CSAR FOCUS

Edition 3, Summer 1999, Editor: Kaukab Jaffri

This issue launches the new look CSAR newsletter, *CSAR Focus*. As well as bringing you an update on news and issues regarding the CSAR service, *CSAR Focus* aims to keep the CSAR community in touch with the world of High Performance Computing.

SOFTWARE UPDATE:
Vampir: speeds up your execution trace

PEOPLE FOCUS:
Head Of Optimization, Dr Mike Pettipher

MRCCS Presents:
HPC Summer School
6-17th Sept. 1999
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Providing High Performance Computing Services *for* the Academic Research Community

CSC THE UNIVERSITY of MANCHESTER sgi

Content

Editorial

CSAR Focus is published four times a year: Spring, Summer, Autumn and Winter. All CSAR users are welcome to participate; all of the editions are available via the web: http://www.csar.cfs.ac.uk/general/newsletter.shtml, as well as this edition being the first to be sent out to all CSAR users.

Regular features include **People Focus** - where we have focussed on CSAR staff up until now, however the next issue will bring you the start of a series of insights into CSAR users and their research interests.

A brand new section - **Software Update** has been introduced, decribing new software that has been implemented onto the CSAR machines. This issue describes Vampir - a software tool that assists the programmer in getting an overview about an execution trace quickly.

This edition's **Feature** concerntrates on the newly formed Manchester Research Centre for Computational Science, or MRCCS as it is known.

The **FAQ** page is updated in each issue, and the **Articles** section brings you a range of of HPC topics, written by CSAR staff/users.

Dr. Nicola Clarkson from EPSRC has a regular feature - in this issue she talks about why it is important to keep your capacity plans up-to-date.

Finally, for anyone who wishes to contribute to the next edition of *CSAR Focus*, which will be in the Autumn, the last date for contributions, be they articles, comments, dates for the Diary, is Friday 24th September.

I look forward to hearing from you!!!

Disclaimer

Articles are the responsibility of the individual author: the Editor and the CSAR Service assume no responsibilty or liability for articles or information appearing in this document. Opinions expressed in some articles may not reflect those of the CSAR Service.

We welcome you all to participate in this publication, with any articles of interest to other CSAR users, or comments on any aspect of HPC.

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Establishing CSAR: A Personal View or Anything that can go wromg did!

W T Hewitt
Head of Scientific Support for CSAR

Early 1997, Smith Systems Engineering Limited were appointed by the Research Councils to manage the procurement of a new High Performance Computing Service for UK Academia. They called the project HPC'97.

By the time you read this, the CSAR service will have been officially live for six months, and the editor asked me to review the first six months. For me though it seems more like a lifetime.

June 1997

In June, Smiths' issued a Request for Information (RFI) and we returned our 13 page response on the 30th July. We addressed such questions are "What do you perceive as the advantages and disadvantages of the private finance initiative approach?". I won't bore you with the reply! Well whatever we said got us through to the next round, where we provided another 40 page document in October 1997, our response to the Statement of Requirements. As part of the review of that document, the service providers and the hardware providers were being assessed separately, and Dr Alison Wall from EPSRC and Dr Adrian Colbrook from Smith's came to benchmark our service in November 1997

November 1997

We had prepared a presentation for them and had made copies for staff locally and beautiful colour copies for our visitors. About 10 minutes before their arrival we noticed the cover page said "A Ward" instead of "A Wall". Clearly such a faux pas could not be entertained and I rushed around collecting the all the copies, rushed off to my office to make a new cover, rushed off to the print room for the new covers to be printed.

As I was walking back with the new copies I met Alison and Adrian walking through the building.

Now they know why I was looking a bit harassed.

Needless to say the day went very well and on the 28th November 1997 Smiths informed us that "following the evaluation of your response to the Statement of Requirements and the benchmarking, you have been shortlisted as a service provider...".

From then on the pace quickened. At this stage we were asked to form consortia of technology suppliers and service providers.

After some negotiating with the other shortlisted suppliers - Computer Sciences Corporation, Silicon Graphics, we came together to form Computation for Science (CfS). Loosely speaking we had to combine three 40 page documents, our individual responses to the SOR to form our answer to the Invitation to Negotiate. Numerous meetings followed with our new partners and with the Smiths. From Manchester many people contributed to the proposal but the main team was Professor providers and the hardware providers were being assessed separately, and Dr Alison Wall from EPSRC and Dr Adrian Colbrook from Smith's came to benchmark our service in November 1997.

Robin McDonough, Louis Blanchet, Julia Chruszcz, John Brooke, Mike Pettipher and myself. Most of these meetings were in Guildford, Reading or Farnborough, and some of us became regulars on the Manchester to London Heathrow British Airways shuttle.

On one trip Julia Chruszcz and I arrived for the 0830 shuttle, and were told it was delayed, so we went off to the café to wait. We got engrossed in something, probably about kids, but we should at least pretend it was something to do with HPC'97. Eventually I realised that the departure time had passed, and we had not heard an announcement about it. We approached the British Airways staff who pointed not only that there had been an announcement but also the plane was just leaving. Seeing the prospect of being at least two hours late for the meeting Julia phoned the other members of the team already in Reading to inform them of the delay. Meanwhile we could see the plane about 50m away from the gate, and we started to panic. The truth will remain a secret but Julia said on the phone to our boss "Terry's thumped the table and they are bringing the plane back". Well the plane did return to the gate and we did get on it and we did make that meeting in time.

March 1998

Christmas came and went and though we were busy, the deadline of Monday 17th March 1998 for the next 80 pages seemed far away. Well of course it caught up on us, and Robin and I spent a week in Farnborough with another six of our partners to put it all together. Well Saturday came, and I saved the latest copy on my laptop, on a floppy disc and on one of the Farnborough fileservers. Three copies must be enough I said, and off we went for curry and a rest. Sunday last day not much left to do and I thought I would do the next few edits just before breakfast.

I made the edits, breakfast suddenly seemed more important, so I clicked save and Word97 for collapsed and refused to save the document. "Oh well, I've only wasted five minutes editing, I can do those again and if there are real problems I've got two other copies."

To cut a long story short, all three versions of the document would not save! For about two hours I looked at all sorts of ways of solving the problem. I was thinking, "How long will it take to re-type these 80 pages? Can we manage it in the next 24 hours? This document is only worth £26M". Luckily at such times of panic, I was sweating a lot by now, the simple solutions worked. John Rawlins from CSC saved the day, as I explained the problem to him he said "Is that all? That's easy. To fix it..." and about 5 mouse clicks later I had saved the document and the rest of the day passed in a haze of edits, and numbers for the costs that made you look at them twice to make sure you weren't imaging things. Then three of us checked them; one digit wrong in £26,000,000 could cost you a lot of money.

