

Essential Enzyme Research Gets Boost with SHARCNET

BY MITCH RITTER, CO-ORDINATOR OF SPARK (STUDENTS PROMOTING AWARENESS OF RESEARCH KNOWLEDGE), UNIVERSITY OF GUELPH



James Gauld, Windsor researcher and SHARCNET Fellowship holder

Imagine being able to produce therapeutic drugs specific to certain viruses. Or using science and technology to better understand brain development. Or helping keep patients with high blood pressure healthy and in check. Now, a team of SHARCNET

researchers are using computational chemistry to realize these goals, and more.

Dr. James Gauld, Assistant Professor in the Department of Chemistry and Biochemistry at the University of Windsor, along with a team of researchers, is applying computational chemistry to gain a better understanding of how biocatalysts such as protein enzymes, ribonucleic acid catalysts (ribozymes) function.

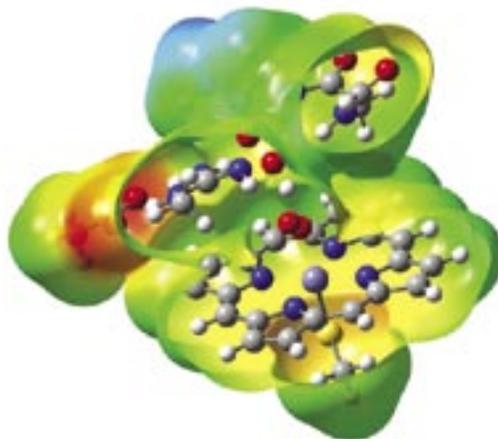
"This research will enable us to better understand the function of a particular enzyme in the development of therapeutic drugs," says Gauld. He notes that almost 70 per cent of all current therapeutic drugs are enzyme inhibitors; by researching computational chemistry, Gauld and his team hope to further understand the properties and

chemistry of new and novel biochemical catalysts found within living cells.

In particular, their research focuses on the unique catalytic mechanism of the class of enzymes known as nitric oxide synthases (NOSs). These enzymes play an important role in the synthesis of nitric oxide (NO), a chemical that serves a vital function in life processes such as brain development, embryo formation and blood pressure regulation.

In addition, Gauld and his team of researchers are interested in explaining the mechanisms of catalytic ribonucleic acids (RNA), ribozymes. RNA has long been known as an essential building block of life; now, it turns out it also has a key role in the life-cycles of some

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An electrostatic potential map of the catalytic active site with the substrate bound, of the enzyme Nitric Oxide Synthase.

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Message from the Chair of the Board



Ted Hewitt

“This partnership and infrastructure expansion is another huge milestone for SHARCNET as our vision of creating an organization with “Power, Partnership and Performance” is realized.”

On behalf of the Board of Directors, I am pleased to welcome the addition of three new academic partners – Lakehead, Laurentian and Trent universities – who are just joining the SHARCNET consortium. This will bring the total number of institutions involved with the SHARCNET to 14, double the size from where we started in 2001. Without question, this expansion positions SHARCNET as the largest HPC consortium in Canada. SHARCNET also added Silicon Graphics Inc. as an industrial partner earlier in 2005.

SHARCNET is currently in a state of significant transformation as a massive infrastructure upgrade is underway as a result of funding provided by our industry partners (Hewlett Packard and SGI, in particular) and substantial national and provincial grants provided by CFI, MEDT and OIT. The support we receive from both industry and government is very much appreciated and is a critical component of our success.

