CSAR

# FOCUS

Edition 10
Summer 2003

high performance computing at Manchester ~ taking research into the future

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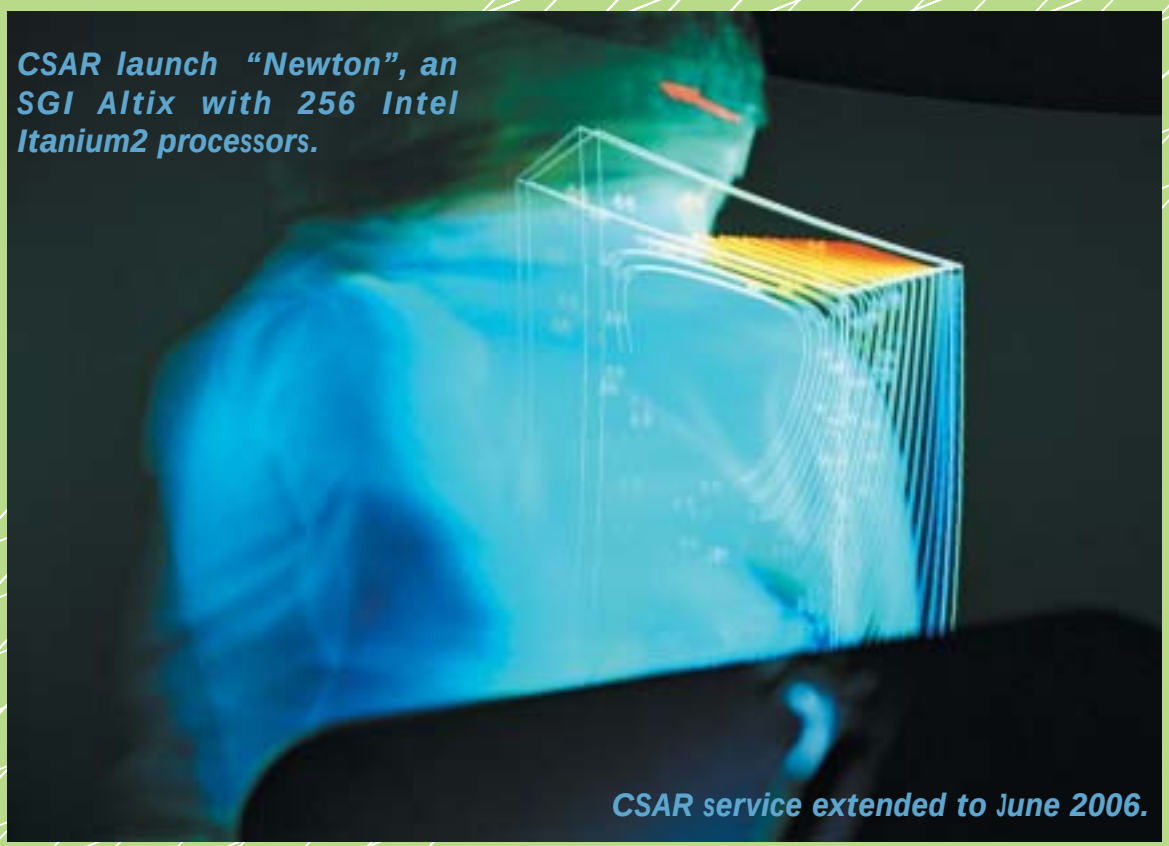
## CSAR install 256 processor Altix system



*CSAR launch "Newton", an SGI Altix with 256 Intel Itanium2 processors.*

*CSAR service extended to June 2006.*

THE UNIVERSITY of MANCHESTER

CSC

sgi

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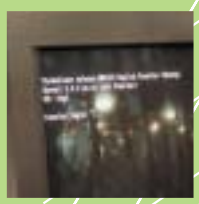


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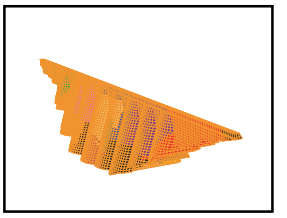

7: Finite Element Analysis

14: Parallel Support Toolkit for AVS/Express

# Editorial

We are delighted to announce that the Research Councils have extended the CSAR contract by eighteen months to June 2006. This extension enables us to add an SGI Altix to the service, Andrew Jones introduces the new machine "Newton" to you in our special report on page 4. Newton will be introduced into full service by 1st October - you can apply for resources on the system now.

The new system, along with the introduction of the HPCx service, has meant that changes have been made to the application process for HPC resources within the UK. Deborah Miller of EPSRC explains in this issue (page 6) how these changes will affect the user community and also provides a forward-look at the next national HPC service, due to start at the end of 2005.

Also included is "A New Look at Tropospheric Chemistry" from Glenn Carver and Fiona O'Connor who detail their experiences in running their "TOMCAT" 3-D model - used to study the role of the ozone in the troposphere - on green. If you would like to highlight your successful research on our machines in the next edition of *CSAR Focus*, or have any other articles you would like to submit, please do not hesitate to contact me.

A one-week Summer School will be held at the University of Manchester in the week commencing 1st September. The Summer School will focus on high performance computing in finite element analysis and is free to CSAR users - we look forward to seeing you there.

Claire Green
Editor, *CSAR Focus*

# CSAR launches 256 processor Itanium2 Altix supercomputer

***Andrew Jones***
***HPC Team, Manchester Computing, University of Manchester***

The Research Councils have extended the CSAR contract by eighteen months - the CSAR service will now run to June 2006. This announcement demonstrates the continuing confidence of the Research Councils in the CSAR service. The extension enables CSAR to introduce "Newton", an SGI Altix supercomputer with 256 Itanium2 processors. This system, the largest Altix in the world, will be released into full user service by 1st October 2003. [1]

## *Benefits for CSAR users*

The 256 Itanium2 processors, globally shared memory of 384 GB (more per processor than any of the current CSAR or HPCx systems), and SGI's NUMAflex interconnect (the lowest latency architecture currently available) is expected to give the Altix a user performance at least double that of the Cray T3E-1200E "Turing". (Turing is now scheduled to be removed from service on 31st December 2003).

CSAR's two flagship machines - Green (512-processor Origin running IRIX) and Newton (256-processor Altix running Linux) - will continue to deliver a flexible and simple world-class national supercomputing service for world-class research including:

- Computational Fluid Dynamics (CFD) and Aerodynamics
- Molecular Dynamics
- Bioinformatics or Computational Biochemistry
- Numerical Algebra
- Computational Chemistry
- Materials Science
- Atomic and Molecular Physics
- Environmental Sciences, including weather predictions
- Parallel finite elements
- Computational Electromagnetics (CEM)

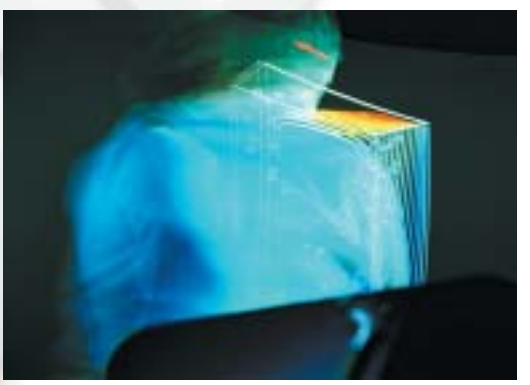

Figure 1: Parallel Finite Element Analysis at CSAR

Simplicity across the service will be achieved through both main systems using the common SAN (Storage Area Network) for home filestore, common batch system, LSF, common scheduling policies, common user/project management system and both supercomputers being large globally shared memory systems.

Flexibility will be achieved through the availability of 2 different operating systems, 2 different processor types, and 2 different processor/memory/interconnect speed balances.

## *Record Performances*

Both the Itanium2 processor and the Altix system have created impressive – industry leading – benchmark results on standard benchmarks and on real applications [2, 3].

Many of these benchmarks show that the current "McKinley" version of the Itanium2 is the fastest scalar processor available. Newton will use the next generation "Madison" processors, running at 1.3 GHz. These 5.2 GFLOPS

peak CPUs will be connected together by SGI's industry leading low latency high bandwidth NumaLink interconnect. Thus, Newton will have a theoretical peak of 1.33 TFLOPS and an expected sustained performance of 1 TFLOPS Linpack Rmax.

## Most major application codes available

Intel and SGI (and others such as HP) have been working together with the ISVs (Independent Software Vendors) to ensure that over 300 major HPC applications and tools have been ported and optimised for the Itanium2, including Gaussian, Amber, Abaqus, Totalview, FASTA, Star-CD, LS-Dyna, Castep, Gamess and NAMD. Porting for many others, including CFX, Fluent and BLAST are under way. Some of these have shown excellent performance on the Altix platform [3, 4].

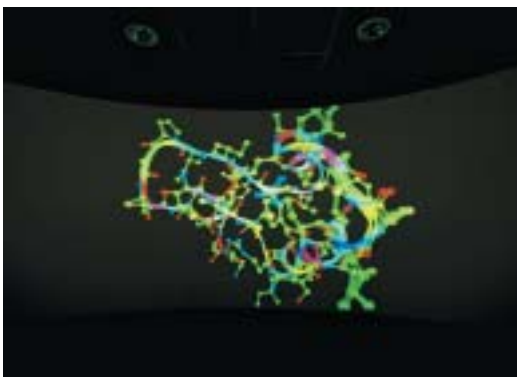

Figure 2: Molecular Visualization at CSAR

The CSAR support team will also be working with suppliers and users to port and optimise the main codes in use on CSAR (Origin 3800 and Cray T3E-1220E) to the Altix – the intention is that by the launch date all supported applications available on the Cray or Origin will also be available on the Altix, in addition to the codes of any user who wishes to contact us to have their code ported.

## Benefits for all UK national HPC users

This highly capable new system will offer both short term and strategic benefits to the UK HPC user community. You, the HPC community, will have access to 3 major supercomputer architectures at CSAR (SGI Altix/Itanium2 and Origin/MIPS) and HPCx (IBM Power4), enabling you to employ the architecture best suited to your own code and science needs – to best undertake your world class scientific research.

## Find out more

Finally, we have created a web page [5], which will be updated frequently with the latest news and progress on the new system. We encourage you to visit this page regularly to keep up to date.

For further information, please contact the CSAR helpdesk at: 0161 275 5997 / 6824 or csar-advice@cfs.ac.uk.

## References


[1] http://www.sgi.com/newsroom/press_releases/2003/april/manchester.html

[2] http://www.sgi.com/newsroom/press_releases/2003/january/altix.html

[3] http://www.sgi.com/newsroom/press_releases/2003/may/madison.html

[4] http://www.sgi.com/newsroom/press_releases/2003/may/mfg_altix.html

[5] http://www.csar.cfs.ac.uk/newton/

# News from EPSRC

***Deborah Miller***
***Associate Programme Manager, High End Computing, EPSRC***

## *Next national HPC service on the horizon*

Although the next national HPC service is not expected to begin until the end of 2005, the procurement process for this service is well underway.