Another panic at about 7 in the evening took a long time to fix, as there were too many of us trying to fix it! By about ten o'clock at night, we printed the master, and passed it to the photocopier. It finished making all the necessary copies some time Monday morning and a despatch rider picked them up at 0900 and they were duly delivered to Smiths' on time.

After bursts of activity there is a quiet spell while Smiths and the Research Council teams review all the submissions and think of hard questions. We worry about what we left out, will they see through what we wrote about something, could we really deliver what we said. The timing of these projects is just right, because as you have just about forgotten about what you wrote, caught up on your other work, a fax arrives with a number of questions.

June 1998

You don't get a fax saying you've won, or anything as simple as that. We are told that we are the "preferred bidder". To me it sounded a bit dubious, but others were more confident than I was. They next thirty days were taken up in creating a contract between CSC and EPSRC, and two sub-contracts with CSC and us and CSC and Silicon Graphics, each of which is about 200 pages. I'm glad to say others did that, and I seemed to have quiet month.

July 1998

The contracts were signed on the 30th June. At last we could go public. We were all a little frustrated that we had not been able to go public during the celebrations of 50 years since Professor

The planning started, and I listed 183 things that needed to be done, such as install battery back up, recruit staff, install software, write documentation, so life really started to get hectic. The tasks are shared out, and I'm glad I got the tasks I did, some of the other ones were much harder!

The advert for the twelve staff appeared in the newspapers and the phoned rang for weeks with queries about the posts.

I was allowed out for four days, (one was a Sunday), when I flew to Minneapolis, to join some others on the team from Silicon Graphics and CSC. On the Monday we drove to the factory, two hours each way. We had some lectures about the T3E, and its future, a tour of the facility, and much to my surprise they showed us our machine, built and working. It was naked and under test. The black outer casing is not put on until it is shipped, to avoid scratching it. At last it is real, it's not just a pile of submissions!

I had a good look at the machine and there was one of the Cray engineers reading his email on it, oneof the most powerful computers in the world.

Well what else could they do with it? That evening we managed a visit to Mall of America, the biggest shopping centre in the world, for dinner and next day visited the Cray software development facility at Eagan. More lectures about their future plans. Its all non-disclosure stuff, so I can't tell you about it - luckily for you. Tuesday evening I'm on the plane back to the UK. I arrive early Wednesday morning and to impress everybody I go straight into work, and there into shower to freshen up and change into clean clothes. There I am - no clothes on and the fire alarm goes off. Somebody doesn't like me.

August 1998

We've now got four ring binders of application forms to go through. In another hectic month we managed about five days of interviewing, including one person who was interviewed over the phone. I'll actually meet him next week! By now I'm getting about 100 emails a day to do with HPC'97.

19th August sees three big lorries arriving and several people from Silicon Graphics USA, including the one who uses it for email, and its one of the days we are interviewing, so I missed the great unpacking.

Within a couple of days it's switched on and we are getting itchy fingers to get the software installed...

The tape silo arrived in flat pack boxes. It looked more like it had come from MFI. Within a few days that was built, and Danielle, my seven year old daughter, managed to get inside the silo before it was closed and the robot arm started. She still thinks she's the only one to have been inside. Hopefully it will be many years before she finds out the truth.

The software is installed and we get some users having a go, and more phone calls and emails with challenges. (We don't have problems we have challenges.)

October 1998

Smiths 44 separate acceptance tests were agreed, from counting the processors and making sure there were 576, to verifying we did have 4 TBytes disc space, to the CVs of all the support staff.

Most of the tests we got through in the two days allocated by Smiths to review them. The others dragged on until mid-November, the date from which the consortium started to get paid. The "go-live" date was still set at 1st January.

Still no time to relax as the official opening will be by Lord Sainsbury, Minister of State in the Office of Science and Technology. Robin has some good ideas about how to make the opening of the service interesting. I got the job of making a video. To be honest I had tried to avoid it but I couldn't. Anyway as with all of these things, with the help of many people we managed to make this video in about 10 days and the master tape arrived the day before the event.

My jobs on the day seemed straightforward enough. Keep out of the way and then show the minister around the computer and demonstrations in the machine room. Up until that point I felt it was all under control. I showed the minister some demonstrations, and as he was being photographed, I stood in the corner out of the way. About two hours and six TV interviews later, it was suddenly all quiet and peaceful. What had happened? I thought.

January 1999

For me the "go-live" date was a non-event. By now many other people were rushing around doing all the hard work.

So I started looking at what's called the added value stuff, summer schools, international collaboration, the future. What sort of system should we have in one year's time, two years time...?

May 1999

Well here we are now. The most powerful computer available to academia in the world, capable of a peak performance of 700 GFlops, 4 Terabytes of disc space, 125 Terabytes of tape store, some 38,000 files transferred for one group alone from Rutherford. Over fifteen world class staff working on it. But it still doesn't make the tea!

What have I got to show for it? Most of the CVs we shredded, but the stack of paper for this project stands at about 2 feet high, emails I guess must run into Gigabytes, more grey hair, and still five and a half years to go.

On Sunday I'm off to Minneapolis again, this time for the Cray User Group. I'll tell you all about it in the next newsletter.

Conclusion

There were and still are many people involved from Computer Sciences Corporation, Silicon Graphics, and The University of Manchester, and they have all made contributions bigger and better than mine. Maybe they too have some good stories!

EPSRC Feature: The Importance of Keeping Your Capacity Plan Up-to-Date

Dr Nicola Clarkson, EPSRC

The capacity planning facilities on the CSAR web pages are designed for the PI of each User Group/Project to specify how they intend to use their service tokens over the lifetime of their grant. This information, if kept up-to-date, is useful to help CfS with their overall capacity planning for the service to ensure that the resources required are there when needed.

When generic service tokens have been awarded to a new grant, CfS will initially enter the resource profile given on the CSAR application from into the capacity plan. The PI needs to confirm this estimated resource usage profile within 3 months of the announcement date of the grant. PIs will not be committed to this profile, but are strongly encouraged to keep their capacity plan updated regularly if their resource usage profile changes significantly. By doing this, the need for 'scheduling' of resources (as we have done for the EPCC T3D and EPSRC/NERC T3E facilities) is removed. PIs are able to use their resources as they wish throughout the lifetime of their grant.

Trading is linked to the capacity planning in such a way that a PI need not re-trade if he/she just wants to re-plan when the User Group's resources will be used. Trading is only required if the PI wishes to change the balance of resources between resource types, e.g. to swap T3E PE hours for disk space.

