

SHARCNET Awards Funds for College Research Chair



Ed Sykes, SHARCNET College Research Chair

SHARCNET is pleased to award \$80,000 in funding, over two years, for its first College Research Chair at Sheridan College. This funding will be supplemented with a \$10,000 Fellowship from the Colleges Ontario Network for Industrial Innovation (CONII) and a \$10,000 Proof of Principle award from CONII.

The position will be filled by Dr. Ed Sykes, from the Sheridan Institute of Technology and Advanced Learning in the School of Applied Computing and Engineering Sciences (ACES). The SHARCNET College Research Chair is a two-year research secondment, commencing January, 2009.

Dr. Sykes is a Professor of Computer Science and holds a Ph.D. in the field Cognition and Learning with emphasis on machine learning algorithms. Granted in 2006 by Brock University, his Ph.D. work involved designing, developing and assessing the Java Intelligent Tutoring System (JITS) which focused on a unique e-learning tutoring system. The innovative design elements created within JITS won him the highly competitive and prestigious 2003 IASTED Best Ph.D. Award. Dr. Sykes has a strong research background in Human Computer Interaction (HCI) and e-learning systems and has published extensively during the last several years in this area. He has been involved in the research department at Sheridan for nearly seven years and has been Principle Investigator for several projects.

Dr. Sykes' current research interests involve algorithmically determining opportune times to interrupt users performing computer-based tasks. The algorithm he is designing will use artificial neural networks and dynamic Bayesian networks which are scalable through the use of MPI on large scale SHARCNET supercomputers.

In his new role as SHARCNET College Research Chair, Dr. Sykes will contribute to the advancement of SHARCNET's aims and objectives by leveraging the value of enhanced College participation. As a SHARCNET College Research Chair, Dr. Sykes aims to:

- i) Conduct high caliber research and publish in top journals;
- ii) Forge new inter-institutional linkages;
- iii) Encourage and enhance research in SHARCNET College members; and
- iv) Increase the number of HPC Highly Qualified Personnel by involving outstanding students in research projects.

"I am very excited about this SHARCNET College Research Chair position. I will strive over the next two years to conduct high caliber research and publish in highly recognized conferences and journals. I am also very motivated to encourage others to use SHARCNET, in particular Fanshawe and other colleges in Ontario. Additionally, I am also interested in establishing relationships with local companies to encourage the use of SHARCNET facilities for industrial-oriented HPC research," says Sykes.

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Dr. Sykes will be conducting visits and talks at other colleges in Ontario to foster HPC research initiatives. Fanshawe, George Brown, Conestoga and other colleges have already approached Dr. Sykes and have expressed an interest in HPC research. Closer to home, Dr. Sykes believes Sheridan is an excellent candidate for conducting Digital Humanities research as Sheridan is world renowned for its Arts and Animation. Fostering the use of HPC in the Digital Humanities at Sheridan and other institutions will be another objective of this Chair position. Dr. Sykes also wishes to pursue establishing relationships with local companies to encourage the use of SHARCNET facilities for industrial-oriented HPC research.

The SHARCNET College Research Chairs Programme is a pilot initiative, building on the existing SHARCNET Chairs Programme targeted at the universities. Its primary goals are to encourage and enhance research by the colleges; forge new inter-institutional and industrial linkages; and help build a community of expertise in HPC.

SHARCNET wishes to acknowledge **Hewlett Packard** and **Silicon Graphics** for their financial contribution which provides funding for this initiative.



Ted Hewitt,
Chair of the Board

“We rank as one of
the top HPC Centres in
Canada, providing Ontario
and Canadian researchers
with an internationally
competitive computational
infrastructure.”

Message from the Chair of the Board

It is my pleasure to present another issue of SHARC Bytes to the broader research community, institutional representatives and our funding agencies.

As is highlighted throughout this newsletter, SHARCNET has and continues to excel in the primary elements of its mission: providing high-performance computing infrastructure and services to support innovative, world-class research; training of highly qualified personnel skilled in advanced computing techniques in a variety of disciplines; and creating a culture of high-performance computing within Ontario.

We rank as one of the top HPC Centres in Canada, providing Ontario and Canadian researchers with an internationally competitive computational environment. SHARCNET is eager to continue on its forward trajectory, by offering the highest quality HPC facilities and services. However, to stay in this position, it is important that funding for HPC continues. We believe that the use of HPC in Canada is far from saturation, and in this context, we expect SHARCNET's user demands to continue to increase substantially over the next four to five years.

