

Computer Simulations Accelerate HIV/AIDS Research

BY LISA LABELLE, DEPARTMENT OF COMMUNICATIONS AND PUBLIC AFFAIRS, THE UNIVERSITY OF WESTERN ONTARIO



Lindi Wahl, Western researcher

By focusing on one of the most prevalent diseases of our time, Lindi Wahl, a professor at The University of Western Ontario, applies her expertise to an expanding issue that demands international attention. The HIV/AIDS

contagion has led Wahl to work on developing better therapies aimed at reducing drug dependence and the amount of medication required for treatment, while preventing drug resistance.

Wahl uses SHARCNET to identify how drugs can lower the viral load, which is the amount of virus in a patient's blood, and keep patients alive longer. The idea with drug sparing regimens is to design therapies that provide breaks from medication, which makes taking antiviral drugs easier for the patient; other traditional approaches may require patients to take up to 18 pills a day, which is close to impossible to achieve.

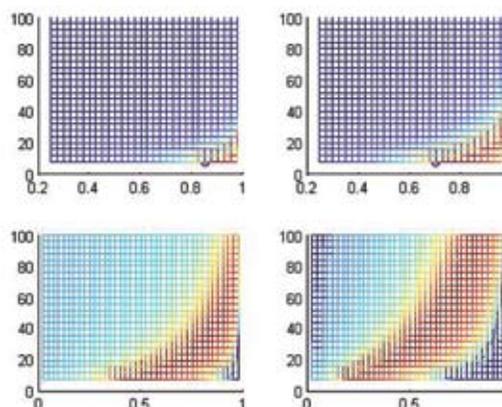
To identify effective ways to incorporate drug holidays in a drug regimen, Wahl uses computer simulations of infected patients. This allows her to model the virus, the infected cells and the immune system to study how the drugs will affect the virus. This is too complicated to do analytically, so by performing evaluations using the computer, she is able to make real-world predictions. Drug regimens with holidays have been tried before,

usually for periods of a month or more, both on and off therapy. "The model is predicting that regimens that are as short as four days on and one day off are better, so we think some clinical trials should be started with these shorter periods on and off because that's what's coming out of our models," says Wahl.

Another research project attempts to model the viral load. Wahl can predict what the patient's viral load will be, but also how it will fluctuate over time. Knowing how big these fluctuations might be over time is critical, because measures of viral load are used to decide how sick the patient is and how well therapy is working.

Both of these projects use a technique called Monte Carlo simulation which simulates behaviours of physical systems at the level of individual cells or virus particles. By using SHARCNET, the Monte Carlo simulations

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For four different antiviral drugs, the x-axis shows the amount of drug per pill, while the y-axis shows the number of hours between successive doses. Colours indicate the overall benefit of therapy; red areas are the best ways to deliver these particular drugs.

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Message from the Chair of the Board

On behalf of the SHARCNET Board, I am pleased to welcome the Ontario College of Art & Design (OCAD) and Perimeter Institute as our newest academic partners. This partnership was formally announced at SHARCNET's Phase II Launch held on May 30th at Western. SHARCNET is growing on a number of fronts, and this latest expansion only underscores our continued success – particularly in the Arts and Humanities.

As has been reported previously, both the federal and provincial governments have taken a fresh approach to how HPC will be funded in the future. One aspect of this was CFI's creation of the National Platforms Fund (NPF) and on the provincial side, the creation of the Ontario HPC Council. The Council, which has met twice since January, will provide a key interface between the three HPC Consortia and the Ontario government, assisting in the development of long-range planning and funding policy and ensuring the best use of resources across the system.

On the international front, representatives from SHARCNET visited the Shanghai Supercomputer Center last Fall, and as a result of this connection, an MOU is being finalized in order to explore areas of potential collaboration.

