

# INDIVIDUAL GRANT REVIEW. DETAILED REPORT FOR GRANT GR/M78069/01: THE COMPUTER SIMULATION OF CONDENSED PHASES (CCP5 1999-2002)

## 1.1 The CCP5 Project

CCP5 started in 1980 to promote computational developments in studies of condensed phases, for which a wide range of techniques are available. These include Molecular Dynamics (MD), Monte Carlo (MC), Lattice Dynamics (LD), Lattice Statics (LS), Brownian dynamics (BD) and quantum methods such as path integral Monte Carlo (PIMC) and Car-Parrinello (C-P) simulations. Areas of application include simple and complex liquids, metals, ceramics, semiconductors, polymers, glasses, organic and inorganic solutions, surfaces, catalysis, surfactants, bio-macromolecules, liquid crystals and powders.

The activities of CCP5 are managed by an Executive Committee composed of six elected academic researchers and an elected chairman, plus two (permanent) members of CCLRC's Department for Computational Science and Engineering allocated part-time to support the project. The committee meets at least three times a year and responds to the opinions and wishes of the simulation community through its meetings, publications and electronic broadcasts. The project's Annual General Meeting also serves as a public forum for the initiation of new activities. The current chairman is Dr John Harding of University College London, who succeeded Prof. D. Heyes of the University of Surrey in 2000.

CCP5's importance to the academic community (not only in the U.K.) is considerable. Over the past 20 years it has been in the forefront of software development, the promotion of advanced techniques and the exchange of scientific knowledge. It is a valued resource to all its members.

In the period 1999-2002 CCP5 has promoted the following activities:

*Conferences to highlight research by simulation methods;*

*Workshops to promote development of computational methodology;*

*Sponsorship of eminent scientists to visit UK universities;*

*Travel funds to enable 'first contact' between collaborating groups in the UK;*

*Training opportunities in simulation methods through the CCP5 Summer School, workshops and short courses. Also, assistance and advice is made available to individuals and groups.*

*Provision of advanced simulation software; and*

*Production of newsletters, program documentation, bulletins, and other electronic information to assist scientists active in the field.*

CCP5 has a number of resources at its disposal. The first of these is the financial support awarded by EPSRC, which is managed by Daresbury Laboratory under the direction of the CCP5 Executive Committee. The part-time assistance of two scientists at Daresbury helps to maintain the continuity and structure of the project. The CCP5 Program Library

contains approximately eighty codes covering a wide range of applications. CCP5 also supports and develops the general-purpose code DL\_POLY [1], which was the first major parallel MD code and has a user base of several hundred users world wide. CCP5 also produces a WWW site [2], and maintains a large repository of past newsletter articles [3] and documentation for DL\_POLY [4].

## 1.2 Project Activities 1999-2002

### 1.2.1 *The Work of the Daresbury Support Staff*

Dr W. Smith has been associated with CCP5 since 1980 and Dr M. Leslie since 1983. Both are allocated 50% to the project and provide technical, scientific and administrative support. Their work in the period 1999-2002 is detailed below.

#### 1.2.1.1 *Dr. W. Smith*

##### *Technical Support:*

Dr. Smith's primary role has been the development of the general- purpose simulation code known as DL\_POLY [1].

- Development of a DL\_POLY Java graphical user interface;
- Incorporation into DL\_POLY of Smoothed Particle Mesh Ewald and Hautman-Klein-Ewald methods for electrostatic systems periodic in 3D and 2D respectively;
- Production of DL\_POLY documentation;
- Adaptation of the DL\_POLY code for National Supercomputers;
- Adaptation of DL\_POLY to parallel-vector computers, in collaboration with RIKEN, Japan.
- DL\_POLY user support and advice;
- Development of the domain decomposition variant DL\_POLY\_3;
- Development of DL\_POLY analysis tools;
- Maintenance and extension of DL\_POLY benchmarking suite;
- DL\_POLY user registration and licencing.
- Development of the DL\_DPD dissipative particle dynamics program.

##### *Scientific support:*

- Computer simulation of powders. In collaboration with C. Yong (Daresbury), K. Kendall (Birmingham) and L. Woodcock (UMIST). An EPSRC funded project to determine the properties of granular materials from first principles.