We will continue to work alongside Compute Canada and the Ontario High Performance Computing Council to ensure this essential research resource is able to expand and flourish.

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

As a result of a Strategic Planning exercise completed over a year ago, SHARCNET has put a significant amount of effort into a number of key initiatives over the last several months. These include: providing increased leadership in national and provincial HPC initiatives; documenting and communicating the importance of HPC; growing the pool of HPC skills and expertise; and expanding outreach efforts.

A new initiative, the SHARCNET College Research Chairs Programme, was launched as a pilot in order to build on the existing Chairs Programme targeted at the universities. Its primary goals are to encourage and enhance research by the colleges; forge new inter-institutional and industrial linkages; and help build a community of expertise in HPC. The position was filled by Dr. Ed Sykes, from Sheridan College, and is highlighted on the cover of our newsletter.

We have taken a leading role in creating links between HPC and the Digital Humanities Community in Canada. SHARCNET held a workshop on HPC and Digital Humanities last April to explore how best to support the Digital Humanities and to foster links between SHARCNET and non-traditional HPC disciplines. This small workshop brought leading researchers from the Humanities, with computational problems and potential, together with computational expertise from SHARCNET. This led to several initiatives and activities including a paper at the Congress of the Humanities in Vancouver last summer and a new SHARCNET Fellowships Programme to help support the use of HPC in the Humanities. Further details of these activities are available on the SHARCNET website.

We were delighted to partner with the Ontario College of Art & Design (OCAD) to present a one-day visualization workshop ("VizDay") at OCAD on November 5th, 2008. The workshop brought together researchers from a range of disciplines including the arts, humanities and science. Presentations from several leading practitioners, both from within Canada and internationally, illustrated the potential of visualization techniques to build bridges among disciplines. The success of this workshop has led to discussion about a follow-up workshop this year.

Plans are underway for "SHARCFest 2009", our annual outreach campaign of open houses, training events and symposia held during the month of May to help educate the broader community on the uses and importance of high-performance computing to research. We are currently working on a number of activities including a second symposium on GPU and CELL computing at the University of Waterloo on May 20th and Research Day on May 21st. The anchor event for

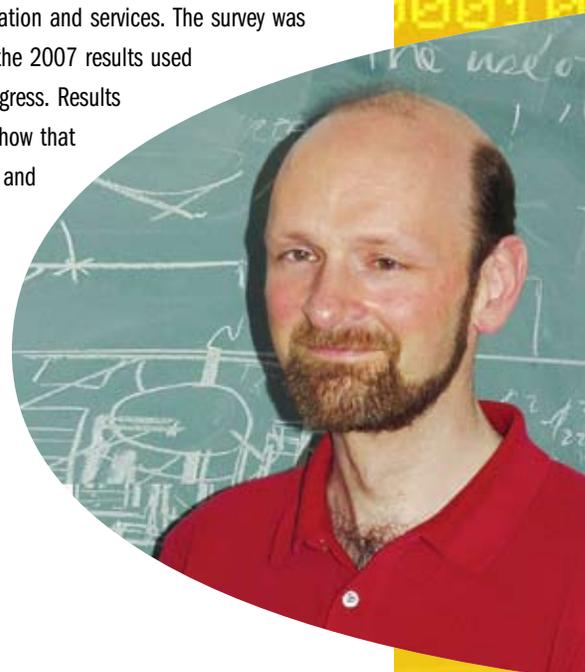
SHARCFest will be our annual HPC Summer School scheduled from June 1-5 at Sheridan College. Watch the SHARCNET website and events calendar for more information!

On the systems side, we are pleased to advise the community of several new additions to SHARCNET's infrastructure suite:

- "Saw" (2600+ cores with an InfiniBand interconnect): Saw is our new general purpose cluster for parallel jobs, resulting from an RFP issued last fall. For users running larger jobs, this should ease the load on narwhal and requin and reduce queue wait times.
- "Hound" (128gb ram/node): Hound is our experimental cluster, and is considered a fat node cluster. Each node of this cluster contains a large amount of memory and more CPUs than any of our other clusters (either 16 or 32 cores per node).
- "Angel" (gp gpu): Angel is one of SHARCNET's specialty systems. It is a cluster that permits the use of graphics cards to greatly speed up certain applications.
- "Prickly": Prickly is a new specialty system which contains IBM's CELL processor (SIMD architecture) which, like the graphics cards in angel, can greatly speed up certain codes.