The next national HPC service is intended to meet the needs of all the Research Councils, with EPSRC acting as the Managing Agent (as it does for CSAR and HPCx). It is likely to have an initial capability of a peak performance in the range of 50 to 100 TFlop/s, doubling to 100 to 200 TFlop/s after two years and doubling again to 200 to 400 TFlop/s two years after that. Other possible components of the service are one or more hardware systems, large capacity data management, visualization facilities, computational science and engineering support and training.

The cost of providing this sort of performance (even with Moore's Law) is likely to exceed that of HPCx by a wide margin, so EPSRC is exploring a possible partnership with DEFRA, which has a requirement for a high performance computer for climate change research of a similar capability, and within similar timescales.

Progress to date includes alerting RCUK (Research Councils UK) to the need to include the next national HPC service in the latest version of the Large Facilities Road Map. Inclusion in the Road Map is not a guarantee of funding, but consideration for funding requires that the bid is on the Road Map!

A scientific case for the service will need to be submitted to RCUK in October and this will be prepared using the Technology Watch Panel and the Trends and Opportunities Panel of the High End Computing Strategy Committee.

One of the most important elements in the procurement process is identifying and capturing the needs of users. A start has been made on this by EPSRC staff visiting the existing HPC consortia of all the Research Councils. Each of these visits has included a discussion on the consortium's high-level requirements for the service. The sort of issues we have explored include; their views on what they consider to be a "balanced system" for their research e.g. what is the ideal amount of memory per TFlop/s peak performance, disk and long-term storage requirements and their requirements for computational science and engineering support and how it might be provided.

In addition to these initial discussions with the consortia, Hugh Pilcher-Clayton has commissioned Professor Ian Sommerville from Lancaster University to develop an HPC requirements capture methodology. This is expected to be completed in October and the formal requirements capture process will take place between November and March 2004, resulting in a Statement of Requirements.

EPSRC will also be meeting vendors at SC2003 in November to discuss with them the feasibility of meeting our users' requirements and scientific case.

Assuming there are no hiccups, the OJEC notice will be issued in April 2004.

## *Changes to the application process for CSAR and HPCx resources*

As mentioned in Terry Hewitt's article in the previous issue of *CSAR Focus*, EPSRC has been looking at the application process for resources on CSAR and HPCx.

EPSRC would like to ensure that applicants a) select the most suitable service, and b) that the level of resources requested is appropriate for the research they intend to undertake, so two changes have been introduced to the application process.

Firstly, all applicants will be required to obtain a technical assessment of their proposal from CSAR and/or HPCx

before submitting their proposal to a Research Council. Secondly, applicants who have not used CSAR or HPCx before will be asked to submit a draft case for support, together with code and test data, to both the HPCx and CSAR services. The services will run the test code and will report back to the applicant on the suitability of their service and will provide the technical assessment. As necessary, discussions can follow between the applicant and the centres to determine which service (or possibly services) is best for their research and what resources are required. The applicant will then decide which service they wish to use and finalise their research proposal.

Experienced HPC users, confident of the service they require, will not be required to submit test code to both services, but it is hoped that obtaining a technical assessment of their proposal before submission will open up a dialogue between the service and applicant and allow fine tuning of the proposal.

# Parallel Finite Element Analysis

***Lee Margetts, Mike Pettipher, Ian Smith***
***University of Manchester***

Why are some of the world's leading experts in parallel finite element analysis (FEA) coming to Manchester this summer? Over the past year, there has been growing interest in Manchester's parallel FEA work. So much so that some of the leading names from America, Europe and Japan are going to be teaching here at a week long Summer School jointly organised by the National Science Foundation (NSF) of America and the University of Manchester.

The story starts around 1995 when Ian Smith of the Manchester School of Engineering first approached Mike Pettipher about parallelising one of the programs from his book 'Programming the Finite Element Method'. By this time, the Domain Decomposition techniques popularised in the late 1980's by Farhat with his 'Greedy Algorithm', had grown in maturity. Despite this, the Domain Decomposition approach to parallel FEA never seemed to hit the mainstream, remaining until this day a largely specialist activity. Perhaps the algorithms, basically centred on matrix condensation or tearing the finite element mesh apart and distributing the pieces, were too difficult to master.

Ian Smith focused his attention on an alternative solution strategy whereby the pieces to be distributed are the finite elements themselves. The 'element-by-element' or 'mesh free' approach can be solved by purely iterative strategies. No mesh is ever assembled and consequently does not require tearing apart. The technique is basically the same as 'explicit' methods which have long been considered 'embarrassingly' parallel.

In 1998, EPSRC agreed to fund a joint research project between Manchester Computing and the Manchester School of Engineering. At this time, Lee Margetts joined the team to study for his PhD under the supervision of Ian Smith. The objective was to develop a parallelisation strategy that could easily be applied by a non-specialist to any general finite element problem.

By the end of 2002, the parallelisation strategy first implemented by Mike Pettipher had been successfully generalised and all the MPI coding was hidden away into a library of FORTRAN callable subroutines. This library was used to create a suite of ten example programs covering the three main types of problem found in Engineering: Static equilibrium; dynamics (or time dependent problems) and eigenvalues.

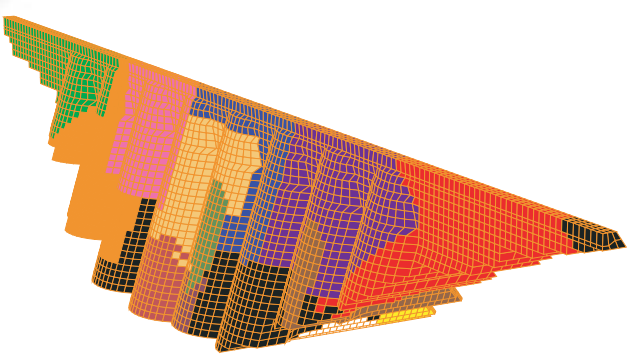

Figure 1: Finite element mesh of a buttress dam used to evaluate the structural response to earthquakes. The mesh is distributed across processors as illustrated by the colouring.

In March this year, a UKHEC workshop introduced the work to non-specialists in parallel computing. As the parallel programs retain the same structure and style of the original serial programs taken from Ian Smith's book, a researcher already familiar with serial FORTRAN programming and finite element analysis should be able to develop his or her own parallel codes. This was the philosophy behind the teaching and practical sessions at the workshop.

An article about parallel computing would not be complete without some performance figures! All the programs scale extremely well over large numbers of processors and for the results presented here, CSAR's 512 processor Origin3000, Green, was used. To give an impression of the scalability, our program for the direct numerical solution of the Navier Stokes equations boasts a speed up of 256 on 256 processors, whilst sustaining an impressive 30% of the machine's peak performance (see table 1). Similar performance is achieved for an elastoplasticity problem as illustrated in table 2. In this case, efficient use of up to 500 processors is clearly demonstrated. To name another example, an 8,000,000 equation eigenvalue analysis recently run on 256 processors found the first 100 eigenvectors in 460 seconds. Programs written to solve problems in heat conduction, dynamical systems and coupled processes such as magnetohydrodynamics show similar results.

| Reynolds Number | 256 processors | Serial | % Peak |
|---|---|---|---|
| 10 | 20 minutes | 2-3 days | 29 |
| 100 | 47 minutes | 8-9 days | 29 |
| 1000 | 180 minutes | > 1 month | 29 |

**Table 1: Direct Numerical Solution of the Navier-Stokes equations – 4,500,000 equations**

| Processors | PCG(s) | MFlops | % Peak |
|---|---|---|---|
| 4 | 2786 | 999 | 31 |
| 256 | 43.4 | 64190 | 31 |
| 500 | 23.9 | 116500 | 29 |

**Table 2: Elastoplasticity – 6,000,000 unknowns**

Why is this method so successful? To cover the three problem types mentioned earlier, three different iterative solvers are used: PCG (preconditioned conjugant gradients) for symmetric positive definite problems; BiCGStab(l) for non-symmetric systems and Lanczos for eigenvalue problems. These all have at their core matrix-vector products and other simple vector operations. Most of the communication and computation may be overlapped. The only possible downside is the unavoidable presence of a few global communications, such as dot products, which on some systems are known to limit scalability. If the problems are large enough, the communication to computation ratio is so low that the technique also works well on networks of PCs connected by Ethernet. This has been recently demonstrated by some collaborative work with the Civil Engineering department at the Universidad Politecnica de Madrid.

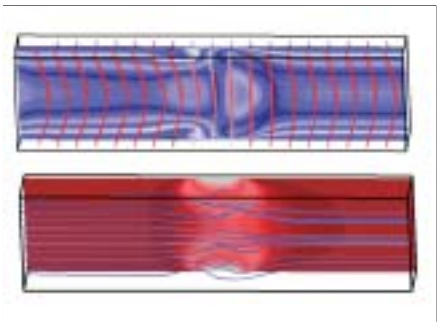

Figure 2: An example of magnetohydrodynamics: The flow of an electrically conducting fluid through an insulated rectangular duct under the influence of an externally applied magnetic field.

Although the parallel programs enable the solution of 3D problems with millions of degrees of freedom, understanding the results can itself present further challenges. Collaboration between the project and staff of the Manchester Visualisation Centre (MVC), in particular Joanna Leng, enabled the development of a powerful and convenient way of presenting and interpreting the results of the simulations. Using the AVS Express toolkit, Joanna produced an application that allows the user to view and manipulate the results of the simulations in stereo, in a virtual immersive environment such as an SGI Reality Centre. To interactively manipulate the largest data sets, ~ 10,000,000 variables, the multi-pipe edition of AVS developed by MVC was required. At Manchester this was run on an SGI Onyx300 with 6 dedicated graphics pipes.

These are exciting times. With the efficient use of powerful HPC resources and advanced visualization tools, scientists and engineers are not only able to investigate more complex models and systems, they are also able to explore their models intuitively and collaboratively through virtual reality visualization. In the future, we will highlight the merits of parallel FEA from another perspective. The same solution strategies can be applied to solve smaller problems very quickly – so fast that the engineer or scientist may be able to interact with their model in real time. This is the aim of the Advanced Virtual Prototyping Research Centre's Virtual Prototyping project in which Manchester are contributing their parallel finite element expertise.

Finally, if you would like to know more, please feel free to contact the authors or better still, enrol on the Summer School - it's free to CSAR users!

Manchester Research Centre for Computational Science

# MRCCS/NSF Summer School
# High Performance Computing in Finite Element Analysis

## 1st - 5th September 2003, University of Manchester, UK
## www.mrccs.man.ac.uk/summer_school/2003

The Manchester Research Centre for Computational Science (MRCCS) in conjunction with the National Science Foundation (NSF) of the USA are jointly organising a one-week Summer School on High Performance Computing in Finite Element Analysis. It will be held from 1st to 5th September 2003 at the University of Manchester, UK. The invited speakers are from Japan and France as well as from the UK and the USA. The format of the summer school will be a mixture of lectures and practical sessions, and will also include demonstrations in the virtual reality laboratory.