As members of the SHARCNET family, we can take great pride in the continued growth of our organization, in terms of equipment, staff, and partner institutions. Together we are making tremendous progress in expanding HPC resources to the benefit of researchers across Ontario. At our last SHARCNET Board meeting at Brock University in June, one of these researchers, Prof. and Board Member Dr. Deborah Stacey, provided a presentation of research highlights from across the consortium to demonstrate the quality and breadth of research being done on SHARCNET systems. The Board was very impressed with the caliber of the research, some of which you can read about in this issue of Sharc Bytes. I encourage you to browse the SHARCNET website (www.sharcnet.ca/Research/profiles.php) to view other examples of the exciting research being done at SHARCNET.

W. E. (Ted) Hewitt, Ph.D
Chair, SHARCNET Board of Directors and Vice-President
(Research & International Relations), The University of Western Ontario



Ted Hewitt

“We can take great pride in the continued growth of our organization, in terms of equipment, staff, and partner institutions.”

Student paper on hydrological modelling using SHARCNET wins commendation

Scientific Director's Message

I am pleased to report that over the last few months, we have made tremendous headway with the implementation of the new SHARCNET systems. Most of the new systems are now finally on-line, including Narwhal (1068 cpu Opteron utility cluster), Bull (384 cpu SMP cluster), Requin (1536 cpu capability cluster), Silky (SGI 128 processor Altix), as well as several of the PoP developmental clusters. The rebuilt Alpha cluster is also rising phoenix-like and is nearing 400 cpus. We expect the remainder of the systems to become available shortly, including Whale (3072 cpu throughput cluster) and the redeployed Itanium2 clusters. If you refer to the SHARCNET website (www.sharcnet.ca/Facilities), you will be able to see at a glance which machines are available. All systems are completing final configuration, software install and hardening.

The next phase of the installation will be the acquisition of the visualization equipment. The details of this are being finalized over the summer and will be rolled out by early Fall. With these components in place, the bulk of the SHARCNET2 infrastructure plan will have been realized.

In addition, many of you will have noticed that AccessGrid equipment is now in place at Guelph, McMaster, Sheridan, Waterloo and Western. The remaining sites are being outfitted as space becomes available, with plans underway to have all sites operational by the Fall. These AccessGrid rooms will, undoubtedly, provide greater opportunity and flexibility for researchers to collaborate and will allow SHARCNET to more easily engage users at remote sites.

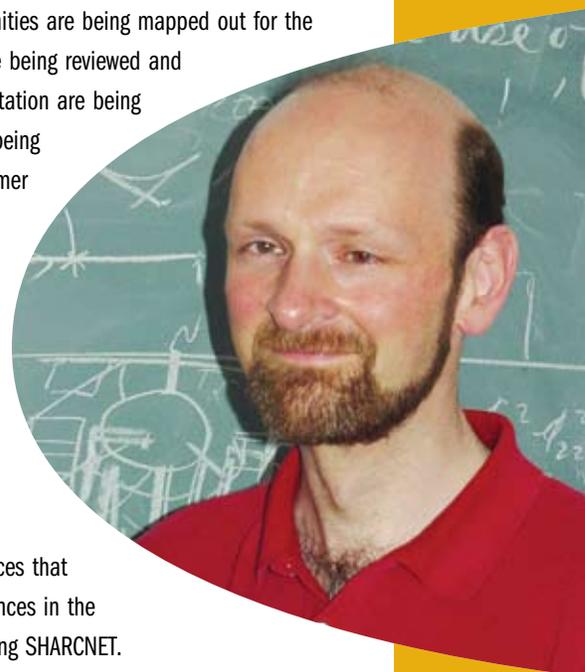
On the national scale, the CFI NPF process has continued with a number of meetings of the National Initiatives Committee (NIC) over the last several months. The proposal deadline originally set

for the end of May was extended to June 30th; the final proposal was actually submitted to CFI June 23rd. The proposal is available at www.c3.ca. On behalf of the NIC, I want to extend my thanks to all of you who contributed to this process. Even if we could not explicitly include your contribution in the final proposal because of the extreme space limitations imposed on us, the many suggestions that we received all contributed to developing a better proposal overall. Thank you!

As we head into the summer months, SHARCNET is ramping up on a number of fronts - new technical staff are being trained; workshops and training opportunities are being mapped out for the Fall; policies and procedures are being reviewed and augmented; masses of documentation are being written; a Town Hall meeting is being planned via AccessGrid; a customer satisfaction survey will be released; and plans for another round of Fellowships are being discussed.

