CHPC CENTRE FOR HIGH PERFORMANCE COMPUTING

NEWS

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Progress towards a cyberinfrastructure for

science in South Africa

WE ARE pleased to announce that the Centre for High Performance Computing (CHPC) is up and running in Cape Town. In the last three months we have seen a huge amount of progress, including:

- The completion of the building modification project at the CSIR site at 15 Lower Hope Street, Rosebank, Cape Town. This project involved extensive remodelling to establish a sophisticated data centre to house the first computer, as well as office space, training areas and user laboratories. This facility, which is conveniently situated close to UCT, the N2 freeway and Cape Town International Airport, will become the national hub for high performance computing in South Africa.
- The first phase of computer procurement and integration was completed in May 2007 and the operations officially started on 1 June 2007. The first phase computer consists of an IBM e1350 Linux computer cluster with 160 nodes. It has passed its initial Linpack benchmark trials according to specification, and shows a rated capacity of around 2.5 teraflops. Eight (8) nodes are equipped with Clearspeed Advance e620 Accelerator boards with Linpack performance of 32.3Gflop/s on a single processor core.
- The selection of and planning for the first three flagship scientific projects which will be run on the computer. These are:
  - a climatology and oceanography project from the University of Cape Town
  - a materials science project from the University of Limpopo
  - a project on cosmology from North West University.

Agreements on the running of these projects have been drawn up, and they will be starting in earnest in the second quarter of this year.

- The recruiting of talented and qualified staff for the CHPC has commenced, and we now have six full-time staff members. We should reach our planned staff complement of 15 by the end of this year.

We have done detailed planning and budgeting for the year ahead, which promises to be a very productive and exciting period in the development of cyberinfrastructure for science in South Africa.

We would like to extend an open invitation to all our friends and associates to come and pay us a visit, see what we are up to and help us plan for the future. □

Above: *Some members of the CHPC Scientific Advisory Committee, from left to right: Dr Happy Sithole (CHPC), Dr Jeff Y-J Chen (CHPC), Prof. Daya Reddy (UCT), Dr. Khomotso Kganyago (CHPC), Prof. Liesbeth Botha (SU), Llewellyn Jones (CHPC), Prof. Colin Wright (Wits), Prof. Mike Inggs (UCT).*

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The CHPC building in progress

IN 1989 the Fishing Industry Research Institute (FIRI) moved into a specially designed building at 15 Lower Hope Street, Rosebank, Cape Town, to serve the technical needs of the food and fisheries industries. Seventeen years later in 2006 this building was modified for the CHPC to house high performance computers for scientific research purposes.

Watch this space and see the transformation from fish processing to supercomputing! □

▶ ***Left:*** *The walk-in freezers and the stainless steel worktop where fish was processed*
Middle: *The demolition work to make space for the supercomputers (HPC Equipment Room G56)*
Right: *The room "as is" before building works and upgrade start in November/December 2007*

Appointment of interim Head of Research

IT IS with great pleasure that we announce that Prof. Daya Reddy of UCT has been appointed interim Head of Research of the CHPC. Although this is only a part-time appointment because of Prof. Reddy's numerous other commitments, he is already becoming involved with the determination of the CHPC's research strategy and plan, and he is providing leadership to the research staff of the CHPC. □

International Supercomputing Conference in Dresden

THE 22ND International Supercomputing Conference (ISC'07) in Dresden, Germany, was attended by 1 213 participants from 45 countries around the world. 144 contributors addressed issues that are expected to impact on the future of high performance computing. 85 exhibitors showed off their products.

What emerged is that it is essential for parallelism and locality to be exposed to the compiler so that the compiler can adapt it to the target system. In parallel languages there are (at least) two promising approaches: functional programming and atomic memory transactions. However, on the one hand functional programs do not allow mutable state, and on the other hand transactional programs implement dependence awkwardly. Therefore it is necessary to support multiple programming styles: functional and transactional, data parallel and task parallel, message passing and shared memory, declarative and imperative, implicit and explicit. □

Visits to the UK and Ireland

DRS KHOMOTSO Kganyago and Happy Sithole visited a number of centres in the UK and Ireland from 1 to 13 July this year. The main purpose of their trip was to meet other scientists in the high performance computing community and discuss possible areas of collaboration. The aim was also to share ideas on the development of high performance computing centres, and to discuss matters of maintenance and user support.

University College of Dublin

We visited Prof. Nick Quirke, President of the University College of Dublin and Professor of Chemistry at Imperial College, London. He was supportive of the CHPC initiative and was prepared to share his experience and assist CHPC management with independent evaluation.

University of Bath

Prof. Steve Parker of the Chemistry Department of the University of Bath is a valuable contact for the CHPC. He has experience in building computers from component level and has developed a widely used code for surface simulation, METADISE, which he is prepared to share with the CHPC and expose its researchers to code development ideas.

Oxford

The Numerical Analysis Group (NAG) in Oxford were prepared to support the CHPC with the benchmarking of the new machines. This group played a role in the CHPC's first procurement and is currently tasked to benchmark the HECTOR project in the UK.

Cambridge University

The visit to Cambridge University was coordinated by Prof. Michael Payne, a well known physicist and the developer of CASTEP, one of the codes used world-wide by academics and industry. Ideas on user management, expansion of facilities and sharing of expertise, especially around code development, were discussed openly with the academic users of the Cambridge HPC and the Director of the Centre. Prof. Payne agreed to assist CHPC users in material science and chemistry codes.

Prof. Martin Dove of Earth Sciences gave a presentation on a database developed for collaboration in grid computing. The Climatology Group discussed advances in this area of modelling.

