CSAR FOCUS

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high performance computing at Manchester ~ taking research into the future

CSAR & HPC(X): The Way Forward

Scalable Molecular Dynamics and CSAR

Multiphoton, Electron Collisions & BEC Consortium

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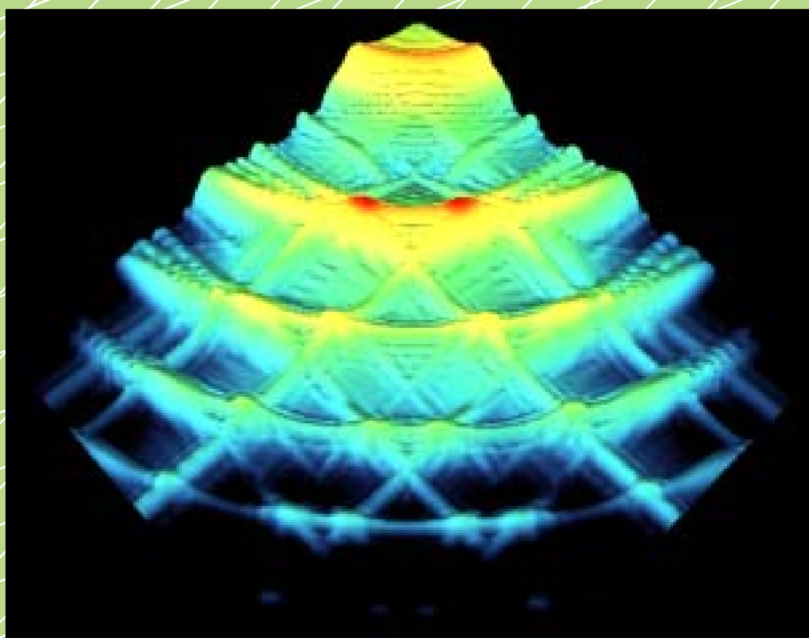

Quantum-mechanical state of helium prepared by a short intense laser pulse produced by the Multiphoton, Electron Collisions & BEC Consortium.

THE UNIVERSITY of MANCHESTER

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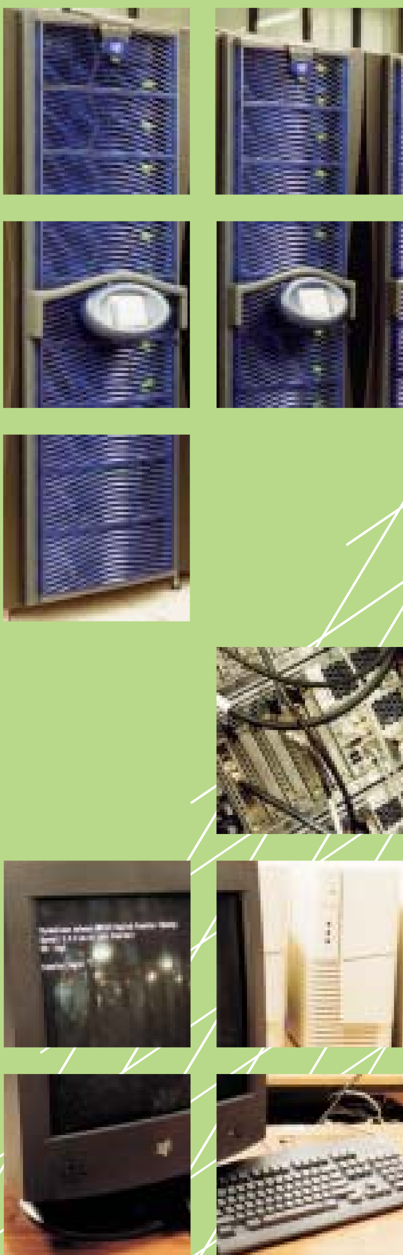

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Editorial Board

Claire Green, Andrew Jones, Mike Pettipher, Terry Hewitt.

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Editorial

This year has seen major developments in terms of the provision of High Performance Computing services for UK academia. The CSAR Service has introduced a new Origin 300 machine - Wren - which has 16 600MHz processors and will provide the the interactive system, enabling Fermat to be purely a batch engine. For details of the life of Wren the human, please turn to page 10. SAN (Storage Area Network) technology has been installed and we have replaced the NQE batch system on the Origin machines with LSF (Load Sharing Facility).

In addition, the new HPC(x) service, provided by a consortium led by the University of Edinburgh, with Daresbury Laboratory and IBM, started its life in December. Terry Hewitt provides an insight into how these two services will work together on the next page.

Please feel free to contact me should you have any comments or suggestions about CSAR Focus. The next issue will be produced in Summer 2003 - articles are very welcome and may be submitted at any time.

Claire Green
Editor, *CSAR Focus*

CSAR & HPC(X): The Way Forward

Terry Hewitt
Head of SVE, University of Manchester

First of all, we must offer our congratulations to Professor Richard Kenway (Edinburgh), Dr Martyn Guest (Daresbury) and Ms Caroline Isaac (IBM) and their teams for their recent success in being awarded the "HPCx" contract. They have passed the acceptance tests and are in full service.

It is good that UK Academia now has access to two world-class HPC services. But from the users' point of view this creates some questions: "Are they competing services?" "How do I choose which one to use?" The aim of this article is to try and shed some light on such questions.

Competing & Collaborating

I'm sure that I speak for both services when I say that our aim is to ensure that you the user can undertake your computational work in the most productive and supportive environment; and that the resources are used in some optimal way to achieve this goal. To help you in this, (as service providers) we must both compete and collaborate! We must compete to ensure we minimise the costs to the user (and thence the managing agents) and we must collaborate where that is beneficial to the user community. Of course, our service being based upon pay per use and the new HPCx service based upon fixed payments, means that it will be a challenge for both the services and EPSRC as managing agents.

However we are more used to collaborating and working together. We are all in a number of collaborative research projects, for example UKHEC which is providing support on high end computing topics to all UK HPC users, RealityGrid, one of the flagship EPSRC eScience projects; and the UK Grid Support Centre.

We are meeting early in 2003 to discuss how the services can better collaborate for the benefit of the users.

How Do You Choose Which Service To Use?

I save this difficult question to last. It is a truism to say many factors influence how well an application runs in a particular environment: and of course HPCx and CSAR offer different environments (as well as different costs!) At the moment the managing agents are reviewing the application process and it is inappropriate for me to say any more. Except that an element of the process is to find a way whereby each service provider gets a fair chance of demonstrating the advantages of their architectures for your science. So you might submit a code and some test case data and each service will provide you with a report detailing how well that application will run on various systems. That report will include details of scaling, single processor efficiency, weaknesses and bottlenecks. It may be that this report identifies resources required to undertake developments to over come bottlenecks or to improve scaling. Subsequently you apply to the appropriate research council for resources from one or more of the services based upon the information you receive in these reports.

Clearly notional costs (or tokens) as well as quality of service and support will be part of your decision making process. I am confident that the CSAR service will do extremely well in all categories. We are always available to discuss and support your new proposals and developments. As always, we are open to review and our web pages contain a wealth of information about our performance as a service. In addition there is material about support and development and some of our own research work. I'm sure you will find this useful in helping you assess which service to use.

I do not envy you in the task of such decisions!

In Conclusion

We (users, services, managing agents) must work together to ensure both services are fully utilised for the maximum benefit of "UK science". In a few years time you the user will need additional resources and the Research Councils and OST will need convincing of the scientific benefit of new investment. You the user will need to know that your codes can expand to fill additional capacity, that your scientific horizons can be achieved with such a facility. That the existing facilities are stretched to beyond their capacity is an important element of that case. The CSAR Service will continue to grow as you confirm the resources needed in your scientific reasearch through your grant applications.

Multiphoton, Electron Collisions and BEC HPC Consortium

Jonathan Parker, Karen Meharg, Daniel Dundas and Ken Taylor
Queen's University, Belfast

In the area of electron collisions, research is focussed on electron collisions with complex atoms, collision induced multiple ionization of helium and positron scattering using parallelised *R*-Matrix and other techniques. The remaining problems are all in the theory of matter-laser interactions: laser-driven helium, laser-driven molecular hydrogen (H_2), *R*-Matrix-Floquet, laser-heating of clusters and laser interactions with Bose-Einstein condensates. All of these efforts involve large-scale time-dependent integrations of quantum mechanical few-and-many-body problems, with the aim of viewing the basic physics of laser-matter interactions in unprecedented detail.

The Multiphoton, Electron Collisions and BEC HPC Consortium has developed a number of highly successful massively-parallel codes in recent years. The most mature of these is the Belfast group's Helium code, which solves the 6-dimensional time-dependent helium-laser Schrödinger equation in its full generality. Thanks to the availability of adequate HPC resources in the UK, the Helium code has enabled the Belfast group to publish the first quantatively accurate helium double ionization cross-section calculations, the first correct predictions of angular-correlation of ejected electrons in double-ionization and the first demonstration of double-electron above threshold ionization (DATI).

DATI is a non-perturbative process in which intense fields violently eject the helium electrons in highly correlated 2-electron wavepackets. It is a process in which all degrees of freedom available to the system are simultaneously exercised and in which all terms of the helium-laser Schrödinger Equation are simultaneously exercised. It is a process of such intrinsic complexity that an accurate theoretical description requires the full sophistication of the Helium code and at present the full power of massively parallel computers.

The figure shows a quantum-mechanical state of helium prepared by a short intense laser pulse. The axes are the absolute value of each electron's momentum (k_1, k_2), which scales asymptomatically as the square root of electron kinetic energy. The circular arcs, satisfying the constraint $k_1^2 + k_2^2$ = constant, represent two-electron wavepackets of constant total kinetic energy. The arcs are separated in energy by a photon's energy, which is the signature of above threshold ionization.

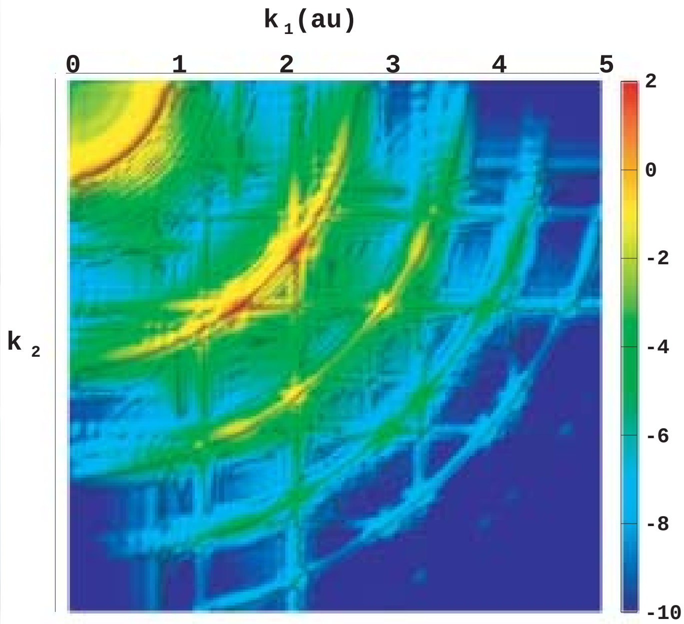

Figure 1 - Quantum-mechanical state of helium prepared by a short intense laser pulse.