I am confident that as we now move into the operational phase of SHARCNET2, you will find that you have access to a range of infrastructure and services that will truly enable significant advances in the research that you can tackle using SHARCNET.

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



Hugh
Couchman

At the biennial meeting of the International Environmental Modelling and Software Society (iEMSs), July 9-13, 2006, Vimal Sharma, PhD student, Computing and Information Science, University of Guelph, received a commendation from the Society for his paper: "Auto-Calibration of Hydrological Models Using High Performance Computing", co-authored with David Swayne (CIS, University of Guelph), David Lam (National Water Research Institute), and William Schertzer (also of NWRI). For more information, refer to the iEMSs website (www.iemss.org). Congratulations to Vimal!

A Watershed of Discovery?

BY MEG ATKINSON, DEPARTMENT OF COMMUNICATIONS AND PUBLIC AFFAIRS,
THE UNIVERSITY OF WESTERN ONTARIO

Ties between high speed computing and environmental protection may not be immediately obvious; however, new research uses technology to solve complex environmental problems.

David Swayne, a Professor in the Department of Computer and Information Sciences at the University of Guelph, uses high speed computing to analyze models used to study watersheds and varying effects of agricultural pollution. He also hopes to standardize the presentation of information required to protect land-lake-atmospheric regions from harmful climate change.

Swayne describes three different components of his research, the first of which is to make virtual models of pollution in watersheds and record relationships between variables in what is called a causal probabilistic network. By running simulations on this network, probability distributions are used to generate distributions for the values of unknown variables. SHARCNET's capacity speeds up this process as many simulations may have to be run up to 1,000 times each. These networks can then be used as specific information becomes known to explore multi-year scenarios or to determine economic penalties incurred by environmentally-based practices.

The second part of Swayne's research requires him to calibrate different local characteristics, or parameters, in particular watersheds. As models become more complicated, they require more complicated calibration and analysis to use them, in his case, in a probabilistic network. "Coming up with a value for models with complex parameters on a single processor can take several days of computing, whereas on a cluster like SHARCNET, the parameters can be found within a few minutes," Swayne explains. This requires investigations of parallel algorithms for the calibration process.

Sharing results is the final component of the research process. SHARCNET's distributed framework allows researchers spanning the network to remotely access the computer where the model is being run. Results are reported seamlessly from desktops all over the province to one master computer.

Swayne says that he and his colleagues are in the middle of this research project. "We're producing some results, displaying them and having them published. Our next step is to deploy this in other places, get more experience and explore parts of the country that haven't yet been modeled in this way."

Swayne hopes his work will provide an efficient, accurate and versatile program used to consider the effects of pollution on watersheds. Domain experts in such areas as sustainable development, pollution remediation economics and environmental conservation will be able to use his programs to calculate and understand the effects of changing variables and implement more successful environmental protection plans.

Swayne cites SHARCNET as a vital resource for his environmental modeling research: "conducting this research is an opportunity that we wouldn't have had without the presence of SHARCNET. The network has been helpful because it allowed us to do proof of concept using a lot of computing horsepower and to develop some algorithms that we wouldn't have had the opportunity to develop without access to the supercomputer."



David Swayne

“Coming up with a value for models with complex parameters on a single processor can take several days of computing, whereas on a cluster like SHARCNET, the parameters can be found within a few minutes.”

SHARCNET Phase II Launch

The SHARCNET Phase II Launch held at Western on May 30th and attended virtually by both McMaster and Guelph universities was a resounding success. With over 75 people in attendance, including researchers, government, and industry representatives, SHARCNET introduced its newest academic partners including the universities of Trent, Lakehead, and Laurentian, and most recently, the Ontario College of Art & Design, and Perimeter Institute.

