SHARCNET™

SHARC BYTES
newsletter

Summer 2009 VOL. 7 ISSUE 1

Harnessing Infectious Disease Modeling for Improving Public Health

BY ARMAND VLADAU, STUDENT COMMUNICATIONS OFFICER, SHARCNET

Chris Bauch
University of Guelph

In the age of routine universal public vaccination programs – implemented to slow the spread of infectious diseases – accurate mathematical models have become very useful. When public health officials are worried about potential disease outbreaks, such as the H1N1 influenza virus otherwise known as "Swine Flu", they often turn to computational models that simulate the rate of spread and extent of an outbreak. Dr. Chris Bauch, from the University of Guelph, uses his research to address these important questions of scientific interest to inform and guide public health policy. With experts predicting the H1N1 pandemic will worsen this upcoming fall and winter, Ontario health officials are seeking input from infectious disease modelers such as Bauch and his team, to model the disease transmission and the impact of control strategies designed to mitigate the pandemic.

Bauch is a professor and researcher in the University of Guelph's Department of Mathematics and Statistics. His research interests lie in theoretical biology, and especially infectious disease modeling where his work focuses on addressing important questions relevant to contemporary health policies. His research work is both impressive and extensive, ranging from creating disease models of measles to smallpox to HIV as well as studying the effects of primary and secondary disease interventions such as vaccination and screening. Bauch's work has also been published in a number of prestigious journals and magazines, such as Proceedings of the National Academy of Sciences, Oikos, The Canadian Medical Association Journal, and PLoS Computational Biology to name a few.

His two most recent projects are focused on assessing cervical cancer screening and predicting the spread of the H1N1 virus. The goal of the CIHR-funded cervical cancer research, he explains, is to use "mathematical and economical models to inform cervical cancer screening policies in the era of cervical cancer vaccination." Although the number of cervical cancer incidents has decreased by nearly 60%, with a decline in the death rate of 50%, since the Papanicolaou (Pap) smear test was first introduced in the 1960s, there has not been much additional decrease since 1990. Bauch believes, however, that recently introduced technologies, specifically new screening tests and a preventative vaccine, "will change the landscape of screening and treatment." Optimistic that a new vaccine against Human Papillomavirus (HPV) – one the major causes of cervical cancer – will continue to reduce the number of cervical cancer cases, Bauch's multidisciplinary team aims to develop a simulation model that "integrates knowledge of economic and epidemiological aspects of disease transmission, cervical cancer progression, vaccination and cervical screening in order to project future cervical cancer disease burden and economic outcomes under various possible alternative vaccination and screening policies."

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Message from the Chair of the Board

Paul Maxim,
Chair of the Board

"HPC is a game-changing technology and desk-top only computing users that fail to adopt it may be at a significant competitive risk."

The U.S. Council on Competitiveness

As the new Chair of the SHARCNET Board of Directors, I am pleased to present the latest edition of the SHARC Bytes newsletter and highlight some key initiatives.

In this issue, we profile three of our medical and bio-informatics researchers who are doing very exciting and topical research in areas such as H1N1 outbreak modeling, human genetics, and DNA analysis. High-performance computing is now at the core of many advanced research programs and is used to address a wide range of problems. SHARCNET provides comprehensive facilities and support services to enable researchers in Ontario and across Canada to use HPC effectively to create advances and breakthroughs in their respective areas. I hope that these highlights will help to underscore the importance of this research to our daily lives.

We also note that SHARCNET has recently awarded fellowships to two digital humanities researchers. SHARCNET's Digital Humanities Fellowships Program is the first of its kind in Canada and we are thrilled to be at the forefront in providing support and programs to this growing group of HPC users. Over the past several years, we have seen a steady increase in the range of research disciplines using SHARCNET. In addition to the traditional disciplines that you would expect, we now have researchers from a variety of research areas including: biological and life sciences, business, biochemistry, environmental and earth sciences, media and the humanities.

On the national front, SHARCNET continues to work with Compute Canada and the other university-based HPC consortia to ensure the global HPC vision and mandate is realized. The National Resource Allocation Committee (NRAC) and the Community Planning and Advocacy Council (CPAC) were struck earlier this year and they are making good progress.

