A forum for computation

For more than 25 years, European researchers have come to CECAM to collaborate on computing problems in atomic, molecular and condensed-matter science. **Stefano Baroni** and **Piet Van Leuven** look at the centre's work and highlight some of its successes

When the European Centre for Atomic and Molecular Computations (CECAM) was founded in 1969, few could have envisaged how different the computing world would be by the mid-1990s. The centre was originally set up to enable theorists to apply computational methods to problems in physics and chemistry. Experimental and theoretical developments in atomic, molecular, and condensed-matter science had reached the stage where large-scale computing was starting to yield meaningful research results, but few scientists had adequate computer facilities at their own universities, and "distributed" computer resources were still a long way off.

CECAM, otherwise known as the *Centre Européen de Calcul Atomique et Moleculaire*, was therefore founded as a truly European initiative, where researchers could meet and exchange expertise and know-how. It was supported by five countries and was based at the University of Paris-Sud in Orsay, where it had close links with the large Paris-Sud computer facility. CECAM focused on developing computer code and providing Europe's scientific community with computing resources.

Since that time, however, there have been huge advances in computational science. The development of fast computer communications and the Internet have made it no longer necessary for researchers to be physically next door to a large computer facility. CECAM now places less emphasis on developing computer programs and has instead widened the scope of its scientific activities. But given the many new developments in computing, its function as a meeting place for collaborating scientists is probably more important than ever before.

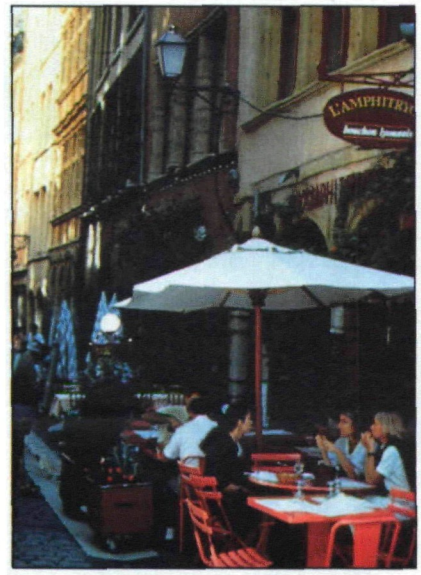
In 1994 the centre moved from Paris to the recently founded Ecole Normale Supérieure in Lyon, France. CECAM is now a consortium of ten European scientific institutions. In addition to the five national funding agencies which founded the centre – the Belgian *Fonds National de la Recherche Scientifique*, the Dutch *Nederlandse Organisatie voor Wetenschappelijk Onderzoek*, the French *Centre National de la Recherche Scientifique*, the Italian *Consiglio Nazionale delle Richerche*, and the UK's Engineering and Physical Sciences Research Council – there are five other members who joined later. These are the French atomic energy authority (*Commisariat à l'Energie Atomique*), the Ecole Normale Supérieure de Lyon, the Greek Foundation for Research and Technology, the Italian *Istituto Nazionale di Fisica della Materia* and the Swiss *Fonds National Suisse*.

Catalyst for growth

So what does CECAM do? The centre is devoted to the entire range of atomic and molecular computation, from the study of single atoms and molecules to research in condensed matter, plasmas, materials science and biomolecules. The emphasis lies in solving complex problems with large computers to give quantitative predictions of the observed properties of real systems (rather than the simplified models of "traditional" theoretical physics) and qualitative insight into the microscopic mechanisms responsible for these properties.

The centre has played an important role in a number of fields, from quantum chemistry to condensed matter physics and plasma physics. However, its greatest success has been the establishment of a strong European community in the field of classical simulations, especially molecular dynamics (MD) and classical Metropolis Monte Carlo. In 1976 the first MD simulation of a protein ever attempted was performed at a historic workshop organized by Herman Berendsen. Since then, many of the ideas which have turned MD from a clever computer exercise into a predictive tool for condensed-matter theory and materials science have been established or put on a firm theoretical basis at CECAM.