Seamless Access to Multiple Datasets

K. J. Cole, M. A. S. Jones, S. M. Pickles, M. Riding, K. Roy, C. Russell, M.Sensier, W. T. Hewitt,
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The objective of SAMD is to integrate and streamline the access to data repositories and analysis engines in a social science context. We demonstrate this using Grid-based modifications to the current National Statistics (NS) Time Series Data interface operated by MIMAS.

Current access to time series in the National Statistics Time Series Data held by the MIMAS service at the University of Manchester is through a web interface (http://www.mimas.ac.uk/macro_econ/ons/), with username/password authentication. Once authenticated the user may search for and select various data series. The process involves several transfers of any selected datasets back and forward between server and client (the web browser) before analysis can even begin. The user is left with one or more files on her local disk, which is not necessarily the system on which subsequent analysis is to be performed. Although adequate for *ad hoc* enquiries, the present situation is not conducive to systematic cross-analysis of multiple datasets, nor to automation of queries that must be rerun periodically (for example, whenever a particular dataset changes) nor even to retrieval of very large datasets (there are faster protocols than HTTP).

SAMD offers a simple solution. It allows databanks to be searched and resulting series to be assembled into and used where required for files ready for analysis. Data files are transferred directly to the HPC engine of choice using GridFTP. The user's proxy credential is picked up by the application authentication in a single sign-on environment.

The demonstrator application transfers multiple time series from MIMAS (a JISC supported national data centre based at Manchester Computing) to an HPC engine for computationally intensive analysis, and then returns the results to the user. The entire operation requires only a single sign-on (grid-proxy-init) on the user's workstation.

With reference to Figure 1, in step 1, the application on the user's workstation searches for and requests one or more datasets via HTTPS with GSI authentication. In steps 2-3, CGI programs running on the web server verify that the user is privileged to access the requested dataset. In steps 4-7, the requested data is extracted from the MIMAS data repository and copied to a short-lived file, and an XML "ticket" is returned to the application.

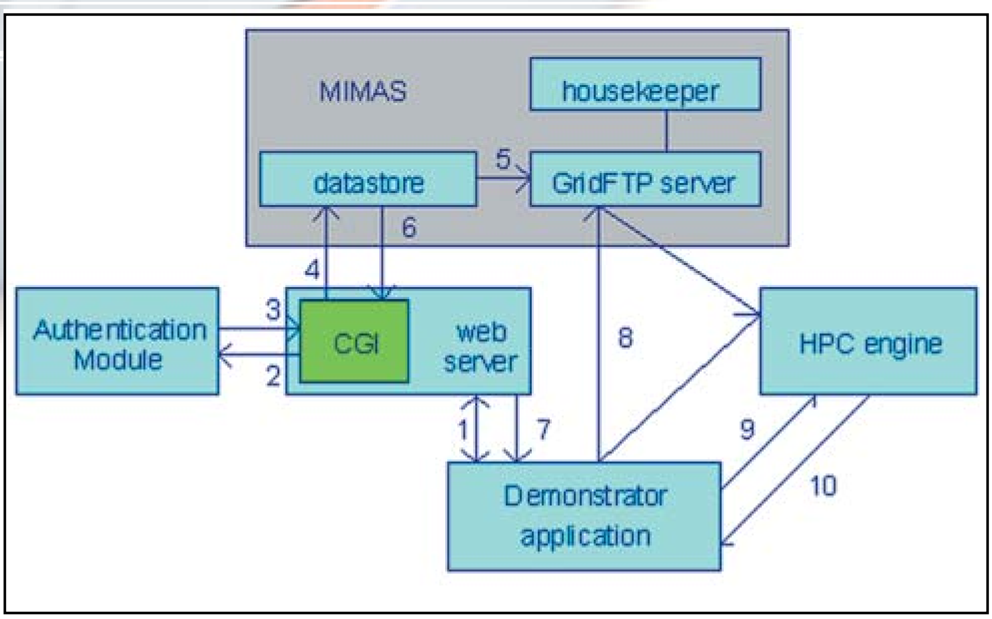

Figure 1: The SAMD Architecture

Actions performed in step 8 are based on information supplied in the ticket, the application uses GridFTP to initiate a third-party file transfer from MIMAS to the HPC engine. Steps 1-7 are repeated for each group of datasets. In steps 9 and 10, Globus mechanisms are used to launch an analysis run on the HPC engine and to retrieve the results. A housekeeping task cleans up temporary files.

User Interface

The user interface, shown in figure 2, has a number of features: "Certification" creates a proxy credential. "Data Acquisition" functionally recreates the current web-based interface to the NS datasets from within the demonstrator application. "Data Analysis" allows the user to search for and select a target HPC machine for the analysis stage, to locate an executable to perform the analysis, to launch the remote job, and to retrieve job status or results. The three list boxes at the bottom of the Data Acquisition panel (left-to-right) are used to show the time series that match the search criteria, select a subset of these, and transfer them to the HPC Engine.

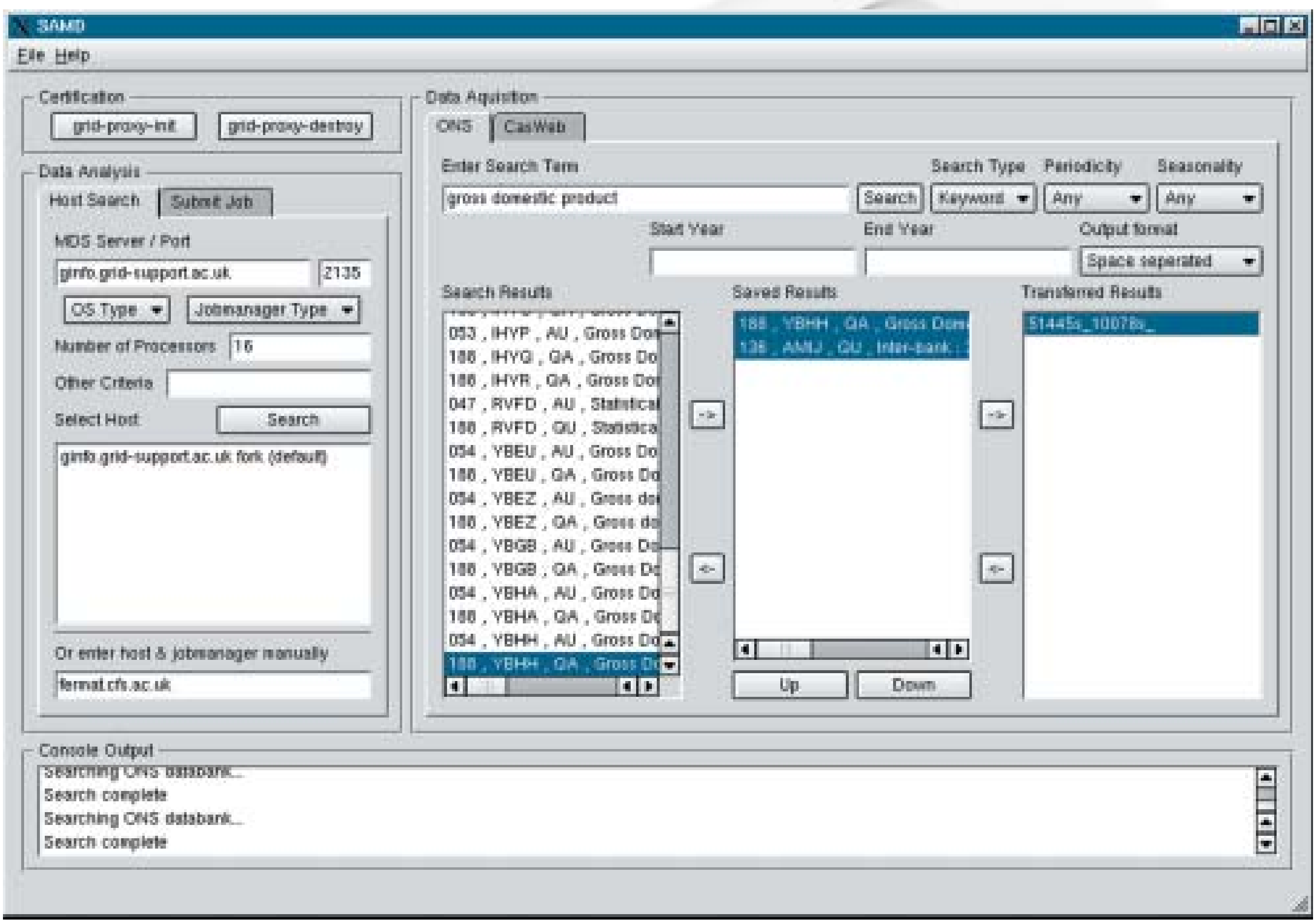

Figure 2 The Graphical User Interface

Computational Task

The demonstrator problem chosen for the SAMD project examines the asymmetric effects of interest rate changes on the UK's GDP. This is a substantive research question of genuine policy interest, and is based on data drawn from the National Statistics datasets hosted by MIMAS. The National Statistics Time Series Data (formerly the NS Databank) contains some 55,000 time series in 34 major datasets from the Office for National Statistics relating to economics, trade, employment and industry. A subset of time series related to interest rates and GDP is selected via the SAMD interface and then sent to an HPC engine on the Grid for analysis – an array of first difference of the logarithm of real GDP is compared to a series of arrays of earlier changes in interest rates. The results show that changes in interest rates have greater effecton output when past growth has been high than when past growth has been normal or negative, i.e. the effect of interest rate changes on GDP varies over the business cycle. A version of the analysis already existed as a Gauss program, taking 40 minutes to run to completion on a small dataset. We re-implemented the algorithm in Fortran 90, and then parallelised it using OpenMP directives. Converting to Fortran 90 improved the performance by a factor of 8 and we observe very good parallel efficiency.

