

ATLAS

Editorial

Formation of the Department for Computation and Information in CLRC

As this edition goes to press a new federal department of CLRC is being created by bringing together the Computing and Information Systems Department at Rutherford Appleton Laboratory and the Theory and Computational Science Division at Daresbury Laboratory (DL). The new Department for Computation and Information will also take on activities from other Departments of CLRC by mutual agreement. The first example is the provision of IT infrastructural support at DL, and others will follow.

The activities of the new Department include the application of high performance computational techniques across a wide range of scientific and engineering disciplines in academic and industrial research, the application of advanced information

systems engineering in collaboration with many partners in the UK and elsewhere in Europe, and the provision of services covering computing, data, information systems and IT infrastructure for customers inside and outside of CLRC. Funding sources include Research Councils, the European Union, and industry.

By creating the new Department a wide range of skills and experience are being brought together within CLRC and this will facilitate further advances in the effective exploitation of advances in computational and information systems to the benefit of CLRC's programmes and partners.

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Developments in HPC

We are pleased to see that it has been announced that a sum of £10m has been included in the UK science budget in the 1997/8 financial year planning figures for capital expenditure on high performance computing. The money is intended for the purchase of one or more major new systems to support Research Councils' programmes needing access to the most powerful computers available.

Following discussions between the Research Councils, PPARC is proceeding to select a specialist system for Quantum Chromodynamics work and EPSRC, ESRC, NERC and PPARC (astronomy) are joining together to select a new system or systems for their research communities with the hope that this will come into service in late 1997.

Some current systems are heavily overloaded. As it will be over a year before a new system can be brought into full production service, the Advisory Body for High Performance Computing approved an interim investment in current systems to provide some additional capacity in the short to medium term. The Cray T3D at Edinburgh Parallel Computing Centre has been

upgraded to 512 processors - this will provide significant extra parallel capacity, and will also provide a new capability to run jobs of 512 PEs and 32 GBytes of memory. The Cray Y-MP8 at RAL has been replaced by a J932/32-4096 system. The peak performance of each processor is slower than the Y-MP8, but since there are four times as many, the new system will have higher throughput and lower running costs. This is an interim service to provide additional capacity until the new system(s) is fully in production - the longer-term requirement for the service will then be reviewed. EPSRC have agreed with RAL and JISC an increase to 9% in Class 3 time on this system.

If you would like to discuss anything raised by this message, please post to our newsgroup at news:uk.org.epsrc.hpc.discussion.

Rob Whetnall and Alison Wall
High Performance Computing Group
EPSRC

For further information on the procurement see <http://www.epsrc.ac.uk/hpc/> and on the newsgroup news:uk.org.epsrc.hpc.news



CENTRAL LABORATORY OF
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High Performance Computational Engineering

More than one hundred people attended this meeting held at CLRC Daresbury Laboratory on 18 and 19 March 1996. The meeting covered the work of the High Performance Computing Initiative (HPCI) in three fields: external aerodynamic flows (under the direction of Prof Brian Richards, Glasgow), Computational Combustion (under Prof Derek Bradley, Leeds) and Turbulence Modelling (under Prof Michael Leschziner UMIST).

External aerodynamics and high lift structures were covered by five presentations including an excellent review by Brian Richards and a paper by Steve Fiddes (Bristol) presenting an interesting approach to compound structures (wing plus leading and trailing flaps) by the use of moving meshes. Two other papers covered similar flows using unstructured grids (Michael Marchant, Swansea) and multigrid methods for unstructured grids (Paul Crumpton, Oxford). The final paper in this session covered the slightly different topic of Computational Electromagnetics (CEM) calculation on parallel architectures. The CEM wave equations are cast in conservative form amenable to solution by finite element techniques. The problem chosen (by Peter Brookes, Swansea) was the outgoing diffracted wave from an annular cylindrical object closed at one end representing an aeroengine intake. From this its radar signature is obtainable.

The second session was devoted to computational combustion with six papers covering such topics as industrial requirements, laminar flamelet modelling, the extremely demanding techniques of direct numerical simulation of turbulent flames and the large eddy simulation of turbulent combustion. The detailed chemical kinetics (NO_x kinetics) was covered by Peter Lindstedt (Imperial College). The reviewer of the session (Barry Moss, Cranfield) emphasised the considerable progress that had been made in this field recently.

The last two sessions were concerned with advanced turbulence modelling LES and DNS techniques. The points of view ranged from Neil Sandham's upbeat paper on the progress towards the use of these models in engineering problems to Michael Leschziner's conservatism in the continuing caution needed in code normalisation and the possible unreliability when large extrapolations are made.