### *Finite Element Method (FEM)*

The finite element method is a general and powerful technique, applicable to a broad variety of mathematical problems that arise in almost all areas of science and engineering:

- Civil, Structural, Nuclear and Bio- engineering
- Mechanical and Aerospace Engineering (Computational Fluid Dynamics - CFD)
- Geology/Geophysics
- Acoustics
- Industrial Forming Processes
- Multiphysics

While some of these areas, such as CFD and the solid earth modelling in the Earth Simulator project, already make use of high performance computers, many of the other applications based on finite element analysis do not as yet make significant use of such facilities.

### *Objectives of this Workshop*

The primary objective of this workshop is to encourage engineers and other scientists using finite element analysis to dramatically extend the range of problems they can study by exploiting the power of the world's most powerful high performance computers. The intention is to bring together students of relevant disciplines, and for specialists in the field of parallel finite element analysis to lecture on their own areas of expertise, so that the students gain an understanding of the different approaches in current use.

### *Subject Areas*

The following topics will be covered in the workshop: computational geomechanics, biomechanics, computational fluid dynamics, tools for parallel computational mechanics and finite element meshes.

### *How to Apply*

An on-line application form is available at the following address:
http://www.mrccs.man.ac.uk/summer_school/2003/Application_Form.shtml

hpc-advice@man.ac.uk

# A new look at Tropospheric Chemistry

*Fiona O'Connor and Glenn Carver*
*Centre for Atmospheric Science, Dept. of Chemistry, University of Cambridge*

## *Tropospheric science*

The troposphere is the lowest part of the atmosphere from the ground up to what's known as the 'tropopause' - a narrow region at roughly 10km altitude across which there is a significant change in atmospheric properties. The chemistry in the troposphere is very complex. Computer models of tropospheric chemistry need to consider emissions from natural (e.g. lightning) and anthropogenic (e.g. industry, transport) sources, gas phase reactions that take place on both short and long timescales as well as heterogeneous gas reactions such as aqueous reactions in clouds. At the Centre for Atmospheric Science, University of Cambridge, scientists are using a range of computer models to study various aspects of tropospheric chemistry and in particular the role of ozone.

Although only a trace gas, ozone plays an important role in the troposphere, both radiatively and chemically. Ozone is an effective greenhouse gas and research suggests that, on recent timescales, it could be at least as important a greenhouse gas as methane. Chemically, ozone is the precursor for the main tropospheric oxidising agents, and hence has a strong influence on the ability of the troposphere to remove atmospheric pollutants. Furthermore, ozone near the Earth's surface is itself a pollutant and is detrimental to people with respiratory problems and to ecosystems. However, there is a still a large uncertainty in the factors controlling ozone in the troposphere.

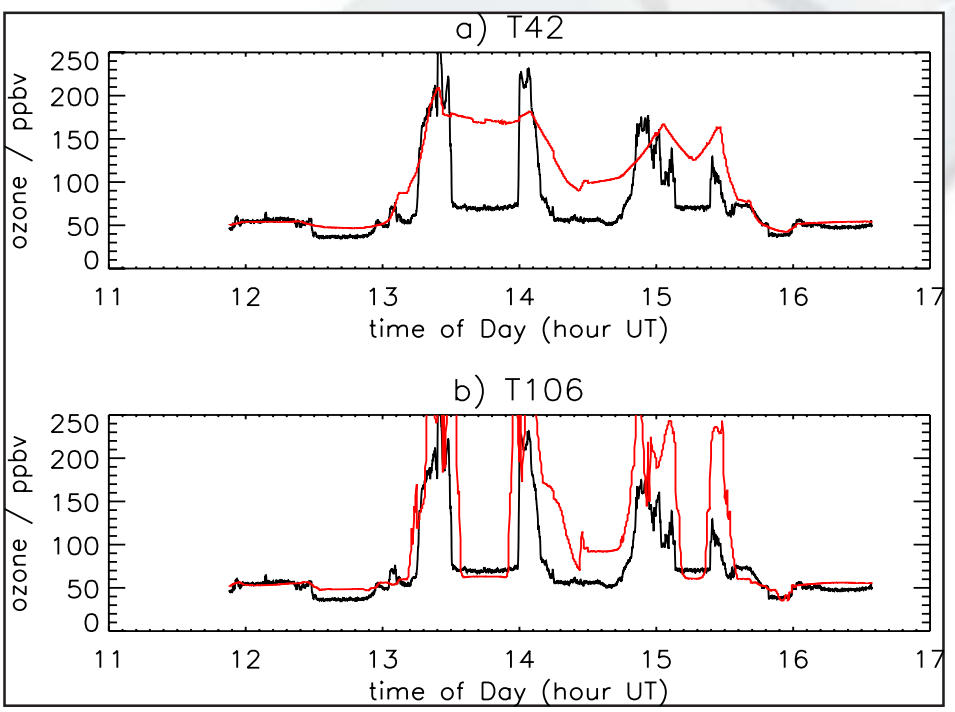


Figure 1: Comparison between modelled (red) and measured (black) ozone concentrations along a flight track from two TOMCAT integrations a) on the 3x3 degree model grid (normal resolution) and b) on the 1x1 degree model grid, made possible by the new model. The flight track is an example of a flight involving the UK Meteorological Office C-130 aircraft during the ACTO (Atmospheric Chemistry and Transport of Ozone) campaign in May 2000, funded by NERC's UTLS (Upper Troposphere/Lower Stratosphere) thematic programme.

## *Tropospheric chemistry modelling research*

One of the main models used is the 'TOMCAT' 3D model of tropospheric chemistry. This is what is known as a 'transport model' in that it uses meteorological analyses, winds and temperatures, to transport modelled chemical species accurately on a 3D model grid representation of the troposphere. Until recently, this model was run on the Fujitsu vector computer at Manchester but the closure of that service prompted the development of a new version of TOMCAT based on MPI. The new version offers substantially improved performance, enabling much faster runtimes than before and new research topics to be tackled. Assistance in porting the model was provided by CSAR.

The TOMCAT model is an ideal tool for carrying out studies of the role of ozone in the troposphere. For example, recent work for the Intergovernmental Panel on Climate Change has examined the impact of increased surface emissions on air quality in the coming century and found that air quality standards, in relation to ozone, will be strongly violated. TOMCAT has also been used to study the impact of subsonic aircraft on ozone. It was found that aircraft emissions result in enhancements to tropospheric ozone and hence contribute to the greenhouse effect. In addition, tropospheric ozone is strongly influenced by transport from the ozone layer above the tropopause. Current research aims to quantify the impact of this transport and the impacts from individual sources such as lightning, aircraft as well as surface emissions from Europe and the other continents. However, such emissions are very localised and the chemical processes acting on those emissions are non-linear. As a result, a crucial aspect in studying the impact of emissions on ozone levels in the current and future atmospheres is the issue of the importance of spatial scales from local, to regional, to continental and global. The new TOMCAT model will, for the first time, allow integrations at high horizontal and vertical resolution to be carried out. The new model offers the opportunity for a major advance in our understanding of the complex scientific problem, a problem of direct relevance to society.

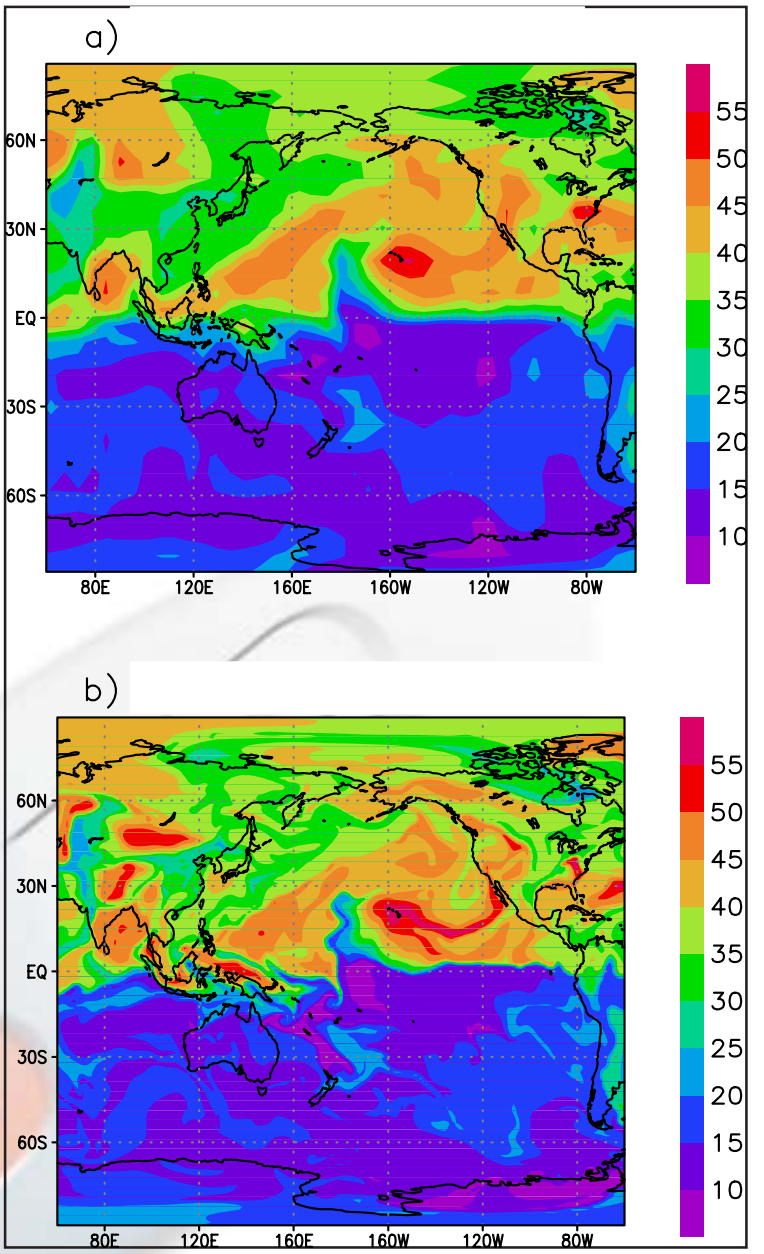


Figure 2: Modelled ozone concentrations at the surface for the Pacific region from TOMCAT a) on the 3x3 degree model grid and b) on the 1x1 degree model grid. Of particular interest is the ability of TOMCAT at high horizontal resolution to maintain features of small spatial scales and to conserve very sharp gradients e.g. near the equator.


## *Acknowledgements*

We are delighted to acknowledge expert assistance from Kevin Roy and Neil Stringfellow of CSAR in developing and debugging this new model.

Glenn Carver and Fiona O'Connor are funded by NCAS-ACMSU.

