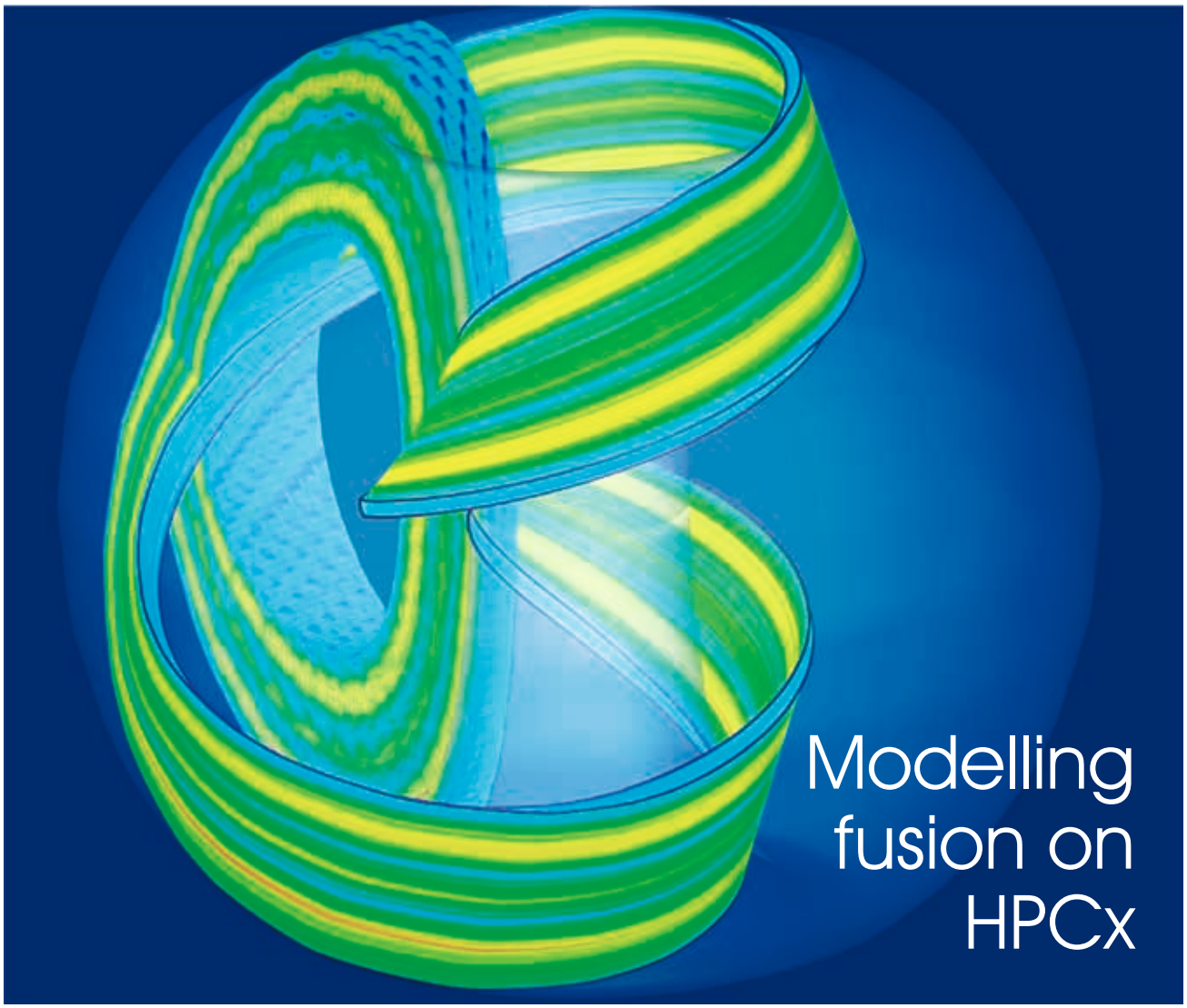
Capability Computing

The newsletter of the HPCx community

[ISSUE 6, AUTUMN 2005]



Modelling fusion on HPCx

CONTENTS

Editorial

Fiona Reid,
HPCx Terascaling Team

Welcome to the sixth edition of *Capability Computing*, the newsletter of the HPCx community. The HPCx user base has continued to grow and we now have over 600 registered users from 64 different projects using the system. We would like to extend a warm welcome to all the projects and users who have joined since the last issue.

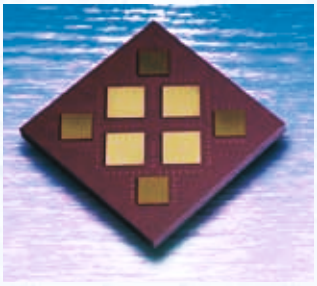
This is an exciting time for HPCx users. We are very pleased to announce that HPCx will shortly be upgraded to a Power 5 system. Further details of the forthcoming upgrade are given below.

In this edition our main theme is capability science on HPCx. We present three science articles from users of HPCx. The articles describe subjects ranging from modelling fusion to investigating radiation damage to molecular dynamics of biomolecular systems.

We also have an article on the new features of the IBM Fortran compiler, xlf 9.1, and an article on task farming on HPCx.

The Third HPCx Annual Seminar titled 'Capability Science on HPCx' is being held in Daresbury on December 5th 2005. The seminar will include talks from HPCx users, HPCx staff and IBM personnel and will be followed by the HPCx User Group meeting. See page 16 for details.

Finally, I would also like to draw your attention to the August 2005 issue of *Philosophical Transactions of the Royal Society of London Series A; Theme Issue on Scientific Grid Computing*. Many of the articles are HPC-related and make use of HPCx. Further details can be obtained from:
http://www.journals.royalsoc.ac.uk/link.asp?id=h88056h75554



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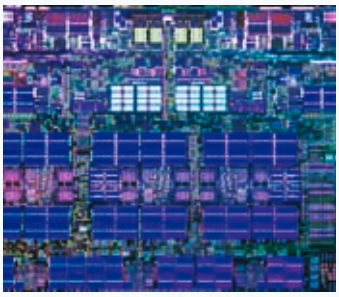
HPCx to be upgraded to Power 5

Alan Simpson, HPCx Project Director

The HPCx consortium has recently had approval from EPSRC for a significant upgrade of the HPCx system. The current Power 4+ system will be replaced by a Power 5 system in November 2005. The Phase 3 upgrade, which is due in 2006, will also now be a Power 5 system.

The Power 5 systems will be based on Power 5 p5-575 dual core compute nodes with a frequency of 1.5 GHz; each node has 16 CPUs and 32 GB of memory. The initial system to be installed in November will consist of some 96 nodes connected through the High Performance Switch making a total of 1536 Power 5 CPUs; this should ensure that the new system at least matches the performance of the existing Power 4+-based system.



Moreover, each processor will have double the memory of the existing processors and the total memory will be more than 3TB, which is almost double the current total. This enhanced memory addresses one of the most important issues raised by users and should allow significant new capability science. We have already been working closely with IBM to plan the upgrade in such a way as to minimise disruption to users and to ensure that the SC2005 experiments are successful. The new Power 5 system will be built alongside the existing one. We anticipate a break in service of a maximum of two days while we transfer to the new system.

The timetable for the Phase 3 upgrade has not yet been finalised but it will happen during next year. This will involve adding additional Power 5 nodes on to the switch infrastructure to roughly double the performance and the total memory.

Upgrading HPCx to Power 5 will allow the service to remain on IBM's key technology curve throughout its lifetime, i.e., until at least the end of 2008. This will ensure that users gain maximum benefit from future improvements in compilers and other tools, libraries and improvements to the switch performance.

Come and see us at SuperComputing 2005 'Gateway to Discovery'

12th-18th November, Seattle, USA

Adrian Jackson and Fiona Reid, HPCx Applications Support Team

Both EPCC and CCLRC Daresbury Laboratory will, as in previous years, be exhibiting at this year's conference for High Performance Computing, Network, and Storage: SuperComputing 2005. SC|05 is being held in the Washington State Convention and Trade Center, in Seattle, from the 12th to the 18th of November. Under this year's theme of the 'Gateway to Discovery', SC|05 promises to be an exciting mix of exhibitions, lectures, tutorials, and technical events from the world of High Performance Computing.

HPCx will also be playing a part at SC|05. It is one of a number of resources that will be used by SPICE (Simulated Pore Interactive Computing Experiment) who are finalists for the HPC Analytics Challenge. SPICE is part of a UK-US collaboration jointly funded by EPSRC and NSF which will be performing a set of steered large scale molecular dynamics simulations using a federated trans-Atlantic Grid combining the UK National Grid Service and US TeraGrid.