SHARCNET is entering a new era of funding for HPC on both the national and provincial fronts. The national Long Range Plan (www.c3.ca/LRP/), which was released at the beginning of November, lays out an HPC framework for the future and proposes a national high-level funding model for sustainability of these essential resources. The need for reporting, reviewing, and vetting processes that will help the Ontario government prioritize its support of HPC resources for research is also critical. The formation of an Ontario HPC Council and an HPC Coordination Committee has been initiated to help meet this provincial need. The Ontario High Performance Computing Council will help affirm and maintain Ontario's national leadership position in research utilizing HPC and will make recommendations to the Ontario government and its associated agencies regarding HPC funding and positioning. The Coordinating Committee (which will include a representative from SHARCNET and the other two Ontario consortia) will be more operational in nature and is expected to do preliminary vetting of provincial HPC grant applications, and coordinate the collection of information and reporting. In this context, SHARCNET has recently submitted a revised application to the Ontario Research Fund (ORF), which replaces the Ontario Research and Development Challenge Fund, to provide renewed operating funding for the expanded partnership and facilities.

I would like to take this opportunity to thank the many faces of SHARCNET, from the Board level, to the HPC Strategic Council, SHARCNET management and staff, and the researcher community at large for their tremendous support and contributions. All have played a role in the evolution of SHARCNET which truly positions us as a world-class HPC resource – something we can all take great pride in.

This partnership and infrastructure expansion is another huge milestone for SHARCNET as our vision of creating an organization with “Power, Partnership and Performance” is realized. I look forward to the months ahead as we continue to aspire to be an HPC organization worthy of national and international attention.

W. E. (Ted) Hewitt, Ph.D

Chair, SHARCNET Board of Directors and Vice-President (Research & International Relations), The University of Western Ontario

Scientific Director's Message

The last six months has seen the beginning of dramatic changes in the HPC landscape at SHARCNET, in Ontario and in Canada. SHARCNET is undergoing a very substantial expansion in terms of members and research capability, and the level of visibility that HPC is attracting provincially and nationally is, at last, seeding the hope that the need to carefully nurture and sustain a competitive HPC environment has been recognized by our funders.

Nationally, the C3.ca Long-Range Plan for HPC - two years in the making - has finally been released. The plan is built around two fundamental realities. First, that HPC is ubiquitous and not to invest in the hardware and people will result in Canada becoming uncompetitive in research, economically and societally. The title of the plan, "Engines of Discovery: the 21st Century Revolution", references the Victorian adage that the steam engine was an "engine of change". Steam power, in many respects, ushered in the modern age; in the same way our ability to compute and analyse systems of previously unimaginable magnitude and complexity is now driving a similar change in all aspects of intellectual and economic endeavour. The second factor is that hardware and the people who support it, support the use of it and who use it, form a tightly coupled system with two quite different timescales. Large-scale HPC hardware has a competitive lifetime of perhaps four years. Although, in principle, an uncompetitive hardware situation can be remedied with the injection of sufficient funds, it will take years to rebuild the knowledge and replace the people who will have left because of lack of resources. Both components must be sustained together.

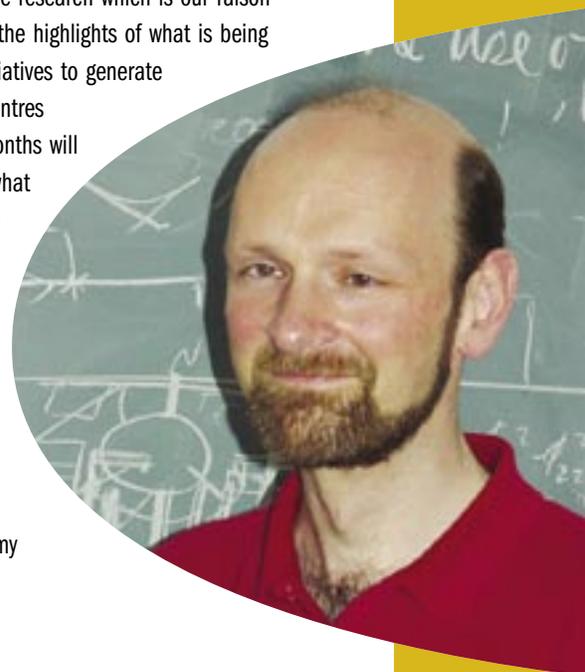
SHARCNET is, of course, a microcosm of these challenges and opportunities. At present, we are in the middle of installing across the partnership over 6,000 new processors and nearly 500TB of storage in a variety of equipment from our partners HP and SGI; are establishing the protocols and software to make it useable; and are deploying the dedicated network in conjunction with ORION that will tie all the components together into a single resource to enable leading research. It is worth emphasizing one of the fundamental principles of the agreement governing SHARCNET: that all of this infrastructure is available to all users irrespective of where the equipment is located. We are also in the process of hiring new staff to support the infrastructure and its effective use. The first of these new staff, Cindy Munro and Robert Schmidt, are introduced in this newsletter. Further staff are envisioned to support the expanded infrastructure and new partners. The new staff will allow us to expand the range of support and services that we offer and they join a truly outstanding team who have worked unremittingly to make SHARCNET a success. The scope of the new equipment has