# Caught in the act – modelling how a biological catalyst works

***Adrian J. Mulholland, School of Chemistry, University of Bristol and Lars Ridder, Molecular Design & Informatics, N.V. Organon***

Essentially all of the multitude of biochemical reactions in a cell depend on enzymes to make them 'go'. Dissecting how these biological catalysts work will be vital to understanding biological processes at the molecular level, and also promises technological benefits in the form of new drugs, genetic analysis and catalytic processes. Central to enzyme catalysis is the nebulous 'transition state' of a chemical reaction, in which bonds are partly formed and broken. Biologists have theorized for many years that enzymes are able to recognise and stabilize transition states, and that this stabilization is at the heart of enzyme catalysis. However, transition states are extremely unstable and short-lived, making it impossible to study them directly in systems as large and complex as enzymes. The challenge is to analyse the groups and interactions involved in a biological reaction 'as it happens' within the protein structure of the enzyme. Now quantum chemical modelling on the CSAR T3E has provided a detailed picture of a reaction in an important enzyme, showing at the atomic level how transition state stabilization is achieved[1].

*Para*-hydroxybenzoate hydroxylase (PHBH) is an important enzyme in the microbial biodegradation of a wide variety of aromatic chemicals, including pollutants and lignin, a major component of wood and so among the most abundant of all biopolymers. PHBH acts by oxygenating its substrates (adding a hydroxyl (OH) group to the aromatic ring), and is a key member of an important class of oxygenase enzymes. Its mechanism has been investigated in a collaboration between computational chemists at the School of Chemistry, University of Bristol, and biochemists and toxicologists at Wageningen University, The Netherlands. Using the computational power of the CSAR T3E it has been possible to model the vital reaction step in the enzyme.

The reaction was modelled starting from a protein structure determined by X-ray crystallography. Using a technique combining quantum mechanics calculations with a simpler ('molecular mechanics') description of the protein, it was possible to model how the bonds break and form, and how the structure of the enzyme and the reacting groups change during the reaction[1].

The results showed that a specific interaction with the enzyme is found only at the transition state. This has the effect of stabilizing the transition state relative to the reactants, lowering the barrier to reaction. A hydrogen bond is formed between a group in the enzyme (the backbone carbonyl of a proline amino acid residue) and the hydroxyl group as it is transferred onto the substrate. The active site of the enzyme is exquisitely well organized to stabilize the transition state, in a way that was not at all obvious until the reaction was modelled. The calculations indicate that this interaction lowers the barrier by a catalytically significant amount. The results also appear to agree well with biochemical experiments[2]. What is particularly exciting is that this catalytic motif seems to be a common feature of this family of enzymes, so the finding may be useful in understanding their biodegradation processes more generally[1,3].

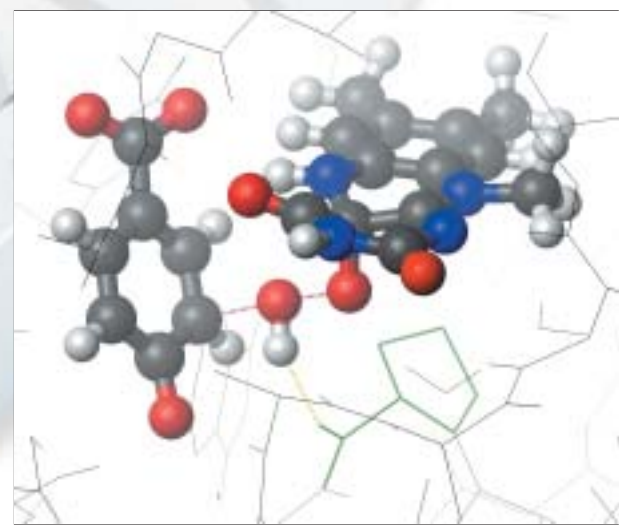

Figure 1: How a biological reaction happens: this picture shows the transition state in the enzyme para-hydroxybenzoate hydroxylase, as found by modelling. An OH group (centre) is transferred from a cofactor (right) to the substrate (left) (reacting groups shown as balls and sticks), and is stabilized by an interaction with a key group in the enzyme (shown in green).

Biological oxygenation reactions are the focus of a lot of current research, both from the point of view of understanding the challenging chemistry involved, and with a view to practical applications of biocatalysts. These computational results show the potential of high-

level modelling for analysing the fascinating and little understood mechanisms of enzyme catalysis.

### *References*


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## High Performance Computing and Visualization - MSc degree courses at the University of Manchester

Most of you will be aware that CSAR and the University of Manchester provide training courses, workshops etc. in the area of high performance computing and visualization. These are primarily of a short duration and aimed at users of existing HPC facilities. However, there are many opportunities to learn about different aspects of HPC and visualization, both theoretical and practical, in some of the MSc degree courses offered at the University of Manchester. CSAR staff teach and supervise research projects on these courses, which include the following:

**MSc in Applied Numerical Computing**
http://www.maths.man.ac.uk/DeptWeb/MScCourses/NA/NewNAMSc.html
The Departments of Mathematics at the University of Manchester and UMIST jointly run an MSc in Applied Numerical Computing that provides training in the use and development of reliable numerical methods and corresponding software. The programme covers the underlying mathematical ideas and techniques, scientific and high-performance numerical programming (including MPI and OpenMP), the use and design of mathematical software, and options in a number of application areas. The course involves both taught work and a dissertation. It is supported by EPSRC and industrial partners.

**MSc in Advanced Computer Science**
http://www.cs.man.ac.uk/Study_subweb/Postgrad/ACS-CS/syllabus/acs/acs.html *&*
**MSc in Computational Science**
http://www.cs.man.ac.uk/Study_subweb/Postgrad/cpn.asp
Both of these courses are taught by the internationally renowned Centre for Novel Computing within the Department of Computer Science, and are supported by industrial partners. The MSc in Computational Science is aimed at graduates in the Physical Sciences, Engineering and Mathematics who have an understanding of the role of differential equations in the modelling of physical phenomena. The course concentrates on the high-performance computational aspects of such modelling and simulation, including algorithmic aspects, visualization, the development of software and the use of massively parallel machines for fast simulation.

Both of these courses combine a wide range of taught modules with a research project. Modules particularly relevant to HPC include:

- Grid Computing and eScience
- High Performance Computing in Science and Engineering
- Fundamentals of High Performance Execution
- Visualization for HPC

THE UNIVERSITY of MANCHESTER

# Parallel Support Toolkit for AVS/Express

*James Perrin*
*SVE Team, Manchester Computing, University of Manchester*

*Bringing multi-processor performance to a leading visualization application*

## Introduction

AVS/Express is a leading visualization and application development package. It provides a visual programming interface where the user connects together modules from libraries of data readers, filters and visualization techniques to create an AVS network (visualization pipeline). AVS/Express is a general visualization package though it is mainly aimed at scientific visualization for engineering, medicine, geology, simulations and other fields. Manchester Visualization Centre (MVC) has extensive experience with the package; using it for many projects and also hosting the International AVS Centre, an internet repository of user submitted modules.

AVS/Express is a well established piece of software, however it has always been single processor based. AVS took its first step towards HPC support with the development of Multi Pipe Express (MPE) which takes advantage of multiple graphics pipes as found on SGI Onyx hardware to render large datasets and enable use in multiple projector environments such as Caves and RealityCenters. MVC has designed and developed both MPE and the soon to be released Graphics Cluster Edition (GCE) for PC clusters, however, the visualization computation is still performed on a single CPU. Users obviously want to utilise the multi-processor systems that they are running MPE/GCE on, hence the conception of the Parallel Support Toolkit for AVS/Express between MVC, AVS, KGT (Kubota Graphics Technology Inc.) and JAERI (Japan Atomic Energy Research Institute).

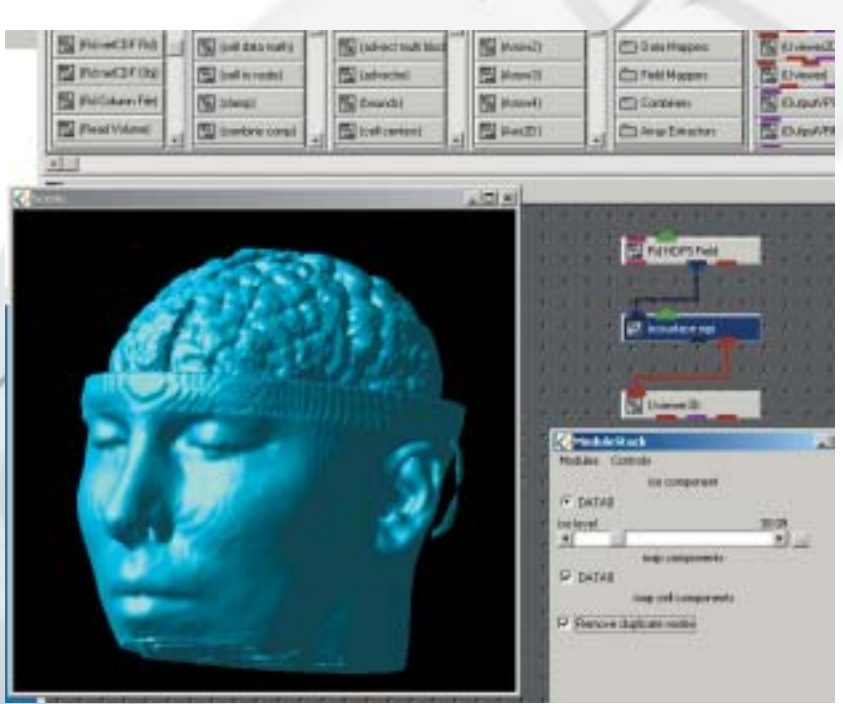

Figure 1: A simple AVS network exploiting the MPI version of isosurface from the feasibility phase

## Overview

Unlike previous attempts to add parallel computation to AVS/Express, such as VIPAR, parallel modules will be aware of other parallel modules in the AVS network so the computation nodes can pass data between computation methods without the need to gather, recompose, decompose and distribute the data as each module is executed. Instead modules will pass tags (meta information) between themselves. These parallel modules can then be used with the standard serial modules to create new AVS networks or integrated into existing networks to enhance the performance of the visualization application.

PST is a multi phased project to run over a course of two years. It will provide developers with a toolkit (API and skeleton code) to enable them to build their own parallel modules for AVS/Express and after the first year a suite of parallel visualization modules will be created to empower the end user with the ability to create AVS networks and applications that harness the power of SMP and cluster based systems. The second year will extend the parallelism paradigms of AVS/Express, optimizing and integrating with current rendering methods and MPE.

The project is currently in Phase 2, the design and implementation phase of the basic PST framework. This followed on from an initial feasibility stage that demonstrated the benefits of parallelization for the

standard isosurface module. PST is being developed for SGI and PC cluster systems and it was originally envisioned that both MPI and OpenMP (on SGI) would be utilised but there are compatibility issues between MPE and OpenMP. MPICH is being used for the PC cluster version.