Government funding representatives Carmen Charette (Senior Vice-President, Canada Foundation for Innovation) and David Bogart (Executive Vice-President and Chief Operating Officer, Ontario Innovation Trust) spoke about the importance of HPC – to both Ontario and Canada – and echoed their support of the SHARCNET project. With funding of over \$100 million to date from federal, provincial and industrial sources, SHARCNET has been able to construct a leading HPC organization for the recruitment of top scientists and the advancement of research.

SHARCNET was also able to show-case collaborate research being done on SHARCNET systems and illustrate how HPC has practical applications for industry. Paul Paolatto, President and CEO of Keigan Systems, demonstrated the world's first ultra high-speed incident mapping and management application designed specifically for First Responders and Command Centres, which was developed in collaboration with SHARCNET researchers.



Paul Paolatto, demonstrating first high-speed incident mapping and management application



Ted Hewitt

“By pooling resources and strengths across the network, we are able to not only enhance collaborative research efforts, but produce tangible results at a previously impossible scale and put the province on the world map for HPC capabilities.”



SHARCNET Wins Leadership Award

SHARCNET was thrilled to be honoured with the Leadership Award from the Ontario Research and Innovation Optical Network (ORION), presented at a special reception at the Ontario R&E Summit held in Toronto on June 5, 2006. The ORION Awards celebrates Ontario's extraordinary accomplishments in research and education and gives recognition for innovative use of advanced networks and collaborative technologies in three categories –Discovery, Learning and Leadership.

The ORION network provides SHARCNET with the high-bandwidth, point-to-point connections that allow the seamless integration of SHARCNET's distributed architecture. This HPC-Grid allows researchers to efficiently leverage SHARCNET compute resources, which are physically separated by hundreds of kilometres across the province. The network and interconnected computing resources are transforming the way researchers access and use high performance computing. Ontario researchers are using this massive power to advance their work in a range of disciplines – from modeling the movement of pollution and creating more efficient electronics, to achieving greater understanding of the outbreak of disease like SARS and in developing stronger, more lightweight aluminums.



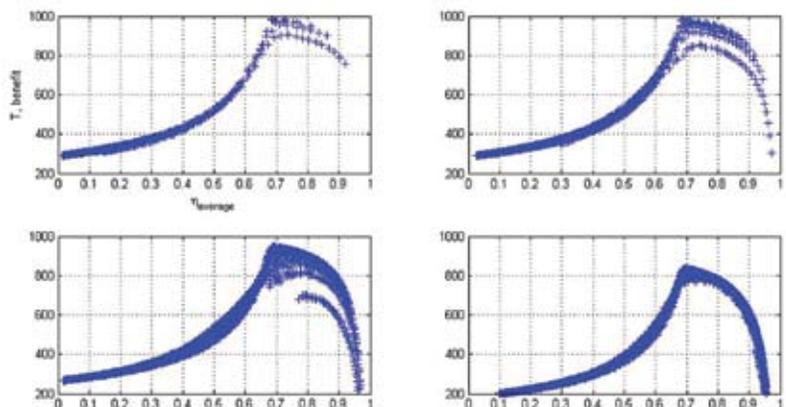
From left, Ontario College of Art and Design President Sara Diamond, SHARCNET Director of Finance and Administration Cindy Munro, Wilfrid Laurier University, Faculty of Science Dean Dr. Art Szabo, SHARCNET Technical Manager John Morton; Parliamentary Assistant to the Minister of Research and Innovation Tony Wong, SHARCNET Scientific Director Dr. Hugh Couchman, and Dr. Stan Shapson, VP Research and Innovation, York University and Chair of ORANO.

Computer Simulations Accelerate HIV/AIDS Research, continued from page 1

help Wahl in her research by allowing her to evaluate, for example, a million different strategies concerning HIV treatment.

In 2003, Wahl contributed ideas to a World Health Organization report titled Adherence to Long-term Therapies, which exercised a huge international effort looking at adherence for eight different diseases, including HIV/AIDS. Wahl explains, "In all of those diseases there are big issues around patients not taking all of their drugs and not being fully involved in their therapy."

Wahl has been able to use SHARCNET for computer simulations aimed at studying how the course of the disease plays out in a single infected individual by simulating physical systems on a very large scale. Without the help of SHARCNET, the ability to create these real-world predictions would never have been possible.