People Focus: Introduction to the CSAR Optimisation Team

Dr Mike Pettipher,
Head of Optimization

The CSAR Optimisation team consists of 3 members from different scientific disciplines plus a team leader, Dr. Mike Pettipher. They also work closely with the Applications support team which has a total of 6 staff, led by Dr. John Brooke (see CSAR Newsletter Edition 2 for information on the Applications Support Team). This article provides information on the role of the Optimisation team, both for and outside the CSAR service, and brief biographies of the members of the team.

The primary role of the Optimisation team for the CSAR service is in the provision of advice, consultancy and programming support in order to optimise the use of the resources of the service. The emphasis is on in-depth coding aspects - choice of algorithm, single processor optimisation, parallelisation and I/O tuning. Such support may require significant effort from one or more individuals, and so would normally start with a visit to the Consortium to discuss the requirements and to agree an appropriate course of action.

Some of you have already requested such support in your CSAR application, but others may be unsure what we can do for you - please contact us for a preliminary discussion (and free quotation!). As an example, one group which is developing some new software asked for help in optimising the single node version. The initial work resulted in a six-fold improvement in performance.

In addition to such direct support, members of the Optimisation team, in conjunction with the Applications team, are actively involved in the development and delivery of training courses, particularly with respect to code optimisation.

Further as mentioned by John Brooke in the last Newsletter, staff from both the optimisation and applications teams are nominated as liaison contacts for each consortium. Current ativities within the group include optimisation work for consortia, installation of additional numerical software and preparations for the HPC Summer School in September.

All members of the Optimisation team are part of the Manchester Research Centre for Computational Science (MRCCS). MRCCS is a focus for high performance computing activities the University of Manchester, bringing together research groups of international standing in high performance computing, visualization, data mining and the applications of such

technology to a range of scientific problems. Thus members of the Optimisation team also have active involvement, in conjunction with other local staff, in the promotion and support of local high performance computing services, which are based around a 40 processor SGI Origin2000 (this system, known as kilburn also provides a National Class 3 service).

People Focus: Introduction to the CSAR Optimisation Team cont.

Dr Mike Pettipher,
Head of Optimization

I originate from a town in the Midlands, Royal Leamington Spa, from where I moved to Hull University for a degree in Mathematics, followed by a PhD at the University of Strathclyde in theoretical population dynamics, perhaps surprisingly in the Applied Physics department.

I then moved to Manchester when our organisation was known as UMRCC

(University of Manchester Regional Computer Centre), and have undertaken a variety of roles, but always with an emphasis on numerical applications software and optimisation. In the early days this involved squeezing programs on to the largest computer in the country (occupying the same floor space now used by turing) - the CDC 7600, with a massive 350 Kbytes of memory!

I was for about five years the CDC Co-ordinator for NAG (the Numerical Algorithms Group), which involved implementing the Nag Libraries on CDC computers, including both the 7600 and the CYBER 70 series. This was a time before Unix, when each system had its own operating system, most of which seem to have been designed to maximise the difficulties in porting between them.

Since that time I have provided support on both the vector and the parallel systems at Manchester Computing. I feel fortunate working in this environment as it provides great opportunites for collaborating with researchers, and this has resulted in continuing work in the development of some parallel finite element software.

My interests outside work mostly involve going up and down mountains, preferably snowy ones, natural history and photography. The three complement each other very well - I never need to admit needing a rest when going up a hill, as there is usually a flower begging to be photographed or a distant object which needs to be investigated with binoculars as it just might be a snow leopard.

People Focus: Dr Martyn Foster

My roots are in Middlesbrough in the North East of England. I lived in this locality before moving away to study at Imperial College in London, and Manchester, where I studied Theoretical Physics. I then went to the North West, to Liverpool University, where I obtained my PhD in lattice gauge theories with the UKQCD consortia.

Here I devoloped an interest in parallel computation being a user of EPCC's T3D. On completing my doctorate in October of this year I returned to Manchester with CSAR in order to further my HPC interests. I work on single node code optimisation and you are liable to bump into me if you attend CSAR's *T3E Development and Optimisation* course which I present.

In my spare time I enjoy playing football and following Boro and when finances permit I also enjoy scuba diving, much of which I have done around the coast of Britain particularly in the Liverpool Bay. I also enjoy travelling and reading (A fan of Armistead Maupin).

People Focus: Kevin Roy

It all began in Malta back in the winter of '75 (although in Malta it wasn't that cold, so it wasn't too bad). However by the time school age arrived, I was living in the West Country. By the time I came to sit my GCSE's I was living in South Wales in my 8th different house and my 8th different school.

When I took my 'A' levels I, had some stability - four successive years in one house and school! Any serious or high level education starts here - a degree in Computer Science and Mathematics was soon followed by an MSc in Numerical Analysis and Computation. Then I end up here, in Manchester, tending this big computer we have.

Well that was the whistlestop tour of my academic life, now what about the rest?

If there is any time left in my days, ironically, I spend it mostly with friends whether it is talking about the issues of the day or any old rubbish. I also spend large portions of my life allowing myself to get kicked from pillar to post playing football, whether at 5-A-side or 11-A-side.

People Focus: Staff Changes

A.N. Other: Please read this item for the missing member of the optimisation team!!

Martin Nygren

As mentioned earlier, there should be 4 members in the Optimisation Team, and up until the end of April, there was. Recently, one member of the team, **Martin Nygren** has left, not just CSAR, and Manchester, but the UK - to return to his native Sweden.

Martin will be know to many of you, particularly for his expertise in computational chemistry. Within a very short time, Martin has forged strong links between CSAR and a number of large consortia. Martin has also been active in developing and delivering training courses, and in other areas of the CSAR service - he is already being missed! It is hard to understand why anybody would want to move from Manchester to Sweden, but perhaps on seconds thoughts.....

We thank Martin for his work.

Mike Pettipher,
Head of Optimisation

New Staff

We are pleased to announce that the vacancy left by Martin Nygren has been filled by Ben Jesson. Ben joined the team on the 1st July, and is also currently completing his D.Phil. in Chemistry from Oxford University.

The CSAR Applications Team have also replaced Dr. Stephen Thompson. Joanna Leng joined the team offically on the 1st June.

Stephen Thompson

Stephen Thompson, from the CSAR Applications Team, left us at the end of May to work as a numerical modeller in Financial Management.

Although Stephen was only with us for eight months, he made a number of important and useful contributions. Firstly, he worked with consortia investigating Lattice-Boltzmann techniques in studying the behaviour of complex fluids. He was the joint author of a paper recently published in Phys. Chem. Chem. Phys., 1999, 1, 2183-2190.

Stephen also put a great deal of effort into work evaluating load balancing software, particularly LSF. This is of considerable interest to CSAR since LSF will become the recommended replacement for NQE on SGI machines.