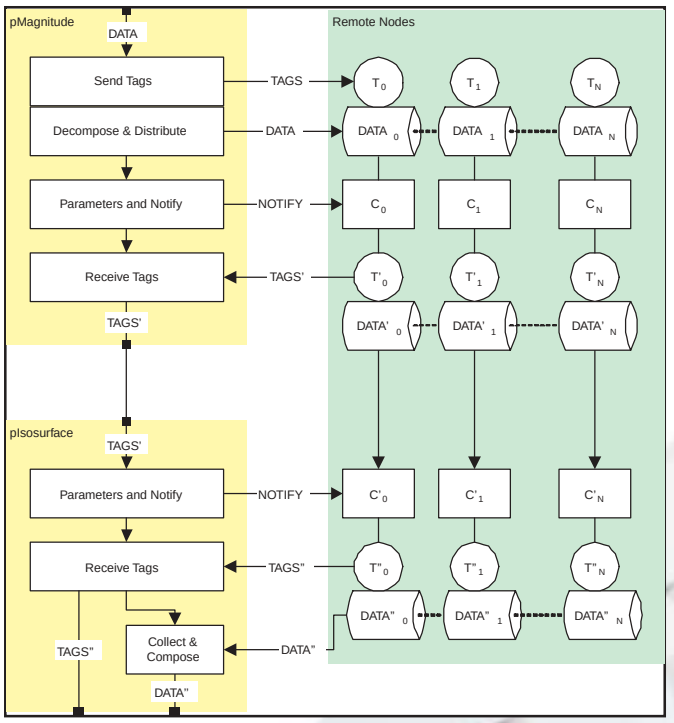


Figure 2: Passing tags rather than data between modules is an advantage over previous attempts to add parallel computing to visualization applications.

## Parallelism, Lots of Parallelism

All the modules will be based on data parallelism. The problem is that different modules may require different decomposition methods; each module therefore has an associated schema which specifies its desired decomposition method (as well as other information about how the module is to be executed). These schema are then resolved to discern where re-composition and distribution is required e.g. a module that requires a domain border of N elements can pass data to a module that doesn't require border elements (assuming the data redundancy overhead being outweighed by not needing to recompose and distribute the data), however the reverse is not true and the schema resolution will force the first module to recompose its data before passing it to the second module. If a set of modules should execute on the same set of nodes, data will be cached on the nodes so that module parameter changes don't require further data distribution. Data only therefore needs to be distributed to and from the first and last modules.

Task parallelism will be implemented at an AVS network level where two or more modules share the same input. Normally these would execute in a serial manner controlled by the Object Manager (OM), but by getting the first module to distribute the data and then return control to the OM after initiating the computation, the next module can start its computation and so on.

Note that each AVS network still executes one cycle at a time, so after a module has executed it has to wait for the remaining downstream modules to complete and the scene to be rendered. By decoupling PST module execution from the OM, when a module has completed execution it can then re-execute if new data is available or parameters have changed. Decoupling modules from the OM enables this "pipeline parallelism" as well as further parallel features and optimization. These features will need to be balanced against the real world advantages that they can provide and the feasibility of adding these to a large and complex serial application within a reasonable timeframe.

## MPE Integration

A driving force behind this work has been users of MPE, as well as increasing the computational performance of MPE. Later phases will integrate PST with the rendering methods of MPE, e.g. modules will be able to pass geometry data directly to the rendering pipes bypassing the re-composition and conversion stages that are used currently.

## Springer Style Final Thoughts

Though there has been much work done in creating specific parallel techniques these have in general been applied to isolated methods such as isosurfacing and have been produced as research projects that only benefit a small number of users. This project aims to bring the fruits of these labours to a larger community and to build on them to produce an end user parallel visualization environment and to enhance the extensibility of AVS/Express with a standardized software toolkit.

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http://www.sve.man.ac.uk/Research/PST/

# Visualization in Earth System Science

*Michael Böttinger, Deutsches Klimarechenzentrum (DKRZ), Martin Schultz, Max-Planck-Institute for Meteorology and Joachim Biercamp, Deutsches Klimarechenzentrum (DKRZ)*

## From Climate to Earth System Models

Traditionally, climate is defined as the statistical collective of the weather conditions of a specified area during a specified interval of time, usually several decades. This definition is currently undergoing a change to place more emphasis on the exchange of energy, momentum, and mass between the different compartments of the Earth System. Although weather is experienced as a pure atmospheric phenomenon with high temporal variability, the long-term changes of mean weather conditions are driven by the dynamics of slowly changing components of the climate system: e.g. the ocean, sea and land ice, and the biosphere.

Several feedbacks between the climate system compartments have been identified. Two prominent examples show links between atmospheric chemistry and the physical atmosphere: the photochemical formation of ozone in the troposphere, which then acts as a greenhouse gas (Figure 1), and the influence of aerosols and their chemical composition on the formation and properties of clouds. In contrast to short-term weather forecasting, where slowly varying components can be prescribed as boundary conditions, coupled global 3-dimensional models of the full physical ocean-atmosphere-sea-ice system are needed for simulations on longer time scales. In the future, we will see even further integration of chemical, biological, and socio-economic models into traditional climate models, ultimately leading to a comprehensive global modelling system termed the Earth System Model (ESM) (Figure 2).

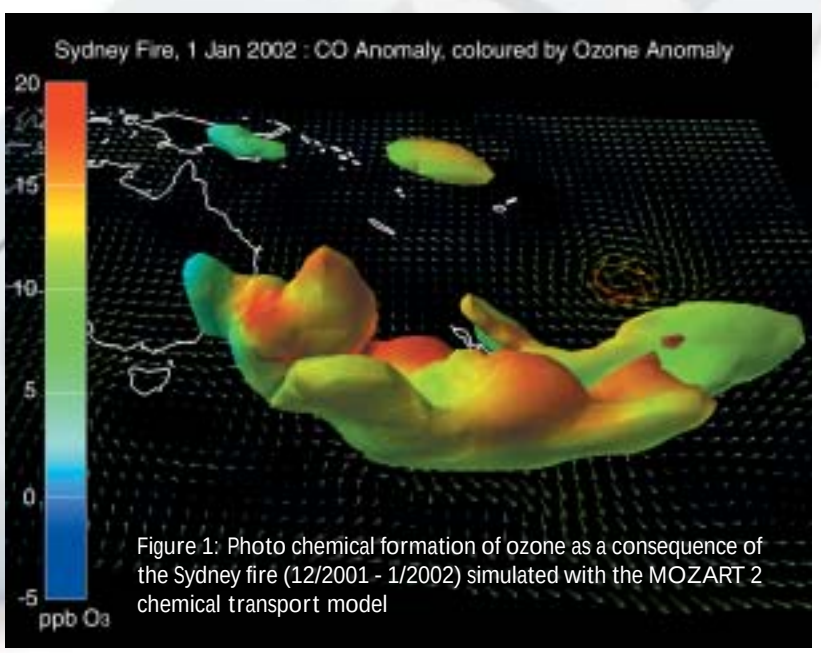


Figure 1: Photo chemical formation of ozone as a consequence of the Sydney fire (12/2001 - 1/2002) simulated with the MOZART 2 chemical transport model

## The challenge

The output from such models can be described as a multitude of time dependent 2D and 3D data sets, each consisting of several scalar and vector variables.

The individual data sets may have different time intervals, and they do not necessarily share a common computational grid. For example, the ocean component may run on an Arakawa-C grid with shifted poles (Figure 3) [1], while the atmosphere is simulated on an almost regular Gaussian grid. New grid structures such as the triangular grid from the GME model of the German Weather Service (DWD) [2] are being developed to remedy some of the problems encountered with regular grids, e.g. the singularity at the poles. Many models use vertically non-linear coordinate systems. Data from atmospheric models is often stored on pressure levels or so-called hybrid levels (topography following levels at the bottom of the model, pressure level at top and a mixture of both in between). Some models like isopycnal ocean models even use time dependent vertical coordinates.

The enhanced supercomputer technology allows us to refine the spatial resolution and to add more processes and variables (e.g. tropospheric and stratospheric chemistry) to the models. The higher resolution has many advantages: small scale processes, which otherwise have to be parameterized, can be simulated directly, and local topographic effects on the atmospheric or the ocean circulation are better resolved.

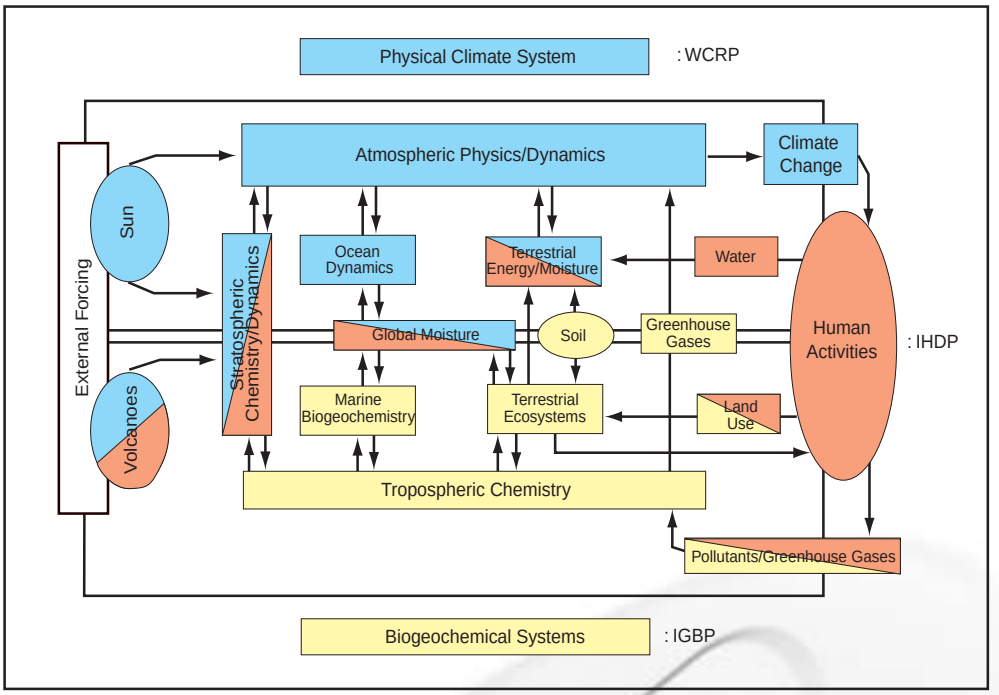


Figure 2: The Earth System: A modified "Bretherton diagram" highlighting some of the linkages between social systems, biogeochemical systems, and the physical climate system. Courtesy Guy Brasseur, Max Planck Institute for Meteorology

So-called Monte-Carlo-simulations (repeating the same simulation with slightly altered initial or boundary conditions) and multi-model simulations are used to quantify the variability of the model simulations and the probability of specific results. Such ensembles further increase the amount and the complexity of model output.