In 2007, we initiated a user satisfaction survey to seek input on all aspects of SHARCNET's organization and services. The survey was repeated again last year, with the 2007 results used as a baseline to gauge our progress. Results have been quite positive and show that SHARCNET is doing a good job and is well regarded by users. For those who are interested, the results of these surveys are posted on the SHARCNET webportal. We plan to run the survey for a third time over the next couple of months and encourage users to respond so that we can get this essential feedback.

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



Hugh
Couchman, Scientific
Director

Visualization Projector Makes an Impact

A stereoscopic projection system installed in the SHARCNET Boardroom at Western is enabling researchers to peer into the complex three-dimensional fluid flow that gives birth to stars.

Shantanu Basu, Associate Professor of Physics and Astronomy, his graduate students Wolf Dapp, Alexander DeSouza, and Nicole Wityk, and SHARCNET staff member Jennifer Berberich, are modeling the fragmentation of interstellar gas clouds to form distinct regions ("cores") that collapse due to the strength of gravity and form stars.

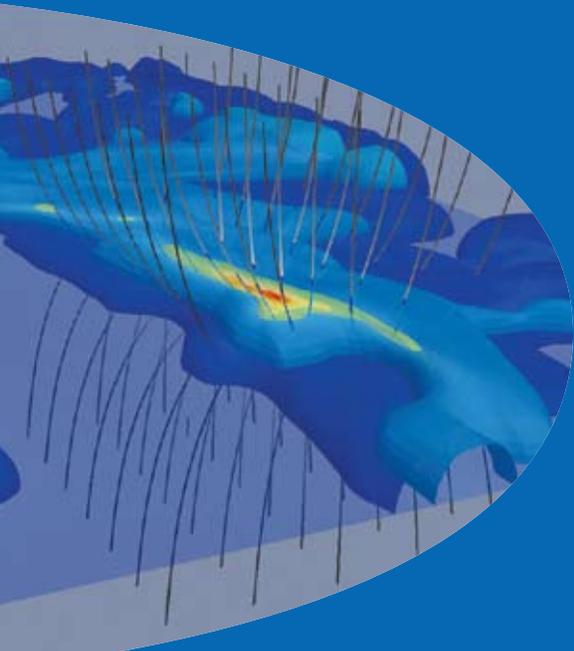
"Our computer simulations reveal the three-dimensional structure of gas and magnetic field in the regions where stars form. Although the actual process of star formation takes millions of years, we can calculate the early stages on a computer and watch animations in real time," says Prof. Basu.

For years, an important paradigm in the field has been that magnetic forces regulate the core formation process, thereby limiting the overall percentage of mass that goes into stars. Observations of stars and gas imply that this number is less than about five percent. Another idea is that stresses due to turbulence are responsible for limiting the influence of gravity. Each idea leads to a distinct three-dimensional structure of the magnetic field, the calculations demonstrate.

By visualizing the three-dimensional structure of the magnetic field, and viewing it from various locations and orientations, the group can better interpret observations of star forming regions. Observed maps of magnetic field structure, measured through polarized emission from interstellar dust, always represents a view from a specific but unknown direction. Models with either strong or weak magnetic field, and strong or weak turbulence, all yield different and observationally distinguishable outcomes.

Basu adds, "We are laying the groundwork for resolving the big questions about which processes regulate star formation, through a combination of computation, visualization, and comparison with current and upcoming observations."

The stereoscopic projection system was jointly funded by SHARCNET and an Academic Development Fund grant from Western.



Gas density in a star-forming interstellar cloud



Graduate student, Nicole Wityk, works with a stereoscopic image of a star formation

Nanoparticles on Display

THEORETICAL PHYSICIST IS UTILIZING MOLECULAR-DYNAMICS SIMULATIONS TO MODEL THE PROPERTIES OF NANOPARTICLES

BY LINDSAY BROWN, STUDENTS PROMOTING AWARENESS OF RESEARCH KNOWLEDGE (SPARK) PROGRAMME AT THE UNIVERSITY OF GUELPH

Tiny particles invisible to the naked eye may be the key to creating more effective medicines, and stronger engineering materials. Research at Laurentian University is advancing our existing knowledge of nanoparticles, so they may transcend across multiple applications.

Prof. Ralf Meyer, Department of Math and Computer Science, is developing more timely and advanced computer simulation programmes that will allow scientists to closely analyze and understand the properties of these infinitely small particles in many different materials.

Meyer is utilizing molecular-dynamic simulations and density functional theory calculations to expand nanotechnology that will provide a better understanding of nanoparticles' properties.