As well as having a booth in the exhibition space, EPCC will also be giving a half-day tutorial on 'Application Performance on the Blue Gene Architecture', presented by Dr Lorna Smith, Dr Mark Bull, and Dr Joachim Hein.

If you are at SC|05, you can find us at booth numbers 136 (EPCC) and 132 (CCLRC Daresbury Laboratory). We hope to see you there!

EPCC becomes one of the two UK High End Computing Training Centres

Adam Carter

EPCC and the Centre for Scientific Computing at the University of Warwick, have been chosen by the UK's Engineering and Physical Sciences Research Council (EPSRC) to be the two UK High End Computing (HEC) Training Centres.

The centre at EPCC will provide postgraduate training at Masters level. Students who come to the centre will be undertaking a PhD in their own scientific discipline at their own UK academic institution, but instead of the usual three-year studentship, they will be on a longer, four-year HEC Studentship programme leading eventually to a PhD. Over the first three years, they will take a number of courses at EPCC followed by an HEC research project. This all leads to an additional qualification: an MSc in High Performance Computing from the University of Edinburgh.

To combine the PhD and MSc programmes successfully, students are formally enrolled as part-time students at the University of Edinburgh. They will usually visit us for two blocks of seven or eight weeks for the taught part of the course, spread out over their first three years of study. This will allow them to meet and share experiences with their fellow MSc students without having to spend too much time away from their home institution where they will be doing the PhD research. Students will spend the first six months at their PhD institution and then come to EPCC for the first set of courses after Easter.

The training that we provide covers a wide range of useful and exciting areas in HEC. This includes how to write high-quality computer programs, how to make programs effectively utilise the world's largest supercomputers, how to use Grid technologies to harness the Internet effectively, visualisation of scientific results and the mathematical tools and techniques that underpin computational science and engineering. Graduates of the MSc in HPC will have acquired skills that make them employable in a wide range of careers ranging from postdoctoral academic research beyond their PhD, to jobs in commercial information technology.

The MSc in High Performance Computing is a well-established programme providing an excellent grounding in HPC technologies and their practical application.

Arithmetising plasma turbulence: the 'final frontier' of classical physics

P J Knight, C M Roach, A Thyagaraja, D J Applegate and N Joiner, UKAEA Fusion, Culham Science Centre

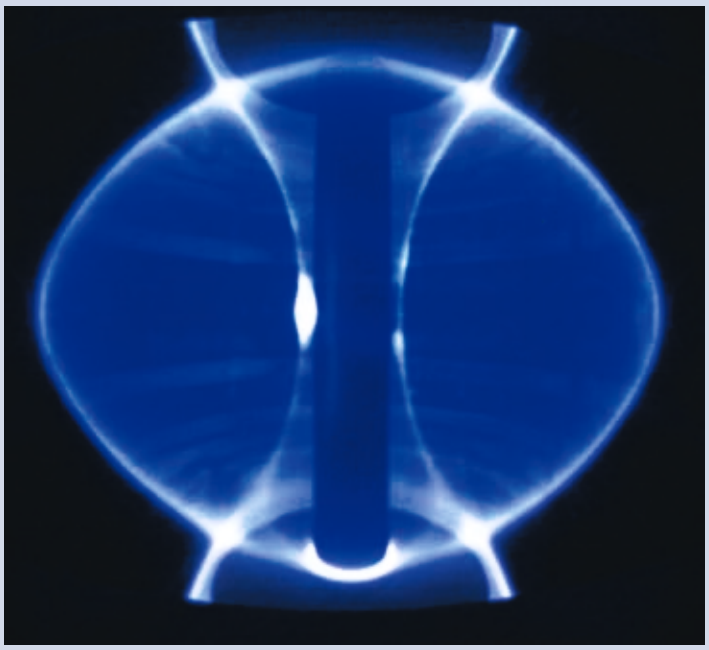


Figure 1 (above): Photograph of a spherical tokamak plasma from the MAST experiment at Culham.

Figure 2 (below): The flux-tube domain of GS2 follows the magnetic field and forms a small sub-region of the plasma.

The late Nobel Laureate, Hans Bethe demonstrated that thermonuclear fusion powers the stars. In July of this year Cadarache in France was chosen to be the site for ITER, the world's largest machine dedicated to research into the production of energy from controlled thermonuclear fusion. ITER is designed to demonstrate that safe, clean electricity can be produced economically. When ITER begins to operate in about ten years it will aim to demonstrate that fusion can fulfil the energy requirements of the modern world without concomitant greenhouse gas production or need for disposal of long-lived radioactive wastes.

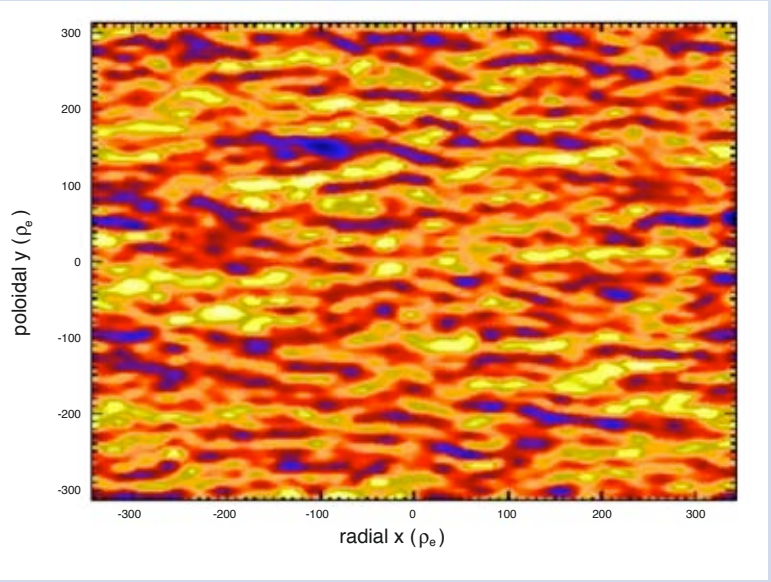
Achieving controlled thermonuclear fusion of light elements on Earth is not easy. In ITER and machines like it, a hot, ionised gas called a plasma must be confined for several seconds in a carefully designed 'magnetic bottle' well away from material walls. For fusion to take place in the deuterium-tritium fuel mixture (these are heavier isotopes of hydrogen, with one and two extra neutrons respectively), the temperature ($\geq 100\times10^6$ °C) must exceed by ten to twenty times that prevailing in the core of the Sun. The high temperature is needed to overcome the 'Coulomb barrier' to nuclear reactions between the deuterium and tritium nuclei. The magnetic fields (~5 Tesla) must be large enough to contain the plasma at a few atmospheres so that sufficiently many reactions can take place and the total power produced by them is significantly larger (>10 times) than that needed to heat the plasma. This plasma confinement approach leads to a doughnut-shaped device known by its Russian acronym, tokamak (toroidal, axisymmetric magnetic chamber).

UKAEA carries out fusion research for the UK Government and EURATOM at the Culham Science Centre in Abingdon, where research in experimental and theoretical physics and engineering tasks in support of ITER is undertaken. Our group's effort is devoted to the problem of understanding electromagnetic turbulence in plasmas, and its undesirable effects on enhancing energy losses (called 'anomalous transport') of the plasma far above those due to collisional processes.

Global tokamak turbulence calculations present truly 'grand challenges' to the most powerful computers in the world such as HPCx and the Earth simulator in Japan. A whole range of linear and non-linear instabilities are involved. The problems are similar in complexity to those encountered in geophysical fluid dynamics/climatology, both in the enormous range of length and time-scales involved and the number of dynamical degrees of freedom modelled. We are, in effect, attempting to 'arithmetise' plasma

Figure 3 (right): Contours in the turbulent electrostatic potential associated with ETG turbulence in the outboard mid-plane show radially extended 'streamer' structures which enhance electron heat transport.

Figure 4 (below): Schematic outline of the plasma coordinate system used in CENTORI. Notice how the radial and poloidal contour lines do not cross at right angles. The current version of the code shares out the toroidal 'onion skins' between the available processors.



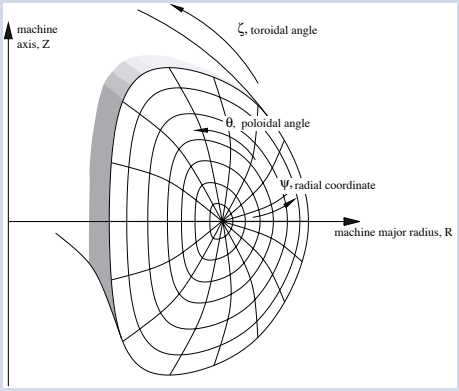
climatology in a tokamak with a supercomputer! We employ two complementary approaches to plasma turbulence modelling at Culham. The kinetic approach focuses on the microscopic spatial scale, exemplified by the Larmor gyration radius of charged particles in the magnetic field, whilst the 'continuum/fluid' method deals with more global scales right up to machine size and confinement time-scale, much longer than the turbulence time-scale.