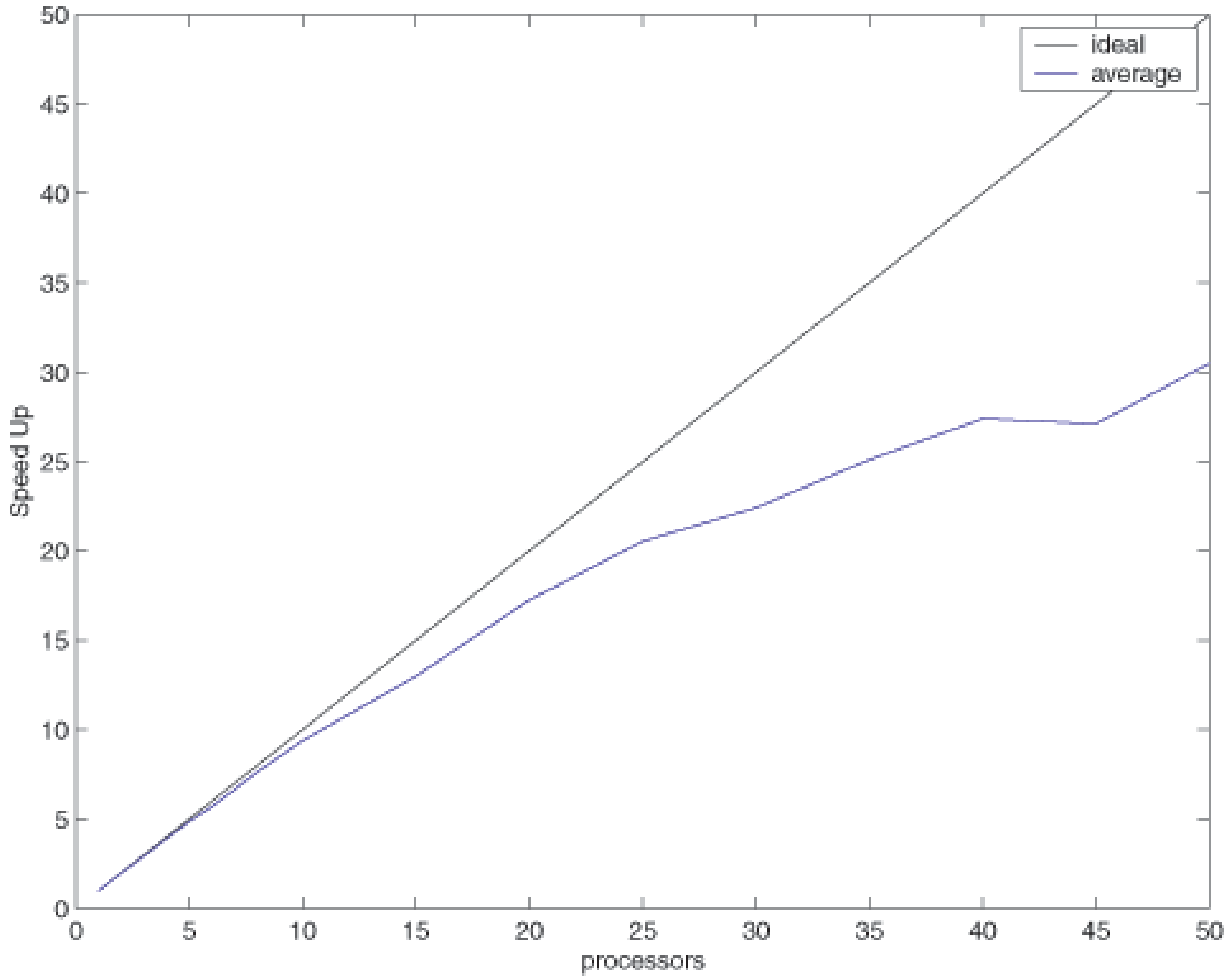

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Figure 3 Parallel Speedup on large processor counts

Authentication and Authorisation

The SAMD demonstrator application communicates with the web server using HTTPS, an approach that permits a high level of re-use of existing CGI code in the server. Authorisation is implemented by an addition to the original CGI scripts. We use standard Apache mechanisms for authentication but found it necessary to make modifications to the SSL module to handle proxy credentials.

Conclusion

SAMD demonstrates the successful incorporation of emerging Grid technologies into an existing social science data service. It shows how the integration of access to both data and computational resources within a single sign-on environment enables the automation of complex workflows, facilitating the scaling up of social science research applications. Finally, it shows how adding programmable interfaces (protocols) to existing services facilitates the development of third-party, value-adding client applications

The SAMD project funded by the ESRC and the DTI (DTI Ref: THBB/008/00082C).

Sir Christopher Wren (1632-1723)

Helen Heath
CSC

Our series of profiles of the mathmeticians who have lent their names to the CSAR systems continues with a look at the life of Christoper Wren - mathematician, astronomer, scientist and architect.

Although these days he is most widely known as an architect and designer, Sir Christopher Wren's career did not begin with training in these disciplines. Before the age of 17 he had invented an instrument that wrote in the dark, a pneumatic engine and a new deaf and dumb language. Among his first contributions to the world was the perfection of a working barometer. His talents were extraordinarily diverse.

Born in 1632 in East Knoyle, Wiltshire, to the Dean of Windsor and his wife, the young Christopher led a privileged early life, despite the death of his mother when he was very young, with the young Prince Charles being one of his playmates.

Figure 1: Portrait of Christopher Wren by Sir Geoffrey Kneller ©

Physically Christopher was a rather frail child who was quite small in stature. He loved drawing from a young age and he developed this markedly as he grew older. Science fascinated him; he showed a natural curiosity in everything around him and loved to conduct little experiments which he devised himself. Christopher had a private tutor during his early years, then when he was nine years old he was sent to Westminster School in London. This school was run by Dr Busby who was noted both for the exceptionally strict discipline he maintained and for his considerable ability which led to great success for many of his pupils. At this school Christopher quickly became proficient in Latin and this is shown by letters he wrote in Latin to his father which still survive.

The Wren family, obviously much favoured by the King, were staunch Royalists. This led to difficulties when, not long after Christopher began his schooling at Westminster, the English Civil War broke out between King and Parliament. Matthew Wren, who was by this time the Bishop of Ely, was imprisoned in the Tower of London for eighteen years. The deanery at Windsor was attacked and Christopher's father was forced to move out. At first he went to Bristol but, when Christopher was eleven years old his sister married William Holder and shortly after this Christopher Wren senior went to live in the rectory in Bletchingham, Oxfordshire, the home of his daughter and son-in-law. William Holder was a mathematician and was to have a very strong influence on Christopher who spent much time at Bletchingham. Holder essentially took on the role of mathematics tutor to Wren and also encouraged him to experiment with astronomy.

In 1646 Wren left Westminster school but he did not enter university immediately. During the next three years he built up a broad knowledge of science. He was employed as an assistant to Dr Charles Scarburgh, helping him with various anatomical experiments. Wren created pasteboard models to illustrate how muscles worked which Scarburgh used for demonstrations during his course of anatomy lectures. The work Wren carried out for Scarburgh was his first significant scientific contribution. After this, and still before entering university, Wren was recommended to William Oughtred, a leading mathematician of the time, as an appropriate person to translate into Latin his work on the mathematics of sundials.

Wren entered Wadham College, Oxford on 25 June 1649, received a B.A degree on 18 March 1651 and his M.A. from Oxford in 1653. He was elected a Fellow of All Souls, Oxford, in 1653 and lived in the College until 1657. At Oxford Wren carried out many scientific experiments. He worked on anatomy, making drawings of the human brain for Willis's Cerebri anatome. He devised a blood transfusion method which he demonstrated by transfusing blood from one dog to another. Perhaps what was most remarkable about the years Wren spent in Oxford was the breadth of his interests. His mind leapt from one topic to another as he came up with ideas such as: an instrument to measure angles, instruments for surveying, machines to lift water, ways to find longitude and distance at sea, military devices for defending cities, and means for fortifying ports.

In 1657 he became Professor of Astronomy at Gresham College, London. He had been making observations of the planet Saturn from around 1652 with the aim of explaining its appearance. His hypothesis was written up in De corpore saturni but before the work was published Huygens presented his theory of the rings of Saturn. Immediately Wren recognised this as a better hypothesis than his own and De corpore saturni was never published.

Wren was part of a scientific discussion group at Gresham College London that, in 1660, initiated formal weekly meetings. He undoubtedly played a major role in the early life of what would become the Royal Society, his great breadth of interests and his expertise in so many different subjects helping in the exchange of ideas between the various scientists. His lectures at Gresham also provided a focal point for meetings of the scientists prior to the formal inauguration of the Royal Society. In fact the report of the meeting at which the Royal Society was founded reads:-

"Memorandum November 28 1660. These persons following according to the usual custom of most of them, met together at Gresham College to hear Mr Wren's lecture, viz. The Lord Brouncker, Mr Boyle, Mr Bruce, Sir Robert Moray, Sir Paule Neile, Dr Wilkins, Dr Goddard, Dr Petty, Mr Ball, Mr Rooke, Mr Wren, Mr Hill. And after the lecture was ended they did according to the usual manner, withdraw for mutual converse."

In 1662 this body received its Royal Charter from Charles II and 'The Royal Society of London for the Promotion of Natural Knowledge' was formed. In addition to being a founder member of the Society, Wren was president of the Royal Society from 1680 to 1682.

Wren became Savilian Professor of Astronomy at Oxford in 1661 and held this post until 1673. It was after this appointment that he made his important contributions to mathematics. Isaac Newton, never one to give excessive praise to others, states in the Principia that he ranks Wren together with Wallis and Huygens as the leading mathematicians of the day.

Wren's fame in mathematics resulted from results he obtained in 1658. He found the length of an arc of the cycloid using an exhaustion proof based on dissections to reduce the problem to summing segments of chords of a circle which are in geometric progression. He was the first to resolve Kepler's Problem on cutting a semicircle in a given ratio by a line through a given point on its diameter. This problem had a basis in astronomy for it had arisen in Kepler's work on elliptical orbits. Kepler reduced finding the mean motion of a planet to that of cutting an ellipse in a given ratio with a line through a focus. In addition to solving Kepler's Problem, Wren independently proved Kepler's third law and, as we noted above, formulated the inverse-square law of gravitational attraction.

Another topic to which Wren contributed was optics. He published a description of a machine to create perspective drawings and he discussed the grinding of conical lenses and mirrors. Out of this work came another of Wren's important mathematical results, namely that the hyperboloid of revolution is a ruled surface. These results were published in 1669. Work on the logarithmic spiral, which had been rectified by Wallis in the late 1650s, led Wren to note that it was possible to consider an area preserving transformation which would transform a cone into a solid logarithmic spiral. This, he remarked, resembled snail shapes and sea shell shapes, ideas which D'Arcy Thompson was to examine 250 years later.

It is not quite clear where Wren's interest in architecture first arose; certainly he read On Architecture by Vitruvius, written in the first century BC, while he was a student in Oxford. In 1661 he was invited to work on the fortifications of the harbour at Tangiers and, although he turned down this request, it is interesting to realise that even at the age of 29 Wren was considered someone who might take on a major architectural project. In 1663 Wren visited Rome where he made a thorough study of the Theatre of Marcellus, examining both the ruins of the theatre and drawings that showed its original form. This was important in Wren's development as an architect and the influence of the Theatre of Marcellus is clearly evident in his early designs. A visit to Paris in 1665 was also influential, particularly the impression that the church of the Sorbonne and the church of Les Invalides made on him.

In 1663 he designed the chapel at Pembroke College, Cambridge, commissioned by his uncle the Bishop of Ely. In the same year he submitted a model of his design of the Sheldonian Theatre, Oxford, to the Royal Society. This project, with its construction beginning in 1664, was the first of his projects to include the design of a dome.

In 1668 building work began on Wren's designs for the Emmanuel College Chapel, Cambridge and the Garden Quadrangle, Trinity College, Oxford.