"Being able to simulate materials, and understand the structure and how the atoms interact within the material, will help many researchers develop better materials across many disciplines, such as medicine and engineering," says Meyer.

The Molecular-Dynamics simulation reveals how thousands or millions of atoms move in a piece of material. The density function theory (DFT) is a quantum mechanical method that studies the electronic structure of a system of atoms and electrons. Meyer is hoping to advance these programmes even further which will allow researchers to do simulations on significantly larger pieces of material containing millions of atoms.

Nanoparticles are extremely small, and vary in size between one and 100 nanometers. But they exhibit properties that differ significantly, depending on the make-up of the material. Nanoparticles can be

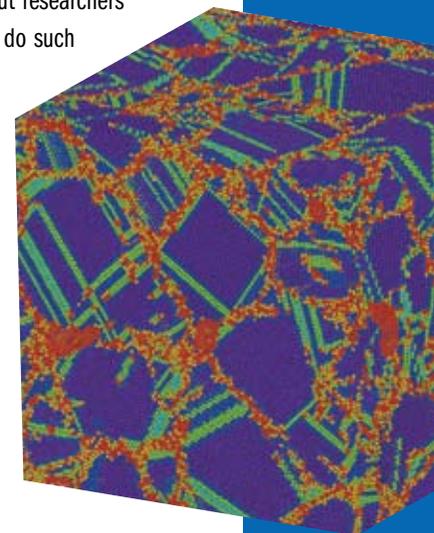
assembled into thin films, or stacks of films, but researchers require very complex computer programmes to do such simulations.

Nanotechnology may be especially useful to the medical field. The tiny particles can be adapted to target specific cells in the body by sensing different environmental conditions. A better understanding of nanotechnology may enhance biomedical research through improving non-invasive imaging tools for scanning internal organs, where the nanoparticles can reveal any abnormalities. Nanotechnology may also improve the effectiveness of many drugs by enhancing their timely relief if the nanoparticles can carry medicinal particles to specific cells or locations within the body very quickly.

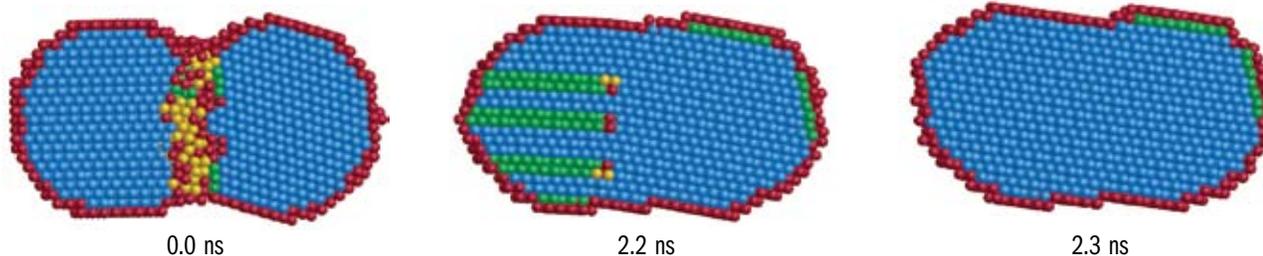
In engineering, nanoparticles would be advantageous to creating materials which require increased strength and resistance to stress. Engineers are creating spherical nanoparticles which absorb stress and disperse it throughout the material. Fast Molecular-Dynamics simulation programmes will enable engineers to know the underlying structure of these nanoparticles and transfer their properties to more resilient, scratch-free coatings on many products.

Meyer is a newly appointed SHARCNET Research Chair within mathematical and computational materials science. Meyer is writing a computer programme which can use parallel computers to carry out DFT calculations on larger sample sizes more efficiently, and at higher speeds than previously capable. He is able to test these programmes on the parallel computer network at SHARCNET.

Funding for this research was provided by the Laurentian University start-up fund.



Molecular-Dynamics simulation of nanocrystalline Cu



Dislocation activity during the sintering of Ni nanoparticles

SHARCNET Awards Additional \$300k for Fellowships

SHARCNET is pleased to announce the results of the Round IX competition for Fellowships and Dedicated Resources. With \$1.7m in funding requests from 85 applications, this was another competitive round.

SHARCNET is awarding \$301,784 over two years for 19 new Fellowships for graduate, undergraduate and post doctoral students. With matching contributions provided by the researchers, the total investment to increasing the number and quality of research personnel using high performance computing is \$600,000.

