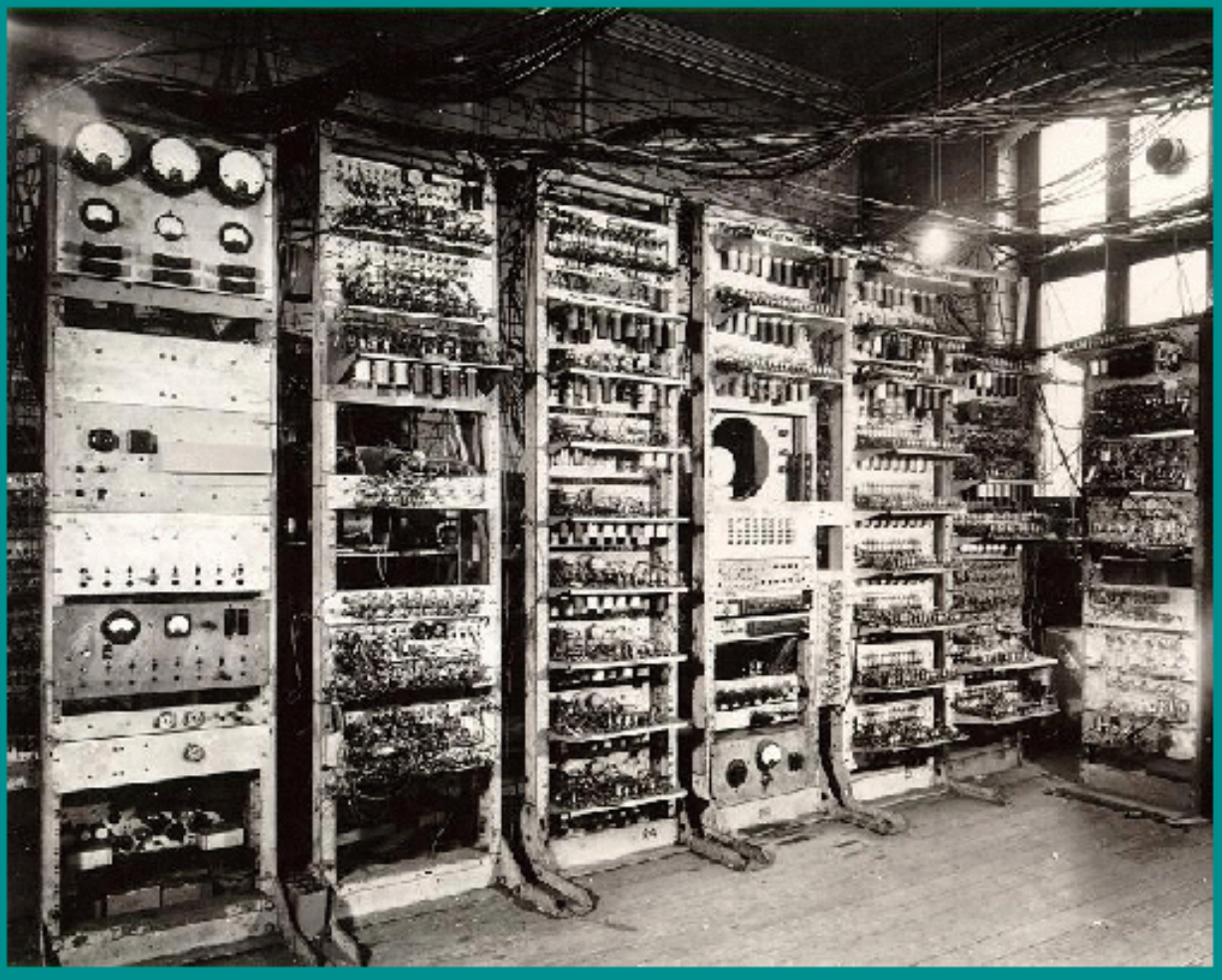
Institute *of* Physics

Newsletter

of

The Computational Physics Group



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Chairman's Remarks

Peter Borcherds (chairman)

To mark the first electronic newsletter of the Computational Physics Group the editor has asked me "for a few words from the chairman".

My experience of electronic computing extends over nearly half a century, and in that time there have been developments which nobody anticipated. Today most of us have on our desks a computer whose cost is about one month's salary, whose processor speed is about 1GHz, with some 100Mbytes of RAM and a hard disc with many Gbytes, many times more powerful than the supercomputers of a generation ago.

I could attempt to predict what the future holds in store, but in a time of such a rapid development in computing, this is unlikely to be of much value. Instead I shall look back and pick out a few developments of significance to computational physics. Much, but not all, of the development has been due to spectacular advances in hardware.