These include the SHAKE algorithm for constrained dynamics by Jean-Paul Ryckaert, Giovanni Ciccotti and Berendsen, and the "substraction" technique by Ciccotti, Gianni Jacucci and Ian McDonald, which enabled the simulation of non-equilibrium phenomena to be started at the same time as similar work at Livermore by William Hoover. The study of rare events by MD has also been pioneered at CECAM by Jacucci and Charles Bennett, as well as path-integral Monte Carlo simulations by Jacucci and Daan Frenkel, and biased-sampling techniques by Frenkel and Anthony Ladd. More recently CECAM workshops have played an important role in establishing new techniques and ideas that had been proposed elsewhere, such as the simulation of different ensembles by Hans Andersen, Suitchi Nose, Aneesur Rahman and Parrinello, and the *ab-initio* molecular dynamics by Car and Parrinello.



Scenic setting – Lyon is home to CECAM, the European Centre for Atomic and Molecular Computations

CECAM's basic aim is to encourage the growth of emerging research fields in computational physics and chemistry. We mainly pursue this by organizing study meetings on various topics (see box). We pay particular attention to those fields where there is a distinct, yet disparate, scientific community, the members of which do not communicate well with one another. We believe we can encourage these communities to grow by lowering the long-standing cultural barriers that have hindered progress in the past. This co-ordination is extremely important in Europe, where cultural diversity is great, language barriers are strong, and political differences have long divided nations. However, we believe that it is important for scientific co-operation to come from the scientists themselves, rather than from any administrative body. In this respect, CECAM is particularly suitable. It is a small institute, the only permanent staff

CECAM's 1996 scientific programme

- Development of transferable intermolecular potentials for phase equilibrium calculations *13–15 May*
- Non-perturbative methods for time-dependent problems of atoms and molecules in strong fields *27–29 May* (to be held in Crete)
- Pattern formation in surface reactions *3–6 June*
- Theoretical predictions of alloy phase stability *10–14 June*
- Algorithms for dynamical critical phenomena *20–22 June*
- Integral equations for classical and quantum fluids *26–29 June*
- Ab-initio phonons *1–3 July*
- Grid, multigrid and wavelet methods in electronic structure calculations *4–6 July*
- Euroconference on the microscopic approach to complexity in non-equilibrium molecular simulations *15–19 July*
- Models and computer simulations for electrokinetic phenomena *22–26 July*
- High performance computational chemistry *5–7 September*
- Going beyond the local density approximation in physics and chemistry *9–13 September*
- Interaction of ultra intense short laser pulses with plasmas *16–20 September*
- Potential functions for simulation of biomolecules *23–25 September*
- Glassy dynamics *30 September–4 October*

The complete programme is available on the World Wide Web at http://www.cecam.fr/worksops/program96.html

member being a secretary, and is run by an acting director (SB) who is a scientist. Interference from the various national science funding agencies that support the centre is therefore reduced to a minimum.

Meeting programme

How is CECAM's research programme decided? Each year, individual scientists (who do not have to be from CECAM member states) present proposals for study meetings to be held the following year. Sometimes these are presented by groups of scientists or by people solicited by the director or the scientific council. The council then examines the proposals, and approves or rejects them based on the scientific opinion of anonymous peer-review referees.

The precise format of the meetings depends on the organizers, but most last between three days and two weeks. Meetings are fairly informal, and have between 15 and 30 delegates. There is usually plenty of time for discussion and personal interaction. Participation is not restricted to scientists from member countries – indeed about half of those who organized or took part in CECAM meetings last year came from other countries.

Each meeting has a budget of FFr 40 000–80 000 (about £5000–10 000) according to its duration and size. CECAM's annual budget enables 10–15 of these meetings to be held each year. We hope that co-sponsorship from other organizations will allow us to pursue more initiatives and to widen their scope.

Small is beautiful

CECAM has recently developed a visitors' programme to promote more continuous research at the centre and effectively turn it into a small international laboratory. The centre now has three kinds of visitor. First (and foremost) are the post-docs and graduate students who stay at CECAM for one or two years. These young scientists are supervised either by the CECAM director or external senior scientists who come for regular short periods. They are the second category of visitor. Finally, there are researchers who are well established in fields that CECAM wishes to pursue, and who have been encouraged to spend a sabbatical year at the centre. Last year, for example, we began a programme on non-adiabatic effects in mixed quantum-classical dynamics by inviting David Coker from Boston University. This year a six-month sabbatical visit is also available.