necessitated a significant amount of disruption and, as a result of various unforeseen problems with equipment availability, substantially more downtime that we had hoped. Many partners have had to renovate space for new systems and to upgrade power and cooling; in one case, at Waterloo, a new building is being constructed! We are trying to minimize difficulties. We anticipate that most of the new infrastructure will be in place by early 2006.

As part of the infrastructure expansion and upgrade we are improving the web site to make it more easily navigated and more useful especially to research users. We will announce these improvements as they come online, but the aim is to make the SHARCNET web portal a simple interface to the very large array of hardware, software and infrastructure that we will offer. We encourage you to visit the website. Some aspects of the new environment are described later in the newsletter.

The installation of new facilities and plans tends to produce a somewhat skewed focus on the minutiae of processors, construction costs, optical fibre etc., but as you will see from the following pages we are still producing the research which is our *raison d'être*. We report on some of the highlights of what is being done at SHARCNET and on initiatives to generate partnerships with other HPC centres internationally. The coming months will see an enormous increase in what is possible with SHARCNET and we urge users to look towards what will be available to them in a few months.

Hugh M.P. Couchman
SHARCNET Scientific Director
Fellow, Canadian Institute for
Advanced Research
Professor, Physics and Astronomy
McMaster University



“All of this infrastructure is available to all users irrespective of where the equipment is located.”

Hugh
Couchman

Financial Math Beyond the Stock Markets:

New math research will help in those challenging situations

BY MITCH RITTER, CO-ORDINATOR OF SPARK (STUDENTS PROMOTING AWARENESS OF RESEARCH KNOWLEDGE), UNIVERSITY OF GUELPH

Wouldn't it be nice to know which stocks to hold to maximize your profit? What about being able to use the same type of theory to mitigate the effects of the next drought in a developing nation? Now, these things and more are becoming a reality with the help of one McMaster University professor who is researching financial derivatives and their effect on various world issues.

Dr. Matheus Grasselli, Assistant Professor, Department of Mathematics and Statistics, is studying financial mathematics and derivatives, and relating them back to real life applications.

"This research has many practical values," says Grasselli. "For example, it can be used to show how executives and employees should exercise stock options given to them as part of their compensation package."

Specifically, Grasselli's research is focused on pricing and hedging techniques in incomplete markets, where the traditional arguments based on replicating portfolios are not applicable. Grasselli's research looks at risk preferences of investors and market participants, to identify the best trading strategies to be followed when non-standard financial instruments are created and introduced.

On a more practical level, Grasselli's research can be used to address socio-economic problems. For example, an innovative United Nations program applies the concepts of derivatives to rainfall levels, to help manage the risk of starvation caused by drought in Africa.

"The same techniques show how market ideas can be used to quantify and manage risks that are not traditionally associated with the financial world, such as environmental or health related risks," says Grasselli.

SHARCNET aids Grasselli's research efforts by generating large-scale simulations of market conditions, on which approximated solutions can be implemented and tested for efficiency and accuracy.

