribution. Daresbury Laboratory has now set up a World Wide Web server and placed the newsletters on it. (See article below).

A small number of people experienced minor problems with the LaTeX file. These were connected with not having the capability for including postscript figures. It should be possible for readers to get the appropriate LaTeX software from one of a number of anonymous ftp site. There were also a small number of problems with postscript printers not being compatible with the postscript sent out.

Back issues of the newsletter will gradually be made available as individual articles rather than as complete newsletters. I will do this if I already have or can easily obtain an electronic copy, but readers should realise that a large amount of the material now only exists on paper. I will also be asking the author's consent to distribute the article in this way. 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).

I will continue to provide postscript and LaTeX, also I will provide compressed postscript.

A need was expressed for the facility to send incoming anonymous ftp; we hope to be able to set this up soon.

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.

Please note that the Daresbury ftp server now has an alias so you will not have to use the actual machine name. At some future date the directory structure of the ccp5 entry will be rationalised, with the two directories ccp5 and ccp5.newsletters appearing as subdirectories of a single ccp5 directory.

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. One of the articles was accepted in WORD format; this has been converted to postscript and made available in this form only.

REQUEST FOR CONTRIBUTIONS

Contributors to the current issue

Our thanks go to:

D. Frenkel G. Mooij	Institute for atomic and Molecular Physics Amsterdam The Netherlands

HOW TO GET THIS NEWSLETTER BY FTP

1.	move to the desired directory on YOUR machine	
2.	type:	ftp ftp.dl.ac.uk
3.	enter userid:	anonymous
4.	enter passwd:	*enter your name and site*
5.	change to ccp5.newsletters/41 directory:	cd ccp5.newsletters/41
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	mget newsletter_part?.ps
	compressed postscript from ps directory	mget newsletter_part?.ps.gz
	latex from latex directory	mget *.tex
8.		quit

M. Leslie W. Smith	DRAL Daresbury Laboratory
M. P. Allen	University of Bristol
D. J. Cleaver	Sheffield Hallam University
D.A. Mac Dónaill and D.A. Morton-Blake	Department of Chemistry, Trinity College, Dublin 2, Republic of Ireland.

The deadline for contributions for the next 2 newsletters will be **1 August 1994 and 1 December 1994** Readers are reminded that contributions are always welcome. Contributions may be sent by Email in LaTeX and we would be prepared to consider other formats on a trial basis.

Address

Dr. M. Leslie	Email	
DRAL Daresbury Laboratory,	INTERNET:	m.leslie@dl.ac.uk
Daresbury	EARN/BITNET:	m.leslie%dl.ac.uk@ukacrl
Warrington	Tel. +44 (0) 925 603334	
WA4 2LR	Fax +44 (0) 925 603634	
UK		

MEETING AND WORKSHOP ANNOUNCEMENTS

HOW TO DERIVE THE INTERATOMIC POTENTIALS NEEDED FOR SIMULATION STUDIES

A two day meeting to be held at Mansfield College Oxford from 12:00 on 4th July to 5:00 on 5th July 1994 Sponsored by CCP5

AIM: To encourage participants to air their results, experience and prejudices concerning the practice as well as the theory of how to derive useful atomistic modelling potentials. Both empirical fitting and ab initio techniques will be represented, as applied to bulk and surface studies of static and dynamic phenomena. Poster presentations are eagerly sought and short manuscripts accepted for the proceedings. The list of speakers includes:

David Cooper, Univ. Liverpool	A modern VB approach for interionic potentials
Julian Gale, Royal Institution	Future directions in empirical potential derivation
Mike Gillan, Univ. Keele	The computer modelling of oxide surfaces
Sally Price, UCL	Anisotropic atom-atom potentials for molecules
David Pettifor, Oxford Univ.	Bond order potentials for the atomistic simulation of covalent stytems
John Murrell, Univ. Sussex	Towards a general strategy for global interatomic potentials for elemental solids and clusters
Mike Payne, Cambridge Univ.	Ab initio data bases for testing empirical potentials
Paul Madden, Oxford Univ.	Realistic description of many-body polarisation effects in simulations of ionic systems

The cost for full board participants is £62 (including dinner on the 4th and lunch on both days). For those not needing overnight accommodation the cost is £42.

Due to the financial support of BIOSYM and Unilever plc. we are able to offer a full board reduced price of £30 for students. Those requiring further information please write to either:

R. W. Grimes
The Royal Institution
21 Albemarle St.
London W1X 4BS

A. H. Harker
Building 424.4
Harwell Laboratory
Didcot, Oxon. OX11 0RA

CCP5 ANNUAL MEETING

ORDER IN LIQUIDS

Sheffield Hallam University
5th to 7 September 1994

The Annual Meeting of CCP5 traditionally provides a forum for the presentation and discussion of the results of molecular simulations across a wide spectrum of scientific problems. In addition to satisfying this more general aim, the special theme of this meeting will be Order in Liquids. Molecular liquids and mesophases exhibit a wide variety of long range and short range order. Many molecular liquids exhibit self assembly and phase transitions in the presence of appropriate thermodynamic fields. The use of computer simulations is now an important tool in investigating these materials and also the way in which the intermolecular potentials yield the observed macroscopic behaviour. It is expected that the meeting will be broadly based but will include discussion of:- molecular liquids, polymers, lyotropic liquid crystals, thermotropic liquid crystals, self assembly, phase transitions, choice of potential, methods of extracting data from a simulation, methods for making comparison with experiment and methods for improving the efficiency of the simulation.

INVITED SPEAKERS

M P Allen	Structure in molecular liquids
D M Cates	Surfactant Solutions
D Frenkel	The escape of the critical point
J Goodfellow	The protein solvent interface
O Mouritsen	Local order in fluid lipid bilayers
M Rodger	Liquid structure and ordered solvation shells
C Zannoni	Computer simulation of some Gay-Berne liquid crystals

Contributed papers are warmly welcomed and there will be poster and oral sessions. The meeting and associated accommodation will be in a pleasant campus environment close to the centre of Sheffield. The meeting will begin with lunch on Monday the 5th September and end with lunch on Wednesday 7th September. The cost of £40 for pounds for non residents includes registration, lunches on all three days and coffee and tea breaks. The fee of £120 for residents includes, in addition, dinner on the Monday evening, the conference dinner on the Tuesday and bed and breakfast for the nights of the 5th and 6th. There is a reduced residential fee of £65 pounds for students whose application is supported by a letter from their supervisor. To book please send the attached registration form as soon as possible.

CCP5 ANNUAL CONFERENCE : 'Order in Liquids'

5-7 September 1994
at Sheffield Hallam University

Registration Form

A Prof./Dr./Mr./Mrs./Ms./Miss (please circle) Surname:

Initials: First Name: Male/Female

B Affiliation:

C Address for communication:

Telephone: Fax:

EMail:

D Conference Fees (please circle appropriate box):

	Non-Student	Student
Resident	£120	£65
Non-Resident (with conf. dinner)	£55	£40
Non-Resident (without conf. dinner)	£40	£25

** £10 discount for residential registrations before 15 July 1994 **

Please indicate if you require vegetarian food (yes).

E Extra Accommodation Requirements (please circle appropriate box):

	Sunday 4th	Wednesday 7th
Evening Meal, B&B	£33	£33
B&B	£22	£22

Total Enclosed (D+E-discount): ....
Please make cheques payable to Sheffield Hallam University.

F Contributed Paper(s) (please give title(s) and enclose camera-ready abstract(s))

Title(s):

Please indicate whether these papers would be oral (O), poster (P) or either (O/P).

DEADLINE FOR REGISTRATION: 15 AUGUST 1994

Please complete and return to:

Trisha Hunt, Conference Administrator,
The Materials Research Institute,
Sheffield Hallam University,
Pond Street, Sheffield, S1 1WB.
Tel: 0742-533500 Fax: 0742-533501

Prof C M Care
Materials Research Institute
Sheffield Hallam University
Pond Street
Sheffield
S1 1WB
Email: C.M.Care@shu.ac.uk
Fax: (0742) 533501

Dr D J Cleaver
Department of Applied Physics
Sheffield Hallam University
Pond Street
Sheffield
S1 1WB
Email: D.J.Cleaver@shu.ac.uk

HIGH PERFORMANCE COMPUTING: A NEW ERA

Notice of Town Meeting 7 July 1994

The Engineering and Physical Sciences Research Council (EPSRC), which oversees the management of the national high performance computing facilities on behalf of all the Research Councils, is holding a Town Meeting on Thursday, 7 July 1994 in London.