The overall benefit of HIV therapy is plotted against the average drug efficacy, for various combinations of dosing times and dosing intervals, and four different antiviral drugs. On the right of each panel we see how doses that are too large reduce the benefit of therapy, due to drug toxicity.

HPCS'06

BY BAOLAI GE, HPTC CONSULTANT, SHARCNET

The 20th International Symposium on High Performance Computer Systems was held at Memorial University of Newfoundland in St. John's, Newfoundland from May 15-17, 2006. HPCS is a multidisciplinary conference held annually in Canada since 1987. It focuses on a broad spectrum of new and exciting scientific and technical areas that utilize high performance computing. This year's conference drew a large attendance of researchers and experts from Canada and other countries. Keynote speakers included Dr. Mark Whitmore from University of Manitoba, Dr. David Hobill from University of Calgary and Dr. Michael Norman from University of California, San Diego. A number of researchers and technical staff from SHARCNET attended the conference and gave talks at technical sessions. Major HPC hardware and software vendors had an exhibition of their products during the conference.

In parallel to HPCS'06, the conference of Open Source Cluster Application Resource (OSCAR) was co-hosted with HPCS. This was the fourth OSCAR conference that had been held in conjunction with HPCS since 2003 and the fifth event hosted in Canada.

OSCAR is a self-installing cluster computing solution that provides a default software stack containing a popular collection of best-known methods for building, programming, and using high-performance computing clusters. OSCAR uniquely permits users to create their own OSCAR-package so that it may be downloaded and automatically installed by others for use on their clusters. OSCAR has been an open source package since its first public release in April 2001.

Also in conjunction with the conference was the annual meeting of the Technical Analyst Support Program (TASP), a program funded by the Canadian High Performance Computing Collaboratory (C3) on Sunday, May 14th. Technical experts in scientific and high performance computing and support from several consortia and institutions across the country attended the meeting. Representatives from each organization reported and exchanged information on the deployment of HPC infrastructure, the usage of resources and the support for research projects. Baolai Ge from SHARCNET gave a presentation on the status of SHARCNET, usage statistics and future plans.

At the TASP meeting, consortia representatives discussed initiatives for collaboration at the national level, such as a

national help desk, resource allocation and collaborative projects. A technical summit on high performance computing and applications was proposed and is set to take place in Toronto in October, 2006.

During the conference, a few other activities also highlighted the event. The C3 annual general meeting was held in parallel to the conference sessions. The first published long range plan on HPC in Canada – a result of collective efforts of researchers across seven consortia in Canada – was presented and discussed. The official launch of the Atlantic Computational Excellence Network (ACEnet) was held at the conference. Like SHARCNET, ACEnet is Atlantic Canada's entry into this national fabric of HPC facilities. It is a partnership of seven institutions, including Memorial University of Newfoundland, University of New Brunswick, Mount Allison University, Dalhousie University, St. Francis Xavier University, St. Mary's University and the University of Prince Edward Island.

HPCS is Canada's preeminent forum for high performance computing in sciences, engineering, mathematics and applied human sciences since 1987. Prior to 1995, the conference series was called Supercomputing Symposium, and was held on a rotating basis between Montreal, Toronto, Edmonton and Calgary, except for 1991, when the conference took place in Fredericton. In 2005 SHARCNET organized and co-sponsored HPCS 2005 (www.sharcnet.ca/events/hpcs2005/) held at the University of Guelph.

For further information, please visit: www.ace-net.ca/events/hpcs2006



HPCS '06:
keynote



TASP meeting
on May 14,
2006

TECC Summit '06

SHARCNET is pleased to be a sponsor of the inaugural Technical Canada 2006 Summit being held from October 23-25 in Toronto, Ontario.