For details of individual awards, please visit: www.sharcnet.ca/research/roundIXresults.html

These Fellowships are made possible through the generous financial contributions of our industrial partners, **Hewlett Packard** and **Silicon Graphics**. Since 2001, over 200 Fellowships have been awarded through eight separate funding rounds. Supporting these individuals allows SHARCNET to increase the number and quality of research personnel involved in HPC.

New Digital Humanities Fellowships Programme Launched

SHARCNET is excited about its recent launch of a new Fellowships Programme targeted at the Digital Humanities. This pilot programme will provide resources for faculty to spend up to a day a week for two terms at one of the SHARCNET centres to work intensively on an HPC-related project. SHARCNET will provide teaching release for up to a course per term for two terms together with access to resources and programming and visualization support. The first call for proposals was announced in February, with applications due by March 31, 2009.

The objectives of the programme are twofold: to allow researchers from the Digital Humanities and Arts communities to undertake projects of exceptional promise that leverage the HPC resources and infrastructure of SHARCNET; and to increase the interaction and integration between the Digital Humanities and Arts communities and the traditional HPC disciplines in the use of SHARCNET's high-performance computing resources and infrastructure. Depending upon the outcome of this pilot and on available funding, additional rounds may be announced in the future. For details, visit: www.sharcnet.ca/Documents/call_for_DH_proposals_i.pdf



SHARCNET wishes to acknowledge **Hewlett Packard** and **Silicon Graphics** for their generous financial contributions which support these very important research programmes.

A banner image showing a person's face in profile, looking at a computer screen, with a blue and white color scheme.

**DIGITAL
HUMANITIES**

Exploring a New Dimension of Differential Equations

BEING ABLE TO LOOK AT TWO-DIMENSIONAL DIFFERENTIAL EQUATIONS WILL GIVE RESEARCHERS ANOTHER TOOL TO MODEL REAL WORLD PROBLEMS

BY ANUPRIYA DEWAN STUDENTS PROMOTING AWARENESS OF RESEARCH KNOWLEDGE (SPARK) PROGRAMME AT THE UNIVERSITY OF GUELPH

Mathematics, science and engineering all rely on differential equations. One type of differential equation, called an integrable equation, only analyzes one spatial dimension and time, and its applications can be limited as a result. A researcher at Brock University is hoping to change that paradigm by adding another dimension to these equations. Because actions unfold in three dimensions, adding another dimension into these differential equations will make the models more representative of the real world.

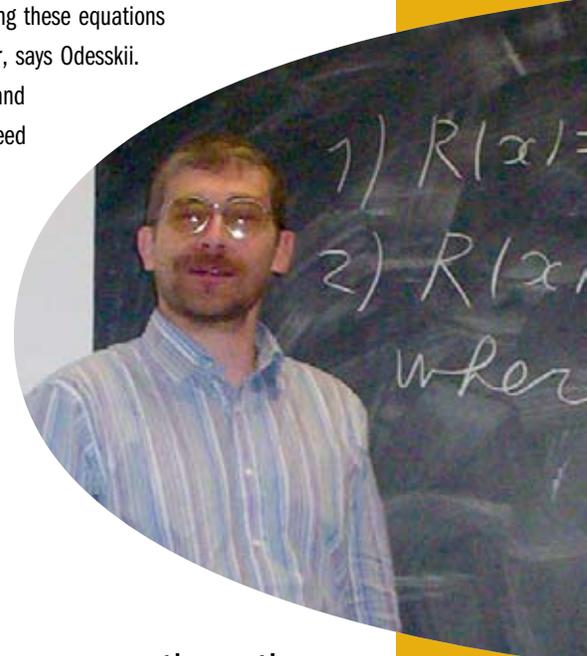
Many mathematical equations form the basis of science and can be used to model several real world problems, but they can be difficult to apply without the help of sophisticated computer software. Dr. Alexander Odesskii is working with SHARCNET to develop new equations that can help solve several real world problems by developing accurate models of real world phenomenon. Exactly where these new equations will be applied is not yet known.

“A new equation in pure mathematics is like working on a piece of art,” says Odesskii. “You can’t focus on the practical applications; they will come once the equations have been sorted out.”

In an increasingly technological society, researchers have come to rely on computer models to simulate complicated real world phenomenon. Pure mathematical equations, such as differential equations, are the key component in modeling natural events as they would occur in real life.

Differential equations accomplish this by using integrable systems to come up with a solution. They also have other applications, such as predicting a soliton – a self-reinforcing solitary wave that maintains a constant speed. These equations are used directly to show how waves lose very little energy even when they travel long distances. Odesskii is hoping to develop a comparable tool with his research in pure mathematics.

