HECToR X2 Vector goes live

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Editorial

Welcome to the autumn edition of EPCC News. In this issue we hope to give you some insight into a few of the projects in which EPCC is currently involved.

The HECToR X2 Vector is now online! The X2 acceptance test was passed successfully back in July and full accounting was enabled in early August. Now some early access users are using the Vector system (see article on opposite page).

While the Condition-Based Monitoring project (see page 15) is coming to an end, many other projects continue and some are introduced in this issue. EPCC has a leading role in a number of current European collaborations, including ADMIRE (page 4) and PRACE (page 10), and we also provide a strong technical contribution to plenty of collaborations, such as OMII-UK (page 12), EUFORIA (page 7) and LSST (page 13).

It is autumn again, so we say goodbye to last year’s MSc students who have just successfully completed their 16-week dissertations (page 6)... and welcome to our new MSc students. Our MSc in HPC is now in its eighth year, while our HPC-Europa visitor programme is now five years old and will continue for at least another four years (page 5).

Sadly Sam Falconer and Margaret Jackson will both leave EPCC at the end of this year (see below) as both of them are taking early retirement. From everyone at EPCC, I’d like to say thanks to Sam and Margaret for your contributions and all the best for your retirement!

Farewell to Sam and Margaret

At the end of 2008, EPCC will say goodbye to two of our colleagues, Sam Falconer and Margaret Jackson, who are both taking early retirement. Sam and Margaret have a combined total of more than 20 years of service with EPCC and 46 years of service with the University of Edinburgh.

Sam Falconer has been responsible for managing EPCC’s accounts since he joined us in 1991. At that time, EPCC was just a fledgling organisation, which had only come into existence the previous year. EPCC was much smaller then, of course, and Sam brought the number of staff to 13 when he joined. That compares to some 75 staff now employed here.

Before joining EPCC, Sam worked for Rank Hovis flour mills for over 20 years, and prior to that he had worked for Lloyds Bank and Scottish Finance.

Sam says he has very much enjoyed his time working at EPCC, and will be sorry to leave us at the end of the year. However, he is looking forward to being able to spend more time with his wife, two children and three grandchildren.

Margaret Jackson joined EPCC in 2005 as the Training and Recruitment Co-ordinator. In addition to co-ordinating the training and recruitment of EPCC’s staff, Margaret is responsible for the administration of our MSc in High Performance Computing.

Prior to joining EPCC, Margaret worked for 10 years in the Department of Forestry and Natural Resources, administering their MSc, and then spent 16 years in the College of Science and Engineering Office, where she was a section manager. She was elected to the University Court as a non-teaching staff representative and was also on the University Expeditions Committee, whose purpose is not to fund expeditions, but rather to determine which expeditions can be endorsed by the University and be allowed to carry its name.

When she leaves EPCC at the end of November, Margaret looks forward to continuing her involvement with the Scottish Gymnastics Association, as a judge and as a tutor for schools gymnastic judging. She has recently set up Team Gym Scotland, which takes roadshows all over Scotland to encourage people to take up gymnastics. She is also looking forward to spending more time with her family (two daughters, six grandchildren and one great-grandchild) and hopes that she will finally be able to find the time to write a book - a work of fiction based on the lowland Scots folklore from the area where she grew up, near the Moorfoot Hills.

We would like to take this opportunity to thank Sam and Margaret for their contributions to EPCC’s success over the years, and to wish them all the very best for their retirement.
The HECToR Vector X2 component successfully passed acceptance back in July. The integration of the X2 with the HECToR XT4 went extremely smoothly thanks to the efforts of all involved. The resulting ‘XT5h’ hybrid supercomputer is the first X2/XT4 integration on this scale.

The Cray vector system – known as "Black Widow" – consists of 28 vector compute nodes, each of which has 4 Cray vector processors, making 112 processors in all. Each processor is capable of 25.6 Gflops, giving a theoretical peak performance of 2.87 Tflops. Each 4-processor node shares 32Gb of memory.

The Black Widow interconnection network has a point-to-point bandwidth of 16 Gb/s and a bi-section bandwidth of 254 Gb/s. The average ping-pong MPI latency is ~ 4.6 µsec.