We are sorry to lose someone with such a good blend of computing and scientific modelling skills. However, in the commercial world people with Stephen's skills and determination are in great demand and we wish him all success in his new job.

An added bonus for Steven is that he will now be working in the city of his favourite Rugby League team, Leeds Rhinos, who you may have seen steamrollering their way to victory in the recent Challenge Cup final at Wembley. In a year when United have won the Treble, Manchester was never going to be easy place for a Yorkshireman!

John Brooke,
Head of Applications

Feature: MRCCS, The Manchester Research Centre for Computational Science.

The Manchester Research Centre for Computational Science (MRCCS) is a focus for high performance computing activities the University of Manchester, bringing together research groups of international standing in high performance computing, visualization, data mining and the applications of such technology to a range of scientific problems.

The core expertise in these technologies is provided through:

* Computational Chemistry Group in the Department of Chemistry led by Professor I Hillier
* The Centre for Novel Computing in the Department of Computer Science led by Dr L Freeman and Professor J Gurd
* Manchester Visualization Centre and CSAR in Manchester Computing led by Professor W R McDonough, with assistance from Mr W T Hewitt

The core staff of MRCCS are hosted in Manchester Computing, Europe's premier university computing facility supporting world class research and teaching in all disciplines. It consists of two groups: Manchester Visualization Centre and the MRCCS optimization team. The optimisation team also provides optimization support to CSAR the new flagship high performance computing service to UK Academia, based around a 576 processor Cray T3E system, (the fourth most powerful computer in the world), and a Silicon Graphics Origin2000 system.

In addition, the University runs a number of other Origin2000 servers as part of its HPC services.

The Computational Chemistry group is one of the largest in Europe and is carrying out research to solve problems in all the major areas of chemistry, including those that impact on biochemistry, catalysis and material science. Their focus is to bring together experimentalists, theoreticians and their own computational and chemistry expertise to provide an integrated approach to the solution of their problems.

The Centre for Novel Computing in the Department of Computer Science aims to help solve the problems most users of high performance parallel systems are finding in effectively exploiting the apparent power of these machines.

They aim to make high performance parallel computing accessible to all users who have a need for the power it can offer.

The Scientific Advisory Board is chaired by Professor Ian Hillier, Department of Chemistry.

The MRCCS have recently announced their first event, the HPC Summer School to be held in Manchester. This event, which runs over two weeks in September, is free for all CSAR users.

For futher information on the Manchester Research Centre for Computationa; Science, and the on-line application form for the Summer School, see the MRCCS web page: http://www.man.ac.uk/mrccs/ or contact the CSAR helpdesk.

MRCCS News: HPC Summer School – Announcement

Summer School

This is the first annual two-week residential event being organised by the Manchester Research Centre for Computational Science. It will be a unique opportunity for you to develop skills so that you can make effective use of distributed programming environments, as typified by the Cray T3E, and to learn how to visualise the results of applications run on such supercomputers. You will

* get to use the most powerful computer available to academia in the world

* meet the international experts who will teach you

* develop contacts with other participants

High Performance Computing Summer School in Distributed Memory Programming and Scientific Visualization: 6th - 17th September 1999, Manchester

Topics and Format

The list of topics, to be presented by speakers from Europe and the USA is

Professor Jack Dongarra	*Systems & Architectures for Distributed Memory Programming
Professor Michael Resch **RUS Stuttgart**	* Distributed Memory Programming * Tools for Profiling & Debugging
Dr Lawrence Mulholland	* Parallel Numerical Libraries for Distibuted Memory Systems
Dr Len Freeman **University of Manchester**	* Parallel Algorithms * Visualization for Multidimensional & Scientific Data
Professor Frits Post **TU Delft**	* Visualization of CFD data (an extended case study)
Mr Terry Hewitt **Manchester Visualization Centre**	* Systems & architectures for Visualization * Computational Steering

The format of the school will be an approximate equal mixture of lectures and practical sessions (roughly 20 hours of each). It is expected that students will use the Cray T3E and other machines for the practical sessions, through the extensive computing and visualization facilities of the University of Manchester.

Personal contact and informal discussions amongst the participants, lecturing and support staff during the leisure time are an important aspect of the School.

Objectives and Audience

The summer school is designed to show how to maximize productivity in distributed memory machines, either highly specialized systems (such as the Cray T3E) or on clusters of workstations and how to visualize their results.

The school is aimed at all graduates, research assistants, and post doctoral research assistants , and industrialists who are thinking of running programs on in such environments, and who need to analyze data from applications run in such an environment.

For further information, see the MRCCS web page:http://www.man.ac.uk/mrccs. The application form can be found at: http://www.man.ac.uk/mrccs/appform.html. If you have any problems finding information or require further assistance, please email the CSAR helpdesk: csar-advice@cfs.ac.uk or telephone 0161 275 5997/6824.

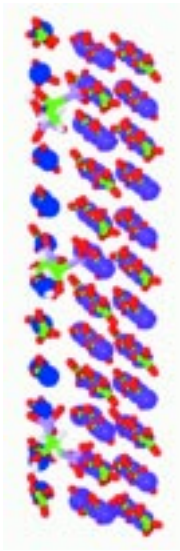
Accommodation and Costs

Accommodation will be provided in a University Hall of residence, within easy walking distance of Manchester Computing where the school will be presented.

The course fee is £750. The fee is waived for staff and students who are users of the CSAR service, and a number of scholarships are also available.

Computational Chemistry's Insatiable Hunger For Computer Resources

Article: Dr. Martyn Nygren



Ball and stick graphical representation showing how HEDP ions fit into steps on a calcite surface

Assume that there exists a scientist who would like to simulate the movements of one mole (18 centi-litres) of water at room temperature and pressure. Treating the water molecules as rigid bodies this gives

6 * 6.023*10^23 degrees of freedom in the simulation. To count from one to

6 * 6.023*10^23 using 512 processors on turing would take at least 186 480 years, this is assuming that every instruction issued is used to increase the count by one.

Our droplet researcher was presumably planning to use classical mechanics to describe the motions of the water molecules.

According to classical mechanics chemical reactions cannot take place if matter is quantized. Many 19th century physicists were therefor critical of Dalton's atomic theory and preferred things like mathematically incomprehensible continuum models suffering from vortex knots. Today there is quantum mechanics, also mathematically incomprehensible, which does allow for atoms to undergo chemical reactions and form complicated molecules.

With chemical reactions theoretically allowed it is reasonable to hope that they can be understood by bone-headed calculation. High accuracy quantum mechanical calculations do in practice struggle with the reaction:

H_2 + O ==> H_2O

and an entire fauna of approximative methods have evolved. A popular choice is to revert to classical mechanics when all chemical bonds are expected to remain intact. An example of what can be done with calculations employing classical mechanics is shown in the picture.

