

Daresbury Laboratory

# INFORMATION NEWSLETTER 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 47

February 2000

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Editor: Dr. M. Leslie

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## General News

### MEMBERSHIP OF EXECUTIVE COMMITTEE

Following a ballot by Email of UK members of CCP5 in September, two new executive committee members have been elected. The executive committee members who have retired are

Dr. J. Harding	Condensed Matter & Materials Physics University College London
Email: j.harding@ucl.ac.uk	
Prof. G.S. Pawley	Dept. of Physics & Astronomy University of Edinburgh
Email: g.s.pawley@ed.ac.uk	

The current executive committee members are

Professor D. Heyes (Chairman)	Department of Chemistry University of Surrey
Email: d.heyas@surrey.ac.uk	
Dr. J. Anwar	Department of Pharmacy Kings College London
Email: jamshed.anwar@kcl.ac.uk	
Dr. M. Dove	Department of Earth Sciences University of Cambridge
Email: martin@esc.cam.ac.uk	
Dr. J. Gale	Dept. of Chemistry Imperial College
Email: j.gale@ic.ac.uk	
Dr. R.L. Johnston	School of Chemistry University of Birmingham
Email: roy@tc.bham.ac.uk	
Dr. J. Melrose	Polymer and Colloid Group, Cavendish Lab University of Cambridge
Email: jrm23@phy.cam.ac.uk	

Prof. A.P. Sutton	Department of Materials University of Oxford
Email: <a href="mailto:adrian.sutton@materials.ox.ac.uk">adrian.sutton@materials.ox.ac.uk</a>	

## **An index of current meetings in the area of computer simulation of condensed phases.**

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A summary table is given, further details may be found by following the links.

- **CCP5 Annual General Meeting 2000**

Molecular Simulation in the 21st Century. University of Surrey  
Guildford, UK.  
UK  
2nd-5th July 2000

- **Modelling Biomolecular Mechanism: From States to Processes at the Atomic Level**

<http://www.mgms.org/diary.htm>  
A meeting of the Molecular Graphics and Modelling Society  
University of York, April 5-8, 2000

- **Psi-k2000 Conference**

<http://psi-k.dl.ac.uk/psi-k2000>  
Schwäbisch Gmünd, Germany, August 22 - 26, 2000

- **Theory and Simulation of Clusters and Nanoparticles**

<http://www.tc.bham.ac.uk/~roy/Summer2000.html>  
Royal Society of Chemistry - Theoretical Chemistry Group  
University of Birmingham 27 August - 6 September 2000

- **6th Granada Seminar on Computational Physics**

<http://ergodic.ugr.es/cp/>  
Granada, Spain, 4-9 September 2000

## **Funds for workshops, visitor proposals and collaborations.**

Applications for funding can now be processed using a WWW form. Copies of these forms may be found on the CCP5 WWW pages. There are copies of the forms on the following pages, these are intended to show the information needed. If you wish to use them please fill in the WWW version.

# WORKSHOP PROPOSAL FORM

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CCP5 organises a programme of workshops on focussed research topics in addition to the annual meeting. It is intended that these should be for a smaller group of people (20 - 30) and concentrate on a specific topic. Speakers may be invited to attend. CCP5 workshops usually last for one to two days (i.e., possibly with an overnight stay). If you have any suggestions for future workshops please fill in the form below, and it will be considered for funding.

Please make every attempt to fill in all of the boxes. If you do not have the requisite information, please leave the box blank.

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## Workshop proposal

<b>Workshop name</b>	
<b>Proposed dates</b>	
<b>Proposed organiser (Optional)</b>	
<b>Where workshop is to be held</b>	
<b>Suggested speakers</b>	

Enter a brief description of the proposal in the box below

## VISITOR PROPOSAL FORM

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CCP5 organises a visitors program which funds the visit to the UK of overseas collaborators. We would normally expect a visitor to visit three sites in the UK and give a lecture at each site. These lectures would be open to all members of CCP5 as well as members of the host university. The visit would normally last between one or two weeks. CCP5 would pay for the cost of travel to the UK (up to a limit of an APEX air fare) and within the UK between universities. CCP5 would expect some contribution towards accommodation expenses at the host university to be met by the university.

If you would like to suggest a visitor, please complete as much of the form below as possible. Additional information may be submitted at a later date. When you have a detailed itinerary, please fill in the details in the visitor itinerary form.