The X2 systems were shipped from Cray’s factory in Chippewa Falls, Wisconsin on Friday 13th June and arrived on site for installation at the University of Edinburgh’s Advanced Computing Facility (ACF) on Thursday 19th June. Specialist temperature controlled air-ride vehicles were used to transport the equipment to Edinburgh from Heathrow airport. The equipment was installed by the local Cray team at the ACF aided by X2 product specialists from Cray in the US.

The HECToR X2 at the ACF

The X2s connect directly into the High Speed Network of the XT4 systems and are located adjacent to the XT4 cabinets. Unlike the XT4 which is air cooled, the X2 uses chilled water for cooling, therefore one of the first tasks was to connect in the water hoses to the cabinets. Once power was applied, the cabinets were allowed to stabilise in the new environment before being exhaustively tested with a suite of diagnostic software.

Integrating the X2s into the XT4s required a service shutdown and a number of configuration changes needed to be made. Full accounting was enabled on the X2 in early August and early access users from a number of projects are currently using the system. These early access projects have been chosen to represent a broad range of sciences from across EPSRC1, BBSRC2 and NERC3 funded research.

To find out more about the HECToR service, including how to apply and the cost of access for both the XT4 and X2 systems, see: www.hector.ac.uk.

1. www.epsrc.ac.uk
2. www.bbsrc.ac.uk
3. www.nerc.ac.uk

Liz Sim, EPCC, and Steve Jordan, Cray Systems
ADMIRE: Making data-mining easier

Ally Hume

Today’s growing wealth of digital data in Europe is poorly exploited. Advances in storage, pervasive computing, digital sensors and instrumentation have led to massive growth in the volume of data collected and the number and complexity of data repositories. This growing wealth of data has an increasing potential to yield great benefits to citizens, science and business as it contains vital hidden knowledge.

Typically, to extract that knowledge requires data-mining combinations of data from multiple data resources. Designers, diagnosticians, decision makers or researchers who need such knowledge face difficult hurdles. To extract information from heterogeneous and distributed sites they have to specify, in great detail, the sources of data, the mechanisms for integrating them and the data mining strategies for exposing the hidden gems of information. Consequentially, with the current state of the art, most of that hidden knowledge remains undiscovered.

EPCC is leading a European Union-funded research project to develop a solution to this huge data challenge. The ADMIRE project (Advanced Data Mining and Integration Research for Europe) will accelerate access to, and increase the benefits that can be gained from, data exploitation for the European citizen and economy. It will achieve this by delivering consistent and easy-to-use technology for extracting information and knowledge. To cope with complexity, change and heterogeneity of services, data, and processes, an abstract view of data-mining and integration will be provided. This will provide power to users and developers of data-mining and integration processes.

ADMIRE will explore two detailed data-intensive scenarios to test the technology:
1. Flood modelling and simulation.
2. Customer relationship management.

The flood modelling and simulation application is a cascade of meteorological, hydrological and hydraulic models, which together allow users to predict flood hazards based on meteorological forecasts. ADMIRE provides an excellent opportunity to advance the model, and provide additional analytical tools which will speed up the simulation process and allow users to take better-informed decisions in controlling the workflow and data management within the application.

ADMIRE - Advanced Data Mining and Integration Research for Europe

Project co-ordinator:
The University of Edinburgh (UK)

Partners:
University of Vienna (A)
Universidad Politecnica de Madrid (E)
Ústav informatiky, Slovenská akadémia vied (SK)
Fujitsu Labs of Europe (UK)
ComArch S.A. (PL)

Duration: 3 years
Total cost: €4,346,077
Programme:
Seventh Framework Programme Theme ICT-1-1.2

Continues opposite.
HPC-Europa 2: 2009 and beyond...

Chris Johnson, EPCC

Many of you will already be aware of the HPC-Europa Transnational Access visitor programme which presently offers researchers from throughout the European Union and associated states the opportunity to visit one of six high-performance computing centres in Europe. Visitors are given access to top-of-the-range computing facilities at the same time as collaborating with a scientific expert.