Entitled "High Performance Computing: a New Era", the purpose of this meeting is to provide a forum for users and providers of high performance computing, including the new CRAY T3D at Edinburgh, to present and discuss a strategy for high performance computing in the UK, and to review developments in high performance computing and networking in a European and International context.

To register an interest in attending the 1994 Town Meeting, please send your full name, postal and email address to:

Mr B Bishop
Room 1130
Engineering and Physical Sciences Research Council
Polaris House
North Star Avenue
Swindon
SN2 1ET

email: sbbi0 @ rutherford.ac.uk

Please note the deadline for registering for this event is 13 May 1994.

International Symposium on Computational Molecular Dynamics

sponsored by

University of Minnesota Supercomputer Institute
Computers in Chemistry Division, American Chemical Society
Division of Computational Physics, American Physical Society
Division of Physical Chemistry, American Chemical Society

October 24-26, 1994

University of Minnesota Supercomputer Institute
1200 Washington Avenue South
Minneapolis, Minnesota

CELLULAR AUTOMATA AND THEIR APPLICATIONS TO MOLECULAR FLUIDS

A conference organised by the Statistical and Thermodynamics Group of the Royal Society of Chemistry to take place in Manchester, U.K. on 19 - 20 July, 1994.

Dynamics of colloidal suspensions	(A. Ladd, Lawrence Livermore, U.S.A.; O. Behrend, Edinburgh; P. Pusey, Edinburgh)
Polymer Dynamics	(X-F. Yuan, Cambridge; J.H.R.Clarke, UMIST)
Flow in Porous Media	(C. Lowe, Amsterdam)
Phase Ordering Kinetics	(M. Ernst, Utrecht; A. Bray, Manchester)
Modelling Chemical Reactions	(B. Boghosian, Thinking Machines, U.S.A.)
Modelling Microbial Growth	(G. Barker, AFRC)
Material Science Applications	(P. Coveney, Schlumberger)
Flow of Immiscible Fluids	(I. Halliday, Sheffield Hallam)
Boundary Effects on Fluid Flow	(D. d'Humieres, Paris)

This is a conference which aims to bring together workers from a wide variety of research fields with a common interest in the dynamics of fluids.
Posters are welcomed describing research in the general field of the dynamics of molecular fluids as well as in cellular automata. There will be a prize awarded for the best poster and a limited number of student travel bursaries will be available.

Symposium organizers: Jan Almlof (University of Minnesota), Evelyn Goldfield (Cornell Theory Center), M. Katharine Holloway (Merck Research Laboratories), William Jorgensen (Yale University), Peter Rossky (University of Texas at Austin), George Schatz (Northwestern University), and Donald Truhlar (University of Minnesota)

The University of Minnesota Supercomputer Institute is hosting an international symposium on Computational Molecular Dynamics, Monday- through-Wednesday, October 24-26, 1994 (with a reception on the 23rd), at the Hubert H. Humphrey Center located on the University of Minnesota campus in Minneapolis. The coverage of the symposium will include all aspects of the dynamics of molecular systems and the use of molecular dynamics simulations-quantum and classical, few-body and many-body, physics and chemistry.

The organizing committee has developed a list of invited speakers that will insure that the program is at the forefront of the field. The list of confirmed speakers includes: Bruce Berne (Columbia University), Emily Carter (University of California,Los Angeles), Jim Chelikowsky (University of Minnesota), Paulette Clancy (Cornell University), Jean Durup (Universite Paul Sabatier), Michael Gillan (University of Keele), Trygve Helgaker (University of Oslo), Jan Hermans (University of North Carolina), Michael Klein (University of Pennsylvania), Ronnie Kosloff (Hebrew University), Uzi Landman (Georgia Tech), Claude Leforestier (Universite de Paris-Sud), Peter Lomdahl (Los Alamos National Laboratory), Paul Madden (Oxford University), Craig Martens (University of California, Irvine), Ken Merz (Penn State), Daniel Neuhauser University of California, Los Angeles), Michele Parrinello (IBM-Zurich), David Pearlman (Vertex Pharmaceuticals), Montgomery Pettitt (University of Houston), Tamar Schlick (New York University), Terry Stouch (Bristol Meyers Squibb), Julian Tirado-Rives (Yale University), Steve Walch (NASA-Ames), and John Zhang (New York University).

In addition to the invited talks, there will also be poster papers to contribute to what we

Cellular Automata and Their Applications to Molecular Fluids - Manchester 1994. Registration form

NAME ____

ADDRESS and AFFILIATION ____

____

____

____

Conference fee	(55.00 pounds)
Accommodation (19 Jul. - lunch, conference dinner, bed and breakfast, 20 Jul. -lunch)	
single room	(53.00 pounds)
en-suite single	(62.50 pounds)
en-suite twin	(77.00 pounds)
Extra accommodation (18 Jul. - dinner, bed and breakfast)	
single room	(28.00 pounds)
en-suite single	(37.50 pounds)
en-suite twin	(52.00 pounds)
Conference dinner only	(17.00 pounds)
total	

Vegetarian meals required YES/NO

anticipate will be a fruitful exchange of information among a broader group of computational chemists and physicists than one usually encounters at a single meeting. Contributed poster papers are invited and strongly encouraged. Confirmed poster contributors at this date include Jan Almlof, H. Ted Davis (University of Minnesota), David Ferguson (University of Minnesota), Evelyn Goldfield, J. Woods Halley (University of Minnesota), Lester Harris (Abbott Northwestern Hospital), Peter Rossky, George Schatz, and Donald Truhlar. Persons who wish to present a poster should send a one-page abstract by July 25, 1994. Late posters will be accepted on a space available basis.

The registration fee for the symposium is $150 for registrations received prior to September 30, and $175 after September 30. A 10 percent discount will be given to members of the cosponsoring divisions of the American Physical Society and American Chemical Society, listed at the top.

To receive more information regarding the meeting, including a list of lecture titles, contact the Symposium Administrator:

Michael J. Olesen
Supercomputer Institute
University of Minnesota

I would like to present a poster(s) YES/NO

(Title of poster(s) ____

____

____

____

I would like to apply for a student bursary YES/NO
(Please include letter from supervisor).
Cheques should be made payable to.... Cellular Automata Conference/University of Manchester, and should be received by 13th May 1994. Participants from outside the UK should make arrangements for payment in pounds sterling.
Please return this form with payment to:

Dr. Andrew Masters,
Department of Chemistry,
University of Manchester,
Manchester M13 9PL, U.K,
Tel. 061 - 275 - 4679,
Fax. 061 - 275 - 4598,
Email: mbdtsam@hpb.ch.man.ac.uk

1200 Washington Avenue South
Minneapolis, MN 55415
phone: (612) 624-1356
fax: (612) 624-8861
electronic mail: olesen@msi.umn.edu

Visitors program

Dr. A. J. C. Ladd

Dr. A. J. C. Ladd will visit the UK in July 1994. The following is the provisional itinerary, subject to confirmation. If CCP5 members not at one of the host institutions wish to attend one of the seminars, please contact the local organiser directly.