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### Visitor proposal

<b>Your name</b>	
<b>Visitor name</b>	
<b>Visitor address</b>	
<b>Proposed dates</b>	

Please give a brief summary of the research area and the timeliness of the visit for UK Science.

I would like CCP5 to ask for suggestions from the members

### Funding

I expect to be able receive part of the cost of the visit from another source. (If this is the case, please send Email to [m.leslie@dl.ac.uk](mailto:m.leslie@dl.ac.uk) giving details)

## VISITOR ITINERARY

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Please fill in a suggested itinerary below, after consultation with the local organisers. If you would like CCP5 to ask for suggestions from the members please check the box at the end. There is space for 5 locations, however CCP5 does not expect visitors to visit more than 3 locations.

Please make every attempt to fill in all of the boxes. If you do not have the requisite information, please leave the box blank.

Host department and Institution	Local organiser (Name and Email address)	Proposed Dates (From - To)

I would like CCP5 to ask for suggestions from the members

### Lecture schedule

Please fill in available information below

Location	Time and Date	Proposed title of lecture

### Funding

I have asked the local organisers if their host universities can pay for the cost of overnight accommodation and other local expenses.

## COLLABORATION PROPOSAL FORM

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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 fill in the form below, and it will be considered for funding.

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### Collaboration proposal

<b>Name and Address of First Collaborator</b>	
<b>Name and Address of Second Collaborator</b>	

Enter a brief description of the proposal in the box below

## **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).

Starting with this issue, the format that is used to distribute the newsletter has changed. The newsletter is still available as a postscript file for downloading as before, also separate copies of the articles. There is also a RTF version for use with MSWORD. The CCP5 WWW pages now point to a HTML version of the newsletter to be viewed online.

## **Distribution of Information by Email**

CCP5 will distribute by Email to the members on the mailing list (about 850 world wide) information which is of interest to our members. Three lists are maintained, for UK members, members in other European countries and all other members. If you have information which you would like sent out in this way please send it by Email to M. Leslie, indicating whether it would be appropriate to restrict its distribution. We also send out post-graduate, post-doctorate and lectureship positions notified to us. Normally the Email messages for post-graduate positions within the UK are restricted to UK members, however if the position is open to non-UK students then Email may be sent to the rest of Europe or the complete mailing list. Messages sent out may be batched together in which case there may be a short delay between the receipt of the message at Daresbury and its transmission. CCP5 no longer places the positions on the WWW or ftp servers but a link will be placed from CCP5's page to a page at a University advertising the position.

## **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).

## **Request for Contributions**

Readers are reminded that contributions are always welcome. Contributions may be sent by Email in LaTeX. WORD documents should preferably be sent in rtf format. Documents for inclusion in the next newsletter can now be sent as HTML.

## MOLECULAR SIMULATION IN THE 21st CENTURY.

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**University of Surrey**

**Guildford, UK.**

**UK**

**2nd-5th July 2000**

The Annual Meeting of CCP5 in the year 2000 happens to be the 21st in the series and also the first in the 21st century. As befits this auspicious coincidence, we plan this meeting to be a rather special occasion, consisting of invited keynote lectures covering a diversity of topics in rapidly moving branches of condensed matter molecular and mesoscale simulation. There will also be opportunities for contributed talks and posters.

An important theme of this meeting is to review the progress made in various branches of what is loosely referred to as 'molecular simulation', and to discuss prospects for and to identify areas that are likely to become of central importance in the not too distant future. The particle-based simulation of liquids, solids and granular materials will be included in the programme. Special attention will be given to methods for expanding the scope of molecular simulation techniques to shorter/longer time and length scales, e.g. biased sampling schemes in Molecular Dynamics and Monte Carlo, and coarse-graining procedures. In the latter case a desire is to retain important aspects of, for example, chemical discernment at the coarse-grained level of description.

### **Plenary Lecturers will include:**

Jean-Louis Barrat	Département de Physique des matériaux Université Claude Bernard Lyon 1	Simulating Non-equilibrium Dynamics in Glassy Systems: Aging, Effective Temperature and Behaviour under Shear.
William G. Hoover	Department of Applied Science University of California, Davis	From Atoms to Continua, using Smooth Particles.
Benedict Leimkuhler	Department of Mathematics and Computer Science University of Leicester	Multiple timescale integrators for Molecular Dynamics Simulation.
Ruth M. Lynden-Bell	Atomistic Simulation Group School of Mathematics and Physics The Queen's University of Belfast	Simulation: How to do things that experimentalists can't do and wish they could.