HPC-Europa’s visitor programme is now in its fifth year and we are pleased to announce that the programme is set to continue for at least another four years, starting in January 2009. The new programme will be both bigger than the present one – with the addition of two new partners, CSC based in Finland and GENCI based in France – and better. We will have considerably more computing time available for visitors than at present as well as the possibility of offering “virtual visits” where successful applicants can apply for computing time and support from one of the HPC centres without the need to travel. This is something which we hope will appeal both to more senior researchers, who may have little time for travel, as well as to other researchers who have already visited a centre and have codes up and running.

Applications can be submitted at any time and the selection panel meets four times per year. The next closing date for applications to visit in 2009 is November 15th 2008. Please see: www.hpc-europa.org

EPCC has run a visitor programme since 1993, having hosted nearly 700 visitors and we will continue to lead the visitor programme for the next four years. However, the HPC-Europa project actually consists of much more than just a visitor programme, with supporting activities covering a whole range of topics related to HPC.

The new project will include joint research activities looking at HPC programming on massive parallel architectures, tools for scientific data services and the setting up of a “virtual cluster” as a way of simulating a parallel environment on a desktop machine. There will also be networking activities focusing on training and the wider HPC community.

EPCC will be involved in all of these activities and in addition to managing the visitor programme we will be leading the training activity where we will co-ordinate tasks providing both on-site and “virtual” training sessions, seminars, tutorials and workshops.

The customer relationship management application provides support to “front office” business processes including sales, marketing and service. Each interaction with a customer is generally added to a customer’s contact history, and staff can retrieve information on customers from the database as necessary. Through integrating the CRM application with ADMIRE the application will be extended from a tool primarily for sales operatives to an analytical tool for managers, allowing them to respond more quickly and accurately to customer needs.

Europe leads the world in its use and development of advanced service-orientated business solutions. By focusing on advanced data-mining and integration, ADMIRE will advance such enterprise systems by showing how an integrated approach can deliver significant new capabilities with which to address the next generation of digital data challenges.

As well as managing the project, EPCC also provides a strong technical contribution based upon previous experience of developing the OGSA-DAI data access and integration technology that will play a major part in the ADMIRE architecture. Additionally EPCC brings considerable data-mining experience from previous commercial and research projects.

www.admire-project.eu
Another year has just started for the MSc in HPC. The programme continues its global appeal; this year we have students from across the UK and mainland Europe, Asia and North America. Meanwhile, last year’s students have now moved on to a variety of jobs and research studentships, including employment here at EPCC.

For many students, a major highlight of the degree is the 16-week dissertation. Projects are available using a wide range of HPC systems and parallel technologies. To illustrate the range of projects undertaken by students, we present here some of the dissertation projects from 2007/08.

**Paul Woodhams: Investigation of Fault Tolerance in MPI Applications**

This project investigated the development of fault tolerant MPI applications. A fault simulation library was designed and implemented, involving the generation of random errors and notification of errors to other processes via a unique global state variable accessed using MPI single-sided communications. The use of this fault simulation library was demonstrated for taskfarm and image processing applications using disk checkpointing as the method of recovery.

**Jim Enright: Vector Processors and Novel Languages**

Four application codes, three computational fluid dynamics (CFD) and one molecular dynamics (MD), were ported to the HECToR system and another vector system, the Cray X1E. A performance analysis of each application was carried out to characterise them to be suitable for the vector or scalar system, including profiling to understand the differences in performance across the systems.

**Thom Haddow: Task Parallel Constructs in Chapel**

This project explored the task parallel constructs in Chapel, a new parallel language from Cray. Performance results were obtained from a suite of benchmarks developed for the language and compared with equivalent benchmark implementations written in C/Pthreads.

**Peter Foster: Parallel Combinatorial Optimisation for Finding Ground States of Ising Spin Glasses**

This project dealt with the Ising spin glass ground state problem. Based on parallel matrix/vector multiplication, cost optimal parallel algorithms for the message passing architecture were developed, using collective or alternatively cyclic communications. Dynamic programming codes were evaluated on a small-scale AMD Opteron based SMP system and on HPCx.

**Ian Kirker: Demanding Parallel FFTs: Slabs & Rods**

The performance of a 3D parallel FFT routine using slab and rod decompositions and the FFT libraries available on each platform were compared on seven different platforms – HECToR, HPCx, Ness, BlueSky, MareNostrum, HLRB II, and Eddie.