Wren's greatest opportunity in architecture came with the rebuilding that followed the fire of London of 1666. Appointed Commissioner for Rebuilding the City of London in that year he carried out a survey of the area destroyed by the fire with the help of three surveyors. Wren replanned the entire city and supervised the rebuilding of 51 churches.

It is worth noting that despite the remarkable number of designs Wren was working on at this time, he still held the Savilian Chair of Astronomy at Oxford. Clearly his love of the academic world made him reluctant to cut his links with it despite his position by this time of Britain's leading architect.

In 1669 Wren was appointed as Surveyor of St Paul's Cathedral. He had been involved in repairs of the old cathedral in 1663 and he was a natural choice to take over this role when, in 1669, he was appointed Surveyor-General of the King's Works.

Wren is best known today as the architect for St Paul's Cathedral. His first design for the new cathedral was rejected by London City Council as not sufficiently grand and Wren produced a second plan together with a model in 1674. This second plan was based on a Greek design which was rejected by the clergy as not in keeping with the proper form of a Christian church. Wren, despite his great disappointment at the reaction to his plans for St Paul's, set to work again and produced a third design based on a Latin Cross with a large dome.

Figure 2: Wren's design for St. Paul's Cathedral

This third design would form the basis for the plans for the Cathedral that stands today but Wren modified them as the work progressed over a period of 35 years. As Wren was already 43 years old when the project began, he might not have been expected to live to see its completion. However, he lived to the age of 90, and St Paul's Cathedral was completed 12 years before his death.

In 1675, the year in which Wren's plans for St Paul's were accepted, he received a commission from Charles II to build a Royal Observatory for Flamsteed who had been appointed as Astronomer Royal in that year. As is so often the case the King was short of money so Wren had to design a building to be constructed 'on the cheap'. Of course Charles II was not having an observatory built to push forward scientific research, rather he wanted a solution to the longitude problem which would give England a huge advantage over its competitors as a sea-faring nation.

Christopher Wren died after catching a chill while travelling to his London home in February 1723 and was buried in St Paul's Cathedral on 5 March under the south aisle of the choir at the east end. Fittingly, he was the first person to be buried at St. Paul's.

I am indebted to a biographical article on Sir Christopher Wren published by the School of Mathematics and Science, University of St.Andrew's, Scotland for most of the information in this article. The rest has come from a variety of sources, including the online BBC History – Society and Culture web page with their biographical overview of Sir Christopher Wren. This may be accessed at: http://www.bbc.co.uk/history/society_culture/art/wren_christopher.shtml

CSAR on the Grid

John Brooke
Manchester Computing, University of Manchester

Realism and Opportunities

It is interesting for me to reflect on two very hectic and exciting years since I became the leader of the Special Projects research team at Manchester and worked in conjunction with my colleagues in the CSAR service and MVC to establish eScience and Grid Computing as a part of the service that we offer to UK High End Computing. From the beginning of the CSAR service we were interested in the possibilities offered by metacomputing, the linking together of computational facilities to provide more than could be gained from a single machine alone. The CSAR service right from its inception had a heterogeneous and differentiated architecture, with an Origin2000 coupled to a T3E. We were therefore interested in the work of other major European and US sites that were involved in metacomputing, such as HLRS Stuttgart, Pittsburgh Supercomputing Centre (PSC) and the Centre for Scientific Computing in Finland.

These contacts proved very fruitful and within two years of the start of the service we had been involved in the prize-winning collaboration in the HPC Games competition at SC99 and were members of the first large scale European Grid project, EUROGRID [1], which specifically concerned itself with linking large centres of computational excellence providing environments for complex problem solving in a variety of areas, molecular biology, meteorology, coupled models in engineering and also provided enabling technology for a European HPC Grid.

Through these contacts we became aware of the intense interest world-wide around the concept of Grid computing. Unfortunately this was a hazy concept, sometime advertised (at that time) as providing cheap, ubiquitous "computing power" on demand and without the user needing to concern him/herself with the origin of such power. The analogy was with the electrical Grid, since then events in the electricity supply industry itself have indicated that even with electrical power things are not that simple, witness the problems faced by the State of California and the Enron crisis. However it was clear that, despite the vagueness of this conception, integrative work of immense value was taking place in large-scale computing. It is greatly to the credit of the Globus project that in the midst of this they produced two very far-reaching research papers, "The Anatomy of the Grid" and "The Physiology of the Grid" [2] that clarified the basis for the developing architecture of persistent distributed collaborations. We were also aware, through EUROGRID, of the work that had gone into the development of the concept of seamless access to complex resources that forms the heart of various projects based around UNICORE [3].

At this time also, the UK eScience programme was initiated by John Taylor the Director-General of the Research Councils and Tony Hey was seconded from the University of Southampton to direct the eScience core programme. We found ourselves working with colleagues at EPCC and CLRC (Daresbury and RAL) to construct a fledgling UK Grid based using Globus. This programme also looked beyond the easy publicity associated with all things Grid, to identify what was the nature of the challenges posed by the integration of computational resources, experimental apparatus and data management and curation. A particular issue identified by the UK was the focus on the data and knowledge levels of the Grid. How does one provide infrastructure for large scale scientific collaboration, how does one ensure that differing data storage formats are made interoperable and what is the computational infrastructure required to support such large scale and persistent collaborations of research groups? These were severe and challenging problems, but because they were identified clearly they offered the prospects of real scientific progress that the vague concepts of a free ubiquitous "power grid" did not. There are now 10 active eScience Centres building the UK Grid, with others constructing regional Grids and a number of projects based on scientific applications throughout the range of disciplines covered by the UK Research Councils.

Current Opportunities for CSAR Users

In the previous section I have tried to show how groups in the UK are combining to form and define what a Grid infrastructure could be and how it could benefit UK science. At CSAR we have a particular focus on the very high-end of the Grid and we regard complexity and problems of scale as part of our particular problem domain. There is a large amount of Grid infrastructure work that is of great importance but does not touch these issues. Thus one can build Grids of clusters of workstations or PCs with a uniform architecture and operating system. This is done in the EU DataGrid project and is clearly the best choice for the problem of handling huge amounts of experimental data. High performance computing centres, however, are not dominated by clusters, they have highly differentiated and specialised architectures and for very good reasons. This has shaped our strategy in terms of project involvement and planning for services.

We are happy to announce that after several years of intensive effort we can now offer CSAR users what we consider to be production level Grid services on our major facilities. These are:

1. The UK eScience Grid links together the 10 eScience Centres all of whom are donating resource to initiate a persistent UK Grid. CSAR is pleased to report that our major resources Turing, Green, Fermat and Wren are enabled to participate in this Grid and have up-to-date and working deployment of Globus as recommended by the UK Grid Support Centre [6]. We have created an experimental project for those wishing to test their application in a Grid context, hopefully involving the participation of other resources at different sites. We are also part of the UK Grid Support Centre along with colleagues at CLRC and EPCC and provide input to the UK Engineering Task Force.

2. The UNICORE service based on the development of middleware to make submission of complex jobs easy for users and independent as much as possible of details of the underlying architectures utilised to run the jobs. It can be thought of as a means of composing complex workflows for solving problems on HPC systems. This allows users the possibilities of conducting experiments across a European High in Performance Grid. A demonstration of the potential scientific benefits of such an approach was given at the recent UK All-Hands Meeting Sheffield (September 2-4 2002) through a collaboration between members of the UK RealityGrid project and the EU EUROGRID project. The application demonstrated was a Lattice-Boltzmann simulation of mixing in two-phase liquids, where the simulation was run on one supercomputer, the visualization modules ran on another and the whole calculation was steered from a laptop on the conference floor with the user having the ability to change parameters and steer the calculation dynamically whilst directly visualizing the changes in the mixing properties of the two-phase fluid and seeing how this responded to the parameter changes. The whole steering was controlled within the framework of the proposed Open Grid Services Architecture [4] and is based on the first working demonstration of a scientific service based on OGSA devloped by Dave Snelling of Fujitsu Laboratories Europe as part of the EU-funded Grid Interoperability Project (GRIP [5]).

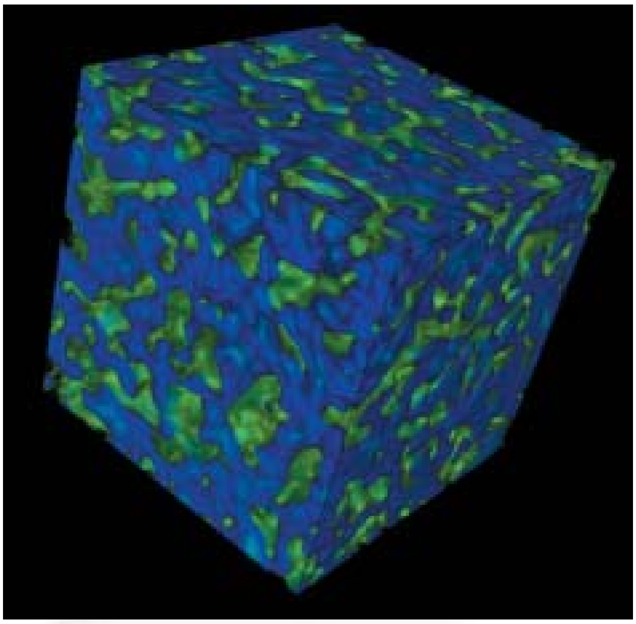

Figure 1: A visualization of data from the early stages of a Lattice-Boltzmann simulation of the phase-separation of an oil/water emulsion on a 256-cubed lattice.

To find out more about these services please contact me via the CSAR Helpdesk. Recently, we demonstrated our Grid technology at Supercomputing 2002, with an enhanced RealityGrid demonstration and demonstrations of metacomputing between world-wide resources to solve problems beyond the limits of a single machine. Some of these demonstrations were shown over the AccessGrid [6].

This is another area where we have successfully pioneered a new service for collaboration, details of this were given in the CSAR Focus December 2001 edition where we described how we organised and presented the UK SCGlobal Constellation Site programme. Our commercial partners in CfS, CSC and SGI very generously donated resources on the CSAR service and facilities at SC2002 which enabled us to provide demonstations comparable in quality and ambition with those being provided by the best centres of High Performance computation in the US, Europe and Asia-Pacific. This work was shown at many locations at SC2002 [7], on our own stand, on the UK eScience stand, the SGI stand, the EUROGRID/GRIP stand and on the stands of our metacomputing partners, such as HLRS Stuttgart, PSC and JAERI and AIST (Japan).

Future Challenges, the Economy of the Grid

As several people (including us) have pointed out, putting resources onto the Grid does not thereby make them free. At present the Grids with which we are working, the UK eScience Grid and EUROGRID have resources donated to them by participants, this generosity cannot survive large scale production use. It is here that the CSAR tokens economy and our experience of it have proved very valuable in helping us to develop proposals for how resources might be traded and exchanged on the Grid. We have been active with our partners in CfS and other UK sites which manage resources for HPC to create a proposal for a Grid Economy that can facilitate the sharing of resources across organisations (the remit is actually wider than this). This project is led by Professor John Darlington of the London eScience Centre and the eScience programme has recently indicated that it will fund the project and it will hold a workshop to publicise the idea and possibility of such exchange. We will work to make this project a success. It will give the UK a lead in this field and will lay the basis for large scale co-operative computing to maximise the UK resources and to provide UK researchers to resources on a global scale.