The Summit

This meeting will bring together technical experts from across Canada, who are building and supporting the nation's high performance computing (HPC) infrastructure with industrial members of Canadian High Performance Computing Collaboratory (C3) in a unique dual-focused summit. The technical experts from the seven Canadian HPC consortia: ACENET, CLUMEQ, SCINET, HPCVL, RQCHP, SHARCNET, WestGrid and other C3 major resource providers (MRPs) will meet and discuss various issues in HPC support and research. One aspect of the sessions will be open discussions on issues relevant to national coordination and planning, with a goal of providing white paper recommendations to C3. Another aspect of the summit will be industry sponsored (potentially NDA) sessions focused on current and future technologies and designed to provide effective two-way technical communication between the C3 industrial membership and the Canadian HPC technical community. All sessions are meant to augment the normal professional development of the Canadian HPC technical community.

Meet and connect with professionals and experts, and experience the current and future technologies that are enabling Canada's cutting edge science and technology research.

Call for Participation

- Regional and national resource allocation and queuing policies
- Building a national HPC benchmarking suite
- National help desk viability
- Collaboration initiatives in Grid and SOA
- Performance evaluation: methodology and tools
- System evaluation for hardware/software acceptance: performance, reliability and stability
- User management, education and training
- Storage, networking and visualization
- Emerging technologies and the future hardware directions for HPC
- Software for management, development and applications

Submit proposals for technical sessions to: tecc2006@c3.ca by September 30, 2006.

Who Should Attend

Software developers, system administrators, IT professionals and managers, as well as researchers in HPC.

Visit the website (www.sharcnet.ca/Events/tecc2006) for more information.

TECC 2006

October 23-25,

Toronto, Ontario

A Technical Symposium

Building the National

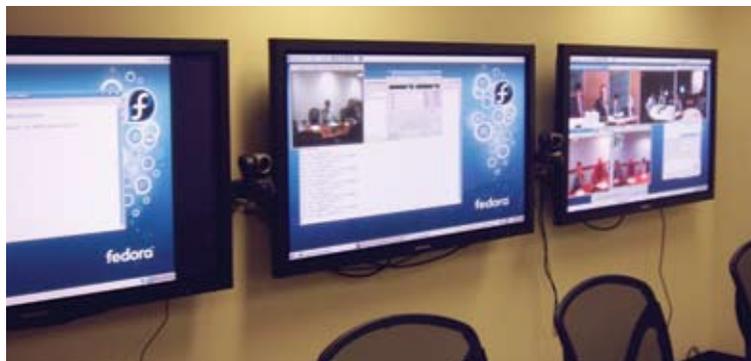
Platform for HPC in Canada

SHARCNET Gets Smaller-

It's becoming a small, small world indeed as SHARCNET deploys video conferencing facilities at each of the SHARCNET member institutions. These rooms will allow researchers to collaborate with colleagues across SHARCNET and can be used for small groups of people at each location to join together for meetings, seminars, conferences and thesis defenses.

The rooms consist of two or three large flat panel displays. These are generally 50-inch plasma screens that provide enough space for a large number of video streams. Two HP servers that also perform the video and audio capture, drive the displays. The rooms provide the ability to share a common desktop across sites to allow a presentation or dataset to be viewed or a document to be edited. Future upgrades may include smart boards, document projectors and high definition cameras.

The software solution installed is called AccessGrid (www.accessgrid.org) which is an open source project and



available for free under an open source software license. Individual users can also download and install the software on their desktop to join conferences from their office. It is a common tool used worldwide by various institutions, including WestGrid (www.westgrid.ca) who uses it for their seminar series.

In any standard video conferencing deployment, there is the potential that a bottleneck is created which slows down all network traffic at a given site. To avoid this, the SHARCNET rooms have been deployed on a dedicated high-speed network. This allows for much higher quality video and audio to be streamed from multiple sites without experiencing much or any delay. The

immediacy of the image and sound help to create the feeling that everyone is truly in the same room.

Standard SHARCNET AccessGrid rooms have been installed at McMaster University, The University of Western Ontario, University of Waterloo and the University of Guelph. Sheridan has a couple of existing AG rooms that SHARCNET will be taking advantage of and the configuration of rooms at York, WLU, UOIT and Fanshawe are underway. Within the next few months, all the current SHARCNET partners will have an AccessGrid room.