**Ali Khajeh-Hosseini: Orchestration of OGSA-DAI Services**

The aim of this project was to provide support in the OGSA-DAI Client Toolkit for the orchestration of OGSA-DAI services. This was achieved by providing users with a higher level of abstraction with which they could create a single high-level workflow that could target individual activities at different OGSA-DAI servers. An Orchestration Engine was developed that processed this high-level workflow and performed the orchestration automatically.

These reports, together with dissertations from previous years, are all available on the MSc website: www.epcc.ed.ac.uk/msc
HECToR X2 Vector goes live

EUFORIA

Adam Carter

EUFORIA is a European-funded project that aims to provide HPC and Grid resources to the European fusion research community. It will provide European fusion scientists with the simulation modelling tools and platforms that they will need to obtain experimental time on ITER (see EPCC News 62).

The project has been running since the start of the year and EPCC has been involved in looking at several different codes in an activity whose primary goals include optimisation and parallelisation of existing fusion codes. To date we have ported CENTORI, GEM, ERO and ELMFIRE to run on HECToR, the national Cray XT5h machine run by EPCC.

These codes vary considerably in both the problem they are trying to solve and the complexity of the existing code. In many cases the code authors have some experience in parallel computing and have taken care to write their codes with performance in mind, but often this has involved optimising the code for the platform which they had available to them at the time. Furthermore, although the authors of the codes are experts in their field and have written quite complex codes to solve their problems, not all of them have the expertise in parallelisation and performance optimisation that the partners in the EUFORIA project are able to provide. The code authors themselves are not directly involved with the project and so we have to take care to ensure that the work we are doing on the codes is both helpful and compatible with their ongoing work in improving and modifying their codes to address different scientific questions.

There are many steps involved in actually creating an optimised version of the code, and much of the first year of the project has been involved in the important ground work required. The first step in this process for us at EPCC has been to ensure that the codes run on the HECToR platform. In some cases the codes have been run on a Cray before, in which case the process is quite straightforward and consists mainly of updating Makefiles to point to the correct libraries. In other cases, the code has not previously run on a Cray system, and it has been necessary to make more major changes to those makefiles which rely on features specific to a certain compiler or machine.

Once the codes were ported, our next task was to understand the current performance of the codes. By using profiling tools such as CrayPAT we have been able to look at the performance of the codes and how this varies as input parameters such as the system size and the number of processors on which the code is run are altered. From this it is possible to pinpoint those routines which are taking the most time and to identify those routines which become increasingly dominant as the number of processors is increased.

We are also able to use other features of CrayPAT to look at the serial performance of the code and symptoms such as cache misses which point to areas of the code whose performance has the potential for optimisation. This more experimental approach to studying the codes allows us to make decisions about those parts of the code which could be improved without having a detailed knowledge of the workings of the code. Once we have identified features of the code which are candidates for optimisation it is possible to combine this information with knowledge of the structure of the codes in order to find ways in which the programs’ performance can be increased.

The next step, which is now beginning, is the difficult step of using this knowledge to actually improve the performance of the codes. The project will identify a subset of the codes under investigation in the project. Efforts will be made to optimise theses codes and the results will form a deliverable which is due at the end of this year.

www.euforia-project.eu/EUFORIA
The Blue Phase of liquid crystals

Davide Marenduzzo and Oliver Henrich, School of Physics and Astronomy, and Kevin Stratford, EPCC

HPC coming to your TV screen soon
The Hector supercomputer service, based at the University of Edinburgh, gives UK scientists the opportunity to look at extremely large and time-consuming computational problems. As one such example, the Soft Matter Physics Group at The University of Edinburgh and EPCC has been using the service to investigate the properties of a number of different types of system, including liquid crystal blue phases.

Liquid crystals are technologically important substances sharing some of the properties of both liquids and crystals. In particular, the ‘crystal’ ordering of the rod-like molecules in liquid crystals is on a length scale which gives them interesting optical properties in the visible part of the spectrum, hence their use in display devices such as televisions.

At high temperature, a liquid crystal is in the “isotropic phase”, with molecules pointing all over the place. On cooling, the molecules orient themselves. For example, in the case where the average orientation, known as the director field, points the same way throughout the liquid crystal is in a nematic phase. In most current liquid crystal display (LCD) devices, a twisted nematic is used in which the director field is made to rotate in a helical fashion about a well-defined axis. However, in the cholesteric phase this helical twist occurs naturally, making them attractive for use in LCD devices.