SHARCNET has recently applied for operating funds from the province to take us beyond our current grant which expires December 31, 2010. These funds are necessary to ensure the essential staff, programs and support services that we have built up over the past eight years are able to continue supporting our leading-edge research. Renewal of major infrastructure is another key issue for SHARCNET as most of our larger systems are aging rapidly, and it is our hope that another call for HPC infrastructure proposals will be announced by the Canada Foundation for Innovation in the coming months.

Paul Maxim
Chair, SHARCNET Board of Directors
Associate Vice-President: Research
Wilfrid Laurier University

Scientific Director's Message

Since the last time I reported, SHARCNET has been busy with a number of activities, including assisting Compute Canada with national HPC efforts, outreach and training events, research support programs, and submitting a grant application to the provincial government for renewed operational funding.

SHARCFest 2009, our outreach campaign of open houses, HPC training events and research talks, was held again over the month of May. Over 20 events were held at various locations across the consortium including a second symposium on GPU and Cell computing, a hands-on IBM workshop, visualization presentations, and our premier event, SHARCNET Research Day 2009, which included a special session on the Digital Humanities. The anchor event for SHARCFest was our annual HPC Summer School, held from June 1-5th at Sheridan College. The response to these events was extremely positive. The annual Summer School, in particular, is gaining in popularity year by year and we are considering ways in which we can expand these sessions in the future, possibly through the use of our remote collaboration, or AccessGrid, rooms. Due to the popularity of these events, plans are already in full swing for SHARCFest 2010.

Most recently, SHARCNET was pleased to be one of the sponsors of the Gregory Chaitin-in-Ontario seminar series, which featured six separate talks over different locations within SHARCNET and Toronto. Gregory Chaitin, IBM T.J. Watson Research Center in New York, is the discoverer of the remarkable Omega number. SHARCNET provides a range of presentations and training opportunities and I encourage you to watch the SHARCNET website for upcoming events.

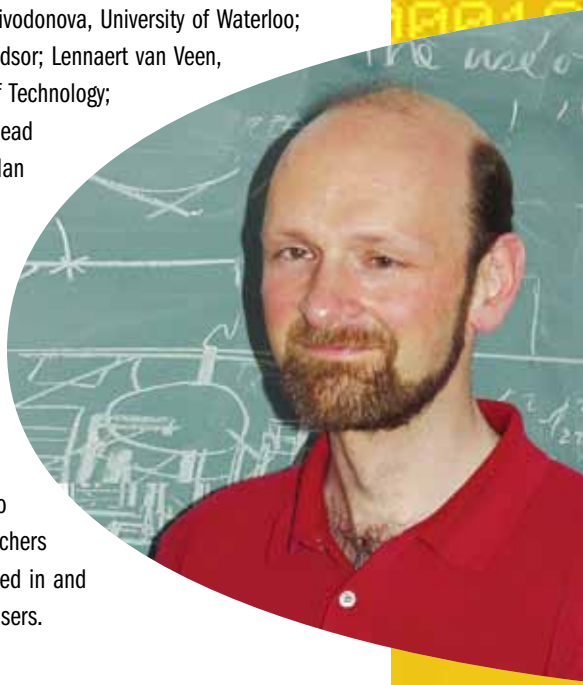
SHARCNET also ran its annual user satisfaction survey earlier this summer. The overall results were very positive, especially the comments we received about the staff, but there is always room for improvement, so we are taking the necessary steps to try respond to this very important user feedback. The survey responses also clearly indicated the growing need for more general compute resources. As you know, to a large extent this depends upon the availability of refresh funding from provincial and federal funding agencies and we are working with Compute Canada to try to secure this. We will also endeavour to ensure that our current resources are used as effectively as possible. For those who are interested, the results of the 2009 survey have been posted on the SHARCNET web portal.

As many of you may have already noticed, a few months ago SHARCNET launched a new look for its website, www.sharcnet.ca. Whether as a direct result of the changes or not, folks have taken notice and the SHARCNET website was listed as the "Link of the week" in International Science Grid This Week, August 19, 2009.

Outreach continues to be a major focus of SHARCNET and the Supercomputer-in-a-Box tours to public and high schools will resume with vigour now that schools are back in session. Large plasma displays are also being installed at Western, Guelph and McMaster initially, so that we can better promote SHARCNET research and activity. If these are successful we will investigate installing further displays around SHARCNET.