We are also working to enable significant codes to utilise such a metacomputing network and will report on this in future issues of CSAR Focus. Our experience confirms that the technical problems of metacomputing can be solved even in demanding environments with machines protected via firewall policies. In particular, PACX-MPI [8] developed by HLRS Stuttgart (partners in our global metacomputing work) has proved itself to be very able to operate in such conditions and we hope to be able to exploit the improved network connectivity of SuperJanet and GEANT. We welcome enquiries from CSAR users who wish to try metacomputing and especially who are interested in collaboration with colleagues who have resources on machines in the UK or outside.

Thus we are able to evaluate Grid middleware from a variety of projects and we are making it available to CSAR users. This will allow our users the ability to make informed judgements about the suitablility of such middleware and will enable them to be able to discriminate among the many claims being made for Grid computing. For our part, we are convinced that the Grid can bring many advantages to users of HPC facilities and look forward to working with you to demonstrate such benefits. The Grid is not the magic solution some people have seemed to claim, more it is a powerful tool which in the right circumstances can bring great benefits to computationally based scientific research.

References

[1] EUROGRID http://www.eurogrid.org
[2] Globus Project http://www.globus.org
[3] UNICORE http://www.unicore.org
[4] Open Grid Services Architecture (OGSA) http://www.globus.org/ogsa
[5] Grid Interoperability Project (GRIP) http://www.grid-interoperability.org
[6] UK Grid Support Centre (GSC) http://www.grid-support.ac.uk
[7] SC2002, Supercomputing Conference http://www.sc2002.org
[8] PACX-MPI, mpi library for metacomputing http://www.hlrs.de/organization/pds/projects/pacx-mpi/

Globus and Unicore are available on the CSAR systems. If you would like to use either of these please do not hesitate to contact CSAR.

Global Climate Visualization for the Hadley Centre

Paul G. Lever
Manchester Visualization Centre, Manchester Computing

The Manchester Visualization Centre has for the past four years been working with the Hadley Centre for Climate Modelling to undertake all their requirements for visualization and computer animation. The Hadley Centre, a division of the UK Meteorological Office, undertakes studies of the global climate using similar, though more extensive, models of the global biosphere as are used by the rest of the Meteorological Office for the prediction of weather conditions. The Hadley Centre's interest is in the long-term prediction of the results of natural effects and human activity on the future evolution of the global climate.

The models used by the Hadley Centre are based on data gathered from the large number of weather stations which have been in place, world-wide, for close to a hundred years and they produce enormous amounts of predicted data which can only be interpreted through the use of visualization techniques. Their predictive simulations are based on HadCM3 (Hadley Climate Model version 3). They have turned to the Manchester Visualization Centre to provide state of the art visualization techniques both for general research work and for use in publicity materials.

The initial phase of the work was to develop a series of data visualizations, supplied as MPEG2 and on video, to be used at the CoP4 (Conference of the Parties to the UN Framework Convention on Climate Change) conference on global warming held in Buenos Aires and attended by representatives of the majority of the world's major governments. These visualizations were demonstrated to the visitors at the conference and were also used at a presentation to Mr. Michael Meacher MP, Minister for the Environment, before the conference. The videos produced were also supplied to news gathering agencies at that presentation and used by both BBC news and Channel 4 news on their evening news broadcasts. Since that conference our work has continued with further productions for the CoP5, CoP6 and CoP7 conferences. In addition MVC also contributed modified visualizations for an episode of the BBC series, "Correspondents".

Throughout the production of material for the Hadley Centre, MVC has strived to enhance the quantity, quality and diversity of the visualization techniques and the video production procedures. MVC has worked closely with the Hadley Centre to develop new visualization techniques and new representations of the data in order to help to make the disturbing conclusions which scientists are drawing from their models clear to the world's leaders. Each year the Hadley Centre has focused on a number of themes, including:

- The global average temperature rise
- Effects on sea-level rise due to gradual warming of the deep ocean
- Severity of El Nino and subsequent climate changes
- Breakdown of the Gulf Stream, due to deep ocean warming and desalination due to the melting of the ice caps and its effect on the UK
- Reduction in size of the polar ice-caps
- Impact on regional climate e.g., cyclones in the Mozambique Channel and the Bay of Bengal and subsequent flooding
- Decimation of South American rainforests and vegetation

As the complexity of the visualizations has increased along with the production quality, the demands on resources have significantly increased. From the initial set of animations which required 400MB of disk storage for the MPEG-2 animations, the most recent set of animations required a storage capacity of 58GB for all the individual frames, movie clips, titles and final digital movies in both uncompressed AVI and MPEG-4. This is mostly the result of increased animation quality, where the visual clarity has been improved through the use of anti-aliasing steps and multi-image composition for titles, labels and visualizations.

Background

The Intergovernmental Panel on Climate Change (IPCC) has published projections of future emissions in their Special Report on Emissions Scenarios (SRES). The basis for these scenarios is a number of 'storylines' describing the way in which the world will develop over the coming century. Assumptions are made about the future including greater prosperity and increased technology. The levels of greenhouse gas emissions are generally less than previous IPCC scenarios, especially towards the end of the 21st century. The emissions of sulphur dioxide, which produce sulphate aerosols that have a cooling effect on climate, are substantially less.

The SRES scenarios are based on recent projections of global population and span a range of potential economic futures. There are four families of scenarios:

Quoted from UK Met Office Web Site:

"The A1 family describes a world with rapid economic growth during the 21st century and a substantial reduction in the regional variations of income per head. Global population rises during the first half of the century, peaks mid-century, then declines. New and efficient technology is rapidly introduced. The A1FI scenario sees the continuation of fossil fuels as the main energy source.

The B1 family describes a world with the same population growth as the A1 family. There are rapid changes in economic activity away from production towards a service economy. Clean and efficient technologies are introduced. Like A1, this storyline describes a convergent world.

The A2 family describes a world that remains heterogeneous with regional identity being preserved and lower income growth per head. Global population rises continuously throughout the century. The introduction of new and efficient technology is less rapid than the other scenarios.

The B2 family describes a world with population increasing throughout the 21st century, but at a lower rate than A2. Levels of economic growth and technological development are less than those of A1 and B1."

Predictions of climate change were made for the A2, B2 and A1FI scenarios using the HadCM3 model to simulate the response of atmospheric concentrations of greenhouse gases and sulphur. The greenhouse-gas concentrations were calculated from the SRES emissions using separate computer models. The sulphur emissions were converted to concentrations of sulphate aerosol particles concentrations within the climate model itself.

Between the present day and the end of the 21st century, the Hadley Centre predict a warming of over 4C for the A1FI scenario; 3.5C for the A2 scenario; 2C for the B2 scenario. From additional calculations warming of just under 2C is predicted for the B1 scenario.

Results

Figure 1 shows changes in global temperature for four SRES (Special Report on Emissions Scenarios) emissions scenarios, known as A1Fi, A2, B1 and B2. The A1Fi scenario in Figure 1(a) shows the simulation starting state with recorded data. Figures 1(b), 1(c) and 1(d) show the unmitigated emissions of pollutants of A1Fi against the other scenarios, the result of which can be seen clearly in 2100 when some areas have risen by more than 12'deg'C. The B1 scenario shows a lesser effect, where emissions have been reduced significantly.

The results for the scenarios show that surface warming is expected over most of the globe, with the largest increase at high northern latitudes. The melting sea ice causes less sunlight to be reflected and more to be absorbed at the surface leading to large warming of the region. The patterns of temperature rise also show a sharp contrast between land and sea, where the land is warming approiximately 80% faster.

Figure 2 shows the effect of pollutant emissions on the Arctic Ice Cap. The size of the ice cap is normally at its greatest in March and at its lowest in September. Figure 2 shows results for two scenarios, A1Fi and B1 for the years 1960 and 2100. As can be seen by 2100 the September ice-cap has all but disappeared and the March ice-cap is considerably smaller. Consequences of this are rising sea-levels and desalinization of the oceans, which in turn effects currents e.g., Gulf Stream.

The HadCM3 simulations predict that the extent and thickness of northern hemisphere sea ice will decrease as temperature increases. By the end of the 21st century the area of sea ice coverage is predicted to fall to around 55% for A1Fi scenario.