However, the process of deriving these equations requires a lot of trial and error, says Odesskii. Several different experiments and formulas are integrated and need to be executed at the same time to see which ones work and which ones need to be modified further. Unique properties and limitations of the equations are also analyzed to determine the future changes that should be made to derive novel equations.



“A new equation in pure mathematics is like working on a piece of art. You can’t focus on the practical applications; they will come once the equations have been sorted out.”

SHARCNET plays a significant role in this discovery by allowing researchers to look at and run several mathematical models efficiently. The network makes it possible to solve the equations, which would otherwise be quite a challenge.

“It would be very difficult to solve these equations with pen and paper,” says Odesskii. “This is when SHARCNET comes to the rescue.”

Odesskii is also a newly appointed SHARCNET Research Chair in high performance symbolic computing. Funding for his research has been provided by both SHARCNET and Brock University.

Alexander Odesskii, Brock researcher and SHARCNET Research Chair



HPCS 2008 hosted by
Université Laval



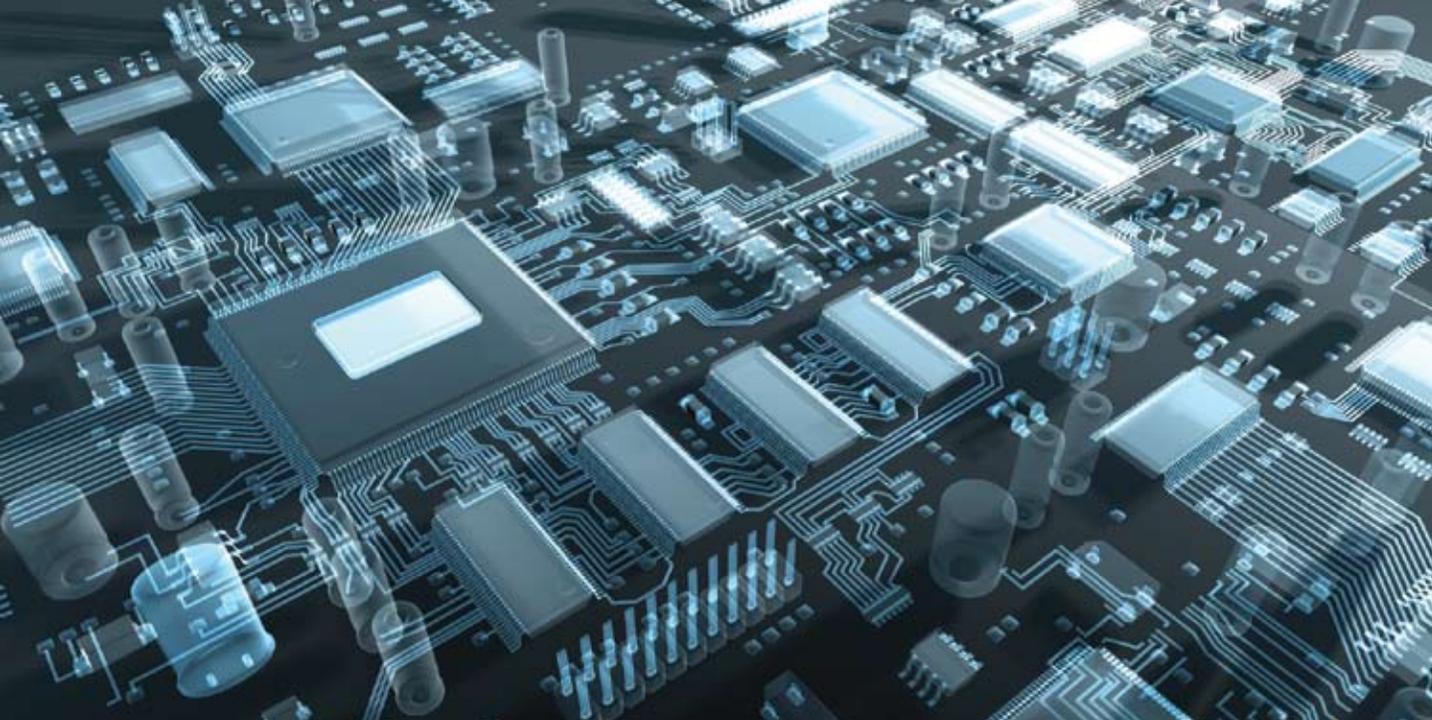
HPCS 2009

SHARCNET IS PLEASED TO HIGHLIGHT HPCS 2009,
BEING HELD JUNE 14-17, IN KINGSTON, ONTARIO.