In addition to Grasselli's day-to-day research efforts, he is also a member of the MITCAS (Modeling Trading and Risk in the Market) project, a network of 12 faculty members, five post-doctoral fellows and 29 graduate students from five different Canadian universities – McMaster, Western Ontario, Calgary, Toronto and British Columbia. Grasselli also maintains scientific ties with research groups in the United Kingdom, Italy, United States, Japan and Brazil.

Grasselli received his PhD in mathematics from King's College London in 2001, and completed a post-doctoral fellowship at McMaster University. Grasselli has also been the SHARCNET Chair in Financial Mathematics since 2003.



Matheus Grasselli

"SHARCNET aids Grasselli's research efforts by generating large-scale simulations of market conditions, on which approximated solutions can be implemented and tested for efficiency and accuracy."

Fellowship Student Wins Best Paper Award

BY ALLAN D. SPENCE, ASSOCIATE PROFESSOR, MCMASTER UNIVERSITY

“Laser Digitizer / Stereo Vision Methods for Simultaneous Measurement / Analysis of Sheet Metal Forming Strain / Geometry”, authored by Harley Chan (Mechanical Engineering and SHARCNET Fellowship student), Philip Mitchell (Electrical & Computer Engineering), Allan Spence (Mechanical Engineering), Mateusz Sklad (Mechanical Engineering), and David Capson (Electrical & Computer Engineering), was chosen from 150 entries to receive the Best Paper Award in the Manufacturing Engineering Division at the ASME International Mechanical Engineering Congress held November 5-11, 2005 in Orlando, Florida.

The research reported in the paper is truly a team effort involving two graduate students and three co-supervising professors with expertise in Dimensional Metrology (Spence), Metal Forming (Sklad), and Computer Vision (Capson). Equipment funding came from the Canada Foundation for Innovation/Ontario Innovation Trust (CFI/OIT), and student funding was provided by the Ontario Research and Development Challenge Fund (ORDCF) - SHARCNET, the Natural Sciences and Engineering Research Council of Canada (NSERC) and Networks of Centres of Excellence - The Automobile of the 21st Century (NCE-AUTO21).



Allan Spence
and Harley
Chan (l-r)

York Hosts Fall Workshop 2005

BY DAVE MCCAUGHAN, HPTC CONSULTANT, SHARCNET

Within SHARCNET, the hallmark of the arrival of fall is the planning and delivery of the annual Fall Workshop. This year's workshop was graciously hosted by York University over three days in October, and explored themes of programming techniques, computational theory and large scale applications.

We are constantly striving to make the Fall Workshop a cornerstone activity for the SHARCNET community. This year was no exception, so while previous year's events have primarily focused on short talks from invited speakers, we made the decision to introduce a significant structured laboratory component, truly making for a “workshop experience” for attendees. Two full days of in-depth workshops organized around the major programming paradigms in parallel computing, clusters and shared memory systems, introduced tremendous value to the users in attendance, and it is our hope that this shift in emphasis triggers the booking of larger laboratory venues in future workshops.

Another full day was dedicated to a slate of distinguished invited speakers from academia and industry, who delivered a quality program of materials relevant to users in their day-to-day endeavors developing the next generation of high performance computing applications and research.

Additional information, including speakers, program and copies of slides and instructional materials can be found online at www.sharcnet.ca/Events/fw2005/.



SHARCNET Visits Shanghai Supercomputer Center

BY BAOLAI GE, HPTC CONSULTANT, SHARCNET

Invited by the Director of Shanghai Supercomputer Center (SSC), Xi Zili, Hugh Couchman (the Scientific Director of SHARCNET), Jeff Chen (the principle investigator for SHARCNET-II for the University of Waterloo) and Baolai Ge (SHARCNET HPTC Consultant), visited SSC from October 24 to 27, 2005. At the conference of High Performance Computing and Applications 2005 co-hosted by SSC and the Chinese Academy of Science, Dr. Couchman gave a keynote speech "The Canadian HPC effort and SHARCNET consortium". Professor Chen gave an invited speech "Understanding the protein folding by computational physics". Ge also gave an invited talk on Fortran threading with POSIX threads on shared memory systems at the two-day conference.