My first active involvement with electronic computing was a vacation job, helping to build an analogue computer: my task was to design and build valve based power supplies to drive the amplifiers used as adders and integrators. A few years later an operational amplifier cost about one month's salary: today it costs a few pence, about the same as a discrete passive component (capacitor or resistor). This enormous decrease in the cost of operational amplifiers has revolutionised the ways in which they are used. For example, op-amps can be used to transform the properties of complex impedances. A negative impedance converter turns an impedance into its negative value, and a gyrator can make a capacitor behave like an inductor of high inductance (e.g. 1 Henry) which has significant implications for analogue computers.

However most computing is now digital.

Forty years ago, in 1961, Hoare developed the Quicksort algorithm. He has described the computer on which the algorithm was developed (Hoare, 1962). It was made by National-Elliott, and had 19 words of immediate access storage for instructions and working space for inner loops. The average access time for an instruction was 0.15ms.

Not all the progress has been through advances in hardware, software development has played a significant role too: the fourier transform provides a good example.

The development of x-ray crystallography led to a large amount of calculation to determine crystal structures. Crystallographers carried out discrete numerical Fourier transforms on diffraction data. In the early days of x-ray crystallography calculations were carried out by hand, (e.g. Whittaker and Robinson, 1924) but later were partially automated using Beevers-Lipson strips (Lipson and Beevers, 1936). The technique of discrete numerical Fourier transforms has been fully automated, and was renamed in 1965 the fast fourier transform (FFT), although the algorithm was known to Gauss 150 years earlier. The use of the FFT on N data points, with its increase in speed of a factor $N/\log(N)$, reminds us how important it is to use efficient algorithms, and how important it is to understand what it is that the computer is doing. A colleague currently wishes to perform an FFT on 60 million data points: for this the FFT will give an increase in speed of a million times over a brute force calculation.

Hoare, C.A.R.: Quicksort. Computer Journal, 5 (1962) 10-15

Lipson, H., Beevers C.A.: An improved numerical method of two-dimensional fourier synthesis for crystals, Proc. Phys. Soc. 48, (1936) 772-780

Whittaker, Sir Edmund and G Robinson: "The Calculus of Observations: A Treatise on Numerical Mathematics", Blackie and Son, London and Glasgow, 1924.

Reports on Meetings

Over the last couple of years several interesting meetings have been organised for the Computational Physics Group. Reports from the organisers of these meetings are presented below.

High Performance Computing in the UK: Present Status and Future Prospects

Organised by: Mike Payne

The meeting was held on the 16^{th} July, 1999, at the Rutherford Conference Centre, Institute of Physics, London.

One of the reasons for organising this meeting was to address the perception that interest in high performance computing (HPC) was declining in the UK. It was certainly true that at the time of the meeting the computing spotlight was predominantly focussed on Beowulf and other cluster solutions. Indeed, the Computational Physics Group organised a meeting on that subject the following year. However, the present meeting concentrated on traditional HPC as the organisers believed that there was still much this technology could offer. The meeting was organised into three sessions which highlighted three basic aspects of HPC: HPC centres, new technology and new applications. A brief description of the talks in each of these sessions is given below.

The meeting was attended by 80 people drawn from a wide range of backgrounds including academic, industrial and government science and computer companies. As is quite common for meetings organised by the Computational Physics Group, a large number of people attending were not members of the Institute of Physics. The meeting achieved its primary objective of demonstrating the strength of HPC in the UK and showing that there were still plenty of opportunities for HPC in the future.

HPC Centres

The morning session focussed on the evolving role of the HPC centre. The first talk was on 'National Provision of High Performance Computing' by Dr. Stewart Cant of the University of Cambridge. Dr. Cant spoke on behalf of the Engineering and Physical Sciences Research Council (EPSRC). His talk included a description of the CSAR service and a discussion of future plans for national provision of HPC. Next Dr. Guna Rajagopal gave a presentation on the University of Cambridge High Performance Computing Facility. He explained how the University had successfully built a world class computing facility with the help of funding from the Joint Research Equipment Initiative and close collaboration with Hitachi and Silicon Graphics. Finally in the morning session, Dr. Alan Simpson explained what the Edinburgh Parallel Computing Centre (EPCC) actually does. Most of the audience were familiar with some of the activities of the Centre, such as running training courses and summer schools but were quite surprised by the range of commercial activities ranging from facilitating HPC usage in small companies to full commercialisation of some of the technologies developed by EPCC.