GS2 – a gyrokinetic code

Kinetic theories model the plasma as a collection of charged particles (~1020) moving in response to self-consistently generated electromagnetic fields. Kinetic equations and Maxwell's equations are solved self-consistently to obtain the time evolution of the particle distribution functions in 6D (real space and velocity space) for each plasma species. Fortunately, in strongly magnetised tokamak plasmas it is possible to average the kinetic equation over the extremely rapid Larmor orbit motions to yield the 5D 'gyrokinetic equation'. This equation faithfully describes short perpendicular wavelength plasma turbulence, which is strongly suspected to underlie anomalous transport in magnetised plasmas.

GS2 [1] is a mature leading-edge plasma turbulence code, developed in the US using F90 and MPI, to solve the non-linear gyrokinetic equation for each plasma species. GS2 is being used to study the microstability properties of spherical tokamak (ST) plasmas, including plasmas from the Culham MAST experiment illustrated in Figure 1. ST geometry presents a challenge for plasma theory, and has important influences on microinstabilities. GS2's domain is a 'flux-tube' sub-region of the tokamak plasma, as illustrated in Figure 2. Domain decomposition is performed in 5D, with care to minimise communications in the directions of the fastest processes along the magnetic field. GS2 has been widely exploited on supercomputers (including HPCx), and with judicious choice of the calculation grids scales efficiently with large numbers of processors.

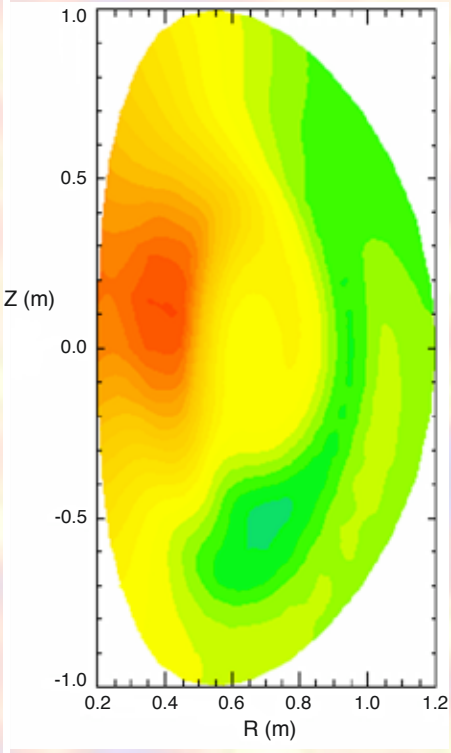
Linear gyrokinetic calculations suggest the existence of key microinstabilities which may ultimately be responsible for anomalous transport of heat and particles. Magnetic field perturbations are found to be particularly important in the ST, and some instabilities are found to tear the equilibrium magnetic field [2]. Fully non-linear calculations are required to predict turbulence saturation levels, and to make contact with experimental observations.

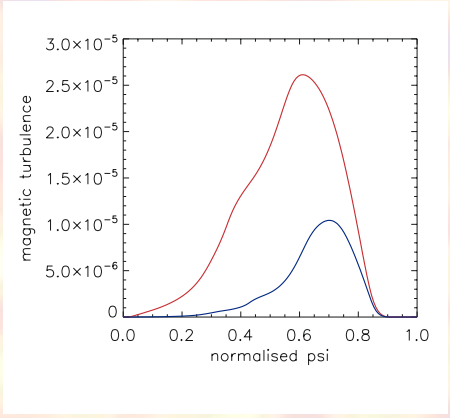


Non-linear GS2 simulations on HPCx have calculated the saturated state of electron temperature gradient (ETG) driven drift wave turbulence in MAST plasmas. These calculations required 256 processors running for approximately 8 hours on HPCx, and predict a level of electron heat transport which is, remarkably, comparable to that measured. This result is of considerable interest as ETG turbulence has previously been dismissed as unimportant! Our recent HPCx non-linear ETG simulations for MAST [2], have revealed that radially extended 'streamer' structures in the electrostatic potential enhance electron heat transport. These 'streamer' structures are clearly visible in Figure 3. In the future it will be important to assess the robustness of these simulations to various approximations, and to find ways of 'tweaking' the plasma equilibrium to reduce the transport levels. We are also presently trying to understand the complicated physics mechanism that drives the instabilities that tear the equilibrium magnetic field lines. Even linear calculations of these modes are challenging computationally, and it will be important to make non-linear simulations to assess the level of transport arising from these modes.

CENTORI – a fluid code

Fluid models contain less detailed physics than gyrokinetics, although many observational phenomena on larger scales are within their ambit. These models represent a tokamak plasma using eight or nine 3D fields varying in space and time. Non-linear balance equations of particle number, momentum and energy for each species and a reduced set of Maxwell equations are derived by suitable averaging of the more exact kinetic description. CENTORI, the global fluid code being developed for use on HPCx, permits calculations of tokamak turbulence evolution and transport





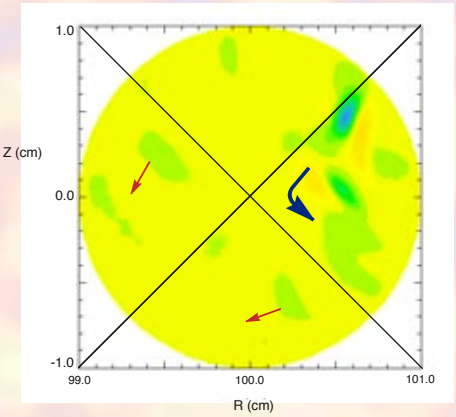


Figure 5 (left): Ion temperature fluctuations in the MAST tokamak (the real plasma is shown in Figure 1), as modelled by CENTORI. Red/orange are high values, blue/green are low.

Figure 6 (above): Evidence for the suppression of turbulence by the presence of a local toroidal flow. The blue curve is the calculated turbulence level when a radially localized region of bulk flow is introduced into the plasma; the red curve is that calculated without such a flow.

Figure 7 (right): Simulation of fundamental plasma ('Alfvén') waves in an X-point configuration. X-points in a tokamak are clearly seen in the top and bottom of the photograph of MAST in Figure 1. The arrows show the direction of motion of the so-called fast waves (in red) and shear waves (blue).

at reasonable resolutions (well beyond current experimental techniques but below those possible with gyrokinetics) for times approaching the typical confinement times.

CENTORI is designed to take full advantage of the parallel architecture of HPCx and Beowulf clusters. It is based on a highly successful serial Fortran 77 code [3] CUTIE (also developed at Culham by two of the authors), which described many experimental observations qualitatively with relatively low resolution calculations. CENTORI improves upon many of the approximations used in CUTIE, and employs a parallel implementation (MPI + FORTRAN 90) of the mixed semi-implicit pseudo-spectral/finite-difference method. Parallel super computing enables us to achieve much higher resolution than possible with CUTIE. CENTORI solves strongly coupled non-linear parabolic differential equations related to the well-known advection-diffusion equation. A plasma-based coordinate system, based on the nested toroidal magnetic flux surfaces is used. The three spatial, plasma-based coordinates are: ψ - labelling the nested flux surfaces, is a measure of the radial distance from the plasma centre to its edge; θ - the poloidal angle within a flux surface; and ζ - the toroidal angle along the torus (see Figure 4). A predictor-corrector, semi-implicit finite difference scheme in ψ is used with fast Fourier transforms in the two angular directions.

Early runs of CENTORI on HPCx have produced promising physical insights. Figures 5 and 6 show some typical outputs from the code, relating to UKAEA Fusion's own MAST experiment, already mentioned (cf. Figure 1). The run demonstrates qualitatively the suppression of turbulence by the presence of a local bulk plasma flow in the toroidal direction. (The phenomenon is known as 'transport barrier formation' and is observed in many tokamaks.) Figure 7 shows the results from another simulation, where CENTORI was used to model Alfvèn wave propagation (so called after their Swedish discoverer Alfvèn) in the vicinity of saddle points ('X-point nulls') in the poloidal magnetic field. In this simulation (a two-dimensional, linear problem) we used 992 processors on HPCx with unprecedented resolution, and the results were in agreement with non-trivial exact solutions of the MHD wave equations [4]. Runs of this kind (only possible on HPCx!) have provided understanding of wave phenomena involved in particle acceleration and the possible loss mechanisms in X-point geometries.