Covered by Chinese news media, the two-day conference was a high profile event attended by researchers, HPC vendors, government officials and invited experts. The conference started with a full day forum of keynote speeches by VIP guest speakers from HPC centres around the world, including San Diego Supercomputing Center, Korea Institute of Science and Technology Information, NCSC, Pittsburgh Supercomputing Center, Ohio State University, Finish IT Center for Science, IBM, Chinese Academy of Science, etc.



Greeted by the Vice Mayor, Yan Junqi, of Shanghai City



Hugh Couchman giving a keynote speech at HPCA 2005

Essential Enzyme Research, continued from page 1

viruses, including hepatitis. In some cases, ribozymes have shown potential as therapeutic agents against life threatening viruses, such as HIV.

"This research will provide greater insights into fundamental chemical principles and interactions," says Gault.

SHARCNET is a vital player in Gault's research efforts. SHARCNET allows Gault and his team to carry out large and complex experiments by providing them with the computational facilities able to house these large-scale projects. More importantly, SHARCNET allows them to use high levels of theory, further enhancing the accuracy and reliability of the results.

Gault is working on two more research projects with colleagues from the university. The first, with Dr. Doug Stephan, aims to develop new organometallic catalysts, particularly relevant to the plastics industry. And another, with Dr. Sirinart Ananvoranich, is setting out to clarify the catalytic mechanism of the hepatitis delta virus (HDV) ribozyme, that plays a crucial role in the reproduction of the hepatitis virus.

Gault received his PhD from the Australian National University in 1997, and held a postdoctoral position at the Institute for Quantum Chemistry at Uppsala University. He then held an Izaak Walton Killam postdoctoral Fellowship at Dalhousie University, working in the research group of Prof. Russ Boyd. Gault joined the University of Windsor in the summer of 2001.

The conference continued on the second day with parallel technical sessions and a round table meeting attended by the invited guests. Three main streams of topics were actively and frankly discussed at the round table meeting: 1) Open and security in supercomputer centres; 2) The sources and models of financial support and 3) The improvement of service: future direction of supercomputer centres.

Before the conference, the VIP guests from overseas were greeted by the Vice Mayor of Shanghai City, Yan Junqi, at SSC.

During his visit, Hugh Couchman had meetings with the executive team of SSC, led by the Associate Director, Wang Puyong. Both parties exchanged information about each organization and discussed potential collaboration initiatives in several areas between the two centers in the very near future.

This was a return visit of SHARCNET to SSC. In May 2005, the Associate Director of SSC, Wang Puyong, was invited by SHARCNET to attend the 19th international symposium on high performance computing and systems at the University of Guelph, Ontario, Canada.

Established in 2000, SSC was 100% funded by the Shanghai municipal government with a total investment of RMB 100 million (20 million CAD) in Phase-I and RMB 150 million in Phase-II expansion with an additional RMB 80 for operational costs. Located in Zhangjiang's high-tech zone in Shanghai, the Center has nearly 60 full-time employees with ~40 technical staff. The mission of SSC is to provide the society with an open platform for HPC demands. Currently SSC serves academia and industry with about 70% and 30% of its resources respectively. In June 2004 the Chinese made Dawning 4000A series deployed at SSC was ranked No. 10 on the Top 500 list.



Pudong,
Shanghai

Collaborative Research Space: AccessGrid at SHARCNET

BY JOHN MORTON, SYSTEMS ADMINISTRATOR,
SHARCNET

Along with a significant increase in processing power, SHARCNET will soon be deploying AccessGrid rooms at each SHARCNET institution. These rooms will be outfitted with equipment to support group-to-group interaction between SHARCNET sites and other AccessGrid equipped facilities, allowing for distributed meetings, collaborative work, presentations and training sessions to take place without participants needing to travel. WestGrid (www.westgrid.ca) has been using AccessGrid technology for a variety of topics including running seminars to audiences spread across several sites.