- Metal particle - metal surface sputtering simulations, in collaboration with K. Kholmurodov, T. Ebisuzaki, K. Yasuoka, at RIKEN, Japan.
- Molecular dynamics simulations of borate glasses, in collaboration with F. Gou, G.N. Greaves and R. Winter (Aberystwyth).
- Molecular dynamics simulation of silicate glasses with M. Dove and K. Trachenko (Cambridge), specifically quantum tunnelling by Path Integral methods.
- Simulation of nanoscale clusters: determination the effective Au-Au solvent mediated cluster potential, with M. Lal (Liverpool).

*Administrative support.*

- Membership of CCP5 Executive Committee;
- Participation in, and organising, CCP5 Summer Schools;
- Organising visits by overseas speakers;
- Support of workshop activities;
- Support of CCP5 Annual General Meetings;
- Maintenance of CCP5 Program Library;
- Contributions to CCP5 Newsletter/Infoweb;
- Maintenance of DL\_POLY WWW site;
- Management of CCP5 funds held at Daresbury.

1.2.1.2 *Dr. M. Leslie*

*Technical Support:*

- Support for the users of the Static Simulation Programs and of DMAREL. (DMAREL is a static lattice, energy minimisation program for calculating the properties of crystalline materials and deriving model potentials.)
- Development of DL\_MULTI distributed multipole molecular dynamics program.
- Adaptation of OXON tight binding program and incorporation into CCP5 program library

*Scientific Support*

- Work on the code DMAREL to simulate crystal structures using potential models with multipoles;
- Collaboration with S. Price (UCL) on molecular crystal morphologies.
- Developing potential models based on ab initio energies derived from the CCP3 code CRYSTAL.

#### *Administrative Support*

- Membership of CCP5 executive committee and minutes secretary;
- Support for workshop activities;
- Support for organisation of CCP5 Annual Meetings including production of delegate handbook;
- CCP5 newsletter editor;
- Maintenance of CCP5 WWW pages;
- Administration of mailing list and Email distribution list.

#### **1.2.2 *The Executive Committee***

The CCP5 Executive Committee comprises a chairman, six academic researchers and two Daresbury staff. The current committee is Dr. J. Harding (Chairman, UCL), Dr. D. Lewis (London), Dr. M. Wilson (Durham), Dr. S. Islam (Surrey), Dr. K. Travis (Bradford), Dr D. Willock (Cardiff), Dr D. Sayle (Cranfield), Dr. M. Leslie (Daresbury) and Dr. W. Smith (Daresbury). Immediate past members include Prof. D. Heyes (former chairman, Surrey), Dr. R. Johnston (Birmingham), Prof. A. Sutton (Oxford), Dr M. Dove (Cambridge), Dr. J. Melrose (Unilever), all of whom served in the period 1999-2002. Prof. D. Heyes was co-opted onto the committee in 2001 to advise on relations with the SIMU European Network.

In the period October 1999-February 2002 Executive Committee meetings took place on: 12/09/02; 20/5/02; 21/1/02; 26/11/01; 19/9/01; 10/5/01; 1/2/01; 3/10/00; 5/4/00; and 22/12/99.

#### **1.2.3 *Annual General Meetings***

The CCP5 Annual Meetings have wide appeal and always attract an international participation. The meetings also serve as a forum for discussion of wider issues in simulation and thus provide a guide to future CCP5 directions. The meetings organised in the 1999-2002 grant period are as follows.

#### *Molecular Simulation in the 21<sup>st</sup> Century*

This meeting took place at the University of Surrey 2-5 July 2000. Principal speakers included R.M. Lynden-Bell (Belfast), L. Gelb (Florida State), R. Sadus (Swinburn), G. Hoover (Livermore), P. Madden (Oxford), U Tuzun (Surrey), S. Reich (Surrey). The meeting covered a wide range of applications of simulation and raised issues likely to be of importance in the coming decade. Mesoscale methods were strongly evident, as were novel integration algorithms, particularly symplectic algorithms, which offer new advances in accuracy and stability. Complex systems, including surface adsorption, interfaces, zeolites, fast ion conductors, ionic melts and corrosion inhibition were presented. Attendance 63.

#### *Liquid and Liquid Interfaces*

This conference took place at Warwick University 16-19 September 2001. The principal speakers were M. Klein (Pennsylvania), M.P. Allen (Bristol/Warwick), M.J. Gillan (UCL), B. Leimkuhler (Imperial College), J. Harding (UCL), D. Cleaver (Sheffield Hallam). The conference covered many aspects of the simulation of liquids and liquid interfaces. The structure of ionic solutions, liquid crystal interfaces and phases, algorithms, grain boundaries in inorganic systems, transport coefficients, polydispersity in solutions, *ab initio* methods, surface tension, biosystems and glass and gel transitions in colloidal systems were all presented. Attendance 58.