HPCS (High Performance Computing Symposium) is a multidisciplinary conference that focuses on research involving High Performance Computing and its application. Attended by Canadian and international experts and renowned researchers in the sciences, all areas of engineering, the applied sciences, medicine and life sciences, mathematics, the humanities and social sciences, it is Canada's pre-eminent forum for HPC.

This year's conference is hosted by the High Performance Computing Virtual Laboratory (HPCVL), in beautiful and historic Kingston. Kingston, the Limestone City, is a city built on a grand heritage and defined by an exquisite ability to blend the beauty of yesterday with the passion and sophistication of today. All of this in a city that dazzles with soaring 19th century limestone architecture and the amenities of a major centre, but retains the allure of a small town.

During the course of the symposium, high profile members of the international research community will present on ongoing projects which use HPC as a research tool. In the past, papers presented have included topics from fields such as Parallel Programming, Molecular Interactions, Biophysics, Environmental Research, Theoretical/Computational Chemistry, Genetic Programming, and Bio-Mechanics. For more information, visit: <http://www.hpcs2009.org/>



Second SHARCNET Symposium on GPU and Cell Computing

Due to the popularity of this event last year, SHARCNET, along with co-hosts the University of Waterloo and Wilfrid Laurier University, is offering its second symposium on GPU and Cell Computing.

This one-day symposium, to be held on May 20th, will explore the use of GPUs and Cell processors for scientific and high performance computing. SHARCNET has deployed high-performance clusters containing both architectures, and this symposium will give researchers the chance to learn about these new technologies from keynote speakers who are at the forefront of research in this field. Researchers working with these architectures are invited to contribute presentations and posters.

Call for Contributions

Researchers interested in presenting their work in the form of a 20-minute presentation or a poster at the symposium are encouraged to submit abstracts for consideration by April 22 to ssgc2009@sharcnet.ca. Submitters are required to register to the symposium before their abstracts will be considered, via www.sharcnet.ca/events/ssgc2009/

A limited number of talks will be selected for presentation at the symposium. Reasonable submissions that are not selected for a talk will automatically be considered for a poster presentation.

Abstracts should be approximately half a page in length for a poster, and up to three pages for a talk.

Important Dates

Note: Please register as soon as possible, as the number of participants is limited.

April 22: deadline for abstract submission (contributed presentations and posters)

April 29: notification of accepted presentations and final programme announcement

May 6: deadline for registration

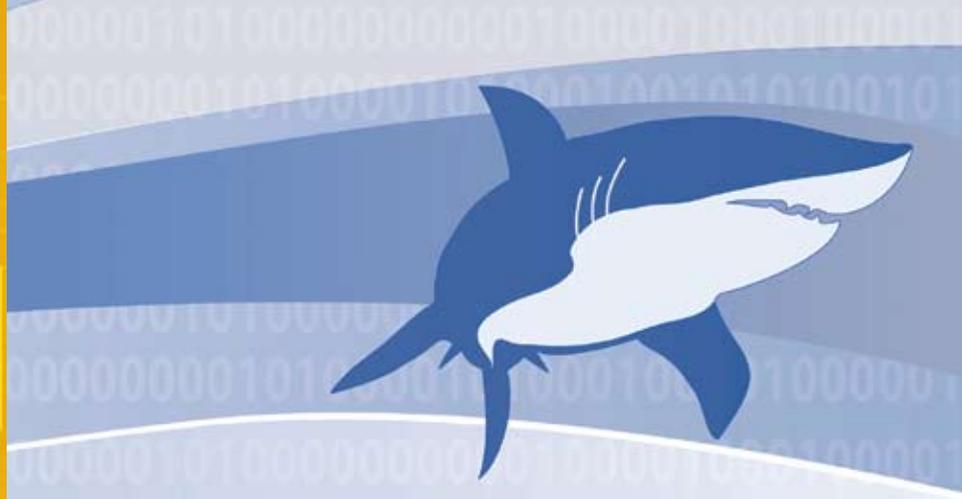




Darryl Willick



Alexei Razoumov



Swimming with SHARCS: New Staff

Recently hired by the Technology Service Centre (TSC) at Lakehead University, Darryl Willick fills the role of Visualization/High Performance Computing Programmer Analyst. Darryl obtained his B.Sc. (Computer Science '88) and M.Sc. (Computer Science '90) at the University of Saskatchewan, where he worked as a Research Officer after graduating. His research focused on modelling High Performance Computer Interconnects and performance evaluation of distributed computer networks. He joined the Materials and Process Simulation Center at the California Institute of Technology in 1993, and has been the Director of Computational Infrastructure since 2001. He has extensive experience building and maintaining High Performance Computer (HPC) systems, managing scientific software, and working with scientists to utilize these tools.