Analysing model results has become a real challenge for geoscientists: the amount of data that is produced by global and regional models has risen exponentially over the past decade (Figure 4). The data volumes generated by an ESM mandate that visualization applications read data in different formats and on different meshes without prior conversion. Data on different geometries and with different dimensions must be compared to each other and to observational data, which is often inhomogeneous in time and space (Figure 5). Geoscientists need data processing and visualization tools, which help them understand the Earth System. These tools must be fast and flexible in order to efficiently support the search for new phenomena and feedbacks, and they must also be able to produce high-quality graphics, which can directly be used in publications (Figure 6).

## *The reality (1) - data structures and formats*

Ten to fifteen years ago, when many of today's visualization packages were being developed, most atmosphere and ocean models had horizontally regular or rectilinear grids. Most of the visualization packages available today are not prepared to deal with irregular grids, which are quickly becoming the standard in Earth System modelling. Hence, such data needs to be interpolated prior to its visualization, which can lead to unacceptable alterations of results.

Over the past decades, two quasi-standard formats have been established, which allow us to write self-describing and machine independent data sets for Earth System science: GRIB and NetCDF. A third format, HDF, is widely used to store satellite data.

Many data sets from atmospheric models have been generated in the GRIB format ([3],[4]). A GRIB record consists of a short descriptive header plus one horizontal layer of one variable. The GRIB header contains a limited metadata set, which for example allows us to read the files without knowing the grid size and structure in advance.

The more general NetCDF format [5] facilitates

random access of individual data records and allows for arbitrary metadata within the file itself. NetCDF is not specifically designed for Earth System requirements, therefore additional metadata conventions are needed to guarantee common names, units etc. In 1995 the COARDS convention [6] has been designed for global atmospheric and oceanographic research data sets. Because of limitations like the restriction to rectilinear grids this standard is not sufficient for many recent models. The CF convention [7] currently being developed is an extension of COARDS which for example adds support for non-rectilinear grids. NetCDF/CF will likely become the quasi standard in Earth System modelling [8][9].

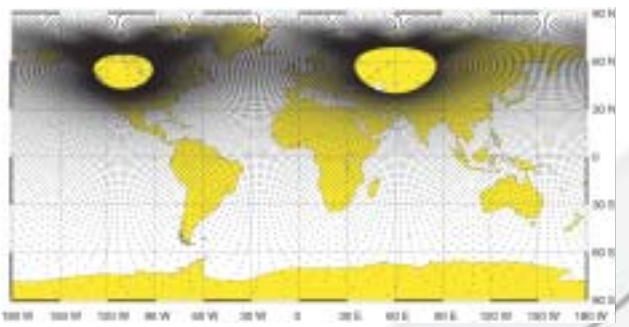

Figure 3: Example for a curvilinear 302x132 grid with the HOPE-C ocean model (GI4). The flexible position of the poles allows for a locally increased grid resolution in the area of interest: in this example the northern North Atlantic (here 30-40 km resolution). Courtesy Uwe Mikolajewicz, Max Planck-Institute for Meteorology

## The reality (2) - visualization software

In terms of algorithm development, the problem "visualization of data that describe the four-dimensional space-time world" is mostly solved. Techniques for the display of time dependent scalar or vector fields have been developed and published years ago. Many of them have been included in commercial and non-commercial data visualization software [10]. But why are these techniques so rarely used by the scientists who generate the data?

Publications of climate researchers seldom include 3D representations of their data. How many 3D images of 3D data are contained in the 881 pages of the last IPCC report [11]? We found none. While we commit that 3D visualization may be more widely used for the interactive exploration of data than for the production of reproducible, quantitatively and scientifically exact graphics, it is nevertheless striking to observe the nearly complete lack of 3D images in climate-related publications. One of the factors, which may explain this phenomenon is the fact that the spatial structure of 3D still images cannot be easily printed. Well-established methods like shadow casting - which would improve the depth perception of 3D images - are not yet available within any scientific visualization package.

Most interactive 3D visualization solutions have very limited 1D and 2D capabilities. Such plots are essential for the quantitative analysis of model output. It is often desirable to interactively explore the data in 3D (e.g. find the ideal location of a slice), before producing a publication quality 2D plot. Currently, this approach usually requires the use of more than one software package with an intermediate "off-line" data extraction step.

*Commercial Software:*
In the late 1980s / beginning of the 1990s several commercial companies started to develop all-purpose 3D data visualization software. Interactive script and command languages like PV-Wave or IDL were extended to provide more 3D functionalities. Modular visual programming environments like AVS, Iris Explorer and IBM Data Explorer or end-user applications like Wavefront's Data Visualizer were expected to revolutionize the way scientific data is displayed [12], and it was believed that they would spread widely enough to provide profits for the companies.

The situation today: Wavefront is gone. IBM stopped further developments of Data Explorer and released it as open source. AVS (now AVS/Express) was rewritten with a more object-oriented approach - which makes it even harder to use. SGI's Iris Explorer was taken over by NAG.

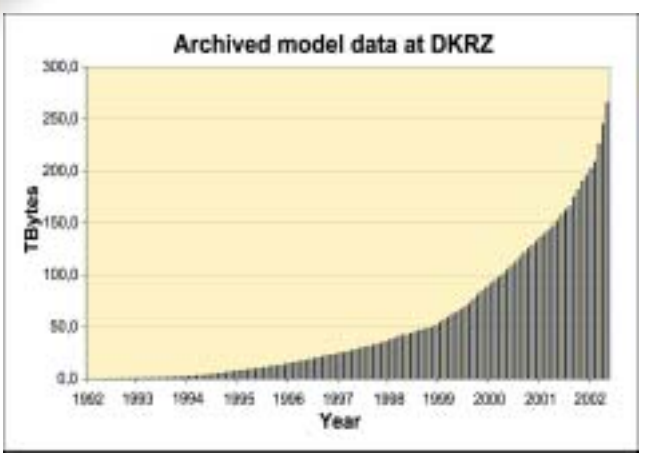


Figure 4: Archived climate model data stored at DKRZ 1992-2002 (without duplicates).

Major developments in these software packages were made years ago. In the last years the advances from release to release were relatively small. Newly developed visualization methods have rarely been implemented; they can only be added by the user with significant effort. The usability has not increased very much. Modules for specific visualization methods (e.g. volume rendering) are very often only applicable for specific data types or grids and users have to be increasingly familiar with the software in order to know in advance which combination of modules might work with their data. Documentation and online help are still an issue: important details are very often not covered. PV-Wave and IDL have grown in functionality. For example, IDL now features an object oriented graphics engine. Both programs are still commercially supported and they are widely used. However, these languages suffer from legacy codes and concepts. In order to use object graphics in IDL, the user has to learn many details about 3D rendering, which distract from the actual task of visualizing scientific data.

None of the commercial products offers a "ready-to-use" visualization application for Earth System modelling; users have to write their own software and learn about the programming language, available libraries, or visual programming environments.

*Free software:*
Based on the insight that commercial software only solved some of the typical problems in the visualization of geophysical data, some scientific institutes decided to develop their own visualization software tailored to their needs (e.g. GrADS, FERRET, NCAR Graphics). These tools were developed in close cooperation with the geoscientists and have therefore enjoyed large acceptance in the community. But considering the challenges of coping with today's model output, it becomes quickly clear that practically all of the freely available plotting packages are too limited in their data model or in the types of plots that are offered. For example: it is impossible to read two data sets with different vertical or horizontal grids into the GrADS software, and to compare the results in one plot. FERRET, GrADS and other software packages can read COARDS NetCDF files, but they often fail if the data was written with other conventions like CF. Except for OpenDX, which appears rather slow with large data sets and requires a large learning effort, hardly any free software package is able to deal with irregular grids. As opposed to most other programs, Vis5D [13] is a very usable and efficient 3D data visualization application for atmospheric data, but it supports only horizontally regular grids, it has only very limited 1D or 2D capabilities, and it has no built-in GRIB or NetCDF data importer. Also, control over the appearance of a plot is fairly limited.

No visualization package fully supports the data formats and conventions applied in ESMs. To use them, a considerable amount of data conversion and module writing is required. Most software is difficult to use for geoscience applications and requires a large learning effort. Expertise in both visualization and Earth System research is needed in order to make full use of the available software, or to develop custom-tailored applications, which can then be used by a small fraction of the community. Bridging the gap between Earth System science and visualization is rarely rewarded, because - from a science perspective - too much time is spent on technical details, and - from the visualization perspective - the focus is too narrow.

## *Conclusion - what is needed*

At present, a patchwork of different tools is needed in order to produce the desired visualization results from ESM output. Data files must be replicated in order to allow for their visualization, and a lot of image manipulation is needed in order to yield publishable results.

Facing the quickly growing data volumes produced with ESMs and their increasing complexity, visualization and data processing must converge into a single system for 1D to 3D visualization. The following list contains key requirements for such a system:

- Cover the whole range from static 1D plots to interactive state-of-the-art 3D visualization methods
- High interactive 3D performance (hardware acceleration)
- Data importer/browser for all major file formats used (GRIB, NetCDF/CF, HDF, IEEE, ASCII)
- Interface to DBMSs
- Capable of dealing with huge data sets
- Automatic use of metadata, including some "understanding" of the meaning of physical quantities
- Access to processing functionality, mathematical functions, statistics
- Support for different geometrical grids, extendable to support future grid definitions
- Multiple data sets on different grids, interpolation between grids
- Easy to use, easy to learn

- Interactive use via GUI and script/batch mode processing
- Extendable to allow for special functions
- Include World Maps and 3D topography, extendable to include e.g. vegetation maps
- Automatic mapping of geo-registered data, arbitrary map projections
- Publishing quality image output with WYSIWYG preview
- Platform independent
- Freely available in order to allow use in education and in developing countries

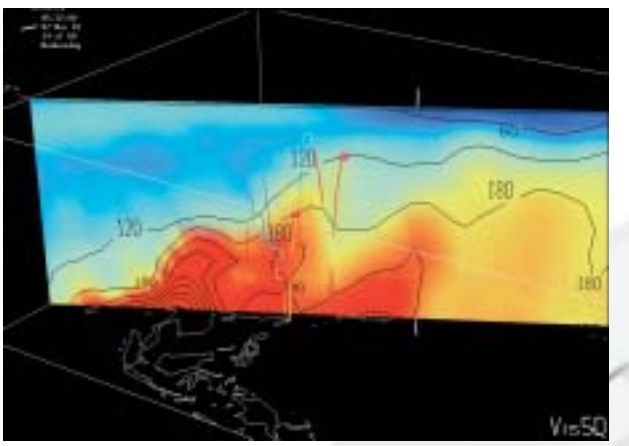

Figure 5: Comparison of airborne CO measurements and model results (TRACE-P).