The blue phases are cholesterics with a twist – both literally and metaphorically. Very close to the transition between the isotropic and cholesteric phases, a simple helical order is frustrated and it is more advantageous for the director field to rotate in a complicated helical fashion named a double twist cylinder.

Topologically, it is impossible to patch together different double twist cylinders without creating defects in between, and this gives rise to the defect or disclination network observed in the blue phases (see pictures), and is responsible for many of their remarkable physical properties.

Blue phases “totally useless” says expert
Blue phases have a fascinating history. They were first reported in the late 19th century by the Austrian biologist Friedrich Reinitzer. Reinitzer was interested in cholesterol in plants, and during his experiments observed under his microscope some of the optical effects we now know to come from liquid crystals. (Unsurprisingly, the blue phases were so-called because of their striking blue appearance.)

Not knowing what to make of his finding, Reinitzer enlisted the help of German physicist Otto Lehmann and so the study of liquid crystal began. However, it appeared that these new substances had no practical use so were forgotten, and remained largely neglected for almost a century.

While an initial theoretical explanation of the appearance of blue phases appeared in the 1980s, blue phases were broadly considered of limited interest, mainly because they were only stable in a very narrow temperature range (about 1 Kelvin) close to the isotropic-cholesteric transition. In 1983, a world-leading expert on liquid crystals, F. C. Frank, said of blue phases: “They are totally useless, I think, except for one important intellectual use, that of providing tangible examples of topological oddities, and so helping to bring topology into the public domain of science, from being the private preserve of a few abstract mathematicians and particle theorists.” In the 21st century, this view has now radically changed.

Important technological advances have increased enormously the stability range to about 50 Kelvin [2,3], and in May this year Samsung presented the first ever blue-phase based liquid crystal display at the SID 2008 International Symposium. This new
Four snapshots of the evolution of a liquid crystal blue phase droplet growing in a cholesteric background, from a simulation on the Hector system. The picture shows the complex topological defect structure which plays an important role in its useful properties.

display is able to operate at an unprecedented frame frequency of 240 Hertz, does not require alignment treatment for the liquid crystal, and may make existing twisted nematic displays obsolete.

However, in order for this exciting technological potential to be realised fully, our understanding of blue phases needs to become as quantitative as that of conventional nematic liquid crystal displays. The Edinburgh Soft Condensed Matter Group, accordingly, has dedicated a significant research effort (funded by a recent 3-year EPSRC grant) to study the dynamics of blue phases with large-scale computer simulations of the sort undertaken on HECToR. These calculations have already shown that they have the potential to improve remarkably our understanding of blue phases [4].

Modelling liquid crystals requires significant computational resources. First, the liquid part of the problem must be accounted for by solving the Navier-Stokes equations for fluid flow. This in itself is a time-consuming problem for which we use the highly parallel lattice Boltzmann method, which discretises the equations on a regular grid. Along with this are the so-called Beris-Edwards equations which, broadly, describe the motion of director field and its interaction with the fluid flow. Representing the director field requires storing a matrix at lattice site in the fluid, which gives rise to a large memory requirement which cannot be satisfied on a serial machine. By examining the properties of the director field, it is possible to work out the location of the disclinations as shown the pictures. It is also possible to use this information to compute how the structures might transmit light, which is important when considering possible display applications.

On HECToR, we have used cubic lattices of up to 256 on a side for this type of calculation. We have run the calculations on up to 4096 processors, approximately half the machine’s capacity. As with any calculation of this type, a large system is required to avoid artefacts associated with the edges of the lattice which would render the results invalid.

Current work in Edinburgh [5] focuses on understanding the growth of blue phase droplets in cholesteric or isotropic background, which has been observed in experiments but never modelled. Work is also planned on the behaviour of blue phases in electric fields, with the goal of understanding the experimental phase diagrams and thus future device design.

References
EPCC leads
PRACE activity
on software for
Petascale systems

Alan D Simpson

EPCC has a leading role in a number of current European projects. In PRACE (Partnership for Advanced Computing in Europe), we lead Work Package 6 (WP6) which is responsible for investigating Software for Petaflop/s Systems.