This ball and stick graphical representation shows how HEDP ions fit into steps on a calcite (CaCO3) surface. Using the good, old trial and horror procedure it has been empirically established that HEDP ions stop calcite crystal from growing. It is also known that the major growth mode of calcite is to add material at steps on the surface. From this it can be figured that HEDP ions ends at the surface doing something, but where did they go and what do they do?

The HEDP ion can enter into a calcite surface by replacing two carbonate ions without breaking or forming any chemical bonds and this process can thus be descibed with reasonable accuracy using classical mechanics. Using classical mechanics, it can be well described which the surface sites that HEDP ions prefers to bind to are. From these calculations it was learned that HEDP ions prefers to be at step sites, as shown in the picture, over the flat surface. Once anchored to the step, the HEDP ion prevents calcium and carbonate ions from binding to the step, thereby poisoning crystal growth.

These calculations, done by researchers at the Royal Institution in London and Curtin University in Perth, Australia, used up several CPU months on Origin 2000 and CRAY-T3E systems. It would of course be very interesting to include water-surface interactions into these simulations. To be able to predict the growth inhibiting properties of various ions, rather than just explain how they work, it would also be necessary to include protonation and deprotonation reactions of anions in aquatic solution. If adequate computational resources had been available; these calculations would, of course, have been undertaken.

Software Update: Vampir- A parallel Profiling Tool

Kevin Roy,
Csar Optimisation Support.

Have you ever had a parallel code and realised that it probably doesn't work quite as well as it could? Running a program and generating the trace data produces reams of information, and for most purposes unintelligible data, is not very useful.

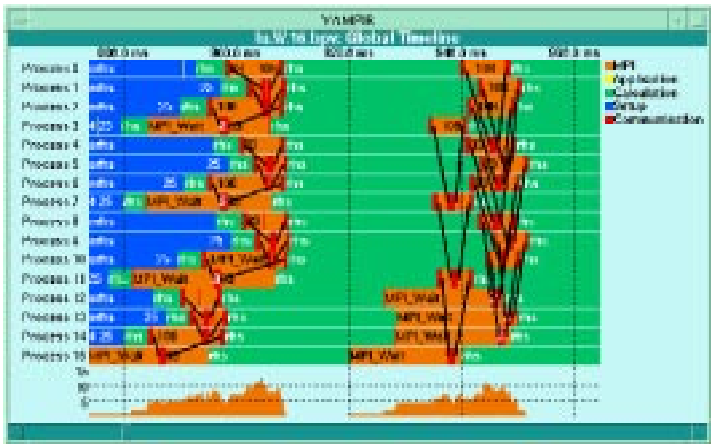
What is needed is a graphical interface that can also, if necessary, go into detail or give a general overview of the program.

Vampir can do this for you!

Vampir is a product from Pallas, an independent high performance computing software company, who have created other software tools such as TotalView (program debugger), Dimemas (performance prediction/ simulation tool) and are involved with Portland Group HPF compiler and the PGI workstation. They are also getting involved in many other projects.

Vampir is a means of seeing the structure of program and specialising in finding communication problems and load balancing problems. The figure below shows the MPI and "user code" sections of a simple program by "zooming in" we can find out exactly what these MPI calls are and what processor is talking to which processor.

Also it is unclear what parts of the code are executing the sections shown, however a little extra programming can leave markers in the trace which vampir can read. This is perhaps one of the pitfalls on the Cray T3E implementation, that the compiler will not help in this way.



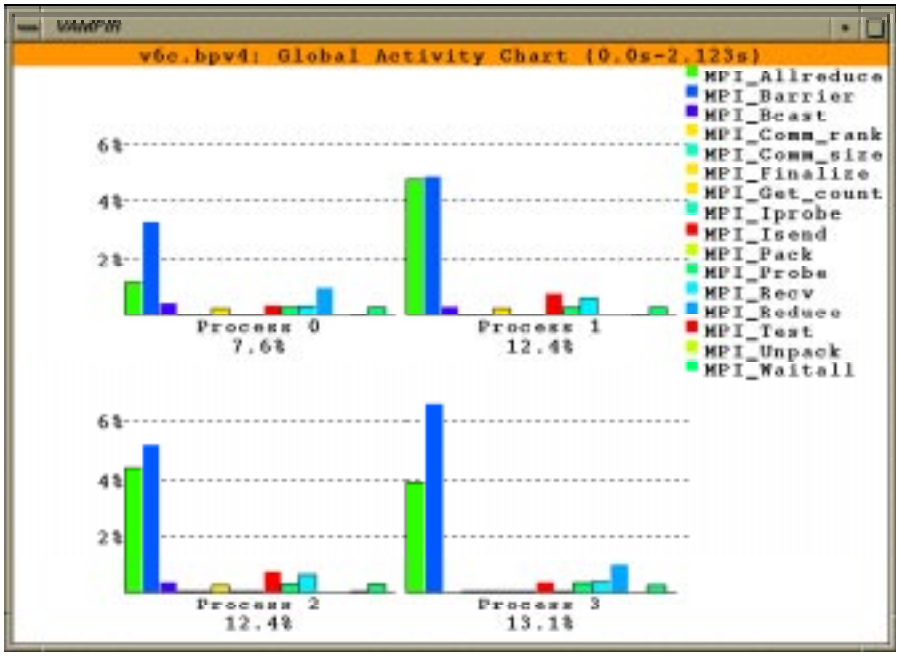
Global Timeline for the LU Benchmark Program

Software Update: Vampir- A parallel Profiling Tool – Cont.

For example the output on a Fujitsu compiled program yields a far more colourful display, there is good news however there may be plans afoot to generate such information. There is also the intention to be able to generate tracefiles from OpenMP source, so it looks like Vampir intends to stay and with such functionality and the non-static production schedule quite rightly so.

It has the ability to make further analysis of codes, for example it is possible to look at the time spent within MPI calls. The diagram below shows a 4 processor program with the MPI_Barrier routine taking up more time on this processor than any of the other routines (perhaps a sign of load imbalancing?).

Try it for yourself!



Global Activity Chart for MPI Communications

Perhaps you'd like to try it for yourself, we have it on turing and fermat (at present for a limited time) see its web page for information on setting it up.

CSAR would like to thank Pallas for the trial software.

Frequently asked questions

Kaukab Jaffri
Editor & CSAR Frontline

This section includes questions, comments and requests received by the CSAR Service. Items have been included based on both frequency and on perceived importance to a majority of users.

Registration/Usernames & Passwords

Can I have a CSAR account?