Dr. Ladd visits Oxford on Monday 11 July, staying overnight and leaving for Bristol late afternoon/early evening of Tuesday 12 July. Seminar in Physical Chemistry Laboratory, South Parks Road, provisionally Monday 11 July at 2.15 p.m. Contact:

Dr. P. A. Madden, tel: 0865 275426
fax: 0865 275410
email: madden@vax.oxford.ac.uk

Dr. Ladd stays the nights of Tuesday 12 July and Wednesday 13 July in Bristol, leaving early in the morning of Thursday 14 July for Cambridge. Seminar in H. H. Wills Physics Laboratory on the Wednesday at 2.15 p.m., title "Computer Simulation of Particulate Suspensions". Contact:

Dr. M. P. Allen, tel: 0272 303885
fax: 0272 255624
email: m.p.allen@bristol.ac.uk

Dr. Ladd stays the night of Thursday 14 July in Cambridge. Seminar in Cavendish Laboratory, Polymer and Colloid seminar room, Friday 15 July at 2.15 pm., title "Computer Simulation of Particulate Suspensions". Contact:

Dr. J. R. Melrose, tel: 0223 337263
fax: 0223 337000
email: jrm23@phy.cam.ac.uk

Prof. P. Vorontsov-Velyaminov

Prof. P. Vorontsov-Velyaminov will visit the UK from Russia this summer. Details remain to be finalised; they will be sent by Email when available. (Alternatively, look at the CCP5 World Wide Web visitors section). A provisional program is given below. He will arrive in the U.K. June 16-18. He will give seminars in

Place	Department	Title	date	host
Oxford	Physical Chemistry Lab.	Polyelectrolytes	June 20th. 2.15	Paul Madden
Cambridge	Physical Chemistry Lab.	Path Integral Simulations with Exchange	June 23rd 2.15	Dr R.Lynden-Bell
Daresbury		Polyelectrolytes	June 27th.	W. Smith
Surrey	Computational Chemistry	Polyelectrolytes		David Heyes

Prof. Vorontsov-Velyaminov has also worked on Free Energy simulations and on Ion Clusters; he will be glad to discuss the above topics with interested persons. If not travelling or staying elsewhere, he will be based c.o. K.Singer 54 Simons Walk, Egham, Surrey TW20 9SQ Tel 0784 432397

The CCP5 Program Library W. Smith

CCP5 Program Library

The CCP5 Program Library provides programs and documentation free of charge to academic centres upon application to Dr. W. Smith, TCS Division, DRAL Daresbury Laboratory, Daresbury, Warrington WA4 4AD, U.K..

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.

THE CCP5 PROGRAM LIBRARY.

Program	Type	Model	Algorithm	Properties	Authors
ADMIXT	MD	LJA MIX	LF	TH MSD RDF	W. Smith
CARLOS	MC	VS AQ		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, J. Mościński
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
MDMEGA	MD	LJA		DD	W. Smith
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
MOLDY	MD PRMD	BHM MIX GEN	BE CP	RDF	K. Refson
NAMELIST	UT	Namelist emulation			K. Refson
NEMD	MD	LJA	SLLOD	Macintosh	D. J. Evans
NSCP3D	UT	Hard sphere packing			M. Bargiel, J. Mościński
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, 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
XEDS	GP				D. Nikolow, W. Alda, J. Kitowski

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
GEN	General Program with many options

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

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
BE	Beeman algorithm
LC	Link-cells MD algorithm
CP	Constant pressure
CT	Constant temperature
TA	Toxvaerd MD algorithm
CA	Constraint algorithm
EM	Energy minimisation
SYM	Symmetry adapted algorithm
RFD	Rossky-Friedman-Doll algorithm
SLLOD	Thermostatted SLLOD equations
DD	Domain decomposition parallel algorithm

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

Programs from the Book "Computer Simulation of Liquids"

F.1	Periodic boundary conditions in various geometries
F.2	5-value Gear predictor-corrector algorithm
F.3	Low-storage MD programs using leapfrog Verlet algorithm
F.4	Velocity version of Verlet algorithm
F.5	Quaternion parameter predictor-corrector algorithm
F.6	Leapfrog algorithms for rotational motion
F.7	Constraint dynamics for a nonlinear triatomic molecule
F.8	Shake algorithm for constraint dynamics of a chain molecule
F.9	Rattle algorithm for constraint dynamics of a chain molecule
F.10	Hard sphere molecular dynamics program
F.11	Constant-NVT Monte Carlo for Lennard-Jones atoms
F.12	Constant-NPT Monte Carlo algorithm
F.13	The heart of a constant μVT Monte Carlo program
F.14	Algorithm to handle indices in constant μVT Monte Carlo
F.15	Routines to randomly rotate molecules
F.16	Hard dumb-bell Monte Carlo program
F.17	A simple Lennard-Jones force routine
F.18	Algorithm for avoiding the square root operation
F.19	The Verlet neighbour list
F.20	Routines to construct and use cell linked-list method
F.21	Multiple timestep molecular dynamics
F.22	Routines to perform the Ewald sum
F.23	Routine to set up alpha fcc lattice of linear molecules
F.24	Initial velocity distribution
F.25	Routine to calculate translational order parameter

F.26	Routines to fold/unfold trajectories in periodic boundaries
F.27	Program to compute time correlation functions
F.28	Constant-NVT molecular dynamics - extended system method
F.29	Constant-NVT molecular dynamics - constraint method
F.30	Constant-NPH molecular dynamics - extended system method
F.31	Constant-NPT molecular dynamics - constraint method
F.32	Cell linked-lists in sheared boundaries
F.33	Brownian dynamics for a Lennard-Jones fluid
F.34	An efficient clustering routine
F.35	The Voronoi construction in 2d and 3d
F.36	Monte Carlo simulation of hard lines in 2d
F.37	Routines to calculate Fourier transforms

Availability of the Allen/Tildesley example programs 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.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. 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.

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.

Problems, questions and comments about STATMECH service on this system should be directed to "statmech-mgr@cheme.cornell.edu".
Steve Thompson, School of Chemical Engineering, Cornell University, Ithaca NY 14853 USA.

Magnetic tape and distribution to commercial users

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.

CCP5 Program Library E-Mail and anonymous ftp Service

It is possible for CCP5 members to get copies of CCP5 programs through E-mail or anonymous ftp *automatically.*

Email

To access the library by E-mail send an E-mail message to **info-server@uk.ac.dl**. The contents of the E-mail message should be as shown in the table. (Note: the use of upper and lower case is significant - this is a unix system!)

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

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

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

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

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

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

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

anonymous ftp

The entire CCP5 program library is now accessible by anonymous FTP. The procedure is as shown in the table.

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

Conditions of use

Neither DRAL, nor the authors of the programs in the above program library guarantee that the programs are free from error and cannot be responsible for any loss or damage as a result of using them. In accepting any of the programs you have agreed to limit its distribution to those engaged in academic research who are authorised users of the facilities provided by your institution, and

1.	move to the desired directory on YOUR machine	
2.	type:	ftp ftp.dl.ac.uk
3.	enter userid:	anonymous
4.	enter passwd:	*enter your name and site*
5.	change to ccp5 directory:	cd ccp5
6.	to list the directory contents:	ls
7.	if desired change to lower directory e.g.	cd TEQUILA
8.	to get a compressed file (.Z)	binary
9.	to get a single file type:	get filename
10.	to get multiple files type:	mget *.*
11.		quit

not to allow the use of the programs for commercial purposes. Any bugs found should be reported to the librarian, for the benefit of other users.

Water Science Network (WSN)
Physics, Chemistry and Biology of Water and Aqueous Systems

WSN is an interdisciplinary forum for scientists interested in physical and chemical properties of water and aqueous solutions, and in the role water plays in biological systems. WSN is created to facilitate communication between experimental and theoretical scientists with different backgrounds, whose research interests are related to:

- water structure and hydrogen bond network
- thermodynamic and kinetic properties of water
- phase transitions in water
- hydrophobic effects
- hydration forces
- water around solutes and water at interfaces
- hydration of biomolecules
- water in membranes
- water in cell
- experimental techniques for studying water properties
- computer simulations of water

Postings to the WSN would contain:

- discussions of new ideas and developments in related fields
- questions and answers about particular problems
- bibliographic information on current and forthcoming books and articles
- information on funding sources
- meeting announcements
- position announcements
- product and service announcements

To subscribe to the WSN, send to listserv@gibbs.oit.unc.edu a one-line message:

subscribe water Your Name

Your e-mail address will be recorded from the header of your message, so all WSN postings would be send to the account where the subscription request came from. Contributions sent to the WSN are automatically archived. Archives would be available for search using various network information search tools. Please feel free to forward this announcement to all interested parties.

WSN coordinator:
Iosif Vaisman (wsn-adm@mmlds1.pha.unc.edu or vaisman@gibbs.oit.unc.edu)
Laboratory for Molecular Modeling
School of Pharmacy
University of North Carolina at Chapel Hill

How to optimize Configurational Bias Monte Carlo? Corrections

Daan Frenkel and Germonda Mooij
FOM Institute for Atomic and Molecular Physics
Kruislaan 407
1098 SJ Amsterdam
The Netherlands

Owing to a data transmission problem with this article from the last newsletter, the equations were not printed with correct superscript characters. The corrected equations are printed below. A complete copy of the corrected article is available by ftp or from the WWW server.