The existing rooms have already been used for a number of SHARCNET staff meetings. They also allowed researchers at McMaster and Guelph to take part in the SHARCNET Phase II Launch on May 30th at Western. A demonstration of the AccessGrid rooms and their abilities can be arranged by contacting a SHARCNET staff member. A virtual open house across multiple sites using the rooms will also be held at a future date. Watch for an announcement coming soon!



Swimming with SHARCS: New Staff

SHARCNET is expanding, again! We have added a number of technical positions over the past few months, to deal with the expansion of SHARCNET's infrastructure and partnership. A few more technical positions will be added in the future, and we plan to supplement administration and management as well. We are pleased to welcome the following individuals to the SHARCNET team.



John Morton

Earlier in 2006, **John Morton** assumed the new role of Technical Manager for SHARCNET. He is responsible for the overall operations of the SHARCNET systems, networks and services and provides guidance and technical direction to the SHARCNET Systems Administrators and HPC Consultants. John previously served as the SHARCNET Systems Administrator located at the University of Guelph.



Thomas Hu

Thomas Hu is a SHARCNET Systems Administrator located at the University of Ontario Institute of Technology, effective January 1, 2006. Thomas is a full-time employee of UOIT who will devote 50% of his time on SHARCNET-related activity. Thomas is a UNIX system engineer who has specialized in designing and deploying UNIX based computing solutions since 2001. Previously, Thomas was a UNIX architecture engineer with CIBC.



Sergey Mashchenko

Sergey Mashchenko, was hired as the HPC Software Specialist/Consultant at McMaster University effective March 1, 2006. Sergey received his PhD in Astrophysics from the Ukrainian Academy of Sciences, Kiev. Prior to joining SHARCNET, he was working on a Post Doctoral Fellowship at McMaster. Sergey has extensive experience in scientific programming and large-scale computation and held Post Doc positions in both Quebec and Montreal.



Kaizaad Bilimorya

Kaizaad Bilimorya joins SHARCNET as a Systems Administrator, located at the University of Guelph, effective April 24, 2006. Kaizaad is a graduate of Brock University with a BSc in Computer Science. He spent the last 5 years working in the ITS Department at Brock.

Fraser McCrossan, joins the technical team as a Systems Administrator, located at The University of Western Ontario, commencing May 1, 2006. Fraser received his BSc in Computer Science and Microprocessor Systems from the University of Strathclyde in Glasgow, Scotland. Prior to joining SHARCNET, Fraser was a Senior Systems Administrator for TVWorks.



Fraser McCrossan

Dan Beamish joins the SHARCNET technical team, located at York University, commencing June 1, 2006. Most recently, Dan was a postdoctoral fellow at the Academy of Mathematics and System Sciences, Chinese Academy of Sciences, Beijing, China. Dan received his Master of Arts and Bachelor of Science in Pure Mathematics at York University.



Dan Beamish

Paul Chapman also joins the technical team, located at Brock University, commencing June 19, 2006. Paul is a Unix systems administrator who has specialized in science and engineering support since 1997. He has previously overseen the development of high-performance computing facilities at the Bedford Institute of Oceanography and at the European Space Agency.



Paul Chapman

Weiguang Guan has recently been assigned to SHARCNET to support visualization efforts. Weiguang is a Visualization Research Engineer in the Research and HPC Support Department at McMaster University. He will be working on graphics programming and visualization projects for SHARCNET researchers. He has a Ph.D in computer science and research and development experience in many fields including image processing/analysis, machine vision, pattern recognition, and volume visualization.



Weiguang Guan

Doug Roberts will fill the new full-time technical position based out of Wilfrid Laurier University, effective August 1, 2006. Doug formerly provided HPC and systems support for both the universities of Windsor and Wilfrid Laurier in a shared capacity. SHARCNET is currently in the recruitment process for a full-time position at the University of Windsor.



Doug Roberts

On behalf of the SHARCNET team, have a safe and relaxing summer holiday!

Board of Directors

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Hugh Couchman (Scientific Director), SHARCNET
Cindy Munro (Secretary), SHARCNET
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