#### *Advances in Simulation of Molecules and Materials*

This conference was held in Durham University 10-12 September 2002 and exemplified a broad range of applications of atomistic simulation. The invited speakers were Neil Allan (Bristol), Gerbrand Ceder (MIT), Julian Clarke (UMIST), Jon Essex (Southampton), Adrian Mulholland (Bristol), Friederike Schmid (Bielefeld) and Claudio Zannoni (Bologna). Attendance 60.

### **1.2.4 Workshops**

#### *Ions in Solids and Liquids and at Interfaces*

This workshop was held on 5-6 January 2000 and was organised jointly with the The Royal Society of Chemistry, Statistical Mechanics and Thermodynamics Group (SMTG) at Nottingham. Four of the speakers: Rustad (PNL), Lindan (Daresbury), Sprik (Cambridge), and Parker (Bath) addressed the problem of the aqueous interface. Fowler (Exeter) discussed current progress in calculating polarisabilities of ions in solids. Wilson (Oxford) gave a number of examples to show how the correct inclusion of polarisability effects could enable ionic models to reproduce effects traditionally considered to be 'covalent'. Harding (UCL) gave a brief survey of mesoscale modelling at interfaces. Attendance 25.

#### *Long Ranged Forces*

This workshop was held at Daresbury Laboratory on December 12 2000. It brought together two distinct 'camps' in molecular simulation with a common difficulty - how to incorporate long ranged forces into microscale simulation most effectively. For some

simulators it is electrostatic forces that give rise to difficulty, while for others, particularly those interested in colloids and bio-polymers, it is hydrodynamic forces. The meeting attracted many overseas participants and included G. Kneller (Orleans), R.B. Jones (QMWC), J. Yeomans (Oxford), M. Whittle (Leeds), J. Elliot (Cambridge), M. Jorge (Edinburgh), C. Holm (MPIP Mainz), P. Hunenberger (ETHZ), M. Neumann (Vienna) and M. Leslie (Daresbury). Attendance 20.

#### *Calcite and Related Materials: Growth and Dissolution*

The workshop was held on 4th - 5th January 2001 at the Department of Chemistry, University of Reading. It was held in response to the large amount of work that has been published on the growth and dissolution of materials with inorganic molecular ions such as carbonate, sulphate, nitrate and perchlorate. In addition recent work had concentrated on calcite (and to a lesser extent the other phases of calcium carbonate) because of their importance in biology and geology. This workshop brought together simulators and experimentalists from different disciplines to discuss common problems and initiate new collaborations. The invited speakers were Prof. Susan Stipp, (University of Copenhagen, Denmark) and Dr. Randy Cygan (Sandia National Laboratories, New Mexico). A report of the workshop has been published as a special issue of Molecular Simulation. Attendance 45.

#### *Multiscale algorithms for the simulation of Materials and fluids*

Held at Imperial College 2-4 April 2001 and organised by D. Heyes (Surrey) and S. Reich (Imperial), this workshop addressed new methodologies for particulate simulations including: Dissipate Particle Dynamics (DPD), Smoothed Particle Hydrodynamics (SPH), Lattice Boltzmann (LB), Stokesian Dynamics (SD), Brownian Dynamics (BD) and others. The speakers included P. Coveney (Queen Mary London), C. Care (Sheffield Hallam), P. Espanol (Madrid), H. Posch (Vienna) and B. Sandberg (NRL Washington). Attendance 40.

#### *Statistical Mechanics and Molecular Simulation of Nucleation and Growth*

The workshop was held at King's College London on 2-4 July 2001 and was organised jointly with the SIMU network by D. Heyes (Surrey) and J. Anwar (King's London). 40 people attended. (SIMU is the acronym for a international collaborative programme sponsored by the European Science Foundation - ESF - and whose title is Challenges in Molecular Simulations: Bridging the Length and Time-scale Gap'.)

#### *Computational methods for mineral sciences research*

This one-day workshop on was held on 19 June 2001 in Cambridge and was jointly organised with the Mineral Physics group of the Mineralogical Society.

### 1.2.5 Other Meetings

A **discussion meeting** was held at Daresbury Laboratory on 21/5/2001 to discuss the implementation of force fields in DL\_POLY and other DL codes.

