CCP5: a collaborative computational project for the computer simulation of condensed phases

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CCP5 is a Collaborative Computational Project in the Computer Simulation of Condensed Phases sponsored by the Science and Engineering Research Council of the United Kingdom. Its purpose, organization and the resources available to the participants are described.

Keywords: computer simulation, condensed phases, collaborative computational project

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CCP5 is the acronym for the Collaborative Computational Project Number 5, which is one of eight projects created by the United Kingdom's Science and Engineering Research Council (SERC) to foster the development of computational science in the United Kingdom[1]. Each CCP covers a specific area of computational science, which is particularly important in the research efforts of British universities and to some extent, industrial companies. The projects currently existing are listed in Table 1.

The CCPs are supported by the SERC's Daresbury Laboratory (near Warrington in the UK), where most of them have strong ties with the Theory and Computational Science (TCS) Division. This is a beneficial association which exploits the expertise of the TCS Division in the development of scientific software for a wide range of applications and computers. The Division also interacts with the SERC's experimental projects, such as the Synchrotron Radiation Source (SRS), and consequently is in a unique position to initiate promising collaborations.

Participation in the CCPs occurs on several levels. Those most actively involved collaborate with others to develop new methods and software to tackle specific physical problems. Others attend the workshops and conferences organized by the CCPs to broadcast and discuss new developments, and others simply exploit the availability of the program libraries and the newsletters issued by the CCPs.

The participants in the CCPs are principally scientists working in the UK. However the participation of overseas scientists and scientists working in industry is welcomed. In the case of CCP5 approximately 50% of its participants, which number over 400 scientists, are from overseas. There are no membership fees and the facilities, such as the program libraries and newsletters are available free of charge. (There are some restrictions on the availability of software to industrial and overseas scientists, but these do not hinder a beneficial participation.)

Table 1. Collaborative Computational Projects currently supported by SERC

Title	Topic
CCP1	Correlated wavefunctions
CCP2	Continuum states of atoms and molecules
CCP3	Computational studies of surfaces
CCP4	Protein crystallography
CCP5	Computer simulation of condensed phases
CCP6	Heavy particle dynamics
CCP7	Analysis of astronomical data
CCP9	Electronic structure of solids

The financial resources of each project are modest, but it is not the function of the CCPs to provide financial support for scientific research. Rather their role is to act as catalysts for new and promising research and to this end the SERC makes available manpower and computing resources. The former, often members of the Daresbury TCS Division, work in close contact with the CCPs, assisting the scientific programme and helping with software development. The computing resources consist of program development time on computers at Daresbury, London and Manchester and assistance from members of the TCS Division in developing programs.

The purpose of the CCPs may be summarized in the objectives:

- To provide facilities for the discussion, development and adoption of the best techniques of computational science and to stimulate collaborative research efforts in new and important areas of science.

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Table 2. CCP5 program library