The Accelrys Group discussed with us options of acquiring the codes, one area being the utilisation of Accelrys's expertise in contract research. We also discussed the possibility of acquiring a country-wide licence for their products rather than our users having to buy the codes individually. We also explored the benefits of the CHPC joining the nano-technology consortia, thus providing access for the user community in South Africa.

HPC facility in Cambridge

The last stop was the HPC facility in Cambridge where the Director, Dr Paul Calleja, took us through the facility and discussed in detail areas of possible cooperation. In Cambridge we have collaborators who are willing to share with us their experience and expertise and host our scientists at any time.

Daresbury Laboratories

HPCx is a national facility at Daresbury Laboratories based in Warrington. There we met researchers whose responsibilities are similar to those of our own research officers. The groups of researchers were the developers of DL_POLY, GAMESS_UK; CRYSTAL and ONETEP. They expressed willingness to collaborate with us on our benchmark exercise and to share expertise in user support on specific codes. The possibility of short-term exchange programmes, which do not necessarily require formal collaboration between our centres, was also mooted, without excluding the formalising the collaboration once long-term staff commitments are involved. Prof. Michael Ashworth, who was the overall coordinator, lined up a very useful team for discussion.

Dr Bill Smith, the developer of DL_POLY, and Dr Paul Sherwood, the developer of GAMES_UK, agreed to run workshops in South Africa in this year. We have also established a relationship with Prof. Martyn Guest and Dr Kristen Kitchen who have been assisting some of our users and playing a role in the benchmarking of codes. Prof. Guest is also a member of our Scientific Advisory Committee. We were also honoured to meet the Director of the Centre, Prof. Richard Blake, who discussed the planning of the facilities and the necessity of engaging stakeholders in the successful implementation of HPC strategy.

Details of the visits

The details of our visits will be available in a report which will be placed on our website (www.chpc.ac.za). Members of the HPC community can contact us direct if they are interested in any of the ideas mentioned in this article. We would also like to encourage the user community to liaise with our research officers if anyone needs to collaborate with the people we visited. This will help to coordinate collaboration and ensure maximum exposure of the expertise to South African researchers. □

Second Annual CHPC meeting

THE ANNUAL meeting of the Centre for High Performance Computing will be held on 3 to 5 December 2007 at the Cape Town International Convention Centre. We anticipate hosting 200 delegates from the HPC research community this year. Invited international speakers will address a range of HPC areas, from infrastructure to applications. The Department of Science and Technology will set the stage on the first day of the conference with a discussion on the future of HPC and expectations from the user community. Invitations have also been extended to HPC technology developers to share their latest developments. The second day of the conference will focus on activities of the Special Interest Groups (SIGs) in the form of break-away sessions and a SCAW workshop immediately after the conference. On the last day of the meeting, the groups will be announced which have been granted flagship status and grand challenge funding. Please visit the CHPC's website at www.chpc.ac.za for the conference programme and related activities. We are looking forward to welcoming you to the 2nd Annual Meeting of the CHPC in Cape Town. □

Special Interest Group Workshop on Computational Chemistry

IN CONJUNCTION with the Carrman Physical Chemistry Symposium of the South African Chemical Institute, CHPC hosted a series of computational chemistry workshops.

Pre-symposium workshop: Molecular dynamics is a technique used by researchers to study the time-dependent property of the macro-system using atomistic models. DL_POLY is a parallel molecular dynamics simulation package developed at Daresbury Laboratory to facilitate molecular dynamics simulations of macromolecules, polymers, ionic systems and solutions on a distributed memory parallel computer. DL_POLY DL_POLY is suitable for simulations of the order of one million atoms on up to 1024 processors. The workshop was presented by one of the original developers, Dr William Smith.

Symposium workshop: To promote the use of computational tools in biology and biochemistry-related research, the CHPC invited Schrödinger to deliver a two-day workshop to provide an overview of a wide range of useful techniques. Day 1 dealt with structure-based approaches and on day 2 ligand-based approaches and high-precision methods were discussed. Areas of application for high-precision tools such as quantum-polarized ligand docking (QPLD) were introduced. These interesting topics were presented by Dr Andrew Sparkes and Dr Jean-Christophe Mozziconacci.

Post-Symposium Workshop: ab initio molecular electronic structure is one of the fundamental computational chemistry tools which can assist researchers to gain insight into the electronic behaviour of molecules. GAMESS-UK is one such program, which is capable of performing SCF- , DFT-, and MCSCF-gradient calculations, together with a variety of techniques for post Hartree Fock calculations. Development of the code over the past decade has been coordinated by the Daresbury Laboratory. This workshop was presented by Dr Paul Sherwood, one of the developers.

Some of the workshop material is available from the CHPC. For more information, please contact Dr Jeff Chen (jyjchen@csir.co.za). □

High School Outreach

IN COLLABORATION with the Computer Society of South Africa and the Provincial Government of the Western Cape, a workshop entitled What IT skills do academic and technical universities expect school learners to have and what does it count? was hosted at the CHPC. More than 50 delegates from high schools, universities and governmental participated in this event and grappled with some of the key issues. It is envisaged that the CHPC will continue to provide a suitable environment to facilitate such discussion between the different parties.

The High School Computer Science Olympiad finalists visited the CHPC. These talented young learners toured the CHPC facility and attended a presentation by Mr Chris Jack from the Climate System Analysis Group of the University of Cape Town. The CHPC and the Computer Science Olympiad Committee will be working together and to formulate more high school outreach and education programmes in the future. □

Interaction with the Special Interest Groups (SIGs)

CHPC HAS held meetings with 8 of the existing 10 Special Interest Groups to foster research innovation in each SIG and to formulate a comprehensive training schemes. Each SIG is unique, so each of them has provided different solutions to overcome the hurdles faced by their scientific community. Most of them have also formulated working committees to enhance the development of their scientific fields. □

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