The message from the meeting was very positive; although much has been done more remains to be done. Progress in these fields can only be achieved by access to computational sources of even greater power.

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The Associates Group

As a continuation of CLRC's active policy of supporting our colleagues in Industry a new Associates Group has been created. By becoming an Associate member of CLRC you have a unique opportunity to share in the fruits of our exciting work, to learn about our achievements at the cutting edge of science and engineering as they happen, and to assess how they can directly benefit your organisation. From over 800 qualified professional scientists and engineers you will be able to obtain independent advice and have access to over £60m of specialist equipment and test facilities.

Benefits to members

By becoming a member, you and your organisation will have access to:

- Consultancy service
We will give you an introductory consultancy, without charge, so that together we can examine a particular research area to determine exactly how our expertise can help tackle your problems.
- The Associates Newsletter
You will receive a quarterly newsletter each issue focusing upon a specific technological theme, giving information and highlighting exciting

areas of engineering research. It is specifically written for our Associates Group and tailored to our members' viewpoint and concerns.

- Technical Seminars and Lectures
Our technological base is extremely broad and links to other centres of excellence world-wide. Our facilities are at the forefront of science and engineering and our scientists and engineers are world leaders in their fields. Associates will have access to a programme of seminars and lectures specifically formulated to keep them abreast of the latest results and thinking on particular topics.
- E-mail Information Transfer
By accessing our information network, as an Associate you will have direct contact with us and our work, as it develops, wherever you are.

Joining the Associates Group

The Associates Group subscription is £250 + VAT per annum for each member organisation. To apply please contact Sonia Moon, 01235 445841 or e-mail: Sonia.Moon@rl.ac.uk

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Wider Access to the RAL Supercomputers

Access to the Cray supercomputing facilities at Rutherford Appleton Laboratory, CLRC (RAL) has until recently been restricted to Research Council grant holders and paying customers. With the impending closure of the Convex supercomputer at University of London Computer Centre (ULCC) there is now a new route for academics in the UK to gain access to the Cray J90.

The new mechanism is known as "Class 3" and has been in effect at ULCC and Manchester for some time. It is intended to provide a modest amount of supercomputing time to the academic community outside of the peer review mechanism for research grants. Class 3 would typically be used for speculative projects that have not yet reached the stage where a full research case can be written, for teaching purposes, for comparison of computer architectures, or where a very small amount of time is needed as part of a larger project and may not have been specified on the original grant request.

Class 3 time will NOT be awarded as a "top up" for student use where there is already a fully approved Research Council grant, and will not be awarded on a repeat basis for projects that fail to pass peer review.

Class 3 is limited by the funding bodies to a maximum of 9% of the usage of the J90 and for the first year of open application (some ULCC Class 3 users used the old Y-MP last year) we are limiting a single request to 80 cpu hours on the J90. This limit will be reviewed next year in the light of the number of requests received.

Invitations to bid for Class 3 time are sent to existing Class 3 users and to University Computer Centres. If you are outside the present process and may not be known to your local computer centre then you should in the first instance make contact with them or if necessary contact Margaret Curtis at RAL, e-mail: M.M.Curtis@rl.ac.uk

Class 3 time is issued for 12 month periods from 1st July each year and since the process is not peer reviewed the time will be awarded on a "first come first served" basis provided the request appears to fall within the guidelines given above. Class 3 bids should use the form NS3, which can be obtained from local computer centres and should be sent to Margaret Curtis, R27, Rutherford Appleton Laboratory, Chilton, Didcot, OX11 0QX.

Columbus

We would also like to use this opportunity to remind you that EPSRC grantholders only can obtain access to the superscalar computer "Columbus" under a new mechanism known catchily as "Class 5". This is meant to add a modest amount of supercomputing time to any existing grant and can give you 100 cpu hours for each year of the grant award. Class 5 applies both to research grants and research studentships.

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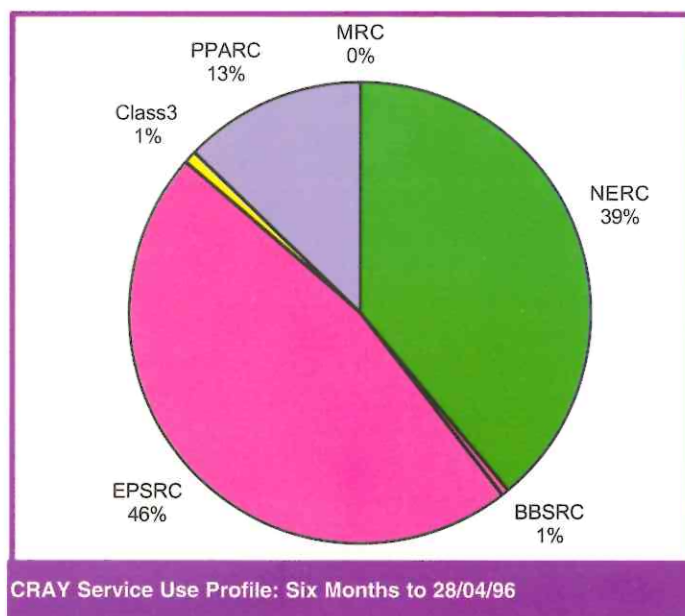
For more details of the above schemes see:
<http://www.cis.rl.ac.uk/services>