AccessGrid (www.accessgrid.org) is an open source software tool that runs on a standard desktop computer. This means it can also be installed on a researcher's computer allowing them to join a meeting or seminar from the comfort of his or her own office. The AccessGrid rooms themselves will be large enough

for four to eight people and have multiple large displays, cameras and microphones.

A proof of concept demonstration was performed October 20 and 21 from four SHARCNET sites (the University of Guelph, Western University, McMaster University and the University of Waterloo) and an existing AccessGrid installation at Sheridan College. The five remote sites were each able to join the session over their standard campus networks with multiple video and audio connections.

The data traffic from each of the SHARCNET AccessGrid rooms will eventually run on SHARCNET's private high bandwidth network to insure superior video and audio performance between rooms.

For more information or if you have any questions, contact John Morton <john@sharcnet.ca>.

SHARCNET Sponsors Quantitative Finance Conference

BY MARK REESOR, SHARCNET CHAIR IN FINANCIAL MATHEMATICS, THE UNIVERSITY OF WESTERN ONTARIO

The Quantitative Finance Conference on Credit Risk took place on November 5, 2005 at The University of Western Ontario. This event attracted 85 people to London Ontario, of which half were students and postdoctoral fellows, with the remaining equally split between professors and practitioners. One of the aims of the conference was to generate significant private-sector participation, something that was achieved by having an equal number of presenters from academia and industry. The topics covered ranged from new frontiers in credit-risk research to some important practical issues from industry.

Kay Giesecke from Stanford University started the day by speaking about a top-down approach for multi-name credit modelling and its application to the pricing of credit default swaps. Michael Walker from the University of Toronto, Alex Kreinin of Algorithmics, and Tom Hurd of McMaster University gave presentations describing different approaches to pricing various Collateralized Debt Obligations (CDOs), currently a hot topic in credit risk research and practice. Michael Gordy of the U.S. Federal Reserve discussed how international regulators determined the new Basel II capital requirements that institutions must hold for their CDOs. Greg Gupton of Moodys/KMV considered the specification and fit of models for the loss given default, a crucial component of any model used for pricing and managing credit products. Niall Whelan from Scotia Capital exposed some of the many computational challenges risk-managers face when dealing with a large portfolio having a large number of risk factors, including the risk of default. He also provided a practical simulation framework to overcome these challenges. Finally, Weidong Tian of the University of Waterloo looked at the issue of capital structure, default and their relation to equity-linked debt products. Feedback the organizers received from academics and practitioners alike suggested that these presentations provided something for everyone interested in credit risk modelling and pricing.

Fields, MITACS, and SHARCNET all generously provided financial support for the conference, with Fields and SHARCNET also providing significant organizational support.



Greg Gupton

“One of the aims
of the conference
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participation.”

SHARCNET is currently in the midst of a major upgrade, during which our CPU count will increase by over eight times to just under 8,000 cpus. In addition to adding dramatically more resources, we're very focused on improving the usability and ease-of-use of SHARCNET's facilities.

USER MODEL: SHARCNET's basic user model is unchanged – request an account via the website, connect to individual clusters using SSH, edit, compile and submit your jobs to that cluster. These steps are being polished though, to improve ease of use.

ACCOUNT SPONSORSHIP: Users apply for an account through a form on the SHARCNET website. Each individual user needs a separate account, since no accounts are shared. Accounts are still structured as a faculty-level sponsor with some number of subsidiary student/postdoc/etc. accounts. The sponsor relationship exists because SHARCNET relies on the sponsor for information about research outcomes and publications. Sponsors are also responsible for re-activating subsidiary accounts each year.