The parallel solvers in CENTORI are being optimised with valuable code development support from Drs Joachim Hein and Lorna Smith at EPCC as part of our EPSRC-HPCx contract. When fully developed and tested, CENTORI will be a powerful capability computing code. Global simulations with it on HPCx will provide new insights into both tokamak physics and plasma astrophysics.

Conclusions

A judicious combination of GS2 and CENTORI on HPCx and its successors will contribute to new understanding of existing tokamaks like JET, MAST and ultimately ITER. Theory and computation are expected to play an essential role in support of experiment and observation in finding a viable new solution to the world's energy problems and in understanding plasma phenomena in the cosmos.

Acknowledgements

This work was funded jointly by the United Kingdom Engineering and Physical Sciences Research Council and by EURATOM. The HPCx computer time was provided under the EPSRC grant GR/S43559/01. We would like to thank Bill Dorland for supplying GS2, George Stantchev for producing Figure 2, and Joachim Hein and co-workers at EPCC for assisting in parallelisation of CENTORI.

References

[1] http://gs2.sourceforge.net/

[2] C.M. Roach et al, to appear in Plasma Physics and Controlled Fusion (2005).

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The latest IBM Fortran Compiler, XLF 9.1

Ian Bush, HPCx Terascaling team

As announced in HPCx user mailing 75 and at the July User Group meeting, IBM's latest version of its Fortran compiler, xlf 9.1, is now available to users as a non-default installation (NDI). Users can invoke this version of the compiler by /usr/local/Fortran/9.1/usr/bin/<xlf version> where <xlf version> is any of the standard xlf variants, mpxlf90_r for example. Users are strongly encouraged to test their applications with the new compiler, and report any problems. If no major problems are found the intention is to make xlf 9.1 the default compiler after the maintenance session on the 14th September.

The new compiler is a major upgrade from version 8.1, the current default. In this article I will indicate some of the new facilities, the major ones being extra compiler facilities, extended language support and, in general, increased performance.

The new compiler facilities include the trapping of quiet NaNs, extra flags to support optimisation and support for the Power5 and Cell processors. The MASS library is also now supported by the compiler group and comes packaged with the compiler. Also IBM has, at last, provided a flag to report the compiler version!

As for language support, the new compiler provides full support for OpenMP 2.0, and partial support for Fortran2003. Full support for the latter will be in xlf11 (xlf10 will be available in 2006).

The Fortran 2003 features supported by the compiler include:

- C interoperability, including the facility to convert Fortran pointers to C pointers, and vice versa
- Access to the command line and command-line arguments
- The `iso_fortran_env` intrinsic module, which supplies implementation specific details such as which unit numbers correspond to standard in, standard out and standard error
- Mixed `Public/Private` components in derived types
- The `Flush` statement
- The `Import` statement to enable host association in interfaces
- The `New_line` intrinsic

Adherence to the new standard may be checked by the –qlanglvl=2003std flag.

Possibly the most interesting of the above to Fortran programmers are C interoperability, command line arguments and details of the implementation. C interoperability is achieved by the use of an intrinsic module, that is one that comes with the language, to provide kinds that map between Fortran and C variable types, and also extension of the interface block to indicate to the Fortran compiler that the subprogram that is being invoked is a C function. A simple example below shows how one might obtain the hostname of the system:

Fortran Side

```
Interface
  Subroutine hostname( host, length, error ) Bind( c )
   Use, Intrinsic :: iso_c_binding
   Character( Kind = c_char ), Dimension( * ) :: host
   Integer( c_int ), Value                    :: length
   Integer( c_int )                           :: error
  End Subroutine hostname
End Interface
..
Call hostname( host, length, error )
```

C Side

```
void hostname( char *host, int length, int *error ){
  *error = gethostname( host, length );
}
```

The `Bind( c )` on the interface indicates that the subroutine hostname is implemented in the C language. The intrinsic module, `iso_c_binding`, provides `c_char` and `c_int` which are used to map the variable types between the two languages. Note only characters of length 1 may be passed. The Value attribute allows arguments to be passed by value, the default mechanism in C, and it should be noted that it may also be used in interfaces to Fortran subprograms.

Also provided by the standard are a number of useful intrinsic subprograms. For instance `c_loc` can be used to obtain a C pointer to a variable, which is represented by the intrinsic type `c_ptr`, and the subroutine `c_f_pointer` converts a C pointer to a Fortran pointer. The whole set of features is very powerful and provides the Fortran programmer with a number of new opportunities, especially with regard to more system-like features. For instance I have implemented a module that allows simple access to Unix shared memory pointers and semaphores by a Fortran program.

Three new intrinsic subprograms provide access to the command line:

- `command_argument_count`
  - returns the number of arguments to the command,
- `get_command_argument`
  - provides access to each of the arguments
- `get_command`
  - returns the complete command line.

`iso_fortran_env` contains a number of symbolic constants detailing certain aspects of the implementation. These include

- `input_unit, output_unit, error_unit`
  – Which units are preconnected to stdin, stdout, stderr
- `numeric_storage_size, character_storage_size`
  – The size, in bits, of storage units
- `iostat_end, iostat_eor`
  – The values returned by `IOSTAT=` for end of file and end of record

xlf 9.1 generally shows improved performance on both benchmark codes and user applications. The SPEC FP Base on Power4 runs, on average, 18% quicker compared to executables generated by xlf8.1. Experience with user codes is limited at present, none have slowed down and some have shown dramatic improvements, with an over 40% improvement found in one case. On average about a 5-10% improvement is observed.

Complete details and full documentation can be found at:
http://publib.boulder.ibm.com/infocenter/comphelp/index.jsp
Slides for the talk at the user group meeting
are at: www.hpcx.ac.uk/about/events/user_group.html

Computing free energies for 'real' systems using molecular dynamics simulations

Shantenu Jha, Shunzhou Wan, and Peter V. Coveney, Centre for Computational Science, University College London.

Classical molecular dynamics (MD) simulations of biomolecular systems have the ability to provide insight into specific aspects of a system at a level of detail not possible for other simulation techniques and often not even accessible experimentally [1]. MD simulations can be used to study a wide range of problems, but arguably one of the most important applications is the use of MD simulations to compute free energies (FE) – which for many problems of interest is the most important thermodynamic variable. Computing FE is critical to understanding many phenomena in biological systems. For example, FE calculations have provided invaluable insight into transport phenomenon [2,3,4], protein-folding [5] and ligand-binding [6], to name just a few.

The use of MD simulations to compute FE (MDFE) in real systems, however, is not trivial. A potential drawback of many computational approaches, and certainly of MDFE, is that it is rather difficult to establish an estimate of systematic errors. One of the most common sources of systematic errors in MD simulations arises due to the uncertainty in the correctness of interaction potentials or forcefield parameterisations. In addition to performing validation tests of the same system for different forcefield parameterisations [7], it is critical to compare computational results with experimental data. Thus there arises the rather interesting situation where computation and experiment at once compete against and complement each other.

Experience [8,9] teaches us that FE techniques which work well for smaller and simpler systems do not necessarily work for significantly larger and complex configurational changes. In addition to systematic errors and the technical details of the methodology, one of the most common challenges encountered in FE computations is that of performing sufficient sampling, which makes FE calculations amongst the most computationally intensive computational science problems. The problem of insufficient sampling is aggravated when studying larger systems with greater conformational flexibility. Thus as we become more ambitious and set out to simulate ever larger systems and configuration changes, better validation tests and greater caution needs to be exercised. As we shall discuss, however, there are reasons to believe that there has been sufficient progress in the theory and practice of the methodologies used to compute FE, including the performance of scalable codes on massively parallel platforms, that we can now tackle 'real' systems.

Depending upon the system and problem of interest, it may be more useful to compute the FE difference between two states or to determine the functional dependence of FE upon some reaction coordinate. For example, when trying to understand ligand-binding, a FE difference is useful, whilst when studying transport processes the FE profile (FEP) is generally preferred. In this article we shall first discuss a 'real' application involving the computation of FE differences and then one involving the calculation of a FEP. We will show how the use of high performance computational approaches plays a critical role in enhancing our understanding of these systems.

Computing free energy differences in immunological systems

The heart of the immune response is a straightforward molecular recognition event which establishes cell-cell contacts between T-cells and antigen-presenting cells (APCs). There are a growing number of attempts to use computational methods to simulate immune responses based on atomistic and statistical models.