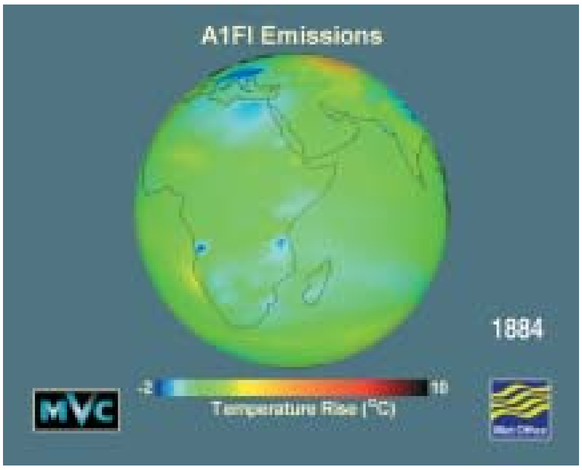

Figure 1(a)
The simulation starting state

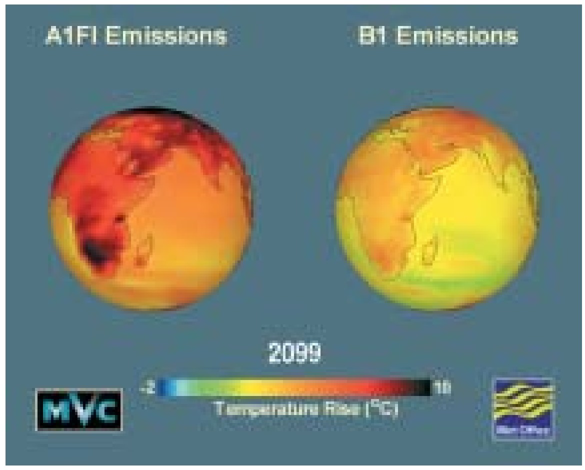

Figure 1(b)
Unmitigated emissions of pollutants of A1Fi against the B1 scenario

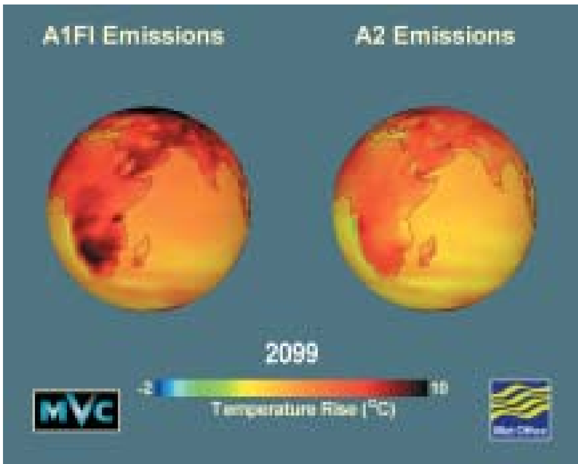

Figure 1(c)
Unmitigated emissions of pollutants of A1Fi against the A2 scenario

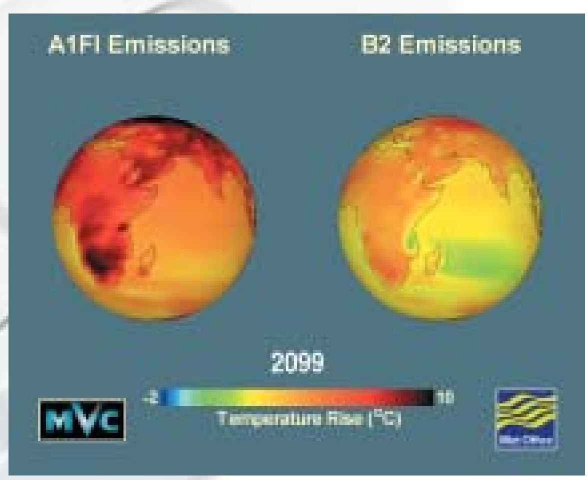

Figure 1(d)
Unmitigated emissions of pollutants of A1Fi against the B2 scenario

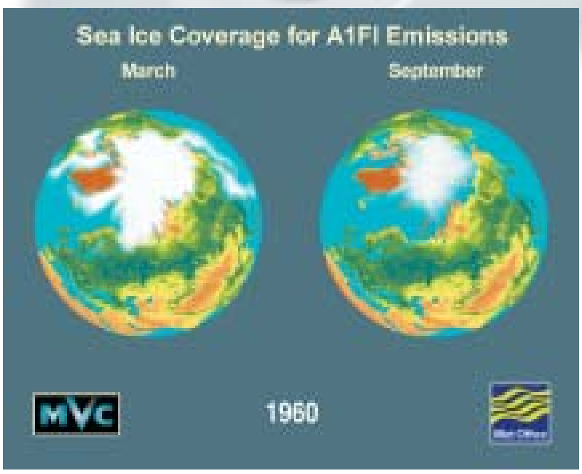

Figure 2(a)
A1Fi scenario - 1960

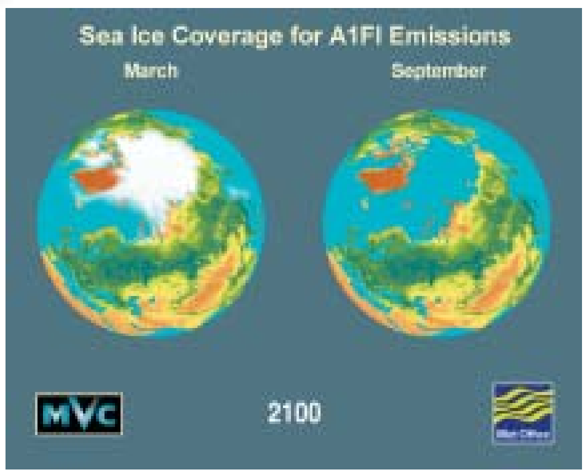

Figure 2(b)
A1Fi scenario - 2100

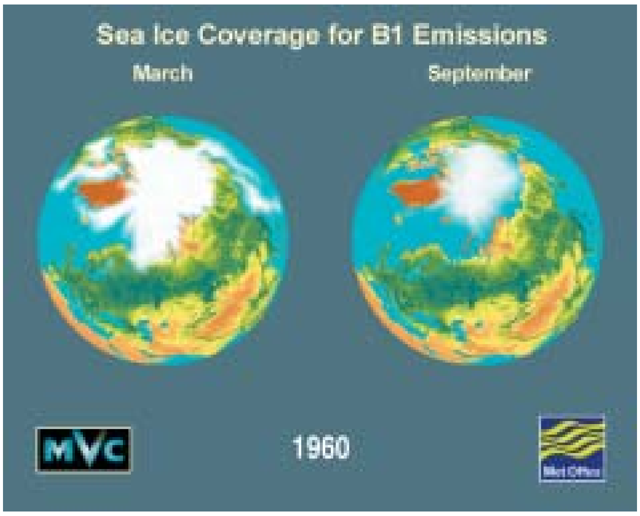

Figure 2(c)
B1 scenario - 1960

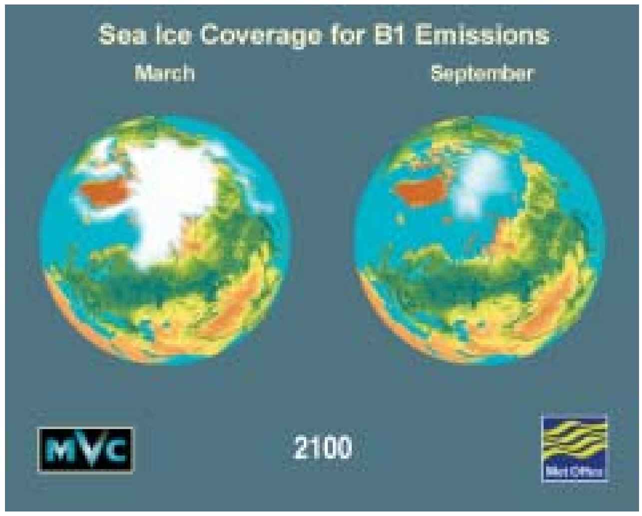

Figure2(d)
B1 scenario - 2100

Figure 3 shows the effect of global warming and human deforestation programmes on the rainforests on South America. The glyph based visualization shows the change in levels of various vegetation that is predicted to occur from the initial starting data of 1860. As shown the rainforest density is radically different by the year 2100.

Figure 3(a)
Levels of vegetation - 1860

Figure 3(b)
Levels of vegetation - 2100

Figures 4 and 5 show a comparison of two models, GCM and RCM. The Global Climate Model (GCM) is of much smaller resolution than the Regional Climate Model (RCM). In this visualization of a cyclone in the Mozambique Channel, it is clearly seen that the GCM does not effectively simulate the cyclone.

Figure 4 shows the wind magnitude and direction for both models from two examples of the various time-steps produced.

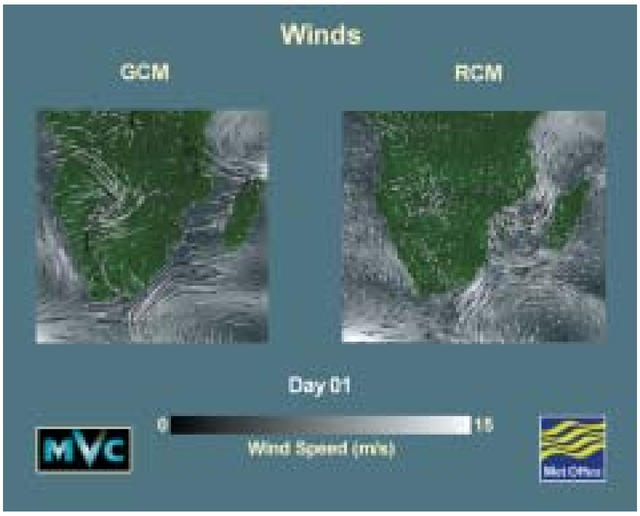

Figure 4 (a)
Wind magnitude/direction - day 1

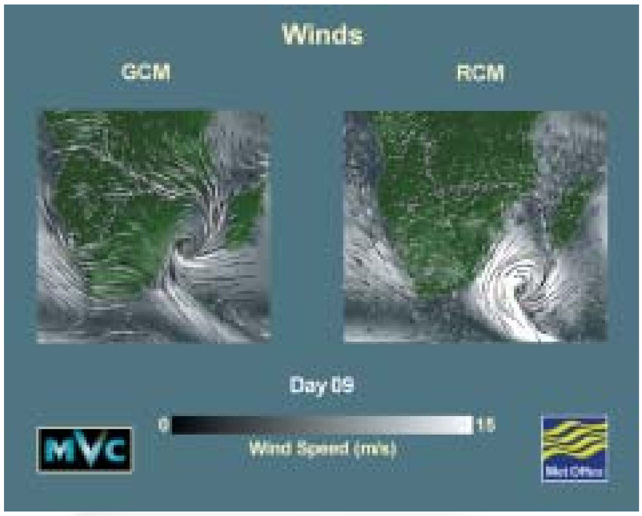

Figure 4 (b)
Wind magnitude/direction - day 9

Figure 5 shows the sea-level-pressure and precipitation for the same simulation, again only two examples have been included.

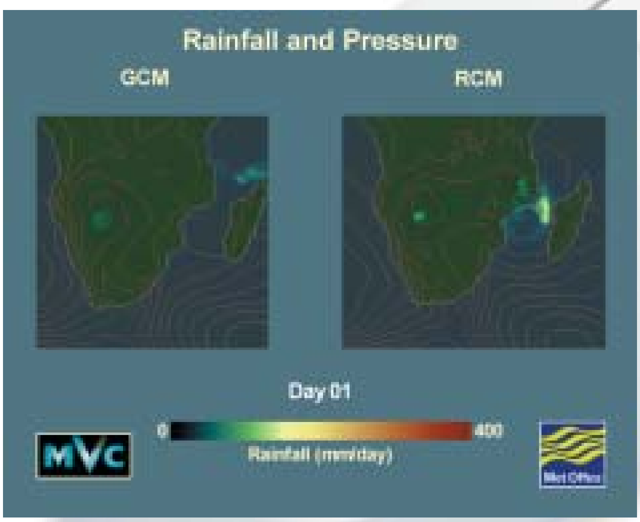

Figure 5 (a)
Sea-level pressure and precipitation - day 1

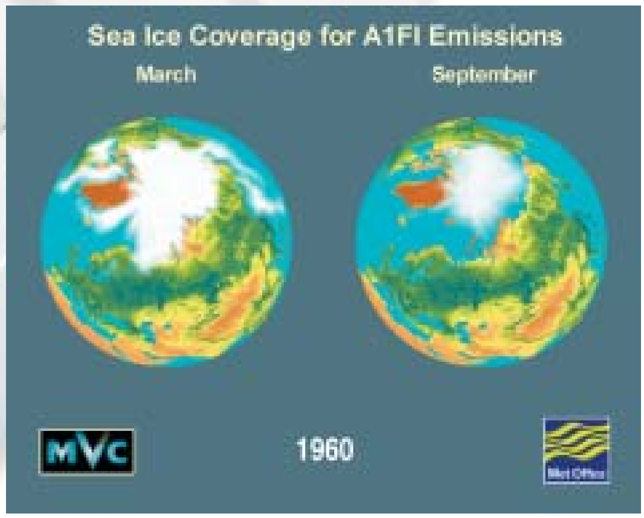

Figure 5 (b)
Sea-level pressure and precipitation - day 9

As can be clearly seen, the higher resolution model (RCM) produces more effective results and will enable the Met Office to conduct more precise predictions in the future, when higher resolution simulations can be used for global rather than regional climate prediction.