On the systems side of things, the SHARCNET "Equipment Needs" Committee has met several times over recent months to flesh out the details for equipment purchases from our share of the most recent National Platforms Fund (NPF) grant. While SHARCNET's share of the NPF grant is relatively modest, we do hope to issue an RFP in the coming weeks for a small general purpose cluster to allow us to meet the growing compute needs of our researchers. Thanks to contributed systems from our researchers, we have a couple of notable additions and expansions. Michel Gingras (Waterloo), has contributed the "*Brown*" system, a 640 core Intel Xeon cluster. A recent contribution from Catherine Beauchemin (Ryerson) has been delivered and will be used to expand "*Goblin*". Our new system from HP, "*Saw*", is proving very useful but as with any large new system, we have had some teething problems to sort out.

There are some changes to the SHARCNET Site Leaders' Advisory Committee to report on. SHARCNET is pleased to welcome several new Site Leaders over recent months, namely: Michael Owen, Ontario College of Art & Design; Lilia Krivodonova, University of Waterloo; Gordon Drake, University of Windsor; Lennaert van Veen, University of Ontario Institute of Technology; and Apichart Linhananta, Lakehead University. Ed Sykes from Sheridan College is the newly appointed Chair of the Committee, taking over for Hans De Sterck from the University of Waterloo. To Site Leaders, past and present, a big thank you for all of your efforts and support of SHARCNET! Having representatives at each site who are connected with local researchers allows SHARCNET to remain tuned in and responsive to the needs of its users.

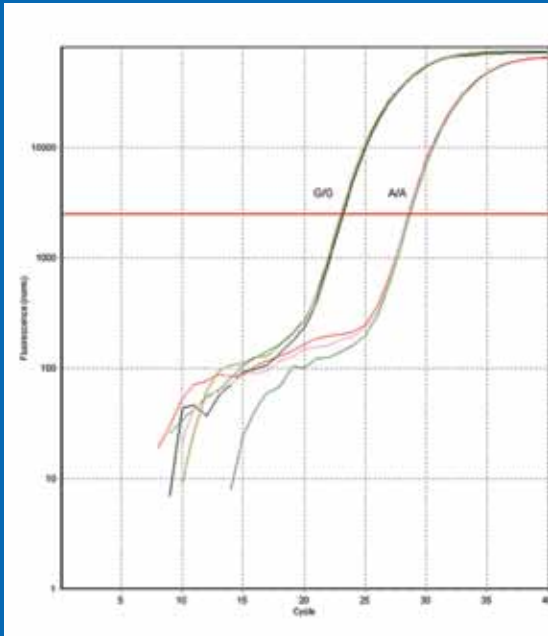


Hugh Couchman,
Scientific Director

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

High Performance Computing Essential for Human Genome Studies

Peter Rogan,
The University of Western Ontario



Results of real-time gene expression studies.

ISOLATED MUTATIONS CAN PLAY A SIGNIFICANT ROLE IN GENETIC DISEASES

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

Human genetic diseases are most commonly caused by mutations that impact specific parts of the genome. These point mutations can alter the way DNA is translated and expressed, leading to the onset of diseases.

Prof. Peter Rogan, Canada Research Chair in Genome Bioinformatics in the Department of Biochemistry at the University of Western Ontario, says specific, individual mutations are linked to the onset of genetic conditions such as lupus, asthma and diabetes. He's collaborating with Tyson Whitehead at SHARCNET to develop software which can quickly identify these mutations and link them to genetic diseases.

"For many years, geneticists thought that we share 99% of our DNA with each other, but we now know that this is a significant underestimate," says Rogan. "We hypothesize that differences in our DNA sequences are the root causes of our predisposition to various common and rare diseases. A goal of our laboratory is to find out which of those differences may be important for disease predisposition."

DNA sequences spell out the diverse genes, each of which provides a set of instructions to produce proteins and RNAs that perform essential operations in our cells. These instructions are sometimes different in different individuals, and even among the two copies of the same gene that we inherit from each of our parents.

In normal individuals, these differences are generally clinically benign. They nevertheless account for features that distinguish our appearance, behaviour, and the response to our environment, including the food we ingest and the drug treatments that we're prescribed.

In other cases, these differences have subtle effects that can be manifested in mild or severe mutations which can affect the processing of the gene products. These instructional errors take only a single wrong letter, or nucleotide, for them to stop making sense. The majority of nucleotide changes are called single nucleotide polymorphisms (SNP). While many of these differences are well tolerated, others can alter the protein, leading to the onset of genetic diseases.