**The London Atomistic Simulation Group (LASG)** met under the auspices of CCP5 on 26 June 2002 at UCL with 35 attendees. In addition to providing a forum for a number of different research groups to meet, this meeting offers a relatively informal occasion for students and PDRAs (particularly those just starting their careers) to present their work. This meeting is now an annual event supported by CCP5.

CCP5 funded **two UK speakers** (CRA Catlow and R Lynden-Bell) to attend the "Exploring modern computational chemistry 2" conference in Nottingham (31 July - 2 August 2002)

### 1.2.6 Education in Simulation Methods

#### *The Methods in Molecular Simulation Summer Schools*

The Methods in Molecular Simulation Summer Schools were initiated by Professors M.P. Allen (Bristol), D.J. Tildesley (Unilever) and J.H.R. Clarke (UMIST) and represent a major educational contribution to the science of molecular simulation. The purpose of the School is to introduce postgraduate students to the fundamentals of molecular simulation through an intensive series of lectures and practical sessions involving real problem solving exercises in applied computational science. The School lasts nine days, the first week is devoted to basic material every student needs to know, followed by two days of specialised, advanced courses on scientific areas of high current interest. Additional plenary lectures by internationally leading speakers introduce students to various research topics. The attendance normally numbers 60 to 80 students from the international community. The Schools are strongly supported by the simulation community, both in the United Kingdom and overseas, as is evidenced by the enthusiastic assistance it receives from speakers from all countries.

The Summer Schools are part sponsored by SIMU (in the form of bursaries to students) and (until 2001) the Statistical Mechanics and Thermodynamics Group of the Royal Society of Chemistry. CCP5 sponsored and organised the Summer Schools at UMIST in Manchester in 2000 and 2001 and at King's College London in 2002. Since the original organisers have now stepped down, CCP5 has set up a sub-committee - the CCP5 Summer School Working Group - to ensure the continuation of the School in the years to come. The working group consists of John Harding (UCL), W. Smith (Daresbury), J. Anwar (Kings London), K. Refson (Rutherford Appleton), P. Lindan (Canterbury) and D. Heyes (Surrey).

#### *Other Training Events*

In response to a growing need in the CCP5 community, CCP5 has organised training sessions in the use of the DL\_POLY simulation code. Two of these have taken place at

Daresbury Laboratory on 14-16 May and 27-28 December 2001. In these sessions, a small number of students (5-10) were given hands-on training in the use of the DL\_POLY code.

### *1.2.7 Visitor's Programme*

CCP5 has always sought to strengthen links between UK simulation scientists and colleagues overseas. An important aspect of this is the frequent invitation of overseas experts to the UK to visit and lecture at several UK Universities. (This being additional to the workshop and annual meeting programmes described above.) As well as providing grounds for future collaborations, the programme helps to promote new and important methods. The invited speakers in the grant period were:

- Prof. Friederike Schmid, from the Max Planck Institute for Polymer Research, Mainz visited 8 - 20 March 2000. Professor Schmid visited Reading University, Imperial College, Bristol University, Leeds IRC in Polymer Science & Technology, Sheffield University and Edinburgh University.
- Prof. Stephen Berry, James Franck Distinguished Service Professor at the University of Chicago, visited 18-27 May 2000. Professor Berry visited the University of Birmingham, Oxford University, Cambridge University and the University of Sussex.
- Dr Mark Tuckerman from New York University visited 14-21 July 2000 and lectured at Cambridge University, Edinburgh University, Daresbury Laboratory and Bristol University.
- Dr John S. Tse of the Steacie Institute for Molecular Science, National Research Council of Canada visited the UK 22 - 29 January 2001. He lectured at University College London, Daresbury Laboratory and the Universities of Warwick and Edinburgh
- Prof. Scott Auerbach of the Department of Chemistry and Department of Chemical Engineering University of Massachusetts, visited the UK from 4-8 June 2001. He gave lectures at the Royal Institution, Oxford University and Daresbury Laboratory.
- Prof. Stefan Estreicher of Texas Tech USA visited from 11-15 June 2001. He lectured at Exeter University and King's College London, and also visited Reading University and Rutherford Appleton Laboratory.
- Prof. Jose Alejandro, University of Mexico, visited and lectured at the Universities of Surrey, Bristol and Oxford and UMIST Manchester 2001.
- Prof. Billy Todd, Swinburne University Melbourne, visited the UK in July 2002 and lectured at Bradford University, Warwick University Imperial College and the University of Surrey.