PRACE is intended to make preparations for the creation of a persistent pan-European HPC service, based on an infrastructure of around 4–5 Petaflop-scale supercomputers. There are PRACE partners in most European countries who work on activities ranging from the governance and legal framework for the future infrastructure, through dissemination and training, to a number of technical activities looking at possible hardware and software for Petascale systems.

EPCC has overall responsibility for WP6, which is the largest technical activity and involves all the PRACE partners. WP6 is responsible for investigating the software on future Petaflop systems and its primary goal is to identify and understand the software libraries, tools, benchmarks and skills required by users to ensure that their application can use a Petaflop/s system productively and efficiently. Analysing the application requirements for these systems is a major challenge but is vital to ensure the systems meet the needs of European researchers.

The prevalence of multi-core technology indicates that future Petascale systems are likely to have hundreds of thousands of cores. Many heavy-used applications codes are not yet able to effectively exploit these large numbers of cores. A key element of WP6 is ensuring that we understand how the major applications codes used across Europe can exploit these large systems.

The initial tasks have been in the identification of the applications’ requirements. These are an important input into another work package that will translate the identified applications’ requirements into architectural requirements for prototypes and future production systems.
So far in WP6, we have performed and analysed surveys of:
1. the major European HPC systems
2. the key applications
3. the major users of such systems.

This should help build up a complete picture of the requirements for future production systems. As discussed in the last issue of EPCC News, WP6 has already used these survey results to identify a list of applications that:
• are representative of the current usage of HPC systems in Europe
• span the scientific areas which exploit HPC
• include examples of the various classes of algorithms
• are widely used across Europe.

Much of the rest of WP6 will be working with these representative applications. They have already been used to analyse the key characteristics and requirements of European applications, and communicating these to the work packages responsible for prototype hardware.

During the remaining 15 months of PRACE, the initial analysis of the applications will develop into more detailed work in Petascaling and optimisation for these applications as well as a general investigation into the techniques required to exploit future systems. We will also investigate the software libraries and programming models required by the applications and how this will translate to the Petascale domain.

The representative applications are intended to form a benchmark suite that will be packaged up by WP6. This benchmark suite will be used to evaluate prototype systems, and may also be used in future Petascale procurements.

PRACE is a great opportunity to demonstrate that Europe’s top HPC centres can collaborate effectively to the benefit of researchers. EPCC is happy to be active in this collaboration and to take responsibility for an important work package ensuring that applications codes can efficiently use future Petascale systems.
OMII-UK: enabling e-research

Mario Antonioletti

OMII-UK is a partnership between three successful UK e-Science projects and it came into being as a virtual organisation in January, 2006. Collectively this group, under the OMII-UK banner, encompasses a significant body of knowledge, expertise and talent. The partners are:

- **OMII at Southampton University.** Originally tasked with curating, hardening and providing support for software produced by projects funded through the UK e-Science Grid Core Programme as these projects came to an end. The UK e-Science Grid Core Programme aimed to give the UK global prominence in establishing frameworks and pilot studies for distributed collaborative science, which it succeeded in doing.

- **The myGrid team.** Based at the University of Manchester. It is responsible for, among other things, Taverna – a client-based workflow-authoring tool and enactment engine widely used within the Biosciences community and now with users in several other research fields.

- **The OGSA-DAI team** at EPCC and the National e-Science Centre in Edinburgh. OGSA-DAI provides a data access and integration middleware platform that grid developers may use to solve their data access and integration requirements.

OMII-UK’s remit under its current director, Neil Chue Hong, is to enable e-Research, both within the UK as well as further afield. Instead of focusing solely on the archiving of software, OMII-UK liaises with researchers, developers and funders to provide the expertise and services required to grow the e-research community.