Statistics on WWW

We maintain on the World Wide Web some reports about the services we provide for the scientific community. At the moment these cover the Atlas Data Store and the Central Computer Services. The information is updated to coincide with the publication of ATLAS.

An example is shown here of the pie-chart reporting the profile of utilisation of the CRAY service by scientists funded by the various Research Councils and the Class 3 service which is provided for small and beginning users for research and training.

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For more details about the stats see:
<http://www.rl.ac.uk/cisd/services/stats/>

The CLRC WWW

Most ATLAS readers should be familiar with the CLRC corporate publicity material on the World Wide Web (WWW). This month marks the first anniversary of the CLRC WWW, which was commissioned by CLRC's Chief Executive Officer Dr Paul Williams. Tony Buckley of CLRC Press and Public Relations is responsible for the content of this WWW, in collaboration with the Advanced Hypermedia Systems Group.

Over the last year the CLRC WWW has been very well-read. In just March 1996, visitors external to CLRC numbered 2393, reading a total of 13394 pages. Not surprisingly perhaps, a large proportion (43%) of the WWW's visitors are from the UK, but there were many visitors from other parts of the world including Germany, France and Italy, and even South America, Kuwait and Japan.

We have been keeping an eye on which sections of the WWW are read the most, and which are read the least so as to try and improve them.

A few months ago we noticed that a large number of people were accessing the "How to gain access to CLRC's facilities" page but did not seem to be interested in reading further. We eventually concluded that this was because the link text

promised some form of guided tour of the facilities so we reworded the link to "Contact names for CLRC's facilities". But the idea of a guided tour intrigued us, so we are in the process of assembling a photographic virtual tour of some of the facilities, enabling readers to click on different parts of the photographs to discover more about the equipment and experiments. A guided tour of ISIS should be ready soon, followed by the other facilities in turn.

Other sections planned for the very near future are the on-line publication of LabNews, the forthcoming quarterly newsletter "CLRC Science & Technology", and various annual reports. Daresbury and Rutherford Appleton Libraries are coming more fully on-line, and have published their Customer Care guidelines, as well as providing on-line access to some of their publication databases.

The CLRC publicity pages will continue to evolve so take some time to surf around!

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For further information see the CLRC publicity pages at: <http://www.cclrc.ac.uk/>

Community Clubs

How do researchers using similar computing techniques in their research but working in different application areas make contact with each other and share information and experiences? The answer is by joining a Community Club. The Engineering and Physical Sciences Research Council (EPSRC) currently supports three Community Clubs in Computational Fluid Dynamics (CFDCC), Visualization (VCC) and Advanced Computing Techniques (ACTCC) which are run on its behalf by Rutherford Appleton Laboratory.

These Clubs run programmes of technical seminars and workshops which provide a focus for meeting and exchanging ideas with other researchers. The programme of each Club is directed by a Steering Group comprising leading researchers from its area of interest. The Clubs maintain good links with industry and so can also assist technology transfer in today's increasingly commercially aware climate.

A major initiative of the Community Clubs is CRISP, the Community Clubs Research Information Service Project. This World Wide Web (WWW) based service will provide links to WWW pages of

individual UK researchers and research groups and to pages about UK research projects. CRISP will be a convenient single point of contact for finding out who is doing what within the UK science and engineering research community.

If you would like to join one of the Community Clubs, please send an e-mail to Virginia Jones (M.V.Jones@rl.ac.uk) or fill in the membership form on the Clubs' WWW pages. The Clubs have just started their own short newsletter, CCnews, to keep members informed about Club events and other topics of interest. If you would like to receive this newsletter in paper form (it will also be available on the WWW), again please e-mail M.V.Jones@rl.ac.uk

These Clubs exist to help you be more effective in your research. Please use them.

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The Clubs WWW pages can be found at:
<http://www.cis.rl.ac.uk/cclubs.html>

<http://www.cis.rl.ac.uk/publications/ATLAS/>

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