In conclusion, the animations produced have proved effective tools for the Hadley Centre to dramatically demonstrate what the future may hold should the governments of this world not take heed of the warnings already evident. The animations have been well received at conferences and have led to the U.K. adopting the proposal to reduce emissions levels to the lowest recommended.

If you would like to know how visualization can help you in your work, please contact the CSAR Helpdesk.

Bringing Scalable Molecular Dynamics to the CSAR Community

Neil Stringfellow
HPC Team, Manchester Computing, University of Manchester

Molecular dynamics (MD) is a computational method which calculates the time dependent behaviour of a molecular system. These systems can be of varying sizes from a few hundred atoms up to large scale systems using tens or hundreds of thousands of atoms, and the time scales for which results are required can be from a few picoseconds (10^{-12} s) to nanoseconds (10^{-9} s) and beyond.

There are several MD codes available on the CSAR systems such as DL_POLY, but the standard package for molecular dynamics simulations involving biological systems which is provided on the CSAR systems is Amber and the latest version of Amber which we have installed is Amber 7.

Amber is implemented using a replicated data model and this produces good performance and allows scalability up to around 16 or 32 processors. However, for large molecular systems which require the memory and computational power of more processors, Amber is limited in its scope.

With the expansion in computing power which has taken place in the last decade, several groups of computational scientists have looked at ways of designing new codes which can solve large problems and are scalable to large numbers of processors. In order to appeal to the wider biological molecular simulation community, these codes have been developed to use many features of some of the older popular codes.

Two new codes from the United States have been provided on the CSAR Origin machines, LAMMPS which was developed by a consortium headed by Sandia National Laboratories and NAMD which was developed at the University of Illinois. The standard input files to these codes consists of Protein Data Bank files and in addition both codes are able to provide compatibility with some Amber input files. The two codes are able to implement the Amber force field, and in addition NAMD can implement the CHARMM and Gromacs force fields and can read the files produced by the related codes.

Testing of the LAMMPS and NAMD codes has shown that they can scale very well, and in the case of NAMD this has been up to the full 512 processor capacity of Green. The scalability of these codes also applies to the number of atoms involved in the simulation and for NAMD tests were carried out on a variety of systems including one of over 300,000 atoms. Timings produced by inputs to NAMD have shown that 1 nanosecond (a million femtosecond steps) of simulation of a 92,000 atom system can be performed in about one and a half days real time, using 256 CPUs on Green. This brings real, large scale simulation of biological molecules within the grasp of the CSAR user community.

For more information about accessing these packages see the CSAR website ~ http://www.csar.cfs.ac.uk/software ~ or contact the CSAR Helpdesk.

Acknowledgements: Professor Peter Coveney, Queen Mary, University of London.

Unified Model

Zoe Chaplin
HPC Team, Mancheseter Computing, University of Manchester

The ongoing collaboration between CSAR and the Met Office has resulted in a copy of the latest version of the Unified Model (UM), version 5.3. This replaces the previous version, 4.5 and represents a complete rewrite for much of the code. It has been in development for approximately 10 years and has only gone operational in the last few weeks.

So why was a new model needed? At 4.5 there is a major approximation in the equations governing the dynamics of the atmosphere. This is that the vertical component of the Coriolis force can be considered negligible and can therefore be ignored (the hydrostatic approximation) which means that vertical velocity (w) need not be explicitly calculated. This is true at large grid scales but, as computing power has increased, the potential to run the model at much finer scales (<10km) has meant that this is no longer desirable. The mesoscale model (this is the version that covers the UK) is already run at 12km resolution and is therefore approaching the limit at which the hydrostatic approximation is no longer valid. The dynamics of the UM has therefore been rewritten to remove this approximation and allow work to be done at scales of 2km or less. The new version of the dynamics code together with a new method of solving the physics equations has had the additional benefit of allowing a longer timestep to be used. This means that, in theory, each run should take less time to complete.

The dynamics has also been written in such a way as to include some implicit diffusion so less explicit diffusion is required. Together with the fact that the poles are now being dealt with in a more efficient manner, this means that less time is spent on calcualation in these areas.

Another major issue concerned how well the model parallelised. Although 4.5 is a parallel version it is based on code that was originally written for a serial machine. It has long been known that the speedup for this version of the model has been abysmal and so it was important to create a new version that was better designed for the sort of architectures that it was going to be run on.

Figure 1 shows the speedup curves for the dynamics and physics sections of both 4.5 and a prototype version of 5.3 on the Met Office T3E. There is clearly a dramatic improvement in the dynamics at 5.3 and there is also significant improvement in the physics. The 4.5 dynamics curve indicates that there was little to be gained from running on more than about 36 processors.

So have these differences improved the model? Well, yes. The latest results show a significant improvement over 4.5, at least in the global and mesoscale configurations. The climate version is still undergoing a lot of development - it's got a tough model to beat as the current version is considered to be one of the best in the world. Researchers at JCMM (Joint Centre for Mesoscale Meteorology) in Reading have already spent a few years looking at resolutions as low as 2km and their results are looking very promising. There appears to be significant improvement over the old model in the way the finer details of the weather are represented.

So when can people start using it? Work is still in progress although 5.3 is available to a limited number of users on Turing. The current release is not portable so it is not yet available for the Origins and it is not an official Met Office release.

Will people notice a difference when running the model? The biggest difference will be in the file sizes. Due to the way the dynamics is now being calculated and with the addition of w as a main variable, the start dumps have increased in size and, for anyone wanting to run a limited area model (such as the mesoscale model) they will find that the boundary condition files are significantly larger. Also, any of the files generated at 4.5 will not be usable at 5.3. And of course, they should notice an improvement to their results!

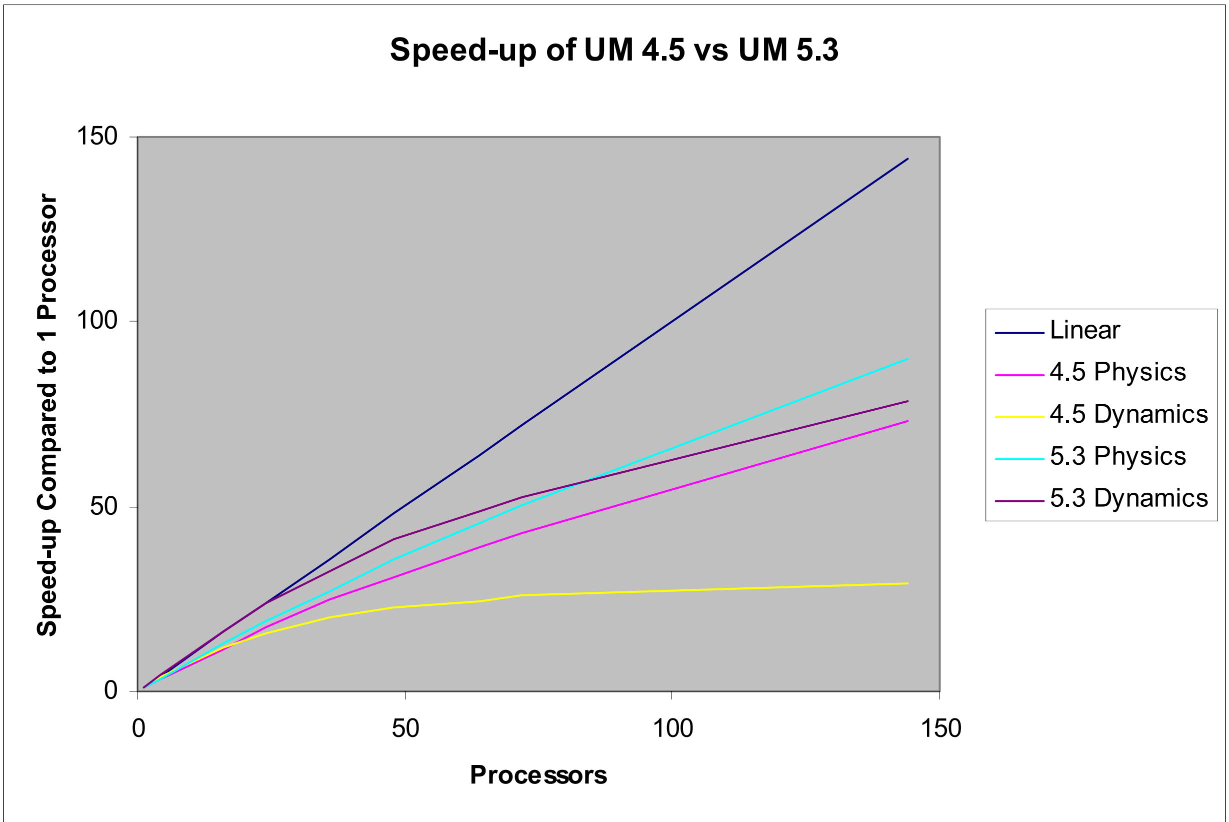

Figure 1

The speed up curves for the dynamics and physics sections of both 4.5 and a prototype version of 5.3 on the Met Office T3E

CSAR User Steering Group Meeting

Claire Green
HPC Frontline Support, Manchester Computing, University of Manchester

The 8th CSAR User steering group meeting took place on Wednesday 4th July 2002, using the Access Grid facilities at Imperial College and the University of Manchester. The meeting is held twice-yearly and is attended by representatives from the User Community, the Research Councils and from CSAR.

The meeting, chaired by Professor Ken Taylor of Queen's University Belfast, contained much discussion regarding the new system developments – the move from NQE to LSF and the new facilities provided via the SAN – as well as providing an opportunity for the user community to bring attention to their views regarding other aspects of the CSAR service.

Dr Lois Steenman-Clark, in her capacity as the Chair of the User Liaison Forum, once again raised the topics that had been commented on by the user community. The SAN and LSF were discussed. Substantial information about both of these is now available on the CSAR webpages :
http://www.csar.cfs.ac.uk/using/san
http://www.csar.cfs.ac.uk/using/lsf/user_guide.shtml

Additional topics include:

Status Page

The weekend is seen as a particular problem by some users in that the Status Page is not manually updated during this period with messages regarding system problems. CSAR have agreed to investigate the implementation of a history of all system-downtimes.

Users of /hold also felt that the inclusion of information relating to /hold within the Status Page would be very useful. Work within this area is now underway.

Scheduling Policy

Dr Steenman-Clark reported that she had received feedback that more guidance regarding the Scheduling Policy was required. Whilst there is already information relating to this on the CSAR website at http://www.csar.cfs.ac.uk/using/man/man_cfsschedule.shtml , the provision of additional information, particularly scheduling policies, is being considered.

Query Management

There have been requests for the introduction of a facility to track the progress of queries that have been submitted to the CSAR Helpdesk. This facility is now available. To check the status of your query, access the User Registration pages at http://www.csar.cfs.ac.uk/admin and choose "Enter the Database", followed by "Details About Yourself". Next click on the link "List problems experienced by <userid>, on any system". This will take you to a screen whereby you can view all of the details of any queries you have submitted that are still open.