Paul Madden	Physical & Theoretical Chemistry Laboratory University of Oxford	Many-body interaction effects on the properties of molten ionic mixtures.
Ugur Tüzün	Dept Chemical & Process Engineering School of Engineering in the Environment University of Surrey	Macromolecular Product Engineering using a Simulation Toolkit.

There are opportunities to give contributed talks and posters (see below).

### Local organisers:

Prof. David Heyes Department of Chemistry University of Surrey Guildford GU2 5XH, UK.	Tel: Fax: Email:	(+44) 1483 259580 (+44) 1483 876851 d.heyes@surrey.ac.uk
Dr. Sebastian Reich, Department of Mathematics and Statistics, University of Surrey, Guildford GU2 5XH, UK.	Tel: Fax: Email:	(+44) 1483 259000 ext. 2638 (+44) 1483 876071 s.reich@surrey.ac.uk

### Other members of the organising committee:

Dr. J. Anwar, Department of Pharmacy, King's College London, Franklin Wilkins Building 150 Stamford Street Waterloo Campus London SE1 8WA.
Dr. W. Smith, CLRC Daresbury Laboratory Daresbury, Warrington, Cheshire WA4 4AD.

Prof. Adrian P. Sutton,  
University of Oxford  
Department of Materials  
Parks Road  
Oxford OX1 3PH.

### **Conference timetable:**

The meeting will start at 09.00 on Monday 3rd July and finish at 13:00 on Wednesday 5th July. For residential delegates, accommodation is provided for the nights of Sunday 2th July, Monday 3rd July and Tuesday 4th July. All accommodation is on the University Campus, a few minutes walk from the lecture theatre.

### **Registration and Accommodation:**

A registration form is available at the CCP5 website (details given below).

The full conference cost (including accommodation, refreshments, meals and conference dinner) is in the range £195-240 per person (depending on the type of accommodation), reduced to £175 for students. For those not requiring accommodation, there is also a reduced conference fee.

There is a £20 supplement for those registering after 1st June.

### **Presentations and abstracts**

An abstract should be sent (preferably at the time of registration and definitely before June 1st) by electronic mail, preferably in LATEX or simply as a text file. If you use MS WORD, please send the abstract as a rtf document. Oral contributions and posters are welcome.

The final date for submitting an abstract for an oral or poster presentation is June 1st.

The abstracts of the talks and posters will be published as part of the conference booklet and also in an issue of the CCP5 quarterly newsletter. Delegates are also encouraged to submit a longer account of their work for publication in the newsletter. Postscript diagrams are acceptable.

### **Registration Form:**

We **must** have a paper version of the registration form sent in the post to David Heyes, for all methods of payment.

## **WWW information**

Up-to-date information about the meeting can be found at

<http://www.dl.ac.uk/CCP/CCP5/meetings/ann2000.html>

where there is also a postscript version of **this information**

<http://www.dl.ac.uk/CCP/CCP5/meetings/ann2000.ps> and registration form.

### **Postscript**

<http://www.dl.ac.uk/CCP/CCP5/meetings/registration2000.ps>

### **Rtf**

<http://www.dl.ac.uk/CCP/CCP5/meetings/registration2000.rtf>

The University of Surrey at Guildford is close to London and is conveniently situated for two of London's major airports, Heathrow and Gatwick. It is readily reached by public transportation from within the UK. A train from central London takes about 35 minutes. Details of how to travel to the University of Surrey may be found at the WWW address:

<http://www.surrey.ac.uk/Where/directions.html>

David Heyes February 2000

# **REGISTRATION FORM**

## **CCP5 ANNUAL MEETING 2000**

## **MOLECULAR SIMULATION IN THE 21st CENTURY**

at

**University of Surrey, Guildford, UK.**

2nd-5th July 2000

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SURNAME: (Prof , Dr , Mr , Mrs , Ms *) (BLOCK letters please). (* Please delete as appropriate)		MALE <input type="checkbox"/>
INITIALS:		FEMALE <input type="checkbox"/>

BADGE: Please indicate how you wish your name to appear on your badge (e.g. David HEYES).