Currently, climate research institutions and research projects rarely provide any significant funding for the development of suitable visualization applications. Infrastructure programmes like PRISM [8] and ESMF [9] do have data processing and visualization on their agenda, but the resources attributed to these issues are far too low. Processing and visualization of Earth System data must be recognized as a challenging engineering problem similar to the construction of a sophisticated scientific instrument. Because many visualization concepts are not known to geoscientists today, they should receive better and earlier training in data processing and visualization techniques (e.g. at university courses). A highly efficient, easy-to-use, and flexible visualization tool would likely boost the productivity of scientists working in climate research. The building blocks are out there: now the architect and the sponsor are needed to bring it all together!

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[7] http://www.cgd.ucar.edu/cms/eaton/cf-metadata/index.html

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[13] http://www.ssec.wisc.edu/~billh/vis5d.html, http://vis5d.sourceforge.net/


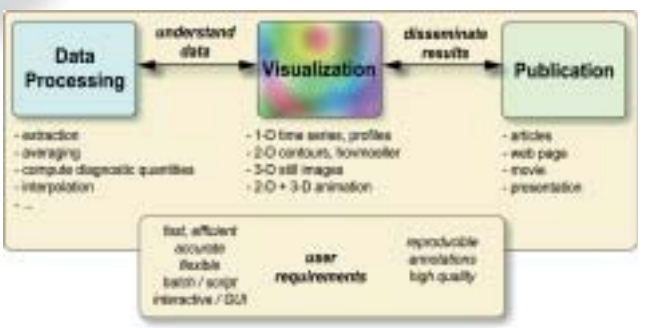


Figure 6: The role of visualization in the geosciences in between data analysis and publication.

# Cray X1 Scientific Library Optimisation

***Adrian Tate***
***HPC Team, Manchester Computing, University of Manchester***

Figure 1: Cray X1

At the Cray User Group Summit in Columbus, Ohio, Cray Inc. announced that the tuning of parallel subroutines within a future release of the X1 scientific library will be carried out by staff of the SVE group at the University of Manchester. This builds on previous work for several CSAR consortia in which the performance of parallel numerical library routines has been successfully increased. By the autumn, ScaLAPACK will be part of the LibSci release, a subset of which will perform optimally after the communication procedures have been overhauled by SVE staff.

The Cray X1 has a number of major architecture differences to its predecessor – the T3E. The distributed-shared memory system is similar to that of a an SGI Origin, but unlike the Origin (or any other system to date) the X1 couples this DSM architecture with 16 vector registers on each processor and with a clock speed of 800 MHz, giving a peak performance of 12.8 Gflops per processor. The system has been designed with MPI codes in mind, but Co-array Fortran, UPC and SHMEM can offer extremely good performance.

Cray are keen to market the machine as highly suited to existing distributed memory applications, and as such are keen to incorporate DM numerical libraries that are efficient and scalable. SVE were selected by Cray because of their experience in creating one-sided communication procedures using SHMEM and Co-array Fortran and because of their knowledge of the complex internal workings of ScaLAPACK and its dependent PBLAS and BLACS libraries. UPC, Co-array and SHMEM operate at very low latency on the Cray X1 and are implemented in such a way that remote data does not enter a local processor's cache but is loaded directly into vector registers. This feature prevents cache invalidation by remote data which has been a problem with implementations in the past, and allows very high speed message passing. In addition, Cray have worked heavily on the Co-array Fortran compiler within Ftn and can enforce pre-fetching with any Co-arrays that appear in an application. Hence, a Co-array version of ScaLAPACK is an attractive prospect and is likely to offer extremely good performance.

An initial pilot project will involve a revision of the communications procedures within the LU factorisation routine pcgetrf/pzgetrf. This will involve complete replacements to four BLACS communication routines and some major alterations to the PBLAS, which govern the communication patterns necessary to achieve parallel execution of Lapack routines. Communications will be a mixture of SHMEM and co-array Fortran, the initial testing of BLACS replacements looks very promising. A longer project will involve a much deeper restructuring of comms patterns within Scalapack, with much work to decrease the programming complexity of specific operations by the capturing of useful functionality into a comprehensive library of efficient programming tools. In addition, Cray are aware of the limitations and restrictions that accompany Scalapack usage, and are interested in the enhancement and development of the user interface to develop a highly tuned, accessible library that may allow less rigorous distribution methods that suit better the attributes of the application.

If you are interested in this work please see the next *CSAR Focus* for an update, or contact Adrian Tate directly:

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# HPCx: Towards Capability Computing

***The HPCx Terascaling Team [1]***
***CCLRC Daresbury Laboratory and the University of Edinburgh***

During the next few decades, advances in computing technologies will increase the speed and capacity of computers, storage, and networks by several orders of magnitude. At the same time, advances in theoretical, mathematical, and computational science will result in computational models of ever increasing predictive capability and utility. The key goal for computational scientists and engineers is then to harness the power offered by present and future high-performance computers to solve the most critical problems in science and engineering. Such a goal demands a capability-driven approach, an approach in which the full power of a Terascale computer is bought to bear on a given scientific problem through effective utilisation of all available resources - CPUs, memory, and in many cases high levels of I/O performance. The primary mission of HPCx is that of Capability Computing, an approach reflected by our drive to ensure that the majority of jobs on the IBM SP/p690-based system are capable of utilising at least a significant fraction of the available resource. In this article we briefly describe the initial progress towards this goal by illustrating the current levels of delivered performance on HPCx from two well-known codes, CRYSTAL and POLCOMS (see [2] for more details).

## *Application Performance; CRYSTAL and POLCOMS*

CRYSTAL [3] permits the calculation of wave-functions and properties of crystalline systems, using a periodic Hartree-Fock or density functional Kohn-Sham Hamiltonian and various hybrid approximations. The wavefunctions are expanded in atom centred Gaussian type orbitals (GTOs) providing a highly efficient and numerically precise solution with no shape approximation to the density or potential. Recent enhancements to the parallel distributed data version of the code, MPP CRYSTAL, include the incorporation of a somewhat faster, and more numerically stable version of the parallel Jacobi diagonaliser [4], the rationalisation of the memory management within the code, and the avoidance of disk access through either the recalculation, or, for distributed objects, storage in memory. Recent benchmark calculations on the IBM/p690 for crystalline crambin [5] performed in basis sets of increasing quality reveal excellent scalability that is enhanced with improvements in the basis set. Thus the 6-31G (7,194 GTOs) and 6-31G** calculations (12,354 GTOs) yielded speed-ups of 573 and 688 respectively on 1024 CPUs. These are some of the largest ab initio electronic structure calculations reported to date.

The Proudman Oceanographic Laboratory Coastal Ocean Modelling System (POLCOMS) has been developed to tackle multi-disciplinary studies in coastal/shelf environments [6]. The central core is a sophisticated 3-dimensional hydrodynamic model that provides realistic physical forcing to interact with, and transport, environmental parameters. In order to study the coastal marine ecosystem, the POLCOMS model has been coupled with the European Seas Regional Ecosystem Model (ERSEM) [7]. Studies to date have been carried out, with and without the ecosystem sub-model, using a shelf-wide grid at 12km resolution. In order to improve simulation of marine processes, we need accurate representation of eddies, fronts and other regions of steep gradients; the next generation of models will need to cover the shelf region at approximately 1km resolution.

In order to assess the suitability of the POLCOMS hydrodynamic code for scaling to these ultra-high resolutions we have designed a set of benchmarks which runs (without the ecosystem model) at grid sizes representative of resolutions from the current 12km down to 1km. Runs on the HPCx system reveal, as expected, that, as the grid size increases, the ratio of communication to computation in the code improves and so does the scalability. At high resolutions the code is scaling almost linearly, delivering speed-ups of approx. 870 and 950 on 1024 processors for resolutions of 2km and 1km, respectively, on the IBM SP/p690.

Figure 1: HPCx is based around a 40-compute node IBM p690 cluster whose configuration is specifically designed for high-availability computing.

## Summary

A significant number of key user applications have already been ported to HPCx. The initial benchmark results from this process and the performance levels achieved have highlighted a wide range of performance, with some algorithms scaling far better than others [2]. What is clear is the limited scalability likely to arise on the HPCx system in any application that involves global communication routines, or a dependency on linear algebra routines with extensive communication requirements. This comes as little surprise given the known limitations of the present Colony-based interconnect. Within the HPCx Terascaling Team there is currently a major focus on algorithm development designed to remove existing dependencies on collective, global operations. Where this has been addressed, e.g. CRYSTAL and POLCOMS, we find excellent levels of scalability and performance.

Finally, it is worth noting that change will be endemic to high-performance computing in the next decade. Although we are currently on a plateau in the evolution of parallel supercomputer architectures (clusters of shared memory computers), this will not last long. New architectures are already on the drawing boards that will be capable of a quadrillion arithmetic operations per second (petaops). Such computers cannot be built using the same technology in today's teraops computers - they would require too much space and consume too much power. The technical problems to be solved are formidable for such computers (typified perhaps by the cellular architecture-based Blue Light and Blue Gene projects from IBM). We are confident that the type of developments currently underway within the HPCx Terascaling team will prove invaluable in assisting the UK community to be ready for these challenges downstream.

## References


[1] The HPCx Terascaling Team, with contributions from Mike Ashworth, Stephen Booth, Ian J. Bush, Martyn F. Guest, David S. Henty, Martin Plummer, Lorna Smith and Andrew G. Sunderland.

[2] Capability Computing News, 1, June 2003

[3] The CRYSTAL code is developed within a long standing collaboration between the Theoretical Chemistry Group at the University of Torino, Italy, and the Computational Materials Science Group at Daresbury Laboratory.
See www.cse.dl.ac.uk/Activity/CRYSTAL and www.chimifm.unito.it/teorica/crystal

[4] http://www.cse.clrc.ac.uk/arc/bfg.shtml

[5] The structure of Crambin is derived from XRD data at 0.52 Å. This crystal structure contains 1284 atoms.

[6] Coupled Marine Ecosystem Modelling on High-Performance Computers, M. Ashworth, R. Proctor, J.T. Holt, J.I. Allen and J.C. Blackford in Developments in Teracomputing, eds. W. Zwieflhofer and N. Kreitz, 2001, pp. 150-163, (World Scientific).

[7] A highly spatially resolved ecosystem model for the North West European Continental Shelf, J.I. Allen, J.C. Blackford, J.T. Holt, R. Proctor, M. Ashworth and J. Siddorn, SARSIA 86 (2001) pp. 423-440.

# CSAR User Survey 2002

**Claire Green**
**HPC Team, Manchester Computing, University of Manchester**

## Background

The CSAR User Survey held for 2002 took place between 22nd November and 13th December 2002. As in previous years, an online form made up of questions designed to encourage feedback on the various aspects of the service was made available for completion and submission via the CSAR website at http://www.csar.cfs.ac.uk/admin/forms.shtml

This time around the survey was publicised by two emails from Dr Neil Pratt of EPSRC, rather than by the usual emails issued by CSAR. Users were also given the opportunity to send their forms directly to Dr Pratt rather than to CSAR, although no one chose to do so. We received 59 completed forms, representing approximately 11% of all Class 1, 2 and 3 users, a figure much higher than that received for 2001 where only 24 users responded. Many new users took the opportunity to complete the survey, with 27% of the respondents having started using the CSAR service during 2002.