Rogan is following changes in SNPs that affect the processing of gene transcripts, many of which appear to be linked to well known genetic diseases. By analyzing SNPs using Shannon information theory, his team has recently predicted SNPs that increase the likelihood of developing lupus erythematosis, hypertension and gastric cancer, among others.

Lupus, an autoimmune disease, has long been suspected to have a genetic connection, but only now has that suspicion been confirmed by the software his team has developed. With new SNPs being discovered constantly, there's a high demand to link them to diseases they could be causing.

Currently, Rogan is looking at these SNPs to determine the most obvious links to known genetic diseases. But with the help of SHARCNET, he'll be able to process SNPs much quicker through the new program.

"Previously, it would have taken us one minute to process one SNP," says Rogan. "With the new SHARCNET software, it takes only five hours to process four million."

John Mucaki in Rogan's laboratory has carried out wet-bench studies, which have confirmed information theory-based predictions for a series of mutant SNPs. The work will be presented at the American Society of Human Genetics meeting in October 2009. His lab is gearing up to scale the laboratory analysis of predicted mutant SNPs using expression microarrays with content derived from the results of his recent SHARCNET analysis.

The technology and software are not just applicable to humans. SNPs are responsible for different traits in plants and animals as well. "We anticipate that not only will we be re-running the software as we discover more SNPs, but it will be useful for other analyses of genetic variation in other genomes besides humans," says Rogan.

Being able to identify these genetic disorders can play a huge role in selecting plants and animals with the most desirable traits for breeding or to select those with natural resistance to pests and infections.

Rogan's research is supported by SHARCNET, the Natural Sciences and Engineering Research Council, Canada Research Chairs and the Canada Foundation for Innovation.

Harnessing Infectious Disease Modeling..., continued from page 1

In simulating these large, computationally taxing agent-based models of infectious disease transmission and intervention strategies, Bauch uses the powerful high-performance resources provided by SHARCNET.

"You need SHARCNET", he explains, "because there is a significant amount of uncertainty about aspects of cervical cancer progression and how it is tied to the underlying HPV infection–there are certain things we just don't know – so we need to run a lot of simulations for a number of different scenarios, where each one may be equally plausible, in order to discern whether there are any robust and general conclusions to be drawn." Ultimately, Bauch hopes that his research will effectively aid provinces in developing new screening recommendations that can significantly reduce the number of patients suffering from cervical cancer in Canada in a cost-effective way.

More recently, Bauch and other infectious disease modelers in Ontario were approached by health officials in Ontario to work on the transmission of the H1N1 virus. In a collaborative effort, with researchers from Emory University, Georgia Institute of Technology, and the University of Toronto, Bauch is developing a computational model to describe the spread of the virus. The team hopes that developing these models quickly will help determine how best to lessen the impact of the H1N1 virus this fall. Both his research on cervical cancer vaccination strategies and his work with the H1N1 flu, may be important to the development of immediate and relevant public health policies in Ontario.

For more information about Dr. Bauch or his research, please visit: http://www.uoguelph.ca/~cbauch/.

SHARCNET Awards First Digital Humanities Fellowships

SHARCNET is pleased to announce the results of SHARCNET's Round I competition for Digital Humanities Fellowships. SHARCNET has awarded $74,000 in cash and technical resources to the following researchers:

- Philosophy Professor, Dr. Marcello Guarini, from the University of Windsor will be using SHARCNET to test a theory that computational neural modeling might provide a way of understanding how an individual can learn to classify moral situations without using substantive principles.
- Economics and History Professor, Dr. Kris Inwood, from the University of Guelph, plans to use SHARCNET to track several million Canadian individuals across eight Canadian and two U.S. censuses from 1852-1916. Such data will help Dr. Inwood's team to understand how previous actions, experiences and family circumstances affect life-course behaviour and outcomes.

Along with matching contributions of $30,000 provided by the researchers and/or their home institution, the total investment for these two projects is over $100,000.

About the SHARCNET Digital Humanities Fellowships Program

This is a new SHARCNET research support program, initially being run as a pilot. The objectives are: 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 resources and infrastructure.

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

Tiny Molecules hold Big Responsibility

BY NATALIE OSBORNE, STUDENTS PROMOTING AWARENESS OF RESEARCH KNOWLEDGE (SPARK) PROGRAM AT THE UNIVERSITY OF GUELPH

Unraveling the mysteries that lie in the smallest strands of DNA is essential for understanding cells and the way living organisms function.