SINGLE SIGN-ON: A SHARCNET account is managed from a central database, and permits login on any cluster as well as the web portal using a single, synchronized password. Users may also configure their accounts to use SSH public keys for login, which is often more convenient and secure than passwords. Often a user does not require the full flexibility of a terminal-like login session, in order to check job status, or to start another job for example. To make these cases easier, we're also developing a full-featured web portal, which will allow secure access to your account, down/upload of files, job status and even a persistent session like a login.

DISPARATE JOBS: One lesson learned from the first generation of SHARCNET machines is that our users run quite disparate kinds of jobs: some users run a few jobs, each of which use many cpus; others run many single-cpu jobs. Some need very little memory, but others are primarily limited by memory size. Even for two users who both run the same-sized MPI jobs, they may differ dramatically in how tightly-coupled the CPUs are.

FINDING CLUSTERS: SHARCNET already has a significant number of clusters, making it a bit of a challenge for a user to find the right cluster to run jobs on. With the expansion, SHARCNET has deliberately specialized clusters to suit certain kinds of jobs.

UNIFORM JOB SCRIPTS: To address this, SHARCNET will provide a uniform set of job-submission and control scripts, which will be usable on every cluster. Users will be able to “`qsub -o outfile -q parallel -n 4 ./prog`” on any machine. We will eventually offer global scheduling across the SHARCNET clusters, so you can submit a job anywhere, and expect it to run on the most appropriate cluster.

UNIFORM COMPILE SCRIPTS: During the initial phase of SHARCNET, existing and new clusters diverged, so it became difficult for users to know how to compile their code on each cluster. Many of the new clusters will be relatively compatible, but there are still differences. To mitigate this complexity, we have developed a script which supplies cluster-specific compiler parameters. This means that “`f90 *.f90 -lmpi -o prog`” will actually compile and run on any cluster; “f90” is implemented by a script that knows which cluster you're on, which compiler to use, can choose sensible default optimization flags, and

which can also supply the right flags to link with MPI.

UNIFORM /home: Another way we're trying to address this complexity is to arrange for you to have a single, same home directory available wherever you login. The intent is that you'll store your source code and configuration files there, but that anything involving major IO will happen on per-cluster storage available as `/work/username`. `/home` will be limited by quotas to a moderate size such as 200 MB, but the intent is that you run jobs from `/work`. The tradeoff here is that it's impractical to share `/home` across all clusters unless it's relatively low-IO, and that for high-IO, we need per-cluster `/work`.

ACTIVE PORTAL: Ideally, a user would like to trigger jobs, not have to worry about where they should run, and have them run immediately. The latter depends mainly on how many other users want to run jobs, and we can reduce the amount of concern for where jobs run. One way to do this is have the user log into the web portal, rather than individual clusters. We already do provide some useful job-monitoring features under MySharcnnet on the existing website. In the near future, we will expand these, as well as providing an “active” portal to allow users to start, control and monitor their jobs. This portal will let users up and down-load files as well. Besides managing jobs, we've found that it's important for users to monitor and control their space usage: the active portal will provide a convenient way to gain an overview of their file usage.

Swimming with SHARCS: New Staff

SHARCNET is growing – not only on the computational side, but on the human side as well. Staff recruitment has been underway over the last few months. Additional technical positions, including a Technical Manager, will be added in the near future.

Cindy Munro rejoined SHARCNET on October 17th as the Director of Finance and Administration. Many of you may remember Cindy from her former role as SHARCNET Administrative Officer (2001-2004). Her involvement with SHARCNET has been crucial in very many areas particularly in efficiently managing the complex financial and administrative aspects of SHARCNET. Along with her previous experience with SHARCNET, Cindy also brings extensive administrative expertise in academic and information and technology environments. From 1984-2001, she was employed with Information Technology Services (ITS) at Western.