Resources on CSAR systems must be applied for using the CSAR Resource Application form available on the Web: (http://www.csar.cfs.ac.uk/general/forms.shtml). There is full information there on the different classes of use.

What do I need to do as a project PI?

When we receive details of the new grant, the PI is contacted via email and given details required to set up their projects. Full information of the tasks required are given at: http://www.csar.cfs.ac.uk/service/PI.shtml. If you require us to perform any of the PI tasks, please contact the Helpdesk.

Can someone else in my project be the CSAR PI?

Yes, but please inform us of the nominated PI for your project, and forward the email containing the access username and passwords to the new PI.

Why does the registration form ask for existing username? What is the site code?

If the user already has a Unix account at Manchester their details are already in the database (which includes a number of Manchester machines). This saves effort and avoids multiple entries in the database. The site code is the prefix for your username and relates to your home institution – the database will supply the appropriate site code.

Frequently asked questions – Cont.

Can I have the same username for different projects?

This is unfortunately not possible due to the need to account all resource usage (including disk/tape) to the appropriate project.

Can I have access to the Fujitsu VPP system?

Access to the Fujitsu machine is subject to some restrictions - please contact the Helpdesk for more information.

I've forgotten my password.

Your PI has the authority to re-set your password. You can also contact the Helpdesk who will do it for you.

Managing Resources

What resources should I bid for, and what do they cost?

We can help with completion of the CSAR Application form. The notional cost of resources is subject to change occasionally, but will be shown in the on-line resource calculator.

What do we do with our generic tokens?

The PI must trade all of their generic tokens for actual resources using the "Trading Pool", accessible from their project's database pages (see the summary guide: http://www.csar.cfs.ac.uk/service/PI.shtml). You may trade again after 3 months to adjust your resources.

If a serious mistake is made in the trade, can it be rectified?

Yes, we will re-enable trading. Please ask the Helpdesk.

Can we have more resources?
The CSAR Service cannot award additional service tokens. Applications must be made to EPSRC.

We want to use fermat for disk only - do we require any fermat CPU time?
Yes - a nominal amount of time is required.

Will resource token exchange rates change at all?
Exchange rates may change, but only very occasionally. Any changes would be as a result of significant changes in the market price of any of the resources, and would be in consultation with EPSRC.

Can projects trade resources with other projects?
No -- the trading pool is not in any way like the stock market! It is intended to provide flexibility for projects in the way that they use their resources.

What resources can be allocated to users?
Sub-allocation is mandatory for certain resources, and possible for others. The PI must allocate some disk resource (quota) to users by way of sub-allocation of the project's disk quota on each machine. If the user will require tape space (the HSM facility which includes /hold areas on disk), they must be sub-allocated some of the project's tape resource. Note that the tape sub-allocation is in units of GByte Years. Once a user has been allocated some tape resource, s/he has an unlimited tape quota; their tape usage is limited by their allocation in GByte Years. Optionally, sub-allcation of CPU time can be made to the users. If no sub-allocation of CPU time is made then the user will have unlimited access to the project's CPU time.

Can we have sub-projects?

Yes, please see http://www.csar.cfs.ac.uk/service/subprojects.shtml.

How do we see how many resources we've used, and what happens if we run out?

PIs can view resource allocation and usage (from the start of the project) on their project's page in the registration database. Users can see their individual usage in the registration system too (by viewing their details via the registration pages). Information on monthly usage is available on turing using the command 'lac' (see man lac), and also in the monthly service reports for all projects and Research Councils, which are available on the Web at http://www.csar.cfs.ac.uk/reports. For projects and users, a more comprehensive web-based system for viewing usage over any period is available at http://www.csar.cfs.ac.uk/reports. Warnings are issued when project/user usage approaches resource limits. In extreme circumstances, batch jobs will be suspended until action is taken to correct deficits in resources.

I need more disk quota

If you are a user (not a PI) you should ask your PI for more disk quota. PIs have the authority to change their project's quota (both up and down) in order to enable them to control their project's rate of usage of disk resources, which is calculated as quota multiplied by time. Initial allocation of disk quota to projects is based on information received with the grant details, if available. There is a physical limit on disk quota available and projects' quotas must sum to less than this amount. For this reason some quota changes may be disallowed by the registration database. Please contact the Helpdesk should this be the case.

Files and Disks

The man pages on turing (and on the Web) give information on files and hold etc. (man cfsfiles).

I need scratch space with non-zero residency time.

The formal policy for /tmp is one of zero residency. in practice this is rarely enforced and the current procedure is that files not accessed for 10 days are regularly deleted. There is an alternative area $DUMP2HOLD where files can be left for 24 hours after a job has finished. (Note that users are responsible for moving files to hold areas).

I can't use hold/tape.

Users must have been sub-allocated some tape resource by their PI - if you are not sure, please check your registration record and ask your PI to allocate some tape resource to you if necessary. If you have a tape allocation, please note the following restrictions for the hold areas:

1. the number of files in the hold areas is limited to avoid delays caused by searching large numbers of small files, hence it is recommended that you tar small files before moving to hold.
2. files should not normally exceed 50 GBytes in size - please contact the Helpdesk if this limit is causing problems.

Frequently asked questions – Cont.

Batch Jobs

Where can I find information on batch jobs/queues/scheduling/priority etc?

The man pages on turing give information on all these aspects – 'man cfsqueue' givesinformation and the full list of man pages relating to jobs, batch queues, scheduling etc. The man pages can also be accessed via the Web at: http://www.csar.cfs.ac.uk/service/docs.shtml.

How do I get information on queue status?

The recommended command is 'qs' (see man cfsqs), and there is also queue status information on the status page on the Web.

Can my job be prioritised?

In exceptional circumstances the priority of a job can be raised. Please ask the Helpdesk.

Training

Can I book a place on a CSAR course and how much does it cost?

Courses are chargeable by way of CSAR training tokens in general, and charges for attendance on courses by non-users of CSAR would be considered on a case-by-case basis. Full details about courses are available on the Web:

Frequently asked questions – Cont.

Documentation

Where can I find CSAR related documentation?

The CSAR Web pages are the primary source of information on all aspects of the CSAR service. Downloadable documentation can be found on the Web:
http://www.csar.cfs.ac.uk/service/docs.shtml.
Requests for additional information should be made to the Helpdesk.

General Queries

I can't log into the systems (turing/fermat)

Please first check the status page on the Web. Scheduled maintenance is normally Tuesday evenings and will be advertised via email and on the systems. Any downtime can affect all systems due to the cross-mounting of file space.

What counts as 'Application Support'?

Only anticipated or pre-arranged in-depth support is chargeable. Helpdesk support on simple and/or unanticipated problems is completely free on charge.