The contribution of each i^{th} segment to this Rosenbluth weight is equal to the average of the Boltzmann factors of the trial positions for this segment:

$$W_{\Gamma_i} = \frac{1}{k_i} \sum_{j=1}^{k_i} \mathrm{e}^{-\beta U_{\Gamma_{ij}}^{\mathrm{nb}}}, \tag{1}$$

where $\beta = 1/k_B T$ and $U_{\Gamma_{ij}}^{\mathrm{nb}}$ is the non-bonded energy of the j^{th} trial direction for the i^{th} segment. The Rosenbluth weight of the total configuration Γ, is the product of the weights of the individual segments, including the Boltzmann factor of the energy of the first segment, U_{Γ_0}:

$$W_\Gamma = \mathrm{e}^{-\beta U_{\Gamma_0}} \prod_{i=1}^{\ell} W_{\Gamma_i}, \tag{2}$$

where ℓ is the chain length.

$$\langle P_{\mathrm{add}}(k_{\ell+1})\rangle = 1 - \langle (1 - P_{\mathrm{add}}(1))^{k_{\ell+1}} \rangle \,. \tag{8}$$

$$\langle P_{\mathrm{add}}(k_{\ell+1})\rangle = 1 - (1 - \langle P_{\mathrm{add}}(1)\rangle)^{k_{\ell+1}}. \tag{9}$$

Figure 1: The efficiency, as defined by equation 7, for inserting a hard dimer (———) and a fully flexible trimer of hard spheres (– – –) into a fluid of hard spheres at several densities $\rho\sigma^3$, over a range of k-values.

CCP5 information on the Daresbury World Wide Web server

Maurice Leslie

1 Introduction

The CCP5 community is widely distributed throughout the world and serves readers with computing facilities from the most sophisticated to very basic. This article has two sections. The first describes what World Wide Web is and gives sufficient information for readers to set up their own servers if they wish. This is followed by a description of information which may be obtained about CCP5 from the Daresbury server.

1.1 What is World Wide Web?

By far the easiest way to find out about World Wide Web is to use it. The following is therefore primarily aimed at those of our readers who do not have access to World Wide Web, or who's sites are not connected to Internet. In order not to interrupt the flow of the document too much I have included a glossary of the large number of terms and acronyms at the end.

World Wide Web (W^3 or WWW) aims to give access in an uncomplicated way to information stored on a computer system anywhere in the world. The project was initiated at CERN with a view to coordinating the high-energy physics community. Consider as an analogy reading a scientific paper in your university library. Two of the activities which you will find yourself needing to do most frequently are to look up a cross-reference in the document and to search an index for a particular keyword. World Wide Web is designed to mimic both of these human activities.

To carry out the cross-referencing activity, World Wide Web documents are written in **hypertext**. This is just the same as ordinary text, except that it contains references within the text which are designed to be interpreted by the computer. These references are called **hypertext links**. They may refer to a separate part of the same document, another document on the same file system, or a document on another file system anywhere in the world. The hypertext links could refer to the author, giving background information, or to the institution. One consequence of this is that documents cease to be static; in the CCP5 library page described below the link from a program name will always point to the most up to date version. The cross-referenced documents may themselves have links; in this way the user is rapidly able to traverse the globe through the Web. Links in documents need not refer to items which are text. It is possible to refer to an item which is a graphical image, an audio sample or a movie, for which the term "hypermedia links" has been coined. Links can also refer to "virtual documents", created by running some program as a result of activating the link.

The activities of providing information and accessing information are kept distinct in WWW. Information providing programs, called servers, provide data requested by information gathering programs called clients. Accessing information is done by means of a 'browser' program, of which there are a number available. The most popular is "Mosaic" written by NCSA. This will run on most UNIX platforms, IBM-compatibles running Microsoft Windows and Macintoshes. There are also browsers for vt100 terminals and line-mode terminals. The fundamental difference between the browsers lies in how the hypermedia links are presented to the user and activated. In the case of mosaic, which is the only browser for which I have personal experience, links are highlighted using different colours on a colour screen and by underlining on a monochrome screen, and are activated using the mouse. When a browser is started, the users terminal will display a home page containing links to other documents. In the case of mosaic, by default the NCSA home page is displayed. In order to view other documents, the user either follows a link or provides a URL from the file menu.

It was a design aim of WWW that it should run on a wide variety of platforms. In order to achieve this aim, a number of new protocols and conventions needed to be established. WWW uses a hypertext data format called HTML, which is defined in terms of SGML. HTML is a simple text formatter with capabilities for document title, headings, lists, verbatim text, embedded images and character fonts. HTML also contains anchors, which mark the beginning (or occasionally the end) of a hypertext link. An anchor which is the beginning of a link will contain a document reference and sensitive text which will be highlighted by the browser that the user is running. The document reference needs to refer in an unambiguous way to the document to which it is linked. This is done by supplying a URL. A URL has a number of components, not all of which need to be given, within an anchor in a HTML documents. These components are

- A protocol which the client will use to obtain the document.
- The Internet address of the computer where the document is stored.
- The location of the document within the filesystem.
- A fragment-id, pointing to a location within the document.

A new network protocol HTTP was defined by the WWW project to give features not otherwise available. This is a protocol not only for the transfer of hypertext, but also it permits the client and server to communicate via the Internet, prior to sending the document, and agree on the most appropriate form of data transfer. Documents transferred need not be written in HTML, they can for example be in postscript. Examples in the next section should clarify this. WWW is able to access a wide number of existing services, including Gopher, anonymous ftp and WAIS.

In order to obtain further information, for readers without a WWW service, use anonymous ftp to

Site	Directory	Information supplied
info.cern.ch	/pub/www	Transfer and read README.txt
ftp.ncsa.uiuc.edu	Web	Transfer and read README.Mosaic

1.2 CCP5 information on WWW

This section is written to describe verbally the contents of the CCP5 WWW page, although it will be much simpler for readers with WWW browsers to try it out. The URL for the CCP5 home page is

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

I will now describe some of the contents using mosaic; readers should be aware that different browsers may behave differently. There is a brief introductory paragraph, followed by a menu of items (history of the project, organisation, research interests, library, meetings and workshops, visitors, index of newsletter articles, copy of recent newsletters and registration form). To get this newsletter, select the *newsletters* option. Follow the directory path 41/ps and select the file newsletter_part1.ps.gz. This is a compressed postscript file. The client program at Daresbury transfers the compressed file, opens an external viewer and displays the newsletter. (Other browsers may not perform all of these operations). The newsletter can then be read on the screen. Suppose the user selects *library*. A new document is displayed with information about the program library. Further down this page is an index of programs in the library. Selecting *directory* in the introductory paragraph will display the entire directory in which the program library is stored. If you move *back* to the library page and select the entry MDMEGA, the code for the program is displayed on the terminal. To transfer a copy to the local host, open the file menu and use the save as option. You will be prompted for the name of the local file. Look at the entry for the program MOLDY. If the link BE is followed, the user finds that the Beeman algorithm is used. Move *back* to the MOLDY entry and follow the *manual* link. This link executes an anonymous ftp transfer to the program author's host computer, where the most up-to-date version will always be stored. Now move back to the library page and look at the NEMD entry. This is a binhexed Mackintosh file (binary and manual) (.hqx) The Daresbury browser in this case just requests a filename to download the file for subsequent processing as there is no sensible way to display the information.

The other capability of WWW is its ability to carry out searches of data. This is carried out using either its own search protocols, or by acting as an interface to one of the existing information services. (Gopher, xarchie, WAIS). A WWW browser can send a request to a client to search a document for a keyword. However, the whole question of how to create an index of information on WWW is currently under active debate. A number of projects have been set up in which a *robot* automatically scans documents, following links in them, extracting titles and header information, or information contained within URL's within the documents. However, such programs can impose a heavy load on the Internet and it is not at present clear that this will be the best way to create indices. The information returned by the robot is often of limited use to the subsequent search of the database, being geographical in nature or covering too broad an area. Readers with WWW browsers are referred to the two documents below; the first is a general description of robots and the second is a useful searchable index.