Roof with a view – CECAM moved to Lyon in 1994

In the past year, seven post-docs and graduate students have worked at CECAM on a diverse range of subjects, including the simulation of the photosynthetic reaction centres in biomolecules; non-adiabatic effects in chemical reactivity; large-scale electronic structure calculations; and *ab-initio* molecular dynamics simulations. Although some of these young scientists have been partially or totally supported by external institutions and/or by EU research programmes, we hope that, in future, member and external institutions will contribute more to the centre's visitors' programme.

Growth targets

What does the future hold in store? CECAM wants to strengthen its commitment to research areas that have been not so well represented in the past, such as the study of quantum processes and mechanisms in condensed phases. We also want to maintain the levels of excellence that we have already established in other fields, such as classical simulations.

And although our most important goal is good science, a major concern of ours is to extend participation in CECAM to those European countries who are not yet represented on the centre's scientific council, such as Germany, Scandinavia, and the nations of Eastern Europe. Readers who believe that their research community would benefit from joining CECAM are encouraged to get in touch with the present director of the centre. Our goal is to transform CECAM into a centre made by Europe for the whole of Europe.

Stefano Baroni is director of CECAM and professor of solodstate physics at the *Consiglio Nazionale delle Richerche* **Piet van Leuven** is president of CECAM's scientific council and professor of physics at the University of Brussels

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IN BRIEF

Women experts brought to book

A European handbook of women experts in science, engineering and technology (SET) has been launched by WITEC, the network that supports women across Europe. Designed to raise the profile of eminent women working in science, engineering and technology,, *European Handbook of Women Experts in SET* aims to increase the participation of women on European and national government committees, working groups and R&D programmes.

The book features the CVs of over 1300 women experts from 14 EU member states, including 325 from the UK. Each country was responsible for selecting its own national experts. Brief overviews of expertise and experience are also included. The handbook will be constantly updated and developed, and possibly extended into a full database.

Further ideas on how it can be used to promote women in SET are welcomed. Copies are available from WITEC, Sheffield Hallam University, Heriot House, City Campus, Sheffield S1 1WB, UK (tel. +44 (0)1142 532041; fax +44 (0)1142 532046).

Self-organized theorists

In response to the continued growth in condensed matter physics, a new Group of the Institute of Physics has been formed. The Theory of Condensed Matter (TCM) Group hopes to attract a range of physicists, from those interested in statistical mechanics to those studying strongly correlated electron systems, and from material scientists to electronic band structure theorists.

As well as organizing meetings and symposia at the annual Condensed Matter and Materials Physics conference, a proposal to relaunch the TCM summer schools for first year graduate students is being drawn up. The group also intends to focus the discussion on future directions of TCM research in the UK.

A steering committee has been set up. Its members are Alan McKane, chairman (Manchester), Colin Lambert, honorary secretary (Lancaster), James Annett (Bristol), Mike Cates (Edinburgh), John Chalker (Oxford), Mike Gunn (Birmingham), John Inglesfield (Cardiff), Peter King (BP), John Pendry (Imperial College), Terry Shepherd (Malvern), Ben Simons (Cambridge) and Marshall Stoneham (University College, London). The membership of this committee has been set at a maximum of three years to ensure that all aspects of the subject, and most UK university research groups, will be adequately represented over time.

Members of the Institute may join the Group free of charge for the remainder of 1996. Thereafter the standard annual subscription (currently £3) for Group membership will apply. Those wishing to join the group should contact the Membership Department, the Institute of Physics, 76–78 Portland Place, London W1N 4AA, UK (tel. +44 (0)171 470 4800; fax +44 (0)171 470 4848).