--

<b>Address</b>		
<b>City:</b>		<b>County/State:</b>
<b>Postcode:</b>		<b>Country</b>
<b>Tel:</b>		<b>Fax:</b>
<b>Email</b>		

Please indicate if you have any special dietary requirements

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To help us advertise our events more effectively in the future, we would appreciate, as an optional question, to discover where you learnt about this conference

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Please send this form, together with any payment details to:

Prof. D.M. Heyes,  
 Department of Chemistry,  
 University of Surrey,  
 Guildford GU2 5XH  
 United Kingdom.

## CONFERENCE COSTS (Prices are in Pounds Sterling (£).)

WE OFFER THREE POSSIBLE PACKAGES.

### PACKAGE A

RESIDENTIAL DELEGATE (includes accommodation on the nights of Sunday, Monday and Tuesday 2nd-4th July, teas, coffees, lunches on 3-5th July, evening meal on Monday 3rd July and the conference dinner on Tuesday 4th July.)

full	(standard University room)	£195.00	<input type="checkbox"/>
full	(Room with En-suite bathroom)	£240.00	<input type="checkbox"/>
student	(standard University room)	£175.00	<input type="checkbox"/>

En-suite rooms have washbasin, shower and wc. Standard rooms have a washbasin.

### PACKAGE B

NON-RESIDENTIAL DELEGATE WITHOUT CONFERENCE DINNER (includes teas, coffees, and lunches on 3-5th July)

full		£95.00	<input type="checkbox"/>
student		£85.00	<input type="checkbox"/>

### PACKAGE C

NON-RESIDENTIAL DELEGATE WITH CONFERENCE DINNER (includes teas, coffees, and lunches on 3-5th July, and conference dinner on Tuesday 4th July.)

full		£130.00	<input type="checkbox"/>
student		£120.00	<input type="checkbox"/>

Late registration, for all categories (after 1st June 2000)	£20.00	<input type="checkbox"/>
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TOTAL PAYMENT:	£	
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Payment method (in Pounds Sterling (£) only):

**Cheque:**

I enclose a cheque for £

payable to 'University of Surrey' and crossed. The reference: "DHS25B/CCP5/NAME", where NAME is your family name in capital letters, should be mentioned in any accompanying letter with the cheque.

Cheques from outside the UK must be made out in Pounds Sterling (£) and drawn on a UK branch of a British Bank.

**Credit Card:**

We can ONLY accept Mastercard, Visa or American Express credit cards.

**Credit Card Payment Details**

I authorise the University of Surrey to debit my  
Mastercard/Visa/American Express (delete as appropriate)

the sum of £ \_\_\_\_\_

Account Number: \_\_\_\_\_

Expiry Date: \_\_\_\_ / \_\_\_\_ Date:

Name on card:

Signature:

Credit Card Billing  
Address: \_\_\_\_\_  
\_\_\_\_\_  
\_\_\_\_\_  
\_\_\_\_\_

## CONFERENCE PRESENTATIONS

I would like to submit a presentation	YES	<input type="checkbox"/>
	NO	<input type="checkbox"/>
I would prefer a presentation which is	ORAL	<input type="checkbox"/>
	POSTER	<input type="checkbox"/>
Please tick as appropriate		

TITLE	
Lead author (presenter):	
Address:	
Co-author(s):	
Address:	

Special visual aids required (overhead projector is available).

35mm Slide projector:	YES	<input type="checkbox"/>	NO	<input type="checkbox"/>
Data projector:	YES	<input type="checkbox"/>	NO	<input type="checkbox"/>
VHS video playback PAL: (UK)	YES	<input type="checkbox"/>	NO	<input type="checkbox"/>
VHS video playback NTSC: (USA)	YES	<input type="checkbox"/>	NO	<input type="checkbox"/>

An abstract should be sent at the time of registration by electronic mail in LATEX, HTML or as a text file to David Heyes, (d.hey@esurrey.ac.uk).

The abstracts will be published in the conference booklet and also as part of an issue of the CCP5 quarterly newsletter. Delegates are also encouraged to submit a longer account of their work for publication in the newsletter. Postscript diagrams are acceptable.

Closing date for receipt of contributed papers is 1st June 2000. The registration cost after 1st June is increased by £20.