URL	Document Title
http://web.nexor.co.uk/mak/doc/robots/robots.html	World Wide Web Wanderers, Spiders and Robots
http://www.stir.ac.uk/jsbin/js	JumpStation Front Page

I have constructed a list of links I have found which are relevant to CCP5. This is not complete, but I hope it will quickly give new people an idea of the scope of WWW. Readers are welcome to contribute to this list if they wish. I would also welcome comments from users of WWW on this article, either for information or for publication in this newsletter, by Email to m.leslie@dl.ac.uk.

Glossary

anchor	A point in an HTML document where there is a hypertext link.
browser	Interface between the user and the systems WWW client program.
client	Program run to access WWW information.
Gopher	A menu-driven information service.
HTML	Acronym for HyperText Markup Language, the data format used for hypertext on all WWW systems.
HTTP	HyperText Transfer Protocol.
hypermedia link	A link from a document to some form of information, stored elsewhere. (synonym hyperlink)

NCSA	National Centre for Supercomputing Applications
robot	A program which recursively follows links in documents in order to build up a database of information about the whole or part of WWW.
server	Program which supplies information.
SGML	Standard Generalised Markup Language, an ISO standard for defining structured document types and markup languages.
URL	A Uniform Resource Locator, a syntax for expressing the names and addresses of objects on the network.
WAIS	Wide-Area Information Service

Resolving Torques in Rigid Multicentred Molecules

W. Smith

The purpose of this note is to resolve the problem that arises in simulating rigid multicentred molecules, where the 'centres' are not necessarily simple atoms, but may be complicated entities such as a multipoles, which themselves experience torques in addition to simple site forces. The problem is how to exploit these torques in computing the dynamics of the molecule as a whole.

We begin with the simplest case, a set of point particles $\{i : i = 1, \ldots, N\}$ arranged in a rigid framework. It is assumed that each particle is subjected to a force $\mathbf{F}_i$. What is the torque of the system about an arbitrary point?

If each particle is located at a point $\mathbf{R}_i$ defined with respect to an arbitrary origin $\mathbf{O}$, the torque *about the centre of mass* of the system ($\mathbf{T}_c$) is given by:

$$\mathbf{T}_c = \sum_{i=1}^{N} (\mathbf{R}_i - \mathbf{R}_c) \times \mathbf{F}_i \tag{1}$$

where the centre of mass $\mathbf{R}_c$ is given by:

$$\mathbf{R}_c = \frac{1}{M} \sum_{i=1}^{N} m_i \mathbf{R}_i \tag{2}$$

with

$$M = \sum_{i=1}^{N} m_i \tag{3}$$

being the total mass of the system.

Equation (1) can be expanded as follows:

$$\mathbf{T}_c = \sum_{i=1}^{N} \mathbf{R}_i \times \mathbf{F}_i - \sum_{i=1}^{N} \mathbf{R}_c \times \mathbf{F}_i$$

$$\mathbf{T}_c = \sum_{i=1}^{N} \mathbf{R}_i \times \mathbf{F}_i - \mathbf{R}_c \times \mathbf{F}_c$$

where

$$\mathbf{F}_c = \sum_{i=1}^{N} \mathbf{F}_i \tag{4}$$

is the sum of the forces acting on the whole system. Hence:

$$\sum_{i=1}^{N} \mathbf{R}_i \times \mathbf{F}_i = \mathbf{T}_c + \mathbf{R}_c \times \mathbf{F}_c$$

or

$$\mathbf{T}_o = \mathbf{T}_c + \mathbf{R}_c \times \mathbf{F}_c \tag{5}$$

where

$$\mathbf{T}_o = \sum_{i=1}^{N} \mathbf{R}_i \times \mathbf{F}_i \tag{6}$$

is the torque about the arbitrary point **O**

Thus for this case we arive at a simple rule: *The torque of a system about an arbitrary point is the the sum of the torque about the centre of mass and the torque due to the net force acting on the centre of mass of the system.*

A more complicated case arises when each point particle is replaced by some other entity, such as a small, rigid cluster of points (i.e. a compound particle), which experiences a torque in addition to the net force acting on it. How are these forces and torques to be combined into a total torque for the full assembly?

We begin with the compound particles. Each has a torque about its centre of mass $\mathbf{T}_n$ which we can write as:

$$\mathbf{T}_n = \sum_{i=1}^{P_n} (\mathbf{R}_i - \mathbf{R}_n) \times \mathbf{F}_i \tag{7}$$

where the centre of mass $\mathbf{R}_n$ is of course given by:

$$\mathbf{R}_n = \frac{1}{M_n} \sum_{i=1}^{P_n} m_i \mathbf{R}_i \tag{8}$$

with the total mass of the compound particle being:

$$M_n = \sum_{i=1}^{P_n} m_i \tag{9}$$

The vectors $\mathbf{R}_i$ are again specified with respect to an arbitrary origin **O**

Once again, we may expand this expression to give:

$$\mathbf{T}_n = \sum_{i=1}^{P_n} \mathbf{R}_i \times \mathbf{F}_i - \sum_{i=1}^{P_n} \mathbf{R}_n \times \mathbf{F}_i$$

and we can form the vector sum ($\mathbf{T}_P$) of all such torques for the entire system (P being the number of compound particles):

$$\mathbf{T}_P = \sum_{n=1}^{P} \mathbf{T}_n = \sum_{n=1}^{P} \sum_{i=1}^{P_n} \mathbf{R}_i \times \mathbf{F}_i - \sum_{n=1}^{P} \sum_{i=1}^{P_n} \mathbf{R}_n \times \mathbf{F}_i$$

or

$$\mathbf{T}_P = \sum_{i=1}^{N} \mathbf{R}_i \times \mathbf{F}_i - \sum_{n=1}^{P} \mathbf{R}_n \times \mathbf{F}_n \tag{10}$$

where we have simply expanded the double summation in the first term on the right, so that $N = \sum_{n=1}^{P} P_n$, and where $\mathbf{F}_n$ represents the net force acting on each compound particle i.e.

$$\mathbf{F}_n = \sum_{i=1}^{P_n} \mathbf{F}_i$$

Equation (10), with a little rearrangement, may be rewritten as:

$$\mathbf{T}_o = \mathbf{T}_P + \sum_{n=1}^{P} \mathbf{R}_n \times \mathbf{F}_n \tag{11}$$

where

$$\mathbf{T}_o = \sum_{i=1}^{N} \mathbf{R}_i \times \mathbf{F}_i \tag{12}$$

is once again the total torque of the system about the arbitrary point $\mathbf{O}$. The equation (11) has an obvious physical interpretation: *The net torque of a rigid system about an arbitrary point* $\mathbf{O}$ *is the vector sum of all the torques* $\mathbf{T}_n$ *acting on individual sites plus the sum of the torques arising from the net force* $\mathbf{F}_n$ *on each site acting about the point* $\mathbf{O}$. (It should be apparent that this follows logically from the rule given in the previous simple case.)

It should be noted that this result will hold, even if the 'arbitrary' point is the centre of mass of the whole system. It will also apply if the compound particles are replaced by equivalent point particles possessing multipolar attributes, such as point dipoles and quadrupoles.

METHODS IN MOLECULAR SIMULATION
CCP5 Spring School 11–15 April

Mike Allen

The Spring School was held at Southampton University, with lectures in the Chemistry Department each morning, hands-on computer workshops in the afternoon at the University's Data Visualization Suite, and a 'guest seminar' before dinner each evening. The principal lecturers were Mike Allen (Bristol), Julian Clarke (UMIST) and Dominic Tildesley (Southampton), with supplementary lectures from Tim Forester (Daresbury) and Stephen Warde (Molecular Simulations). Evening guest seminars were given by Julia Goodfellow (Birkbeck), Geoffrey Luckhurst (Southampton), Paul Madden (Oxford) and Mark Rodger (Reading).

The course began with lectures and workshops on basic and advanced techniques in Monte Carlo and molecular dynamics, and then moved on to topics in molecular modelling and scientific data visualization. Towards the end of the week, more specialized subjects were introduced: nonequilibrium methods, phase transitions, and Fortran 90. For each afternoon, a selection of exercises was provided: enough to give a reasonable choice of new material, while still permitting the student to look back at work from earlier in the week. For almost every exercise, a 'solution' was provided about two-thirds of the way through the afternoon. This allowed students to look at problems that they did not wish, or have time, to attempt, as well as being able to check their own work. The early part of the week concentrated on programming and simulation algorithms, but from Wednesday onwards other software was introduced. Cerius^2 (Molecular Simulations) was used to model zeolite adsorption, Collage (NCSA) was used to visualize large data sets, Iris Explorer (SGI/NAG) was used to illustrate module assembly for visualization, and PV-Wave (Precision Visuals) was also made available. The DL_POLY package was used to run example simulations of water and valinomycin. Finally, on the Friday, there was an exercise involving the progressive introduction of Fortran-90 constructs into a Fortran-77 molecular dynamics program, and an exercise involving programs run on several workstations at once, with message-passing by PVM.