ADMIXT	[MD, LJA/MIX, LF, TH + MSD + RDF] W Smith
CARLOS	[MC, VS + Aquo, TH] B. Jonsson/ S Romano
CARLAN	[DA, CARLOS structure analysis] B Jonsson/ S Romano
CASCADE	[LS, DIL, EM, TH + STR] M Leslie/ W Smith
CURDEN	[DA, Current Density Correlations] W Smith
DENCOR	[DA, Density Correlations] W Smith
HLJ1	[MD, LJA, LF, TH + MSD + RDF] D M Heyes
HLJ2	[MD, LJA, LF, TH + MSD + RDF + VACF] D M Heyes
HLJ3	[MD, LJA, LF/LC, TH + MSD + RDF] D M Heyes
HLJ4	[MD, LJA, LF/CP + CT, TH + MSD + RDF] D M Heyes
HLJ5	[MD, LJA/SF, LF, TH + MSD + RDF] D M Heyes
HLJ6	[MD, LJA, TA, TH + MSD + RDF] D M Heyes
HMDIAT	[MD, LJD, G5 + Q4, TH + MSD + QC] S M Thompson
HSTOCH	[MD/SD, VS + BA, LF + CA/RF, TH] W F van Gunsteren/D M Heyes
MCN	[MC, LJA, TH] N Corbin
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
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
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 and D Fincham
MDPOLY	[MD, LJS, G5 + Q4, TH + MSD + QC] S M Thompson
MDMULP	[MD, LJS + PD + PQ/MIX, LF + QF, TH] W Smith
MDTETRA	[MD, LJT, G5 + Q4, TH + MSD + QC] S M Thompson
MDZOID	[MD, GAU, LF + QF, TH + MSD + RDF + VACF] W Smith
SCN	[MC/RFD, LJA, TH] N Corbin
SURF	[MD, BHM/TF/2D, LF, TH + RDF] D M Heyes
SYMLAT	[LS, PIL, EM + SYM, TH + STR] Harwell
THBFIT	[LS, PIL, EM, Potential fitting] Harwell
THBPHON	[LS, PIL/3B, EM, Phonon dispersion] Harwell
THBREL	[LS, PIL, EM, TH + STR] Harwell

KEY:

Program types:
- MD — Molecular dynamics
- MC — Monte Carlo
- LS — Lattice simulations
- SD — Stochastic dynamics
- DA — Data analysis

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
- 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

Algorithm used:
- G5 — Gear 5th order predictor–corrector
- Q4 — Quaternion plus 4th order Gear P–C
- LF — Leapfrog (Verlet)
- QF — Quaternion plus Fincham 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

Properties calculated:
- TH — Thermodynamic data
- MSD — Mean-square displacement
- RDF — Radial distribution function
- VACF — Velocity autocorrelation function
- QC — Quantum corrections
- STR — Lattice structure
- STF — Structure factor

- To encourage the adoption of good computational practice and encourage the efficient exploitation of new and powerful computers such as the Cray 1s, Cray XMP/48 and Cyber 205 and attached processors such as the FPS 164 and ICL DAP.

In achieving these objectives, each CCP has taken on its own character and operational structure. The remainder of this article describes the structure and operation of CCP5.

CCP5 PROJECT

The need for a collaborative project in the field of com-

puter simulation arose naturally out of the rapid growth in the application of simulation methods to the study of bulk properties of materials. Since the 1950s when the Monte Carlo and molecular dynamics methods were finding their first applications, methods have evolved with the advances in computer technology to the stage where they are considered essential to the understanding of the properties of every kind of material: solids, liquids, gases and plasmas, in fact wherever the bulk properties of materials prove difficult to reduce to atomic or statistical mechanical interpretation. As these methods grew in power and versatility their use spread through the academic community. In the UK some means of pooling the amassed expertise and of fostering the development of the newest and best methods became of great importance. The creation of CCP5 was a direct a response to this need.

The project began in 1980, when it initially concentrated on the computer simulation of liquids using the Monte Carlo and molecular dynamics methods. This is a continuing activity in CCP5, since it provides the most powerful technique for studying the thermodynamic and dynamical properties of liquids and also for assessing model intermolecular potentials. Much of the early effort of CCP5 was directed towards exploiting the power of the Cray 1 s computer then housed at Daresbury and as a result a very useful program library was developed (see below).

At the time of its renewal in 1983, the scope of CCP5 was extended to include the calculation of lattice properties by energy minimization methods. This extremely important area of research has many applications in both academic and industrial laboratories. The skills required in these different areas are highly complementary; the search for good model potentials and the application of both techniques to studies of the dynamical properties of crystals are two examples of where a combined approach can be of great benefit.