The use of scalable atomistic MD codes running on state-of-the-art high performance computers (HPC) enables us to compute biomolecular properties deemed inaccessible some years ago. Our recently published work [10,11] has investigated the binding to the T-cell receptor (TCR) of two peptides complexed to the major histocompatibility complex (MHC) protein by means of MD simulations (Figure 1a). There are approximately 100K and 50K atoms for the bound and unbound systems, respectively. The total time simulated is 35ns, required 80,000 CPU hours on a variety of HPC systems and generated 40 gigabytes of data. HPC resources enabled us to simulate larger, more realistic biological systems for longer durations without the imposition of artificial constraints. The computed FE differences are in qualitative agreement with experimental results [10,11].

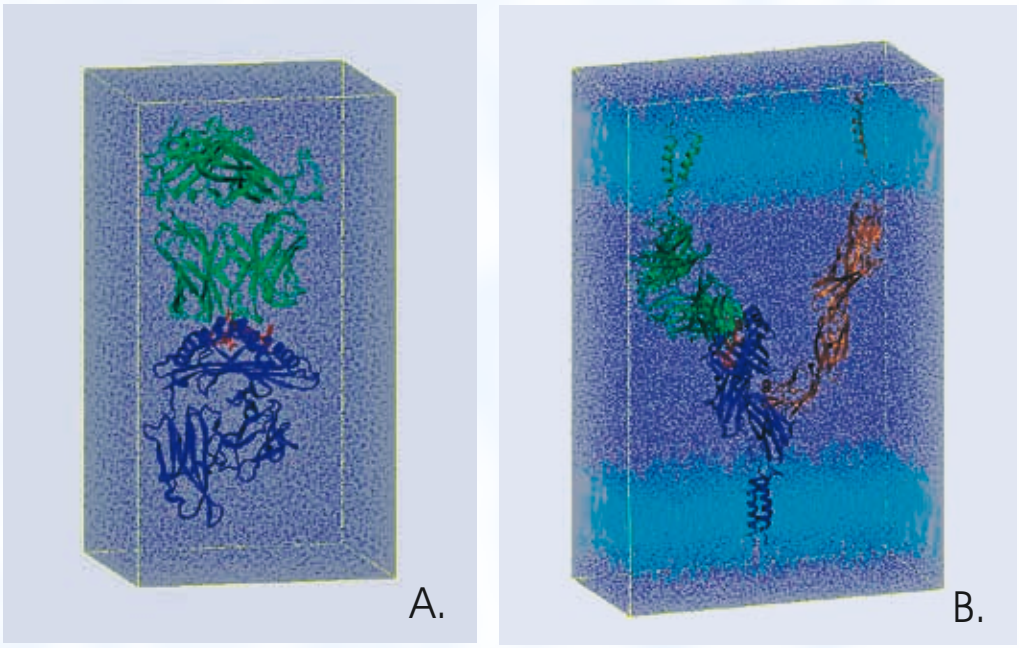

Figure 1: Structure of a) the TCR-pMHC complex, b) a TCR-pMHC-CD4 membrane model. The TCRs are coloured green, the MHCs blue, the peptides red, the CD4s orange and membranes cyan. There are about 100,000 and 330,000 atoms in a) and b) respectively including explicit water molecues as solvent.

To our knowledge, this is the largest system reported for a FE calculation using the thermodynamic integration method. Although our model is more realistic than those used previously, it nevertheless remains limited in its description of the system. Indeed, the recognition process is not an isolated event: when peptide-bound MHCs (pMHCs) are recognised by TCRs, many other co-receptors and accessory molecules, such as CD4 and CD8 proteins, become involved.

To study the recognition in a more realistic biological condition, we have been doing a series of MD studies for the TCR-pMHCCD4 system [12], complexed between two adjacent membranes which mimic the T-cell and APC. The system is embedded in explicit water molecules (Figure 1b), comprising in total about 330,000 atoms. The use of NAMD [13] – a highly scalable parallel MD code – for models of this size leads to a Gold Star rating on HPCx, which in turn provides a 30% discount on net-CPU cycles consumed.

Tuning immune responses involves the formation of the so-called immunological synapse [14], a highly organised, spatiotemporal arrangement of receptors and accessory molecules. We are planning to use the information obtained from this 330,000 atom model, to build a model that attempts to include more components of the immune system. Such a model will reach the 1 million atom level. Simulation on this scale will focus on how components interact to give rise to a typical immune response rather than describing the properties of individual components.

The thermodynamic integration [15] (TI) methodology for computing the binding FE of large systems has been validated with experimental results by Wan *et al* [10]; thus there are reasons to be confident that the basic TI methodology used is not only essentially correct but also highly reliable. [16] discusses the methodology and infrastructure which establishes the proofof-concept that HPC grids can be used to perform FE of binding calculations for small systems on highly reduced timescales. Given that the FE methodology is correct and there are no obvious limits to the scalability of the grid approach – beyond the availability of sufficient computational resources – the next step is to merge the two efforts and use HPC grids to compute the binding FE of large, complex real systems on timescales that are comparable to bench experiments. TI calculations as enacted via HPC Grids [16], afford us an unprecedented opportunity to predict epitopes both *de novo* (without knowledge of existing binding data) and *in silico* (entirely computationally). We can tackle problems head on, using increasingly realistic representations of the system in terms of greater size and duration of simulations. This will represent significant progress and will have important consequences both for fundamental and applied problems.

Using free energy profiles to understand the translocation of biomolecules across protein pores

The transport of biomolecules like DNA, RNA and polypeptides across protein membrane channels is of primary significance in a variety of areas (see Figure 2a). For example, gene expression in eukaryotic cells relies on the passage of mRNA through protein complexes connecting the cytoplasm with the cell nucleus. Although there has been a flurry of recent activity, both theoretical and experimental [17,18] aimed at understanding this crucial process, many aspects remain unclear.

To appreciate why there has not been any signficant computational contribution to understanding the dynamical aspects of the translocation problem, it helps to do a back-of-the-envelope estimate of the computational resources required. The physical time scales for translocation of large biomolecules through a transmembrane pore is typically of the order of tens of microseconds. Simulating one nanosecond of physical time for a system of approximately 300,000 atoms on current high-end platforms requires approximately 24 hours on 128 processors. Thus it takes about 3000 CPU hours – or a similar net number of computer hours for a different number of processors – on a *tightly coupled machine* to simulate 1ns. Therefore a straightforward 'simple' MD simulation will take 3×10^7 CPU hours to simulate 10 microseconds. This remains beyond the reach of even the best endowed computational collaborations. Thus there is a clear motivation, if not an urgent requirement, to attempt an approach which is 'smarter' than classical equilibrium MD simulations.

Computing free energies for 'real' systems using molecular dynamics simulations
continued

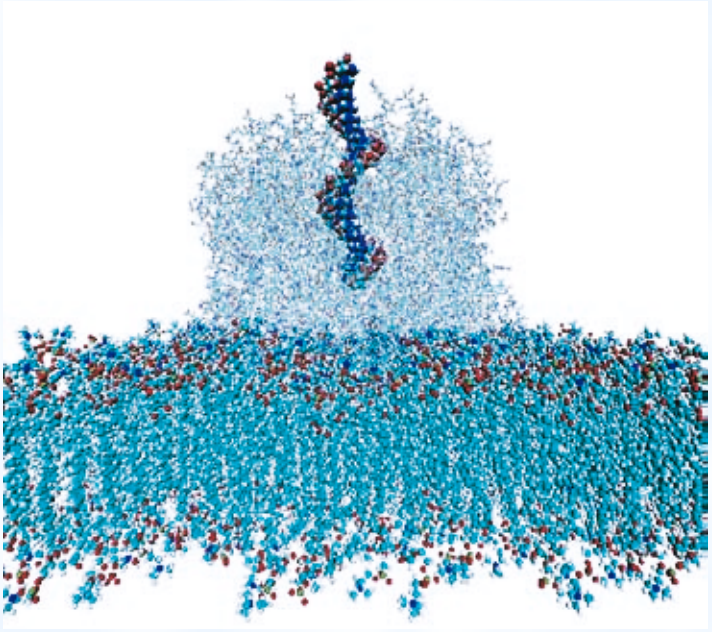

Figure 2a: Snapshot of a single stranded DNA polymer beginning its translocation through the alpha-hemolysin protein pore which is embedded in a lipid membrane bilayer. Water molecules are not shown.