This was an ambitious and intensive programme for both students and lecturers. The 16 Silicon Graphics R3000 Indigos worked almost faultlessly (just one machine was out of action for about an hour). The software was also extremely reliable: Cerius^2 crashed once or twice due to running out of swap space, but otherwise performed very well, and there was a minor glitch with the DL_POLY programs which needed to be recompiled on the R3000-chip Indigos (binaries from an R4000 turned out not to be compatible). None of these minor hiccups caused any real problems. After the course the students were allowed to copy their work, the original exercise programs, and the solutions to all the exercises, back home by ftp.

At the end of the course, the students filled in, anonymously, a set of questionnaires. These will provide some useful feedback and information essential to the planning of future courses, and they will be studied in detail. The overall tone was very positive indeed: all the students seem to have enjoyed their week, and gained something from it. The 'guest seminars' especially were appreciated: they were all delivered in an enthusiastic and inspiring manner. The food and accommodation at Glen Eyre hall of residence also received general approval.

One or two points emerged that need further consideration. There was a larger split than anticipated in background and expectations between 'programmers' and 'package users': if this had been fully appreciated we could have targetted and tailored the course a little better. This split is itself something that needs some attention: our contacts with the commercial sector of molecular modelling suggest that there is a need for more Ph.D.'s who know something of what is inside these packages, rather than just knowing how to use them. Secondly, the students would have appreciated an afternoon off (to see Southampton), and a few more informal opportunities (round tables, poster sessions) to discuss simulations with the lecturers. It would be very desirable to include these in a future programme, but the Spring School would have to extend beyond one week, or we would have to trim down the material to be covered. Additional comments on the questionnaires concerning the level and pace of lectures will also be very useful to us.

I would like to thank my co-lecturers, all the 'guest seminar' speakers, and our two supplementary lecturers, for the effort they put in to present all this material in an interesting and informative way. Dominic Tildesley also deserves thanks for handling registration and all the domestic arrangements. Southampton University provided the lecture theatre and visualization suite free of charge. We could not have mounted this course without the assistance of Southampton Computer Centre staff, notably Ian Hardy, who helped set things up on the DV Suite machines, and worked behind the scenes during the week to keep things running smoothly. Thanks are also due to Mike Stapleton, Stephen Warde and Jeremy Turvey of Molecular Simulations for allowing us to use Cerius^2 during the workshops, and (to Stephen and Jeremy) for setting up the zeolite exercise, and attending the afternoon session to provide advice; to Robert Morell of NAG for allowing us to use their Fortran-90 compiler; to Jeremy Walton of NAG for files and advice on the Iris Explorer exercise; and to Tim Forester of Daresbury Laboratory, for providing the DL_POLY exercise and attending in the afternoon to help with it. Finally, thanks to the students, who, to their credit, attended every lecture and every workshop session, in a packed programme, and demonstrated plenty of enthusiasm and team spirit.

Report on CCP5-Sponsored Meeting of Liquid Crystal Simulators
Sheffield Hallam University
17th March 1994

Doug Cleaver

This meeting of a loose consortium of liquid crystal / complex fluid simulators was held at Sheffield Hallam University, and attracted representatives from Bristol (Mike Allen), Derby (Maureen Neal), Lancaster (John Wheeler), Manchester (Andy Masters), Sheffield (George Jackson and group), Sheffield Hallam (Chris Care and group; Doug Cleaver) and Southampton (Andy Emerson). As on previous occasions, the main purpose of the meeting was to disseminate recent results and discuss the work in progress in the various groups.

Following announcements regarding the conferences to be held at Manchester in July and Sheffield in September, the meeting got underway with a description from Mike Allen of the history and progress of the T3D project. He explained that SERC had, at short notice, sought proposals from the CCP's to cover the first year of the machine's use. The CCP5 steering committee had decided that its main bid should be based on the DL_POLY routines, with an emphasis on the modelling of biomolecular systems. A second bid based on liquid crystals / complex fluids was also deemed suitable, however, and so Mike had coordinated a joint proposal put forward by the consortium as a whole. This bid had detailed five systems suitable for simulation on this scale, namely: a chiral smectic; a disclination defect (in a large system); the biaxial nematic phase; a polymer liquid crystal; and various surfactant phases. A brief discussion followed regarding the options available for any future bids for this facility.

Following this, there were four short presentations of work based on lattice model systems. Chris Care described a microcanonical MC technique which enables efficient calculation of the density of states through the measurement of a transition matrix. This technique was shown to compare favourably with the multiple histogram techniques when applied to the 2-d Ising model. More extensive comparisons of the two methods were being planned, involving larger system sizes and models with continuous energy spectra. Leila Ayat (SHU) then described how she had applied Chris' microcanonical technique to the Lebwohl-Lasher liquid crystal model. She showed energy distribution functions, specific heat curves and the roots of the partition function for different system sizes. The transition temperatures given by these three indicators all extrapolated to a common value in the infinite system limit. The results were in excellent agreement with those of previous studies of the model, and appeared to indicate the first order nature of the transition at smaller system sizes than did other techniques.

Next, Doug Cleaver described an initial study he had been performing on a variant of the Lebwohl-Lasher model which incorporates random anisotropy. This model is thought to simulate the behaviour of a liquid crystal confined in a randomly interconnected porous network (systems which have generated recent experimental interest). The simulation results showed that the first order nematic-isotropic transition is suppressed by the anisotropy, the specific heat peak being broadened and shifted to lower temperatures. Also, the orientational correlation function was shown to take a qualitatively different form from that of the Lebwohl-Lasher model: it decayed algebraically rather than exponentially, indicating that there is no long ranged order (i.e. no nematic phase) in the infinite system limit. Finally, in this section, Jean Desplat (SHU) described the extensions he is making to a lattice model of surfactant behaviour. This model, originally developed by Chris Care and David Brindle, uses short, fully flexible chain molecules composed of 'head' and 'tail' sites arranged on a simple cubic lattice and moved using reptation With the 3-d version of this model, micellar, cylindrical, bicontinuous and lamellar phases have been observed. The planned extensions will involve increasing the coordination number of the underlying lattice, incorporating a term into the Hamiltonian to take account of chain bending energies and implementing the configurational bias technique for performing moves. The model will then be used to investigate the properties of non-ionic surfactants and mixtures thereof.

The afternoon session was dedicated to discussion of off-lattice simulations. First to speak was Maureen Neal. She described work being performed as part of a collaboration between Derby, SHU and Hull, in which a simple model is being sought for triphenylene. This molecule, whilst not being a mesogen itself, does form the core of a wide range of discotic and calamitic liquid crystals. The development of this model is seen, therefore, as a step towards the simulation of more ambitious and complicated systems. The model was developed in a two step process. First, the actual molecule was compared with a model involving 30 Lennard-Jones sites and 3 quadrupoles. A 4-site arrangement of hybrid Gay-Berne Luckhurst-Romano (HGBLR) potentials was then mapped onto this intermediate model through comparison of the interaction between pairs of molecules at seven different relative orientations. MD simulations of 256 and 108 of these 4-site molecules have shown no indication of any thermodynamic singularities. Diffusion measurements suggest that there may be a sharp change in the dynamical behaviour, although the radial distribution function is virtually identical on both sides of this change.

Dominic De Luca (SHU) described how a similar approach had been used to investigate the molecule p-terphenyl by taking it to consist of two coplanar end rings with a central ring rotated by 39° about the para axis. In this case, the intermediate model used was one of 32 Lennard-Jones sites and the final one was a 3-site HGBLR arrangement. Simulations were performed with this three site model both with and without the 39° twist. In both cases, an ordered low temperature phase was formed with a director *perpendicular* to the molecular long axes. This indicated that the dominant ordering field was that between the constituent rings rather than that due to the molecular shape anisotropy. When quadrupoles were incorporated into the intermediate model, the intermolecular potential was found to alter considerably. Incorporation of quadrupoles into the three site model was not a viable option, so instead a modification was made to the well depth ratio of the three HGBLR sites. MD runs on this system have indicated no ordered phases to date.