HPC/CSAR Course Calendar 1st Semester 99/00

The course calendar for next semester - 99/00, is now available. Bookings for courses must be made in advance via the CSAR Helpdesk: csar-advice@cfs.ac.uk. All the courses will be held at the University of Manchester.

Courses are available to everyone. There will be a charge of £5 per day, payable in advance, for non-CSAR users.

High Performance Computing Courses

October 1999

6
Introduction to High Performance Computing - **F.Costen**

7
Computer Architecture for Science & Engineering - **R.Pinning & K.Roy**

15
Introduction to Using the SGI Origin2000 - **R.Pinning**

25-27 (3 days)
SGI Origin2000 Optimisation and Parallellisation - **M.Bane, J.Brooke, R.Pinning**

28-29 (2 days)
C++ for Scientific Applications - **J.Brooke**

November 1999

15
Utilising Clustered Systems - **M. Pettipher**

24
Introduction to Programming with MPI - **S.Pickles**

25
Advanced MPI - **S.Pickles**

HPC/CSAR Course Calendar
1st Semester 99/00

December 1999

6
Shared Memory Parallelisation with Open/MP - **M.Bane**

7
Shared Memory Parallelisation with Threads - **J.Brooke**

8
Introduction to LSF for Clustered Systems - **M.Pettipher**

9
Introduction to High Performance Computing -**F.Costen**

14
Java for High Performance Computing - **A.Dodd, D.Kidger**

15
Introduction to High Performance Fortran - **K.Roy, Pettipher**

January 2000

10-12 (3 days)
SGI Origin2000 Optimisation and Parallelisation - **M.Bane, J.Brooke, R.Pinning**

17-19 (3 days)
Porting/Optimising for the Cray T3E - **D.Kidger, M.Foster**

24
Introduction to Programming with MPI - **S.Pickles**

25
Advanced MPI - **S. Pickles**

26
Shared Memory Parallelisation with Open/MP - **M.Bane**

HPC/CSAR Course Calendar
1st Semester 99/00

CSAR Courses

October 1999

5

Using the CSAR Service **- D. Kidger**

18-20 (3 days)

Porting/Optimising for the Cray T3E **- D.Kidger**

21-22 (2 days)

Parallel Vector Processing on Fujitsu VPP 300 **- D.Kidger, M.Pettipher**

November 1999

23

Using the CSAR Service **- D.Kidger**

December 1999

13

Using the CSAR Service **- D.Kidger**

17-19 (3 days)

January 2000

17-19 (3 days)

Porting/Optimising for the Cray T3E **- D.Kidger**

Introduction to High Performance Computing

Prerequisites: Fortran or C programming experience.

This is a one day seminar for new and potential users of the CSAR service, and for other people who are interest in the topic of High Performance Computing. The following topics will be covered:

- Need for HPC
- Vector and parallel computing
- Parallel decomposition
- Parallel programming paradigms

Introduction to Programming with MPI

Prerequisites: The ability to program in Fortran and C and familiarity with Unix. Some acquaintance with the terminology of High Performance Computing, such as that covered by the Introduction to High Performance Computing course, is also desirable.

A one day workshop with lectures and practical sessions.

MPI (Message Passing Interface) has emerged as the de-facto standard for writing portable, message-passing programs in parallel processing environments. This course introduces the basic essentials of MPI, yet the material covered is sufficient to parallelize a wide range of serial codes. Topics covered include:

- The message-passing paradigm
- Point to point communication
- Synchronisation
- Basic collective communication (reduction operations, broadcast)

Advanced MPI

Prerequisites: Attendance at the Introduction to Programming with MPI, or a good working knowledge of the topics covered. The ability to program in Fortran or C and familiarity with Unix.

A one day workshop with lectures and practical sessions.

This course covers advanced features of MPI (Message Passing Interface), including the following topics:

- MPI derived types
- Groups, Contexts, Communicators
- Process Topologies
- More collective communication
- Future developments (MPI-2)

Introduction to High Performance Fortran

Prerequisites: The ability to program in Fortran or programming experience in other high level languages.

High Performance Fortran (HPF) is a superset of Fortran 90 containing extensions to Fortran 90 to support data parallel programming. HPF allows programmers to produce portable code for parallel machines, without the difficulty of providing explicit message passing calls. This one day 'hands-on' course provides an overview of the HPF language. Major topics include: relevant features of Fortran 90, the HPF model, HPF directives, data distribution, data parallelism, intrinsic and library procedures, extrinsic procedures and subset HPF.

Shared Memory Parallelisation with Threads

Prerequisites: The ability to program in C and familiarity with Unix.

Multithreading is a modern programming paradigm for implementing parallel applications on shared memory multiprocessors. This 1 day course is targeted at individuals with not previous MT programming experience. Topics covered include:

- Parallel computing and multithreading
- Multithreading basics
- Creating and managing threads
- Synchronising threads

On line access with examples and exercises is an integral part of the course.

Shared Memory Parallelisation with Open/MP

Prerequisites: You should have used either Fortran 77 or Fortran 90 to write programs. Familiarity with Unix, emacs or vi, and the X Window System is highly desired.

OpenMP can be used to run Fortran and C programs in parallel on a shared memory computer, such as the SGI Origin2000s kilburn.mcc.ac.uk and fermat.cfs.ac.uk. The OpenMP specification is now widely accepted and suitable compilers are now provided by all major hardware vendors, including SGI, Sun, Compaq/DEC, Intel, HP and IBM.

To use OpenMP you simply add directives to your code. This 1 day course will cover all the important directives and include plenty of hands-on exercises for you to learn how to parallelise your code. Where appropriate, emphasis will be given to the practical use of OpenMP.

The day will also include a very brief overview of concepts of parallel programming and an introduction to the performance analysis tools perfex and SpeedShop.

About a third of the day will involve practical exercises. Note that the examples will be in Fortran only, and will be run on an Origin2000. C examples will be available on the C++ for Scientific Applications course.

Utilising Clustered Systems

Prerequisites: Familiarity with a high level language such as Fortran or C.

Utilising clustered systems (whether workstations or PCs) for parallel computing has emerged as a key technology over the last few years. This course will present an overview of the current developments in hardware and software and covers system and network configuration, languages, libraries and tools which can be used to develop and utilise these clusters for parallel computing.

An Introduction to LSF for Clustered Systems

Prerequisites: The ability to program in Fortran or C and familiarity with Unix.

When individual systems are combined into a single clustered resource, it is possible to increase the overall throughput of work, and also to run parallel programs which may require more memory than is available on a single system. This can be effectively achieved only via an appropriate Cluster Management System. LSF (Load Sharing Facility) is a widely used and highly regarded system. This one-day course will describe the basic features of LSF showing how it may be used to make best use of a clustered system.