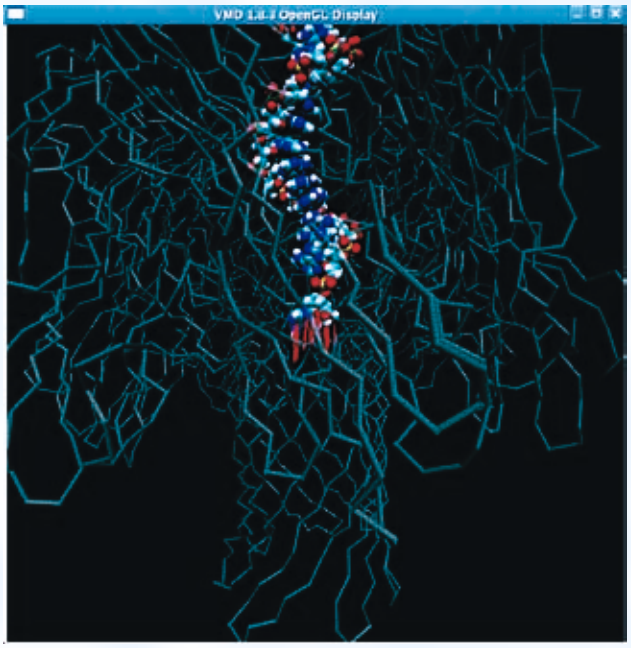

Figure 2b: an interactive steered molecular dynamics simulation in progress. The red arrow-headed lines represent the forces that are applied to the end residues of the DNA to guide and speed up its translocation through the pore.

As part of the SPICE project, we are studying the vital process of translocation of biomolecules across protein pores using a novel algorithmic approach that combines steered molecular dynamics (SMD) simulations and Jarzynski's Equation [19,20] . This approach enables the calculation of the FE profile that the DNA encounters along the vertical axis of the protein pore. Computing this FEP will provide invaluable insight into the details of the transport process.

By adopting the SMD-JE approach, we will be able to reduce the net computational requirement for the problem of interest by approximately a factor of 50. To implement the SMD-JE simulation methodology, however, requires the introduction of two new parameters and a corresponding uncertainty in the choice of the values of these parameters. This situation can be addressed by performing a set of preprocessing simulations, which, along with a series of interactive simulations (see Figure 2b) help inform an appropriate choice of the parameters. Once the right choice of parameters has been determined, multiple short-duration simulations are performed to compute the FEP (as opposed to a single long-running simulation when using standard equilibrium MD simulations).

A standard batch computing approach on HPC systems therefore proves inefficient when using the SMD-JE approach. This is in part due to the large size and complexity of the system being studied, but primarily due to the intricacies of SMD-JE.

Thus, to benefit from the potential advantages of the SMD-JE approach and to facilitate its implementation at all levels – interactive simulations for such large systems, the preprocessing simulations and finally the production simulation set – we use grid infrastructure to optimally utilise the computational resources of a federated transatlantic grid. The grid infrastructure enables us to circumvent traditional constraints of batch computing style HPC by performing distributed large-scale interactive simulations (by coupling geographically distributed visualisation and computational resources) as well as providing the additional computational resources in a uniform, easy-to-access fashion (see [21] and references therein for details).

Grid-techniques also facilitate the use of advanced optical networks [22], which in turn make interactive simulations feasible [23] . HPCx is one of several resources which are being connected to the optically networked Global Lambda Infrastructure Facility [24] (GLIF) via UKLight; all connections should be in place by SC|05. SPICE is the UK part of a joint UK-US high-end computing project funded by EPSRC and US-NSF that will be exhibiting *inter alia* at SC|05.

The investigation of the transport of biomolecules across a protein nanopore by computing the FEP is just one of several large-scale problems that can be efficiently studied using HPC grids. Although the use of grid techniques enables greater resource utilisation than would be possible otherwise [25], there will always be larger and more complex scientific problems of interest which we may be tempted to tackle. Watch this space for further reports of studies that utilise HPC grid infrastructure for studying even larger and more real systems.

Forthcoming events

Supercomputing 2005: Gateway to Discovery
12–18 November 2005, Seattle
http://sc05.supercomputing.org
This conference will include a trans-continental Grid computing demonstration linking HPCx, CSAR and HPC services in the USA, as a follow-up to the TeraGyroid project described in Capability Computing 2: http://www.hpcx.ac.uk/about/newsletter. See also: http://www.cse.clrc.ac.uk/about_us/Frontiers2004

Computational Chemistry on HPCx
30 November to 2 December, 2005, CCLRC Daresbury Laboratory
This course will provide an introduction to the computational chemistry software available on HPCx, with particular emphasis on parallelisation strategies and the kinds of performance characteristics to be expected for particular classes of problem. Codes discussed will include GAMESS-UK, DL_POLY_3, NWChemNAMD and CHARMM. There will be an opportunity to use HPCx during the hands-on session.
Registration details: www.hpcx.ac.uk
A full programme will follow shortly. Places will be limited so early registration is advised.

3rd HPCx Annual Seminar: Capability Science on HPCx
5 December 2005 at CCLRC Daresbury Laboratory.
http://www.hpcx.ac.uk/about/events/annual2005/

16th Machine Evaluation Workshop
6-8 December 2005 at CCLRC Daresbury Laboratory
http://www.cse.clrc.ac.uk/disco/mew16/index.html

21st International Supercomputer Conference
27–30 June 2006, Dresden
http://www.supercomp.de/

ScicomP12 (IBM System Scientific User Group)
17–21 July 2006, NCAR, Colorado
http://www.spscicomp.org/

ICPP-06 (International Conference on Parallel Processing)
14–18 August 2006, Columbus, Ohio, USA
http://www.cse.ohio-state.edu/~icpp2006/

Euro-Par 2006
29 August–1 September 2006, Dresden
http://www.zhr.tu-dresden.de/Euro-Par2006/

Acknowledgments

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DL_POLY_3: science on a grand scale via massively parallelised molecular dynamics simulations

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K Trachenko, MT Dove, University of Cambridge

DL_POLY_3 [1] is a general purpose molecular dynamics (MD) package for simulation of large-scale systems. By inherent parallelism and full memory distribution, DL_POLY_3 excels in performance for large-scale systems on multi-processor clusters. The performance results from intricately interlaced numerical algorithms such as domain decomposition (DD), linked cells (LC) [2] and Daresbury advanced Fourier transform (DAFT) [3]. A reinforced numerical stability so important for highly non-equilibrium simulations, such as radiation damage (RD) cascades [4], is provided by symplectic integration based on Trotter derived velocity Verlet (VV) algorithms [5]. The current version (3.04) is written in suitably modularised FORTRAN90 with embedded MPI and is fully self-contained (no external libraries needed) which makes the code highly platform portable [6].

Science example

DL_POLY_3 offers a wide variety of force-fields and virtually no limit to the system size (current limit of sizes up to 610 million particles) which enable the user to describe complex systems to high accuracy and simulate them in ever-growing realism. At present, it is the availability of HPC resources, high CPU count with extra disk space for output storage that limit the researcher in taking full advantage of the package capability. However, new HPC resources, such as HPCx [7], allow a number of scientists to carry out research on systems from a few hundred thousand to a few million particles [8]. DL_POLY_3 has been routinely used in RD research, where the demand of large size systems is driven by the high energies involved in RD cascades [4, 8-10]. The motivation for such studies lie in the growing need to immobilise radioactive nuclear waste safely by putting it in a waste form that can be an effective barrier to prevent polluting the environment. Safe immobilisation is therefore crucial to the future of the nuclear power industry. Even now, the amount of stored non-immobilised waste is already large enough to pose serious concerns, and is growing.

It is important to assess what consequences high-energy irradiation may have on the performance of the waste form over time, which can vary from about one hundred to tens of thousands of years for different isotopes. To study how properties of waste forms change over time massive parallel MD simulations of high-energy recoils are carried out in materials of interest. A recoil simulates a post alpha-decay event, ie after the alpha particle has transferred most of its energy and impulse to a heavy atom within the host matrix. This causes most of the damage in the structure, resulting in thousands of permanent atomic displacements. In our studies of RD effects [4,9,10] we consider materials related to those proposed to encapsulate highly radioactive nuclear waste (waste forms, glasses) as well as new ceramic materials indicating considerably higher durability. Figure 1 shows how marked the difference in damage (shape- and size-wise) can be for such different materials. These pictures correspond to the settled damage in SiO_2 and TiO_2 after 15 ps from a 50 keV recoil. To simulate this high energy recoil a 2.5 million particle simulation was carried out on 256 CPUs of HPCx running for 90 minutes per each compound.