### *1.2.8 Sponsored Collaborations*

In order to promote new directions in research CCP5 offers limited travel funding (nominally up to £500) to assist collaborations between research groups, subject to a short

scientific case being made to the Executive committee. This funding enables 'first contact' between participants, sometimes leading to a research proposal.

- N.B Wilding, Dept. of Mathematical Sciences, Liverpool University, and P. Sollich, Dept. of Maths, Kings College, London collaborated on the use of Monte Carlo simulations to study the effects of particle size variations (polydispersity) on the phase diagram of a system of hard spheres.
- D.C. Sayle RMCS, Cranfield University Swindon, and G.W. Watson, Trinity College, Dublin collaborated on simulated amorphisation and recrystallisation methodology, to explore structural features that evolve within a supported material.
- Prof. Roger Smith (Loughborough) and John Robertson (Cambridge) studied bonding of a C implant with energetic C atoms in the energy range 30eV-500eV.
- M. Dove and K. Trachenko, Cambridge Earth Sciences collaborated with W. Smith (Daresbury) on quantum tunnelling in silica glasses by path integral molecular dynamics.
- R. L. Johnston, School of Chemical Sciences, University of Birmingham and F. R. Manby, School of Chemistry, University of Bristol collaborated on the simulation of protein structure and folding dynamics
- D. Heyes (Surrey) and J.G. Powles and G. Rickayzen (Canterbury) collaborated on the material properties of steeply repulsive potential fluids.
- J. Titiloye, Aston University, J. Harding, CMMP, UCL, and Prof. S.C Parker, Bath University are investigating the control of calcium carbonate growth with ions, molecules and templates.
- Dewi Lewis (UCL) and Dr R. Ruiz-Salvador (Havana, Cuba) are collaborating on modelling natural zeolites; specifically the absorption/adsorption of drug molecules and surfactants on the surface of hydrated clinoptilolite.

### *1.2.9 Performance Statistics*

The following statistics refer to user access of the CCP5 WWW site, the CCP5 Newsletter and archive and the DL\_POLY WWW site.

#### *Membership List*

CCP5 currently has 953 members. 264 are in the UK, 299 in other European countries and 389 elsewhere. Registration is by electronic submission of a WWW form completed by the new member. The membership list is primarily used to advertise CCP5 activities by Email to CCP5 members.

In addition to CCP5 activities (Workshops, Visitors and meetings) we advertise third party meetings in the area of computer simulation of condensed matter. 25 meetings were advertised in 2001 including those of CCP5.

CCP5 also advertises job vacancies for CCP5 members. These are primarily post-doctoral positions in the UK and Europe, and UK studentships. 98 such positions were advertised in 2001.

### *WWW Pages and ftp server*

The CCP5 WWW pages [2] are used to publicise information about CCP5 activities and contain ftp links to the archive of the program library and electronic newsletters.

There are currently 800 visits per month to the main entry page and 4000 visits per month summed over all pages.

The information page about the program library attracts 400 visits per month, with the meetings, links, newsletter and DL\_POLY pages [3] between 50-100.

There are 2200 downloads per month from the ftp server; 2000 of these are program library files and 200 from the newsletter archive.

There are 700 downloads per month of the files from the textbook "Computer simulation of liquids", which is 20 complete copies.

Between 40 and 50 people per month download the DL\_POLY manuals and licences.

The other programs in the library are downloaded between 5 and 20 times each per month.

Archived articles are downloaded between 1 and 10 times each per month.

### *DL\_POLY*

There are 398 current DL\_POLY licences, ( UK 69, USA 96, France 26, Italy 22, Germany 36, Spain 8 Japan 11, Netherlands 9, Canada 11, China 11, Sweden 9, the bulk of the remainder are elsewhere in Europe and the Far East). 12 industrial companies have licences for the code. There are 658 users on the dl\_poly\_news mailing list, through which they are kept up-to-date about software developments. User applications of the package have recently been documented in a review article [5].

## References

[1] W. Smith and T.R. Forester, *J. Molec. Graphics* **14** (1996) 136.

[2] <http://www.dl.ac.uk/CCP/CCP5/>

[3] [http://www.dl.ac.uk/CCP/CCP5/newsletter\\_index.html](http://www.dl.ac.uk/CCP/CCP5/newsletter_index.html)

[4] [http://www.cse.clrc.ac.uk/msi/software/DL\\_POLY/index.shtml](http://www.cse.clrc.ac.uk/msi/software/DL_POLY/index.shtml)

[5] W. Smith, C.W. Yong and P.M. Rodger, *Molecular Simulation* **28** (2002) 385.