Computer Architecture for Science & Engineering

Prerequisites: Some familiarity with computers and an interest in the area.

This course introduces some of the topics that are mentioned in machine specific courses, such as the T3E and Origin2000 optimisation courses and the Fujitsu course. It looks at and explains the computer hardware and gives an insight into the styles of programming that can be used.

Introduction to Using the SGI Origin2000

Prerequisites: You should have used Unix before and be familiar with Fortran.

This new 1 day course acts as an introduction to using the SGI Origin2000 high performance computer. Topics covered include: overview of the system architecture, making good use of the compilers, performance analysis tools, and running programs interactively and in batch under NQS. There will be a brief discussion of the use of the autoparalleliser.

This is not an introduction to Unix course. For in-depth optimisation and more discussion and practicals concerning shared memory parallelisation, please attend the 3 day SGI Origin2000 Optimisation and Parallelisation course.

SGI Origin2000 Optimisation and Parallelisation

Prerequisites: Practical experience of programming in either Fortran 77 or Fortran 90 is essential. Familiarity with Unix, X Window System, and make/makefiles is required.

This intensive 3 day course will help users understand the key features of the SGI Origin2000 and how to get the most from codes run on this machine.

Issues covered include: system architecture, program development tools, RISC optimisation techniques, performance analysis tools, compiler options, concepts of parallelisation, data dependency analysis and shared memory programming using OpenMP.

The course will be very intensive and include several practical sessions (Fortran only) covering the salient points of the course. C examples will be available on the *C++ for Scientific Applications* course.

Java for High Performance Computing

Java is now firmly established as the language of choice for many application areas, particularly for situations where the code must be extremely robust and portable. It naturally supports multi-threading which allows a code to run simultaneously over several processors. However, currently Java code is slow to run compared to Fortran90 and C.

This course looks at why Java is a good language for 'application codes' such as in computational chemistry or fluid mechanics, and explores how these codes can be made to run almost as fast as if in native Fortran whilst maintaining Java's flexibility and portability, and how the same code can be run on single and parallel architectures.

C++ for Scientific Applications

Prerequisites: Familiarity with the topics covered in the Programming in C++ course or considerable programming experience in C or C++. Familiarity with the topics covered in the Introduction to Unix course.

This course examines the use of C++ in high performance computing applications. The course concentrates on the implementation of numerical methods in C++, and how object-oriented programming can create general classes for scientific applications. The course will be given on a Unix platform.

Using the CSAR Service

Prerequisites: Experience of programming in a Unix environment (Fortran, C, Java etc.).

This is a one day seminar for new users of the CSAR service. It provides basic information on how to use the systems and resources provided by this service. The following topics will be covered:

- Basic hardware configuration
- Files, file systems and tape archiving
- Available software packages (including shells, editors, compilers and applications)
- Compiling a sample program
- Submitting batch jobs on turing, fermat and fuji
- Basic profiling and debugging
- Self registration for new users
- Support (WWW, email, the helpdesk system, specialist applications staff, service quality tokens)

Porting/Optimising for the Cray T3E-1200E

Prerequisites: Fortran or C programmer with message passing experience, Unix.

This is a 3 day workshop which includes lectures and practical sessions.

The Cray T3E, which provides the major computing resource of the CSAR service, is a very powerful, but also a limited resource. This course is designed to provide information and instruction for programmers who wish to use the specific hardware features of the system to maximise the efficiency of their codes.

- System architecture

Parallel Vector Processing on Fujitsu VPP 300

Prerequisites: Fortran or C programmer with message passing experience, Unix.

This is a two day course with lectures and practical sessions which is designed to cover the fundamentals of vector processing, with specific reference to efficient usage of the Fujitsu VPP 300.

The following topics will be covered:

- System architecture
- Vectorisation
- Parallel issues specific to VPP 300
- Optimising tools
- Debugging tools

Forthcoming Events

Check out our list of conferences. This includes not only CSAR related events but details of all conferences related to High Performance Computing:

August 1999

17 - 20

Parallel Computing'99, Delft, Netherlands

31 - Sept 3

EuroPar'99 Toulouse, France

Semptember 1999

6-17

HPC Summer School in Distributed Memory Programming and Scientific Visualization, University of Manchester, England, UK

6-10

Parallel Computing Technologies (PaCT-99), St. Petersburg, Russia

9-10

Fifth European SGI/Cray MPP Workshop, Bologna, Italy

21-24

International Conference on Parallel Processing, Fukushima, Japan.

26-29

6th PVM/MPI European Users' Meeting (EuroPVM/MPI'99), Barcelona, Spain

28

HPC User Meeting, Queen Elizabeth II Conference Centre, Westminister

28 - Oct 3

International Workshop on Global Optimization 1999 - Firenze, Italy

29 - Oct 1

4th international working conference on Massively Parallel Programming Models, Berlin, Germany

30 - Oct 1

First European Workshop on OpenMP, Lund University, Lund Sweden

Forthcoming Events

October 1999

12-16

International Conference on Parallel Architectures and Compilation Techniques (PATC99), California, USA

19-21

The Third International Workshopon Advanced Parallel Processing Technologies APPT'99, Changsha, China

November 1999

13-19

Super Computing'99 (SC99), Portland, US

December 1999

17-20

6th International Conference on High Performance Computing, Calcutta, India

The CSAR Web site (http://www.csar.cfs.ac.uk/) has help and information on all aspects of the service, and includes sections on Software, Training, Courses, Registration & Project Mnagement, and links to other HPC sites.

CSAR Focus is also available to view on the Web: http://www.csar.cfs.ac.uk/general/newsletter.shtml.

CSAR News Pages

All aspects of the service will be described via these web pages (http://www.csar.cfs.ac.uk/general/news.shtml), but we will periodically provide additional information via email, particularly on new developments and other events associated with the service. If you would like to receive such information, please send a mail message to majordomo@mcc.ac.uk, without any headers or footers, with only the following line in the main body of the message:

subscribe csar-update email address

where the email address should only be included if you wish to receive the mail at a different address from that specified in your reply to field.

Getting Help

If you require help on any aspect of the CSAR service, you can contact the friendly CSAR Helpdesk Team. Desirae, Kaukab or Caroline will deal with your query promptly and efficiently.

CSAR Helpdesk by phone: 0161 275 6824/5997

Alternatively, you may contact the CSAR Helpdesk via email, which is just as prompt to respond, as your call will be automatically be logged using the latest call logging system (Action Request System).

CSAR Helpdesk by email: csar-advice@cfs.ac.uk

The CSAR Helpdesk is open from 8.30am - 6pm Monday to Friday, except on Public Holidays.

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