Mike Allen discussed three different pieces of work being performed in his group. The first of these concerned measurements of the Frank elastic constants of the Gay-Berne nematogen. This is being attempted in his group using a constrained director MD technique, and at Southampton/SHU using a similar (but different) MC approach. Both groups are attempting to extract the elastic constants from measurements of fluctuations in the ordering matrix elements. A third measurement of one of the elastic constants by use of twisted boundary conditions is also being performed at Bristol. Mike also reported the findings of his group's shear viscosity measurements in systems of anisotropic hard bodies in the isotropic phase. Previous measurements of this quantity had been found to disagree with Glenn Evans' kinetic theory. These more recent simulations, using extremely long run times, have vindicated the theoretical predictions however; the failure of previous simulations appears to be explained by the long relaxation times required for the orientations of the elongated molecules to equilibrate. Finally, Mike spoke briefly about some even longer runs currently being performed on rather small systems ($\simeq 100$ particles) in order to investigate the free energy associated with the orientation of the director with respect to the simulation box. Analysis of the measured distribution functions is planned for the near future.

Next came two contributions describing the simulation of biaxial molecules using a kinked dimer to represent each molecule. The first of these came from Andy Emerson, who described an initial study of the behaviour of Gay-Berne dimers. His MC simulations have used two 3:1 rod-like monomers per molecule, the monomers being joined end to end at an angle α. Thus far, using angles $\alpha = 109^\circ$ and 150°, no evidence of nematic ordering has been seen for these systems. Andy Masters described a similar project he has been performing in collaboration with Mike Allen using dimers of hard spherocylinders. In most of this work, monomers with $l/d = 2$ were used, the simulations been executed using constant pressure MC. The results indicated stable nematic phases for $\alpha \geq 150^\circ$ but no ordering for $\alpha = 120^\circ$. Once in the nematic phase, little variation was seen in the equation of state with variation of α, the results being in reasonable agreement with Frenkel's for $l/d = 5$ spherocylinders. These systems proved very prone to log-jams, however, and no spontaneous isotropic to nematic transitions were observed. Plans to study this model using theory were also described. In the isotropic phase it is hoped that Wertheim theory can be extended by relating the dimer fluid to the equivalent monomer fluid. Attempts to measure the required distribution function by simulation have proved unsuccessful, however.

The final contribution to the meeting came from George Jackson, and concerned both theory and simulation of hard body systems. The first project he described was based on simulations of linear chains of m tangential hard spheres using the reptation algorithm. This is a long running project which has progressed from $m = 2$ up to (most recently) $m = 7$. For $3 \leq m \leq 6$, these systems have been found to progress from solid to liquid with no intermediate phases (apart from glasses in which the molecules get trapped by the cusps between the constituent spheres). For $m = 7$, a stable nematic *has* now been observed. Comparison of these results with the 'easy' nematic phase formation shown by Mark Wilson's MD on semi-flexible chains with $m = 7$, leads to the conclusion that flexibility aids orientational ordering. A further project described by George is based on large system (1000+) simulations of hard spherocylinders, the aim being to examine the earlier results of Frenkel. For $l/d = 3$, these new results have shown that no smectic phase is formed (Frenkel found one but doubted its validity). For $l/d = 5$, the new results have confirmed the phases seen by Frenkel although slight shifts are apparent.

The first piece of theoretical work described by George concerned a MC annealing technique which can be used to minimise the free energy with respect to the singlet orientational distribution function. Good agreement has been found between the results of this theory and simulations. A specific model which is being studied using theory is that of hard spherocylinders with 'sticky ends' . Here, results predict orientational order even at small l/d as the molecules dimerise to effectively double in length. Reentrant phenomena were predicted to result from this dimerisation. Future work will focus on systems of dipolar hard spherocylinders, using longitudinal, transverse and off-centre transverse dipoles. Again this should lead to dimerisation (though this time it will be side to side rather than end to end) and, again, reentrant behaviour is expected to result.

Polarization Effects on Amino-Acid Conformation

D.A. Mac Dónaill and D.A. Morton-Blake,
Department of Chemistry, Trinity College, Dublin 2, Republic of Ireland.

A modified CNDO/2 method was used to calculate the conformational energy surface of zwitterionic glycine in a simulated polarizable environment. While the calculated global minimum for the *in vacuo* glycine zwitterion corresponds to an eclipsed conformation, the allowance of even a small degree of environmental polarisability inverts the relative stabilities of the staggered and eclipsed forms. The results indicate that *in vacuo* models may be unreliable, even for supposedly 'inert' media, and that the significance of environmental polarizability should be considered in the calculation of short-range potentials.

Key words: Glycine, Solvation effects, Polarization, Virtual charge model, Short-Range Potentials

1. INTRODUCTION

Over the past two decades numerous methods have been developed to account for solvent effects [1-4] which have long been known to play a central role in the structure and function of biological molecules [5]. Nevertheless, *in vacuo* calculations are still commonly pursued in modelling the behaviour of biopolymers [6]. It seems reasonable to wonder whether the interaction between a solute molecule and a postulated inert solvent environment could be sufficiently small that the properties of the solute could be reliably calculated by quantum chemical calculations performed on the isolated *in vacuo* molecule. Clearly, if this approximation is not tenable, doubt is cast on the validity of *in vacuo* calculations, not only by quantum chemical methods, but also by procedures that are based on the representation of intermolecular interactions by simple atom-pair potentials.

In this study we examine a molecule of biological interest, the irreducible element of peptides and proteins - zwitterionic glycine ($^{-}O_2C\text{-}CH_2\text{-}NH_3^{+}$), for which there is disagreement between the results of experimental measurements made in supposedly 'inert' environments and of quantum chemical calculations on the isolated molecule. Molecular conformations are specified using the torsional angles ϕ and ψ in accordance with the IUPAC-IUB convention [7]. In the case of glycine ψ governs the $^{-}O_2C\text{-}CH_2$ bond and ϕ the $CH_2\text{-}NH_3^{+}$ bond.

2. CALCULATION METHOD

Calculations were performed using the CNDO/2 (Complete Neglect of Differential Overlap) method described by Pople and Beveridge [8], and later modified by Constanciel and Tapia [9] to incorporate the VCM (virtual charge model) as a means of modelling solvent effects. CNDO/2 is by definition an approximate method and is not, therefore, quantitatively perfectly accurate. However, for electron-donor-acceptor interactions, particularly for moderately strong intermolecular and intramolecular H-bonds, CNDO/2 is quite reliable [10].

In the VCM [9] a polarizable environment is accounted for by associating with each solute atom A, bearing a partial atomic charge Q_A, a virtual charge Q_A' given by

$$Q_A' = -(1 - \frac{1}{D}) Q_A \qquad (1)$$

where the effective dielectric constant D is related to the bulk dielectric constant by

$$D = \sqrt{\varepsilon} \tag{2}$$

The virtual charges polarize the solute and as required interatomic electrostatic interactions are attenuated by a factor of $1/\varepsilon$. However, the virtual charges polarize the solute, thereby altering the partial atomic charges and consequently the electrostatic interaction energies.

The VCM also includes the Born solvation energy of the partial atomic charges, given by

$$E_{\mathrm{Born}} = -\tfrac{1}{2}(1 - D^{-2})Q_A^2\gamma_{AA} \tag{3}$$

where γ_{AA} is the one-centre coulombic integral

$$\gamma_{AA} = \int \mu_A(1)\mu_A(1)\frac{1}{r_{12}}\nu_A(1)\nu_A(1)d\tau \tag{4}$$

The partial atomic charges are themselves conformationally dependent, resulting in a complex conformational dependence for the total solvation energy. Thus, the action of a solvent on a solute cannot be regarded as simply the attenuation of interatomic electrostatic interactions (including H-bonds) by a dielectric environment.

The VCM considers only bulk or continuum environmental effects and cannot account for specific solvent-solute interactions. However, the method may be usefully applied where either bulk effects dominate the interaction of a molecule with its environment or where one is interested in the bulk component of environmental effects. Our task here is to compare the effect of the bulk dielectric of an 'inert' medium with the results of *in vacuo* calculations, in order to assess the role of the polarizability of the environment, and explain the disagreement between the observed and predicted conformations of zwitterionic glycine.