The results of the User Survey for 2002 are very similar to those for previous years. The full report is available for viewing online at http://www.csar.cfs.ac.uk/admin/reports/user_surveys/

Below are just some of our findings.

## Results

The aspect of the CSAR systems that users are most satisfied with is still service availability with 96% very or fairly satisfied. The aspect that users are the least satisfied with is turnaround times for jobs with 70% satisfied.

The survey highlighted that users are satisfied with the responses that they have received when dealing with the CSAR staff. Most of the users who indicated that they had used the various CSAR feedback mechanisms had done so by contacting the CSAR Helpdesk. The next most popular route proved to be the CSAR Managers, followed by the use of Service Quality Tokens. The level of satisfaction with the CSAR training services remained the same for 2002 as for the previous years – 100% of the users who responded that they had attended the CSAR training sessions had found them useful.

87% are satisfied with the information provided by CSAR to the user community. 87% of respondents also stated that they are happy with the applications software provided on the CSAR systems.

Overall 84% of users rated their view of the High Performance Computing facilities provided by CSAR in 2002 as "Very Good" or "Good". The remaining viewed the service as "Adequate", with no-one responding that it had been "Poor" or "Unacceptable".

## How your feedback helps us to improve the service we provide

User feedback is essential in helping us to improve the service that we provide. This year we noticed through analysing the responses to the User Survey that awareness of the Status Page - http://www.csar.cfs.ac.uk/using/status.shtml - was relatively low at 66%. To increase awareness of this page we now advertise its existence through our monthly bulletins and also through the advisory emails issued to new project PIs.

We provided "Comments" fields at the end of the various sections to encourage additional feedback. Several users made use of these sections to make excellent suggestions as to how we could improve the service, for example, the additional software that it would be useful to install on our systems. These suggestions are being considered and in some cases have already been implemented.

Thank you to all those of you who participated in the User Survey held for 2002. We will be holding another User Survey at the end of this year but in the meantime you can contact us at csar-advice@cfs.ac.uk if you have any problems or suggestions.

# Cray User Group Summit 2003

***Adrian Tate***
***HPC Team, Manchester Computing, University of Manchester***

The format of this year's CUG meeting deviated from that of previous years since SGI have decided to hold a separate user group meeting from 2003 onwards. This gave Cray the chance to give the new X1 machine centre stage for a whole week of presentations and discussions at the Hyatt on Capitol Square, Columbus. Another notable difference from last year's event was the enthusiasm and confidence that accompanied the meeting, with both Cray employees and CUG site representatives showing approval at the early performance of the X1. The enthusiasm is justified since the X1, Cray's first high-profile release since the T3E, has created $100million of income for Cray in just one quarter-year, with more large systems on the horizon. In fact, early in the week, Cray's corporate updates revealed that the next year's product targets have already been reached.

The US DoE's newly installed system at Oak Ridge National Laboratory was of particular interest, since the existing 32 processor system will undergo a series of upgrades, eventually making a 40 Teraflop system that will rival the Earth Simulator for the No.1 slot in the Top 500. Cray are also benefiting from the income and publicity gained from the ASCI Red-Storm project - a $90million project which will create a 40 TFlop/s AMD-chipped system for the US DoE. Cray's established systems such as the MTA and the SV1 were also discussed. MTA technology will form a crucial part of the upcoming Black Widow project.

Representatives from the SVE group at Manchester gave three presentations at the conference. Mike Pettipher discussed CSAR's innovative resource management system and procedures. Jon Gibson's work on finite element analysis codes on the Cray MTA was also presented by Mike Pettipher and Adrian Tate talked about SVE's new project to tune parallel numerical library routines for the X1 scientific library (see page 21 of this issue). All of the SVE talks were enthusiastically received by conference attendees, with many people personally expressing an interest, or posing questions throughout the conference.

The theme of the conference was 'Flight to Insight' which was given some context when Janet Bednarek gave an account of the history of aviation, to which Ohio has a very important role being the home of the Wright brothers. Orville Wright even made an appearance at the CUG night out. Another keynote talk was given by Jeffrey Harrow of the Harrow Group who gave an entertaining and atypical account of the development of technology. Paul Muzio and Richard Walsh gave a total life cycle cost comparison of a Cray X1 and commodity clusters. For a given application, with many factors taken into account, such as purchase cost, necessary support and likely sustained performance, the X1 came out slightly better than a Pentium 4 system.

Representatives of Los Alamos National Laboratory gave a half day tutorial on performance modelling of large applications. These models attempt to give, in advance, some understanding of what the performance of important applications will be on certain architectures. The model is achieved by considering a range of factors and by examining the performance of micro-kernels extracted from the application. Later in the week, these techniques were applied to the Earth Simulator.

Of the technical presentations, there were many important talks on features of X1 programming and optimisation such as an overview of CrayPat - Cray's optimisation tool, a tutorial on X1 optimisation techniques that advocated the use of SHMEM and Co-array Fortran over MPI, and a preview of what to expect in Fortran 2000, which detailed some interesting features such as the lack of constraints on allocatable array and derived type usage, and advanced C-Fortran interoperability. A number of talks gave overviews of the X1 technology's initial performance and reliability.

The most important feature of events such as CUG is to meet and exchange ideas with recognized experts in the field. The CUG social focus and the excellent facilities at the conference centre allowed this practice to flourish. The next CUG will be held at Knoxville, Tennessee, home to Oak Ridge National Laboratory and the new X1. Despite the imminent retirement of Turing, CSAR as part of the SVE group, will continue to play an active role in Cray User group meetings, not least since by the time of the next CUG there will be much to show in the X1 scientific library tuning project.

# SGI User Group

***Andrew Jones***
***HPC Team, Manchester Computing, University of Manchester***

The inaugural SGI User Group Conference was held from 11-13th June, at SGI's headquarters in Mountain View, California. This was the first gathering of SGI's major customers/users after the split of the former Cray/SGI User Group into Cray-only and SGI-only groups last year.

Terry Hewitt (University of Manchester), Andrew Jones (University of Manchester) and Paul White (CSC) attended on behalf of CfS and on behalf of their host institutions.

The week was packed full and included meetings, 2 half-day tutorials and 3 days of technical papers and presentations, many focusing on the new Altix product - in which CSAR is leading the way by introducing a 256 processor system this summer, (see page 4 for further details). Highlights of the technical program included a talk by SGI Chief Technology Officer, Eng Lim Goh, on the future of HPC under strong US Government funding, and how SGI will be a pivotal part of that future; the use of SGI HPC and visualization hardware to design for the America's Cup boat races; Grid activities involving SGI systems; and a talk by Gerhard Wellein from Erlangen in Germany comparing the performance of various state-of-the art processors - the Itanium2, as used in the Altix, winning many of the real user code tests, ahead of its main rivals such as the Power4 from IBM.

The social events (including a tour of the NASA Ames campus) were used to develop relationships with other supercomputing centres.

The organising committee for future User Group Conferences was formed, and includes all three CfS representatives, with Terry being accepted as the Deputy Chairman. The next conference (probably mid May 2004) will be held in Orlando, Florida.

Finally, one of the highlights for me was watching Terry's increasing frustration with the in-seat TV/video/computer on the Airbus flight to the US (economy class - honest!), culminating in him crashing the computer and having to beg the hostess to reboot it. The other 400 passengers managed just fine.

*For more information, see* ***http://www.sgi.com/events/tech_users/usergroup.html***

# *Stop Press:* Capability Computing at CSAR

Discounts for capability jobs are now available on the CSAR systems.

This has been agreed with the Research Councils to encourage greater scientific achievement.

Users are reminded that CSAR is deemed by the Research Councils to be a capability service and thus capability jobs are given priority wherever possible.

This is subject only to urgent work from others, agreed Advanced Reservation slots and over-usage of fair-share work whilst other work is waiting.

The discount rates are as follows:

| *System* | *No of Processors* | *Discount* |
|---|---|---|
| Newton | 192+ CPUs | 15% discount |
| Newton | 128+ CPUs | 10% discount |
| Green | 384+ CPUs | 15% discount |
| Green | 256+ CPUs | 10% discount |
| Turing | 512+ CPUs | 10% discount |

For further information please see:
http://www.csar.cfs.ac.uk/using/capability.shtml or email csar-advice@cfs.ac.uk


2002: MyGrid presentation by Dr Stephen Pickles and Dr Mike Jones

2002: Dr John Brooke broadcasts Molecular Dynamics from Manchester across the Access Grid

**SVE, who maintain the national CSAR facility as part of the CfS consortium, will be exhibiting for the 5th year at Supercomputing 2003. Visit us at booth 3215 in the European Village or join in events via the Access Grid.**


2002: Terry Hewitt and Dr Robin Pinning present RealityGrid on the SGI stand

2002: A hive of activity on the booth

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## CSAR Information

The CSAR Website - http://www.csar.cfs.ac.uk - contains help and information on all aspects of the service, including sections on Software, Training, Registration and Project Management and Accounting.

Additional information, particularly with regards to service developments and other events associated with the service, is also provided via a monthly bulletin issued by email to all users. An archive of these bulletins is available at http://www.csar.cfs.ac.uk/monthly_bulletin

CSAR Focus is published twice a year and is also available to view on the Web - http://www.csar.cfs.ac.uk/general/newsletter.shtml. To change your mailing address please email your new details to the CSAR Helpdesk.

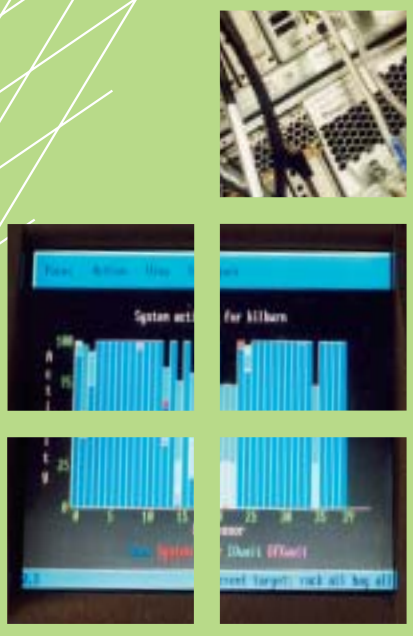
## Getting Help

If you require help on any aspect of using the CSAR service you can contact the CSAR Helpdesk team who will deal with your query promptly and efficiently. The contact details are as follows:

Telephone: 0161 275 5997 / 0161 275 6824

Email: csar-advice@cfs.ac.uk

The CSAR Helpdesk is open from 08:30 - 18:00 Monday to Friday, except on Public Holidays.



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