The activities of CCP5 are organized by a Steering Committee, which consists of about 30 scientists, who work in the computer simulation field. The bulk of these scientists are from British universities, but about 30% of them are based overseas in Europe, or the USA. A small number of industrial scientists are also present. The purpose of the Steering Committee is to organize the scientific programme of the Project and allocate the resources. The current elected Chairman of CCP5 is Prof C R A Catlow, Department of Chemistry, University of Keele, UK.

ACTIVITIES OF CCP5

CCP5 supports the computer simulation community in a number of ways. In general it attempts to promote the development of all aspects of computer simulation, but for the past three years it has worked to encourage the development of four specific areas of simulation, namely:

- Quantum mechanical simulations[2,3], which includes semiclassical molecular dynamics using Gaussian wavepackets, path-integral Monte Carlo methods and the Green's function–Monte Carlo method. These methods are becoming of fundamental importance in the study of quantum systems.
- The simulation of interfaces[4], including crystal surfaces, solid–solid interfaces, solid–liquid interfaces and liquid–vapour interfaces using dynamical, Monte Carlo and static lattice methods.
- The calculation of transport properties[5,6] such as shear viscosity, thermal conductivity, the dynamical structure factor and translational–rotational coupling using a variety of molecular dynamics methods such as Green–Kubo and non-equilibrium methods.
- Solid state simulations using static lattice methods in studies of ceramics[7], silica and silicates[8].

In each of these nominated areas CCP5 has organized a number of workshops, in which a number of scientists gathered together to discuss the methods available, exchange ideas and solve common problems. On occasion foreign scientists eminent in these areas were invited to the UK, either to give seminars or to discuss matters in depth at one of the British universities.

In addition to the informal workshops, CCP5 has organized several formal conferences, which were based on a theme of particular importance or interest. The conferences organized by CCP5 over the past three years include *Phase transitions*[9], *Potential models for computer simulation*[10], *Static and dynamic properties of dense fluids*[11], *Stochastic dynamics and macromolecules*[12] and *The glass transition*[13]. A particularly attractive feature of these conferences has been the strong participation of scientists from overseas. The proceedings of the conferences and workshops are published in the CCP5 newsletter.

CCP5 NEWSLETTER

CCP5 is probably most widely known through its regular newsletter, which is produced at Daresbury Laboratory. The *Information quarterly for computer simulation of condensed phases* is an informal publication, which carries articles on the techniques of computer simulation, proceedings of conferences and workshops and other topics of interest including news of interesting events. The newsletter is issued free by Daresbury and is obtainable on a regular basis on request.*

CCP5 PROGRAM LIBRARY

The CCP5 Program Library is a collection of over 30 computer programs for the computer simulation of bulk phases. The programs are available free of charge to academic establishments from the Theory and Computational Science Division at Daresbury. There are however restrictions on the circulation of certain programs, which have been produced by commercial companies and the applicants are required to sign a declaration restricting the use of all programs to non-commercial research. The programs fall into three broad categories: molecular dynamics, Monte Carlo and static lattice programs. The category of molecular dynamics programs is the largest. Nearly all of the programs have been vectorized to some degree, to allow efficient exploitation of the Cray 1s computer. However, this should not deter potential users with access to scalar machines only, as the majority of the programs may be adapted with little difficulty. Documentation for the programs is also available. The programs are listed, with a brief description, in Table 2. Copies of the CCP5 Program Library can be obtained on request.*

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FUTURE

In October 1986, CCP5 was renewed by the SERC for a further two years. In the extended period CCP5 intends to devote particular attention to newly designated areas:

- simulations of molecular and macromolecular systems;
- simulations of fluid transport properties;
- and simulations of polar solids.

It is intended that these areas of research be supported through workshops and a collaborative effort in the manner outlined above. CCP5 also intends to be active in the important work of assessing the capabilities of the nascent 'parallel processors' and other special purpose computers. In addition, CCP5 will continue to support the simulation community through its newsletter, program library and the distribution of its resources. Every scientist active in computer simulation in the UK or overseas is invited to participate. Those interested should contact the author.

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