OMII-UK is also very active globally, participating in open standards development through the Open Grid Forum, attending many conferences to liaise with e-researchers and providing training events to specific communities. To conclude, OMII-UK is here to help the UK e-research community, which generally means people like you! Visit the OMII-UK website and see what components OMII-UK already provides and how others have used them to help their projects. If you do not find what you require, or if you have a great idea for other components to enable your e-research, get in touch:

info@omii.ac.uk

OMII: www.omii.ac.uk
The Large Synoptic Survey Telescope (LSST) [1] is a US project that is both publicly and privately funded (the private funders include Google and Bill Gates). The telescope will operate in the visible band and be based in Northern Chile. It is expected to see first light sometime between 2013 and 2015 and to start work for ten years from about 2016 onwards. It is to cover the entire visible sky, where the same parts of the sky will be re-visited several times each night (if you wondered what synoptic means).

This project will cover a huge variety of scientific goals:
1. Constraining dark matter and dark energy.
2. Mapping the Milky Way (about $10^{10}$ stars).
3. Exploring the transient sky.
4. Inventorying the Solar System.

The exploration of the transient sky, for example, will allow the detection of objects that change on a small time scale, such as Potentially Hazardous Asteroids (PHAs), and rapidly changing objects, such as exploding supernovae. Alerts for events such as gamma ray bursts are to be launched within 60 seconds to allow astronomers to follow them up by studying them with more specialised telescopes.

The major component of the $37M operational cost per year will be due to data management operations. The LSST is expected to produce amounts of data which are huge compared with today’s standards. Per night about 30 TB of raw image data are expected. This will accumulate to 60 PB over 10 years and more than 30 PB for the online query catalogs [2].

There will be a Mountain Summit/Base Facility at the location of the telescope, a central archive facility and multiple Data Access Centres (DACs). The data will be transported via existing high-speed optical fibre links from Chile to the US.

EPCC, the Wide Field Astronomy Unit (WFAU) at the IfA and NeSc are collaborating under eDIKT2 to assess the data management requirements of the LSST. The goal of this half-year project is to build up the necessary expertise so that Edinburgh (EPCC, WFAU and NeSc) will be in a front-line position among European applicants if the UK is going to buy into the LSST corporation. This will allow European astronomers to have faster access to the data.

EPCC and WFAU are currently assessing the technical requirements to host a DAC. There will be several DACs worldwide, most of which will be located in the US. The purpose of the DACs is to receive the raw data, run analysis code via LSST’s so-called pipeline software and make the released data available to the users: astronomers who want to use the results for their research. These users will access the data through iRODS [3] controlled file access. The acronym stands for `i Rule Oriented Data Systems`. It is an adaptive middleware architecture which extends the functionality provided by Grid middleware such as SRB (Storage Resource Broker). Its purpose is to allow data and metadata sharing where the data are distributed across heterogeneous resources. The adaptiveness of iRODS allows the middleware to be adapted to the users’ needs without having to change the hardwired coding. All changes are set by rules instead.

[1] www.lsst.org
Initially, the PCP client is used to submit a job token, which is forwarded to the first site listed in the clique, which then launches a monitoring subprogram to track the token activity. The NPM is executed, and the token is forwarded to the next site in the clique, and the subprogram goes into a locked state, awaiting the return of the token once it has circulated throughout the clique. The token arrives at the next site in the clique, and the process is repeated. At the last site in the clique, the token is then forwarded back to the first site, changing it to an unlocked state, the NPM is freed to run at the next scheduled time, and subsequently the token is circulated around the clique again, and so on.

The operation of the PCP is based on a system of tokens which can be passed around the sites involved in the NPMs. These tokens can perform a variety of operations, but the main function is the job token. This token contains information such as which NPM is required to be run, how often it is to be executed, and at which sites (referred to as a clique of sites). There can be several such cliques in operation at any given time (see figure).

The PCP token mechanism is important as it provides various benefits. Because a site will not run its NPM until it has received the token from the previous site in the clique, overlapping measurements are avoided. In addition, the measurements can...
EPCC’s engagement in ITI Techmedia’s Condition-Based Monitoring (CBM) Programme is now nearing its conclusion, and it’s been an interesting journey.

The CBM Programme is the sixth research and development programme for ITI Techmedia, the organisation which develops market-driven intellectual property for the benefit of Scotland. CBM is a three-year, £4.75M programme which aims to apply sensors and network technology to develop a condition-based monitoring platform with applications across a range of industries.

From EPCC’s perspective, the programme has consisted mainly of two activities. The first was concerned with the collection of large amounts of sensor data. The second involved the development of analysis techniques to make sense of the data, and find patterns in the data which would allow us to monitor and predict various conditions.