Data from these sort of simulations on various materials are used to quantify a number of properties such as resistance/susceptibility to amorphisation, glass-forming ability, stopping power of irradiation, cascade-quenching, crystalline recoverability (self-healing), etc. These are used to improve scientific understanding

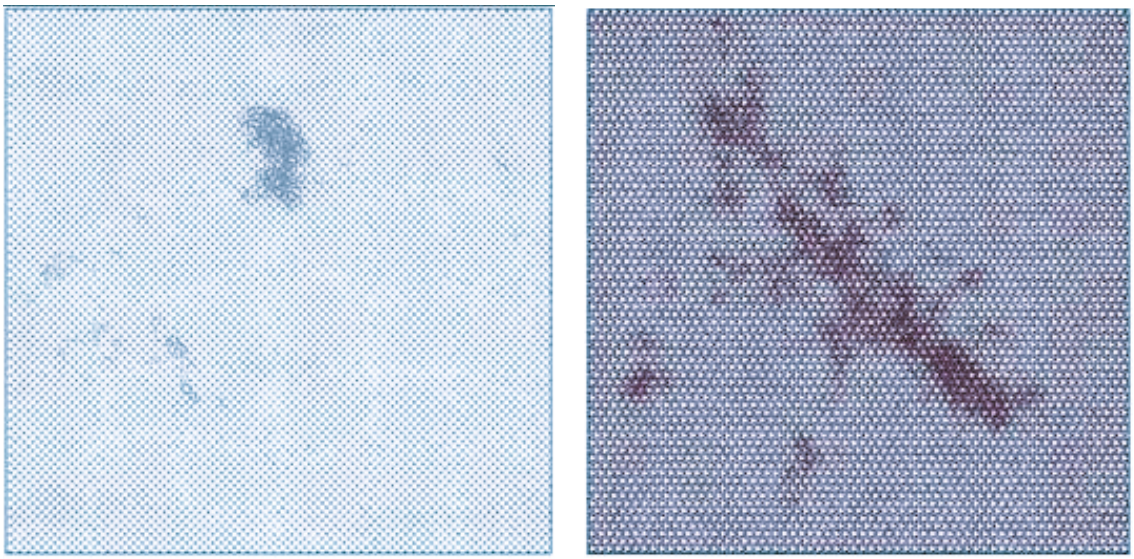


Figure 1: Damage in TiO_2 (left) and SiO_2 (right) after 15 ps from a 50 keV recoil. The simulated system size is 2.5 million particles.

Each simulation was carried out on 256 CPUs of HPCx running for 90 minutes.

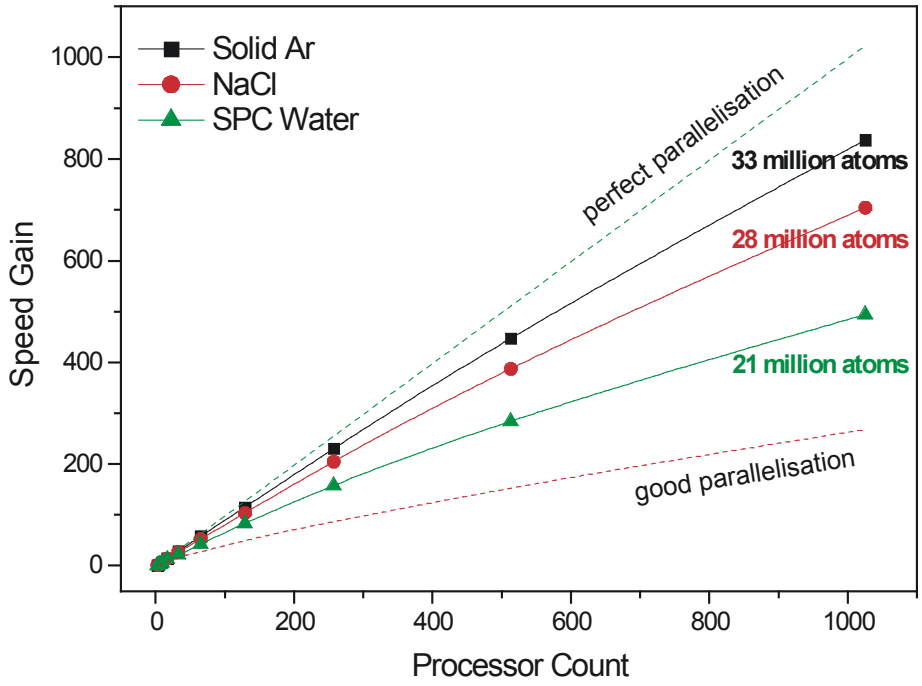


Figure 2. DL_POLY_3 speed gain plotted as a function of processor count. The green dotted line indicates the parallelisation limit also called perfect or embarrassing parallelisation. The red line indicates the standard for a good parallelisation, speed gain = $1.75^{\log_2(\text{CPU count})}$.

and build theories of how the mechanisms of resistance to damage and healing from damage are related to the chemical nature of the material and eventually to suggest better candidates for waste forms [10].

Benchmarking performance

To investigate DL_POLY_3 performance on HPCx we carried out simulations on three model systems as listed in Table 1.

The quality of parallelisation was benchmarked over a large processor count by comparing simulation times per integration timestep as the ratio system size – processor count was kept constant. In such circumstances perfect parallelism would result in unchanged simulation times at any processor count and a speed-gain equal to the CPU count. In Figure 2 the speed gain is plotted as a function of CPU count for the three model systems. Also included in the figure are plots indicating perfect (linear) and good parallelisation. This plot clearly shows that parallelisation performance for each model system is better than the nominal for good parallelisation at any processor count.

The deviation from perfect parallelisation in the case of the Solid Ar system is due to inevitable communication organisation losses which increase with the processor count. The deviation in parallelisation performance between the NaCl and the Solid Ar systems results from the NlogN scalability of the DAFT algorithm with system size (N), which is used for calculation of the long-ranged Coulomb interactions (as part of the NaCl system force-field). The deviation in performance between the SPC Water and NaCl systems comes from the further complexity in the force-field of the former system, which includes constraint bonds. Constraints are handled by the iterative algorithms, RATTLE [11] or SHAKE [13] which involve extra communications at each iteration. Overall, DL_POLY_3 exhibits excellent parallelisation over a wide range of CPU counts for which it has been awarded a Gold Star on HPCx. It is also worth noting that DL_POLY_3 holds the current record for the largest simulation (28 million ions on 1024 CPUs for the NaCl system) by a general purpose MD code including full evaluation of the Coulombic interactions.

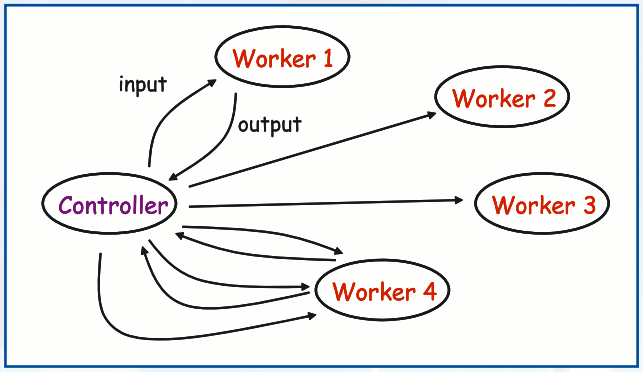
Maximum load test involving the three basics systems were also run on HPCx. We increased the MD simulation size load on one CPU (≈ 0.8 GB memory) incrementally until execution failed. The maximum load for the Solid Ar system was 600 000 particles per CPU. This on 1024 CPUs would add up to ≈ 610 million particles, which is just below the limit DL_POLY_3 can handle before some integer accumulators exceed their 32-bit declaration limit. With a little work this limit can be changed to the real 32-bit limit (2 147 483 647). Even this limit can be exceeded with careful effort and system sizes of 9.2×10^{18} are possible. To achieve this the package must be compiled in 64-bit mode and executed on a 64-bit platform requiring considerable hard disk space. For a 2.5 million particle system a configuration file (lattice parameters, positions, velocity and forces) in textual format is ≈ 1 GB.

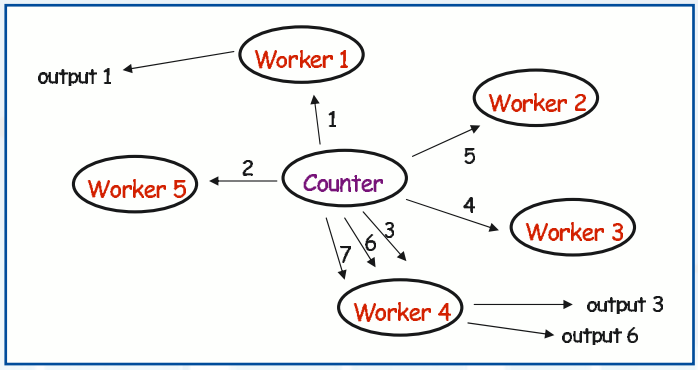
The maximum load per CPU for the NaCl and SPC Water systems amounted to 180 000 and 170 000 ions respectively. These cannot be scaled so directly to 1024 CPUs since some extra memory per CPU will be needed for the 3D FFTs in the SPME summations[13]

Continued on page 14.