The requests from users to CSAR were not the only items discussed at the meeting. The User Steering Group is a means of sharing information between the user community and CSAR, and we took the opportunity to ask for contributions to the CfS Annual Report.

The User Steering Group meeting is considered to be an excellent means of you ensuring that your comments and suggestions are heard by the Research Councils, the CSAR management and by other CSAR users. You can also make your views known by contributing to the Annual CSAR Survey (the results of the 2002 Survey will be published in the next edition of CSAR Focus) and by contacting the CSAR Helpdesk or using the Service Quality Token facility.

The report from the CSAR User Steering Group held on 6 January 2003 will feature in the next edition of CSAR Focus.

ISC 2002 Conference Report

Neil Stringfellow
CSAR Applications Support, University of Manchester

The International Supercomputer Conference, held each year in Heidelberg, Germany, has now developed into an established event on the HPC calendar. For the first time Manchester exhibited with a team comprising of Terry Hewitt, Claire Green, Kaukab Jaffri and myself.

We arrived in Heidelberg at the end of one of the hottest June days in German meteorological records and the whole conference was blessed with glorious sunshine, even if the temperatures made life a little uncomfortable. The event itself took place in the Stadthaus, on the banks of the Neckar river, a venue which is just the right size for the 500 attendees.

Our stand included demonstrations of work carried out at Manchester and displayed information about the facilities and work of CSAR. Most of the surrounding stands were from German supercomputer centres and collaborative grid projects, and whilst we had a good throughput of visitors, our stand became particularly popular on the Thursday lunchtime, as the stand directly opposite from HLRS Stuttgart showed live action from the world cup game between Germany and the U.S.A.

As can be expected at a supercomputer conference, most of the major hardware vendors were in attendance and they all had two opportunities during the conference to talk about their latest offerings, once during the tutorial session to advocate their grid strategies, and once during the main conference to talk about their latest products.

The keynote presentations at the conference began with Monika Henzinger from Google who talked about the challenges of using parallel machines and clusters of PCs for maintaining and using databases of web pages on the Internet, when the number of these pages doubles every eight months. This was later followed by presentations from Jack Dongarra who envisaged problem solving environments for large scale numerical grid applications and Dona Crawford of Lawrence Livermore National Laboratory who talked about computing at the laboratory in the previous 50 years and the future directions for applications and infrastructure.

ISC2002 Keynote Presentation by Monika Henzinger, director of research with Google Inc.

For many people at the conference the highlight was a presentation by Tetsuya Sato, the Director-General of the Earth Simulator Centre who gave a brief overview of the hardware and surrounding infrastructure of the simulator, but who then was able to spend most of his time showing some of the fascinating scientific results which have been produced by the applications running on this machine.

International Supercomputer Conference is a very valuable event. We will be exhibiting at ISC 2003 and hope to see you there. Further information about the event is available at http://www.isc2003.org.

Public awarding of the of the No. 1 TOP500 Certificate by Hans Meuer to Shigemune Kitawaki representing the Earth Simulator Center in Yokohama, Japan

CSAR Support & the SVE Group at Manchester

Andrew Jones
HPC Team, Manchester Computing University of Manchester

There have been some reorganisations at Manchester Computing, along with some new faces in the CSAR support team. This article describes the new structure here and introduces the team.

A long time ago … there was a group called the Computer Graphics Unit (CGU). In time this became the Manchester Visualisation Centre (MVC), headed by Terry Hewitt. A few years ago, MVC (on behalf of Manchester Computing) along with SGI and CSC formed the Computation for Science (CfS) consortium and won the contract from the research councils to provide the UK national academic supercomputing service – CSAR. MVC's main role was to provide the user support component of the service, and thus CSAR user support was provided by staff from MVC. MVC's other roles at the time and since included visualisation research, HPC support for the local university HPC services, grid research, UKHEC, etc.

Recently, however, MVC has been very successful in research and has grown both its activities and staff to the extent where we felt we needed to get some structure. And so was born the Supercomputing, Visualisation & e-Science Group (SVE). SVE is made up of three parts – MVC, the HPC team, and the e-Science team – with a total of around 50 staff.

SVE's management team comprises:

> Terry Hewitt, *Headof SVE, and formally CSAR User Services Manager;*
> Nigel John, *Head of MVC and deputy head of SVE;*
> Yien Kwok, *Deputy for Nigel within MVC;*
> Mike Pettipher, *Head of HPC;*
> Andrew Jones, *Deputy head of HPC;*
> John Brooke, *Head of e-Science, and co-director of the ESNW Centre;*
> Stephen Pickles, *Deputy head of e-Science, and Grid Support Manager.*

Support for the CSAR service is now one of the jobs (the main one) of the HPC team, headed by Mike Pettipher. The HPC team's other activities include supporting local university supercomputing facilities, performing HPC related research and providing support, training and consultancy for the various aspects of HPC and its applications to academic and commercial customers.

We have experience and success with a wide mix of architectures and configurations – CSAR comprises over 1500 CPUs, including an 816 CPU Cray T3E, various SGI Origins (from 16 to 512 CPUs), plus Fujitsu Vector, IBM, Compaq Alpha and Itanium systems. We have experts in a range of parallel methodologies – MPI, PVM, OpenMP, HPF, Mixed MPI/OpenMP, and in all major languages – F77, F90, C and C++. Through CSAR and our other activities, we support a diverse range of HPC applications, including computational chemistry, engineering, finite difference methods, finite element methods, boundary element methods, linear algebra and matrix methods.

Our sister groups within SVE – the MVC and e-Science teams can provide additional added value services to the CSAR community. One example is visualisation support and research – after all why generate many Gb of data on a supercomputer if you never investigate it properly to gain the maximum physical insight? Another example is training courses and advice for HPC related topics such as large dataset visualisation, or use of the GRID in research.

Take a look at our new SVE website at www.man.ac.uk/sve for more ideas and information – including our participation in a range of research projects, staff profiles and details of our services.

Finally, two of the HPC staff (myself and Fiona) arrived since the last CSAR Focus was published and so we have been asked to provide a brief article introducing ourselves to the user community.

Fiona Cook
Frontline Support

I joined the CSAR frontline support team in May 2002. Originally from South Lanarkshire in Scotland, I relocated to the North West in March of this year.

I started out my working life as a civil servant employed by the Inland Revenue. During this period I studied part-time in Edinburgh to attain my BA business studies degree. After almost 7 years in the Inland Revenue, I moved into a semi-technical role working for a local further education college where I was responsible for the day to day running of the MIS department. It was during my time here that I developed an interest in IT and decided to return to full time education to study for a MSc in Information Systems. In Jan 2001 I joined Sun Microsystems at their manufacturing plant in Linlithgow. The primary objective of this role was to provide specialist advice and problem resolution within the Worldwide Application Support organisation for all ERP applications used within Sun's Supply Chain.

Outside of work my main interest is scuba diving. I learned to dive in the Red Sea where I completed my PADI open water course. I completed my advanced diving course this time in a quarry in Wales (not quite the same experience as the Red Sea). I've since dived throughout the UK, my favourite dive site so far is Scapa Flow in Orkney, where I dived what remains of the scuttled German fleet. I'm heading back to the Red Sea later on in the year to dive the World War II British freighter SS Thistlegorm. When I'm not diving I also enjoy badminton, reading and hill climbing. I've also recently taken an interest in a certain Manchester football club (they play in red)!

Andrew Jones
Deputy Head of HPC Team

I joined the HPC group, which provides the user support for the CSAR service at the beginning of May 2002.

My academic background is in science, and in particular physics. My involvement with Manchester has some history – I got my first degree (BSc Physics) from the University of Manchester in 1996.

My last 5½ years were spent at as DERA (which split into DSTL and QinetiQ in 2002). I started out in a research role, and this research theme remained throughout my time at DERA, although in more recent times I took on many other roles. My research was mostly based in computational science, with occasional forays into real experiments, or even full trials.

I have done (doing the hard work myself) or directed (guiding others through the hard work whilst taking all the credit) scientific and engineering research, drawing together a blend of simulation data, experimental data and data from other sources to design and validate algorithms, develop software and design experiments, investigate the limits of the techniques and the technologies, and use the data to further the science and develop new or improved solutions for our particular focus.

Being a computational scientist inevitably meant software development became a core part of my work, and my projects have involved significant software design, development (mostly in C++/Fortran/IDL, sometimes with GUIs in MFC), validation and benchmarking. The nature of our science meant that the high performance computing was essential, and my projects made heavy use of a variety of high performance computers, (including the old Farnborough Supercomputing Centre for those who remember it) and I have managed to play with most common system architectures and development languages.

Of course, as time progressed, I adopted more management and strategic roles. Through need and practice, I became adept at (either doing or delegating and managing where possible) system administration, technical computing procurement and strategy, business cases, project management, people management, financial management, customer relations and product management and other essentials of the business world. Throughout these extra roles, I preserved my scientific and computational research core.

Finally, after the transition from fresh graduate to recognised expert in my particular field, I left QinetiQ to join SVE and the CSAR service, where I look forward to the task of ensuring, along with the rest of the team, that CSAR remains at the forefront of supercomputing services for research and establishes a reputation of being powerful, easy-to-use and flexible – enabling world-class science.

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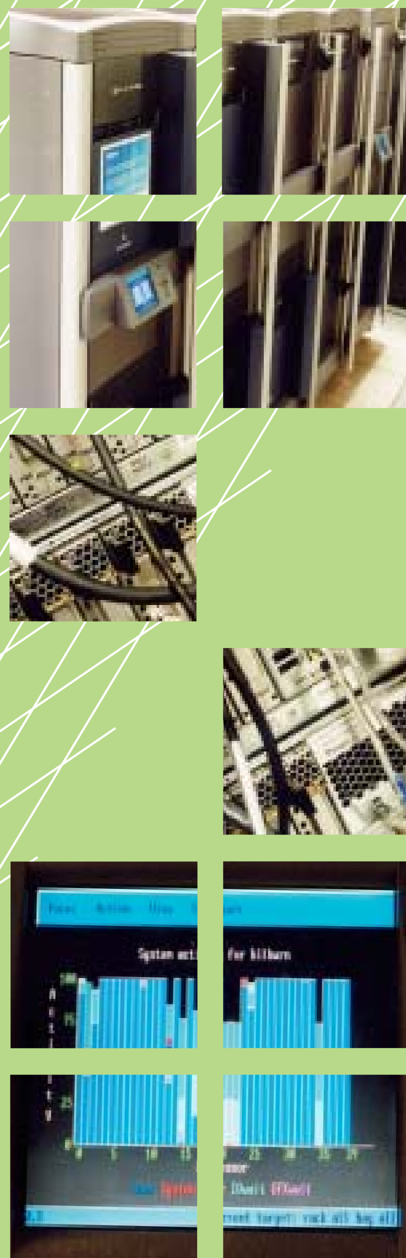
CSAR Information

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.

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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