New Technology

After lunch, Professor Ron Perrott of Queens' University Belfast and Chairman of EPSRC's Technology Watch Panel gave a talk on 'Future Technologies'. Much of this talk focussed on the American ASCII programme, which dominated the top end of HPC at the time of the meeting and, indeed, has continued to dominate it since. His talk highlighted the very different attitude to HPC in America compared to the UK. This talk was followed by presentations from Silicon Graphics, Hitachi, IBM and Fujitsu describing their future plans for HPC.

New Applications

The final session of the meeting concentrated on scientific fields that were relatively new to HPC. Professor Laurie Hall of the Herchel Smith Laboratory for Medicinal Chemistry talked about 'HPC in Medicine and Biology' highlighting some of the opportunities for exploitation of HPC in these fields. Dr. Peter Gill of QChem Inc spoke about 'Quantum Chemistry: The Present and Future' describing how new software packages for quantum chemistry were being written to exploit the power of parallel computers. Finally, Dr. Whobrey of Fujitsu European Centre for IT described some applications of HPC to financial modelling.

Beowulf Clusters

Organised by: Richard Ansorge

A one-day meeting on BEOWULF computing systems took place on 10 February 2000. The meeting was held in the Rutherford Conference Centre and attracted about 100 delegates. The following talks were given:

1. *Welcome and Introduction*, **Dr Richard Ansorge**, University of Cambridge.
2. *General Overview of Cluster Computing*, **Dr Mark Baker**, University of Portsmouth.
3. *Clusters and Experience of Ownership*, **Dr Paul Calleja**, Insilico Ltd.
4. *High Performance Interconnects*, **Dr John Taylor**, Quadrics Ltd.
5. *Computational Chemistry on High-End Commodity Type Computers*, **Dr Martyn Guest**, CCLRC Daresbury.
6. *Windows Clustering, Why, When and How*, **Dr Kenji Takeda**, University of Southampton.
7. *High Performance Bioinformatics Computing*, **Dr Stuart Moodie**, Inpharmatica Ltd.

In addition to the talks, there were lively discussion sessions.

A second Beowulf meeting is scheduled for 6 September 2001 in the Rutherford Conference Centre, details of the program will be available soon.

Modern Software Design for Scientific Applications

Organised by: Andrew Horsfield

This meeting was designed to alert physicists to the gap between the tools they often use to write software, and what is currently available. While using `vi` and FORTRAN 77 is fine for small codes used and developed by one person, larger projects demand more sophisticated tools. The topics focused on in this meeting were: object oriented programming, parallel programming, and software development tools.

The meeting was held on March 31^{st}, 2000, in the Department of Nuclear Physics at Oxford University. It was attended by over 40 people. We had the following five talks:

1. **Sven van den Bergh** spoke on *Java: an object oriented language*
2. **Peter Chow** spoke on *Component approach to building an open software framework for mesh-based multi-physics simulations*
3. **Mike Rudgyard** spoke on *Component approach to building an open software framework for mesh-based multi-physics simulations*
4. **David Bowler** spoke on *Component approach to building an open software framework for mesh-based multi-physics simulations*
5. **Terry Sloan** spoke on *Integrated development environments and source code control*

The overheads from most of these talks are available from the following web site: http://www.fecit.co.uk/ hfield/Talks/talks.html.

There was clear interest in these topics from the audience, but maybe Java grabbed people's attention the most. This is no doubt a result of the enormous publicity this language has received. There are tentative plans to have a future meeting on Java for High Performance Computing. Feel free to let us know if you would be interested in attending (or even contributing to) such a meeting.

Upcoming Meetings

XI Computational Materials Science Workshop

The Euroconference *X*I Computational Materials Science Workshop 2001 will be held from 17 to 23 September 2001 in Villasimius, Sardinia, Italy.

Web page: http://www.dsf.unica.it/CMS2001

9th International Conference on the Applications of the Density Functional Theory in Chemistry and Physics

The *9*th International Conference on the Applications of the Density Functional Theory in Chemistry and Physics will be held from the 10 to 14 September 2001 in San Lorenzo del Escorial, Madrid, Spain.

Web page: http://www.uam.es/dft2001

Local orbitals and linear-scaling ab initio calculations

The workshop will be held at CECAM, Lyon, France, from 3 to 7 September 2001.

This workshop, jointly supported by CECAM and the ESF STRUC-Ψ_k Programme, aims to bring together scientists from a wide variety of communities who use local-orbital techniques for electronic structure calculations and atomistic simulations, with a particular emphasis on linear-scaling methods. This follows on from the successful workshop on localized orbitals held at CECAM in 1998.

Five sessions have been planned:

1. Atomic type orbitals
2. Gaussian type orbitals
3. Real space grid methods
4. Optimized orbitals
5. Linear-scaling methods

Web page: http://www.tcm.phy.cam.ac.uk/LocalOrbital