ANKA's away

The go-ahead for an innovative new synchrotron source has been given by the German superministry for science, education, research and technology (BMBF). The new source, to be called ANKA, will be based at the Karlsruhe research centre. It will mainly be used for commercially oriented research, such as quality control and small-instrument manufacture, and the ministry hopes that 10% of users will come from industry. ANKA will operate as an independent company, owned equally by the research centre and the local Baden-Württemberg region.

"ANKA should be market-oriented, free from bureaucratic regulations, and geared to the needs of users, particularly small- to medium-sized enterprises," said Jürgen Rüttgers, the German science minister. He also believes that ANKA will benefit from the technical backup available at the Karlsruhe lab. The facility will cost an estimated DM 54m (about £24m) to build. Annual running costs will be DM 10m.

California set fair

The Sherman Fairchild foundation has awarded the California Institute of Technology $2.5m (about £1.6m) to support 13 post-doctoral research workers in physics and astronomy. The gift extends over eight years and will support six theoretical or astro-physicists, five observational optical-infrared astonmers, and two others in experimental physics, astrophysics or radio astronomy. The foundation was set up in 1955 by Sherman Mills Fairchild, former chairman of IBM. The first post-docs will begin in the autumn.

COMPUTING

Plus ça change ...

The European Centre for Atomic and Molecular Calculations (CECAM) moves from Paris to the Ecole Normale Supérieure de Lyon in the Rhone-Alpes region of France this month. As part of the move, the ENS will become a partner in the centre. The existing partners are the national funding agencies of France (CNRS), Belgium (FNRS), Holland (ZWO), Italy (CNR) and the UK (SERC), plus the French atomic energy authority (CEA). CECAM director Giovanni Ciccotti also expects the national research councils of Denmark, Greece and Switzerland to apply for membership soon.

CECAM is not a supercomputing facility. Rather, it exists to promote the use of high-performance computing and numerical simulation in various branches of physics and chemistry, mainly through the organization of workshops and meetings. According to Jean-Pierre Hansen, director of research at ENS Lyon, "CECAM is intended to bring users of high-performance computers together. It enables researchers to swap ideas and compare methodology and codes – they do not come to run codes for long periods of time".

Five workshops, typically bringing together 20 or so researchers for about two weeks, and a similar number of planning meetings, have so far been planned for 1994. Attendance at workshops and meetings is not restricted to nationals of the CECAM partners. "The main focus", says Ciccotti, "is the microscopic approach – molecular dynamics and Monte Carlo techniques – to condensed matter physics." This embraces classical and quantum statistical mechanics, solid-state physics, materials and "soft" matter (including polymers and colloids). Coverage also extends to atomic and molecular physics, rheology, quantum chemistry, plasma physics and biomolecules. CECAM has no permanent researchers, but has a part-time director and an annual budget of around FFr 2.5m (about £290k). The centre also currently hosts eight postdoctoral researchers on short-term contracts.

Previously CECAM was housed in the CIRCE supercomputer centre run by the CNRS at the University of Paris-Sud in Orsay. However, in a recent reorganization of French supercomputing, the CNRS decided to replace CIRCE, and two other supercomputer centres, with a new national institute for high-performance computing (IDRIS) in Orsay (*Physics World* December 1993 p6). In addition to operating a Cray C98 supercomputer, IDRIS also intends to foster applications in a manner, and sometimes in subjects, similar to CECAM.

Initially there were discussions between the CNRS and CECAM's Scientific Council about bringing these initiatives together. However, these came to nothing and when the CNRS announced that it wanted the CECAM agreement to be renegotiated, the Scientific Council decided to withdraw from Orsay and ask for possible sites elsewhere in one of the member countries.

Lyon beat Amsterdam and Lausanne in the competition to host the centre. The CNRS's decision to support Lyon is in line with its policy of decentralization. ENS Lyon already hosts a number of CNRS research units in the fields covered by CECAM. Its mathematics, physics and theoretical chemistry laboratories coordinate their numerical modelling activities, whilst the computer science laboratory has set up a collaboration with local parallel computer manufacturer, Archipel.

Ciccotti, who is a professor of condensed matter physics at the University of Rome *La Sapienza*, finishes his term of office in October. His successor will be chosen at the next Scientific Council meeting in April. **Peter Rodgers**