3. ZWITTERIONIC GLYCINE

Microwave studies indicate that glycine does not exist as the zwitterion in the gas phase [11,12]. However, where the angle ϕ has been experimentally determined in the solid phase (in the zwitterion of glycine and related compounds) it is nearly always near 60°, corresponding to the staggered conformation [13]. More specifically, in the case of glycine itself ϕ has been determined by neutron diffraction to be roughly 60° for the α-crystalline form [14].

Most reliable calculation methods (e.g. *ab initio*, CNDO/2, PCILO) yield similar conformational energy surfaces for zwitterionic glycine *in vacuo*, and predict the protonated amino group ($-NH_3^+$) to exist in the eclipsed conformation ($\phi = 0$) reflecting a strong intramolecular H-bond. By contrast, methods using empirical functions predict it to adopt the staggered conformation ($\phi = 60$) [13,15].

If the steric energy is similar to that in ethane [16] one would expect the staggered conformation to be favoured by about 12-13 kJ/mole in the absence of a H-bond. An intramolecular H-bond, typically about 21 kJ/mole [10], should favour the eclipsed conformation. Since the quantum chemical methods referred to 'recognise' hydrogen-bonding they predict the eclipsed conformation to be the more stable, with a low energy barrier to internal rotation (usually about 12-13 kJ/mole or less), reflecting a fine balance between electrostatic and non-electrostatic interactions [13]. (All computational procedures, empirical [15] or otherwise, predict $\psi = 0$ in agreement with experiment [13].)

Clearly some critical factor is being neglected in the calculations;; we now consider the polarizability of an 'inert' environment.

4. RESULTS AND DISCUSSION

In the calculations the crystal lattice is treated as a polarizable continuum and zwitterionic glycine as a 'solute' in a solid 'solvent'. In the absence of experimental data we consider a value of $D = 2$ ($\varepsilon = 4$) as a reasonable one for glycine crystals on the basis of the dielectric constants (at 17° - 22°) of similar systems; solid urea ($\varepsilon = 3.5$), acetic acid ($\varepsilon = 4.1$) and acetamide ($\varepsilon = 4.0$) [17]. Greenberg et al. [18] used a dielectric step function with $D = 2$ for distances greater than 3.5 Å which agrees well with the value used here. However, recognising the inexactitude in the concept of dielectric constant at a molecular level, calculations were also performed using a series of D values.

The CNDO/2 *in vacuo* conformational energy surface for the zwitterion, identified as the total energy of the solute-system, was calculated at 15° resolution using the bond lengths and angles given in [19].

The *in vacuo* global minimum is at ($\phi = 0, \psi = 0$) - the eclipsed conformation in agreement with earlier calculations but in disagreement with experiment. For the condensed phase environment modelled with $D = 2$ ($\varepsilon = 4.0$) the global minimum occurs at ($\phi = 60, \psi = 0$) - the staggered conformation. Clearly even a low dielectric environment, in fact any condensed phase environment whatsoever, is sufficient to reverse the relative stabilities of the eclipsed and staggered forms. In fig. 1 the ϕ dependence of the energy is plotted (at $\psi = 0$) for various values of D and clearly shows the greater stability of the staggered conformation ($\phi = 60$) at very small D values. While one expects a H-bond to be destabilized by a polarizable environment it is striking how sensitive the system is.

One can conclude that even the weak dielectric constant ($\varepsilon = 4$) of crystalline zwitterionic glycine sufficiently weakens the intramolecular H-bond so that the staggered conformation is adopted in agreement with experiment. Intermolecular interactions in crystals may indeed further stabilize this conformation but our calculations suggest that the polarizable environment is alone sufficient to account for the observed structure.

We note that solvation calculations where the partial atomic charges were held fixed at their *in vacuo* values did not reflect the same environmental sensitivity. Partitioning of the calculated energy showed that electron redistribution within the solute glycine on solvation to be a critical component of the total solvent effect.

5. CONCLUSION

Atomistic simulations, originally designed for ionic systems, are increasingly being applied to covalent systems. Our calculations suggest that two-, three- and four-body potentials should be based on quantum chemical calculations which explicitly model environmental polarizability. Modelling of the solvent environment in an atomistic simulation by application of a Born-type model on top of *in vacuo* based potentials may not adequately model solvation.

6. REFERENCES

1. O. Tapia: *Mol. Interactions* **3**, 47 (1982) and references therein.

2. O. Ventura, J. Bartolucci: *Theoret. Chim. Acta* **64**, 229 (1984) and references therein.

3. D. Mac Dónaill, D.A. Morton-Blake: *Theoret. Chim. Acta*, **65**, 13 (1984).

4. R.A. Beckman, L.A. Loeb, *Quart. Rev. Biophys.*, **26**, 225 (1993) and references therein.

5. C. Tanford: *Adv. Protein Chem.* **23**, 121 (1968).

6. C. Aleman, J. Percy, *Int. J. Pept. Prot. Res.*, **43**, 258 (1994).

7. IUPAC-IUB Commission on Biochemical Nomenclature: *Biochemistry*, **9**, 3741 (1970).

8. J.A. Pople, D.L. Beveridge, *Approximate Molecular Orbital Theory*, McGrath-Hill, New York, (1970).

9. R. Constanciel, O. Tapia: *Theoret. Chim. Acta* **48**, 75 (1978).

10. C. Rao, B. Sudhindra, H. Ratajczak, *Molecular Interactions*, **1**, 67 (1980) and references therein.

11. R. Suenram, F. Lovas: *J. Mol. Spectrosc.* **72**, 372 (1978).

12. R. Brown, P. Godfrey, J. Storey, M. Bassey: *J.C.S., Chem. Comm.* 547, (1978).

13. P. Palla, C. Petrongola, J. Tomasi: *J. Phys. Chem.* **84**, 435 (1980).

14. P.-G. Jönsson, A. Kvick, *Acta Cryst.*, **B28**, 1827 (1972).

15. P. Ponnuswamy, V. Saisekharan, *Biopolymers*, **7**, 624 (1969).

16. R. Morrison, R. Boyd: p27, *Organic Chemistry*, 3rd edition, Allyn and Bacon Inc., Boston, 1973.

17. '*Handbook of Chemistry and Physics*', 62nd edition, 1981-1982, eds. R. Weast, M. Astle, CRC Press, Florida.

18. D. Greenberg, C. Barry, G. Marshall: *J. Amer. Chem. Soc.* **100**, 4020 (1978).

19. L. Shipman, R. Christoffersen: *Theoret. Chim. Acta*, **31**, 75 (1973) and references therein.

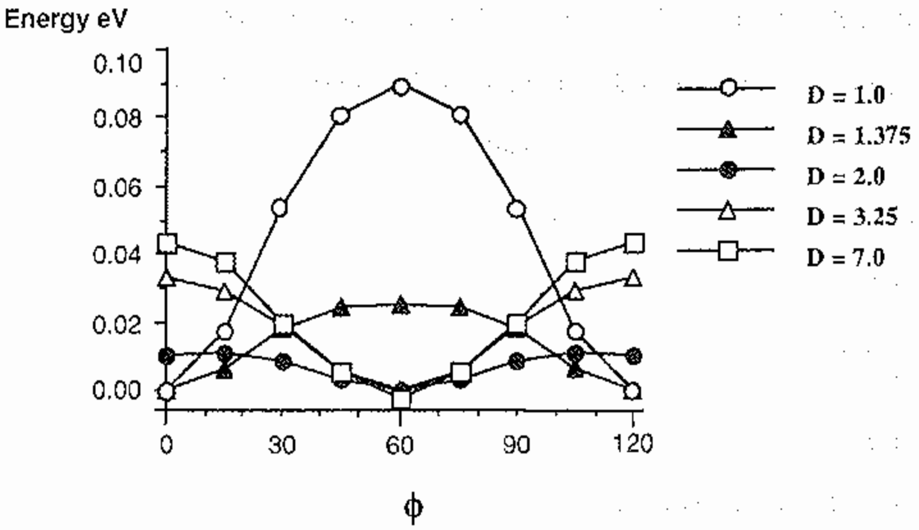

Figure 1. Conformational energy of zwitterionic glycine as a function of ϕ for various dielectric constants, D ($\psi = 0$).