Alexei Razoumov is as our newest HPC Technical Specialist based out of the University of Ontario Institute of Technology, commencing April 1st. Alexei Razoumov has a research background in computational astrophysics, with a particular interest in computational fluid dynamics and numerical radiative transfer. He received his Ph.D. from the University of British Columbia and worked at the University of Illinois at Urbana-Champaign, University of California San Diego, and Oak Ridge National Laboratory. Most recently, he was an ACEnet fellow at Saint Mary's University.

SHARCNET is pleased to welcome both Darryl and Alexei to the HPC community!

The Compute Canada Database Project

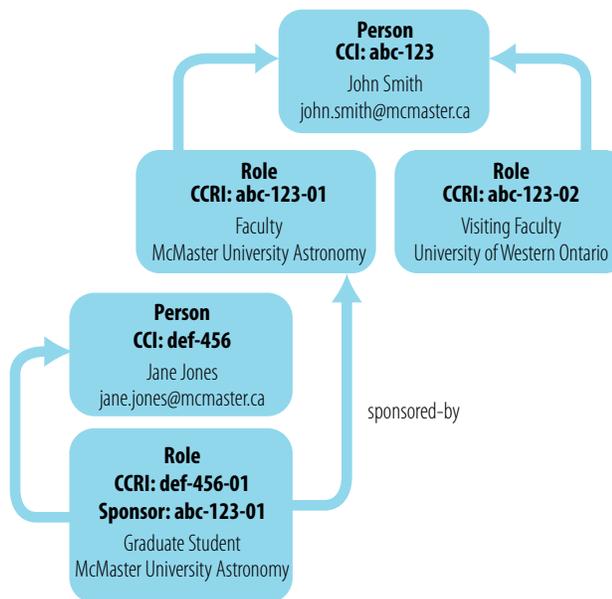
For the next round of CFI National Platforms funding, CFI has asked that all Canadian High Performance Computing consortia work more closely together. In particular, it should be easier for Canadian researchers to access CFI-funded equipment anywhere in Canada, regardless of their home institution or consortium, and it should be possible to generate reports on resource usage across all HPC systems in Canada.

An “Access To Resources” Working Group composed of members from all consortia, including SHARCNET, has taken the first step by creating a Compute Canada Database (CCDB) and associated web portal. SHARCNET has undertaken the actual development of this system based on the design of the Working Group. This CCDB will record every individual HPC researcher in Canada as well as details of their jobs, positions and supervisors.

Each consortium will continue to maintain its own database of user information, but any information in the CCDB will be authoritative – changes in the CCDB will be copied to the local database. This means that even if you use multiple consortia you will only need to update your information in one place, the CCDB.

The CCDB contains a somewhat abstract representation that gets mapped by the consortium into something that makes sense locally. The CCDB contains “People”, identified by a “CCI” (Compute Canada Identifier) and “Roles” identified by a “CCRI” (Compute Canada Role Identifier). These identifiers are then used to get accounts at the various consortia, with the CCDB supplying all of the account information.

It's easiest to explain by example. Consider John Smith, an Astronomy professor at McMaster University, who is also a visiting professor at Western. He supervises a graduate student at McMaster, Jane Jones. The CCDB records might look something like this:



Each consortium will record the relationship between their local user accounts and the CCDB identifiers. For example, SHARCNET might record that the CCI “abc-123” belongs to the username “jsmith”, while RQCHP might have “smithj”. However, since all of the user information will come from the CCDB, Smith would enter this information just once, in the CCDB, and his accounts at each consortium would synchronize any changes.

Over time the CCDB will expand to include lists of resources at each consortium (clusters, software packages), projects and special allocations (known as “Resource Allocation Projects”) and usage statistics from all consortia.

At some time in the coming year, you will require a Compute Canada account in order to apply for a SHARCNET account or to renew your existing SHARCNET account. It might sound like a chore to apply for yet another web account, but this one helps you more easily access systems all over Canada, and helps the consortia to satisfy CFI’s requirements, so that you will continue to have access to high-quality HPC resources in the years to come.

Shared Hierarchical Academic Research Computing Network

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