Robert Schmidt joined SHARCNET as a Systems Administrator, located at the University of Waterloo, on November 21st. Robert is a graduate of the University of Waterloo with a B. Math in Honours Combinatorics and Optimization and has been working for the past two years with Information Systems and Technology (IST) at the University of Waterloo. He held two positions within the IST: originally hired for the UNIX support team, Robert spent a year supporting the central UNIX infrastructure and for the second year worked as a member of the Network support team supporting the campus core network, external access and ResNet.



Cindy Munro



Robert Schmidt



New Building for Waterloo

By Mike Hudson, SHARCNET Site Leader, University of Waterloo

At the University of Waterloo, a new building is being built to house the SHARCNET throughput cluster, amongst other things. The building links the Physics and Engineering buildings on the Waterloo campus. The ground floor of the new building will be a state-of-the-art machine room with raised floors and 150 tons of cooling, and will host several HPC clusters and servers. The second and third floor will serve as a new home for other computing facilities and offices in Science and Engineering, as well as a temporary home for Waterloo's Institute for Quantum Computing, School of Pharmacy and Nanotech programs.

SHARCNET and HPCVL Joint Symposium

BY BAOLAI GE, HPTC CONSULTANT, SHARCNET

A joint symposium on high performance computing and applications was held by SHARCNET and HPCVL (High Performance Computing Virtual Laboratory) at Ryerson University on October 11, 2005. Co-sponsored by ORANO, the carrier of the high speed optical network that connects research institutions one to another in the province, and to the world, the one-day event was attended by ~30 people from 13 institutions and companies. Seven invited speakers from SHARCNET/HPCVL institutions and ORANO gave talks on topics on high performance computing and applications in areas of bioinformatics, astrophysics, medical science, psychology, physics and networking, etc.

The aim of this symposium was to provide a forum for the discussion of the latest developments of computational

technologies and the impact on the advances in computational science and applications. This was the first event jointly organized by the two HPC consortia in a move towards joint efforts in providing HPC support in Ontario. Since the establishment of two consortia, SHARCNET and HPCVL have been serving ~1,600 HPC users in the universities, colleges and research institutions across Ontario, as well as other provinces.

For details about the symposium, visit the web site at <http://www.sharcnet.ca/events/symposium2005/>.

A Prime Example of High Performance Computing:

SHARCNET Used to Confirm a World Record-Breaking Number

SHARCNET computers have confirmed the world's largest Mersenne prime number, comprised of 7,816,230 digits.

Jeff Gilchrist, a graduate student from Carleton University, used a SHARCNET parallel computer to verify the accuracy of the record-breaking figure, discovered in February 2005 by Dr. Martin Nowak, an eye surgeon from Michelfeld, Germany. Employing 12 of the 16 1.2GHz CPUs on SHARCNET's Compaq Alpha GS160 server, Typhon, Gilchrist was able to validate the number in only 15 days.

A prime number is a whole number greater than one, and whose only whole number factors are one and itself (e.g. seven, which is divisible only by one and by seven). If a number of the form $2^p - 1$, where p is prime, is itself prime, then it is known as a Mersenne prime. Mersenne primes are a rare class of prime numbers; $7 = 2^3 - 1$ is the second Mersenne prime. A French monk named Marin Mersenne was the first to study these types of primes nearly 350 years ago.

Mersenne primes are the largest known prime numbers and play a critical role in many applications related to data security and confidentiality. Online banking, electronic funds transfer and stock transaction all require the use of large prime numbers for encryption purposes.

Discovery of primes of this size require computational techniques and cannot be discovered by hand. The new prime was verified using different software and hardware systems to ensure that the initial outcome was not the result of a software bug or calculation error.

The new prime has set a "benchmark for how far computers have come," says Gilchrist. "The process is comparable to finding a needle in a hay stack." The new 42nd Mersenne prime is 225,964,951-1.

High performance parallel computing resources like SHARCNET's dramatically speed up the verification process for Mersenne prime numbers.

Happy Holidays!

The SHARCNET team would like to extend holiday greetings to the community at large, especially to our researchers, industrial partners and granting agencies. We look forward to an exciting and prosperous 2006!

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