Here at EPCC we were able to set up an automated data workflow to capture and store the flood of data collected. The raw data originated at research installations engaged by ITI Techmedia in the Programme. The workflow system provided an easy way for them to transfer this data to us, where it was then automatically checked and archived. Our Advanced Computing Facility was a natural home for both the data and a dedicated compute resource for data analysis. This system became a cornerstone of the project.

As the lead developer for this project, my activities have been many and varied. I’ve spent time herding several terabytes of data, assisting Programme collaborators in the analysis of said data and troubleshooting various parts of the process along the way. The project has been both challenging, interesting and fun.

One of the things which has impressed me about this project is the way that we’ve worked with the rest of the team brought together by ITI. Distributed programmes present their own set of challenges, as both distance and organisational barriers can lead to communication problems. In this programme, we had excellent working relationships with all of the other participants.

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ITI Techmedia: www.ititechmedia.com

One of the key features is support for maintaining a clique despite the failure of one of the sites. If the expected token does not arrive within the pre-determined timeout limit due to a site failure, a new token is generated, the NPM is executed and the regenerated token passed on to maintain the clique. This mechanism can continue indefinitely, so once the failed site is returned to service, the clique still exists and the site will thus receive the token as it circulates, and rejoin the clique.

Of course, the most important feature is the removal of the requirement on having system administrators available in order to set up or change measurement, or manage cliques. These functions can be performed via the PCP client, along with various other administrative activities. There are several other features of the PCP including: support for certificate-based security; a plug-in design for straightforward adaptation to different requirements beyond the field of NPMs; and portability across multiple platforms.

For more information on PCP, or to download the software along with comprehensive user, developer and installation guides, please see:

www.egee-npm.org/pcp

The PCP work was undertaken as part of the Enabling Grids for eScience (EGEE-II) project and jointly funded by the Joint Information Systems Committee (JISC). It is currently being considered for deployment in the Grid Network Performance Monitoring for UK e-Science (GridMon) project.

EGEE: www.eu-egee.org
JISC: www.jisc.ac.uk
GridMon: gridmon.dl.ac.uk
EPCC at SC08
15–21 November, Austin, Texas

Music is in the air at this year’s SC’08, the International Conference for High Performance Computing, Networking, Storage and Analysis.

The conference is being held in Austin, Texas, which is billed as the "live music capital of the world". A number of extra activities have been added to the conference schedule to encourage attendees join in the musical theme, including: ViSCIiTunes, a call for people to add music to their scientific visualisations and submit them to a conference wide playlist; a competition to try to identify songs generated by a computer and those composed with real instruments; and a live music room for attendees to perform in.

Away from the musical theme, SC08 marks the 20th anniversary of the first conference, then known as Supercomputing, held in Orlando, Florida in 1988. A number of events are planned to celebrate this event through the duration of the conference. The conference committee is also looking for contributions from people who have attended all 20 SC conferences. The 20th SC conference also sees a broadening of the scope of the program with two Technology Thrusts, one focusing on renewable energy and energy efficiency research, the second focusing on biomedical informatics including computational and systems biology.

If you are at SC08, you can find EPCC at booth number 2329, alongside STFC Daresbury Laboratory in booth 2325.
www.sc08.supercomputing.org

High Performance Reconfigurable Computing: using FPGAs for HPC
26-27 November 2008, EPCC, Edinburgh

The primary aim of this course is to provide potential users of Maxwell, the 64-FPGA supercomputer, with a solid grounding in getting the most from the machine. As well as providing the necessary background in FPGA and HPC technologies, high-performance reconfigurable computing (HPRC) and the FHPCA Parallel Toolkit (PTK) the material will cover logging in, software development tools, job submission and other key usability topics.

For more details on Maxwell see: www.fhpca.org/maxwell.html
For more details on the course and a registration form see: www.hpcx.ac.uk/support/training

EPCC is a European centre of expertise in developing high performance, novel computing solutions; managing advanced systems and providing HPC training. Our clients and partners include local and global industry, government institutions and academia. EPCC’s combination of advanced computing resources and expertise is unique and unmatched by any European university.

www.epcc.ed.ac.uk info@epcc.ed.ac.uk