Table 1. The model systems simulated using DL_POLY_3.04.

System	Size per CPU [particles]	Ensemble [type]	Force-field complexity	Cutoff [Å]	Temperature [K]	Pressure [k bar]
Solid Ar	32 000	NVE	short range	9	4.2	0.001
NaCl	27 000	NVE	above & Coulomb	12	500	0.001
SPC Water	20 736	NPT Berendsen 0.5 0.75	above & constraints	8	300	0.001





Left: A classical task farm with a separate controller process. Above: a task farm comprising only workers accessing a shared counter.

Task farming on HPCx

David Henty

Although HPCx is primarily intended to run single parallel applications that scale to many hundreds of processors, there are situations where it can be beneficial to run simultaneously a large number of smaller jobs which are loosely coupled. These small jobs could be parallel applications that perhaps do not scale well, or even sequential programs. Typical examples include statistical sampling, ensemble modelling, parameter searches and pre- or post-processing of data.

The way that the parallel environment is implemented on IBM systems means that there is a very tight coupling between LoadLeveler and the 'poe' command (the parallel job launcher). The effect is that it may not immediately be obvious how to do anything other than launch a single large MPI job across all the requested CPUs.

There have been quite a number of requests to the HPCx Helpdesk for assistance with taskfarming, for example:

- Is it possible to run multiple serial jobs?
- Will these jobs be distributed across the whole machine or will they all run on a single node?
- How can I distinguish between jobs so that they can perform different tasks?

To help address these issues, I have written a simple harness called 'taskfarm' that lives in /usr/local/packages/bin/. This allows users to run multiple serial jobs in a straightforward way across any number of processors, and gives each of them access to a unique identifier analogous to the MPI rank. For details, see the FAQ entry 'How can I run a task farm on HPCx ...' at http://www.hpcx.ac.uk/support/FAQ/.

It is somewhat more difficult to run multiple parallel jobs at the same time. This can still be achieved using 'taskfarm' if the jobs are not parallelised with MPI, eg if they use another mechanism like OpenMP or explicit threads. Running multiple MPI jobs, however, requires changes to the source code, but in some cases this can be relatively straightforward. For a general discussion see the talk 'Task Farming on HPCx', which was presented at the HPCx User Group meeting in July and is linked from the FAQ entry mentioned above.

DL_POLY_3 continued

(used for evaluating the Coulomb interactions) if the SPME precision is kept constant. We estimate that we should be able to load such systems on 1024 CPUs to 1000 times the maximum load per CPU.

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SciComP XXL

David Henty, HPCx Applications Support Team

Left: Gary Kumfert, SciComP President
Above: Assembly Rooms, Edinburgh

As part of EPCC@15, a series of events marking EPCC's 15th year, EPCC hosted the 11th meeting of ScicomP in Edinburgh from 31 May until 3 June 2005.

The meeting was co-located with the summer meeting of SP-XXL. ScicomP, the IBM System Scientific Computing User Group, is an international organisation focusing on the performance and scalability of scientific applications on IBM HPC platforms. SP-XXL's interests are similar to ScicomP; however, their focus is more systems oriented whereas ScicomP is more application driven.

Given EPCC's involvement in HPCx, coupled with running the first IBM eServer Blue Gene in Europe, the interests of both groups and EPCC match very well. There was a lot of international interest in both meetings and we welcomed over a hundred participants to Edinburgh. As I was mostly involved with ScicomP, and since SP-XXL is a closed meeting, I will report mainly on events at ScicomP11.

ScicomP11 had three main strands: in-depth tutorials and presentations from IBM on new products and technologies; scientific results from researchers using well-established IBM services such as HPCx; and initial experiences from users of the new Blue Gene systems.

Here I will briefly describe a few talks from each strand that should be of interest to users of HPCx. Copies of the presentations are available from the ScicomP website: http://www.spscicomp.org/ScicomP11/

- Charles Grassl from IBM spoke on 'Power5 processor and System Evolution', which is of particular relevance as HPCx will be moving to Power5 this November. The enhanced memory bandwidth of Power5 should help all scientific users, although the benefits of Simultaneous Multi-Threading (SMT) are yet to be proven for HPC applications.
- Deborah Salmond from the ECMWF weather centre presented results from their major climate model running on a p690+ system. The performance of this code benefits from the use of a sophisticated mixed-mode OpenMP/MPI implementation, although the subsequent talk from John Hague demonstrated that this approach can make subsequent code development quite challenging.
- Stephen Booth and Ian Bush both presented talks from HPCx. Stephen's work on an optimised MPI Alltoallv operation is currently being used to help real applications; Ian's talk demonstrated the benefits gained from the new switch interconnect on HPCx, and compared performance to the CSAR Altix system.
- Lorna Smith of EPCC discussed early experiences of applications performance on Blue Gene. Although the system is still fairly new, real scientific applications are already running in full production with impressive sustained performance. The key to gaining performance on Blue Gene is achieving scalability to thousands of processors, and the challenges that this presents were covered in a number of other applications talks.

As part of the social program, IBM invited everyone to the Surgeons' Hall on Wednesday night. The main social event was on Thursday evening, starting with a walking tour through Edinburgh's Old and New Towns, followed by a whisky tasting reception and a dinner in the Georgian splendour of the Assembly Rooms. All the delegates seemed to really enjoy the opportunity to see many of Edinburgh's historic buildings, despite the best attempts of the Scottish weather to dampen their enthusiasm!

The conference was a great success and full of interesting scientific and technical information for all users of IBM HPC systems. Next year's meeting, ScicomP12, is being hosted by NCAR in Boulder, Colorado. Keep an eye on www.spscicomp.org for details.

NCAR in Boulder, Colorado

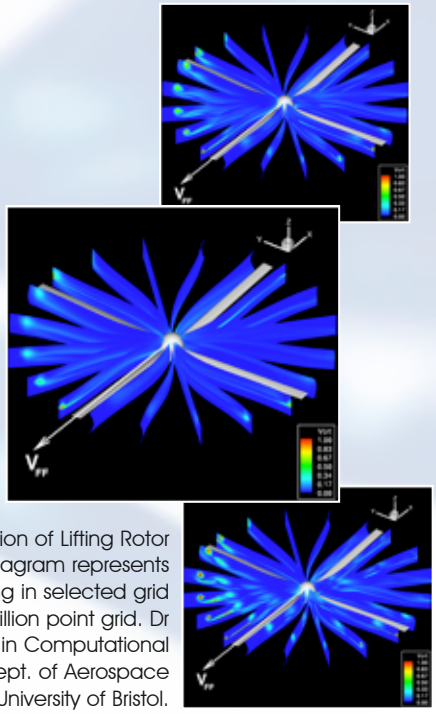
The Third HPCx Annual Seminar: Capability Science on HPCx

5 December 2005, CCLRC Daresbury Laboratory

The 3rd HPCx Annual Seminar 'Capability Science on HPCx' will be held in the Merrison Lecture Theatre, CCLRC Daresbury Laboratory on Monday 5th December 2005.

The seminar will include presentations from HPCx Users and Staff and is the third in a highly successful series of seminars organised by the UK's primary high performance computing service. We are very pleased to announce that our keynote speaker will be Prof. Geerd Hoffmann from Deutscher Wetterdienst (DWD). Attendance at this event is free to all academics.

Further details and registration information can be found at: http://www.hpcx.ac.uk/about/events/annual2005/



'Parallel Simulation of Lifting Rotor Wakes on HPCx'. Diagram represents vorticity shading in selected grid planes for 32 million point grid. Dr Chris Allen, Reader in Computational Aerodynamics, Dept. of Aerospace Engineering, University of Bristol.

16th Machine Evaluation Workshop

6–8 December 2005
CCLRC Daresbury Laboratory

Exhibition

Latest range of UNIX & Linux Workstations, PCs and HPC systems from the leading vendors.

Vendors demonstrating storage and network components, plus developments in graphics and visualisation

Benchmarking

Try out your own code on different machines, which will be accessible over the internet prior to the workshop, as well as during the event.

Commercial Outreach Forum

Thursday 8th December: Commercial Outreach Forum.
One-day meeting of regional (and national) companies to discuss computational requirements to meet the challenges of industrial R&D and to highlight the skill-base at Daresbury Laboratory.

Presentations:

Talks from leading HPC users and vendors in the UK and abroad.

Demonstration:

Software Engineering Support Programme (SESP) will be organising a one-day workshop on software engineering tools for computational science during MEW2005: http://www.sesp.cse.clrc.ac.uk

Further Details:

http://www.cse.clrc.ac.uk/disco

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