Researchers at the University of Guelph have been using SHARCNET to discover the functions of a new and little understood genetic component known as small RNAs. They suspect these tiny molecules, which assist in regulating protein production in both plants and animals, could be a key factor for healthy cell growth and development.

Prof. Lewis Lukens, Department of Plant Agriculture, and graduate student Shuhua Zhan have discovered eight new types of small RNAs, now known as micro RNAs, in plants. He found their functions range from processing sugars - an essential element for plant survival – to assisting in plant development.

> "SHARCNET's capacity for analyzing large datasets was critical for this work," says Lukens.

DNA serves as a set of instructions for cell growth and function. RNA molecules are responsible for reading these instructions and transferring the information, to make proteins which carry out the cell's various functions. Messenger RNA (mRNAs) copy a segment of DNA and then travel to a production site, where specific proteins are made using this piece of genetic information. Small RNAs act on the messenger molecules by attaching to the segment and slicing it, making it unusable and unable to continue producing that protein. Therefore, they're considered a regulatory switch, determining which proteins are made or discontinued within a cell, according to the cell's nutritional or functional needs.

Small RNAs appear to play a significant role in the sequential progression of plant growth. Lukens found that plant mutants lacking small RNAs were stuck in an early developmental stage and unable to progress normally. He suspects the micro RNAs aid in development by acting as garbage disposals for old and unnecessary mRNA segments.

"If you're a cell moving into the next developmental stage, you'll have all these mRNAs from the old stage creating proteins you don't need any more," says Lukens. "At this point, the micro RNAs would be activated to cut them all up, so you could begin making new proteins for the new developmental stage."

Lukens says learning more about small RNAs in plants might also one day help develop healthier or more efficient crops.

He and his team compared mutant and normal variations of the plant *Arabidopsis thaliana* to discover which specific genes small RNAs target. The mutated plants were unable to produce micro RNAs, which led to problems including stunted growth and mismatched tissue development.

The researchers used SHARCNET to form information catalogues, and scanned the plants' mRNA populations, looking for the genes responsible for the differences between the mutant and normal types. By comparing the plants with and without micro RNAs, researchers could learn which traits and genes are affected by the micro RNAs' regulatory action.

Lukens is now investigating whether micro RNAs play a part in plants' responses to environmental stresses. Learning how a plant copes with cold temperatures or drought conditions, for example, could one day help crops' resistance to these stresses.

Lewis Lukens, University of Guelph

"New technology allows us to sequence genomes and mRNA transcripts at a very high rate, but we need to make sense of the huge amount of data we get back," says Lukens. "We couldn't make these important connections between genetic information and cellular functions without the help of SHARCNET's computational powers."

Funding for this study was provided by the Natural Sciences and Engineering Research Council.

HPC to Go: Supercomputer-in-a-Box Tour 2009

BY DAVE MCCAUGHAN, HPTC CONSULTANT, SHARCNET

SHARCNET's
Supercomputer-in-a-Box

While individual sites were busy running events during SHARCFest this past May, another cog in the outreach machine was touring Southern Ontario taking the larger of our two portable supercomputers ("Supercomputer-in-a-Box" or SiB) on the road. This outreach tour was a concentrated effort to cultivate wider awareness of what high performance computing has to offer the more general Canadian academic community. The message we are trying to get across is clear: parallelism is no longer an exclusive resource available only to those in specialized academic or industrial circles. Even inexpensive desktop hardware now provides multiple compute cores so parallelism is no longer on the horizon; it is here for the masses today and cannot afford to ignore it.

The greatest challenge in this sort of outreach is providing compelling, yet accessible examples of HPC in action, as the audience for these talks is typically made up of those new to HPC. We leaned primarily on a ray tracing application that makes use of the physics of light to render graphical images. Ray tracing produces extremely realistic images, but is computationally expensive making the effect of having many processors available to shoulder the load readily apparent to even a non-technical audience. And showing pretty pictures, rendered in real-time, never hurts a presentation it seems.

The SiB Tour 2009 was a tremendous success, with large audiences addressed across the spectrum of academic disciplines, from IT professionals to historians. Spikes in user account creation coincided with tour dates demonstrating the effectiveness of the presentation format in keeping the audience motivated beyond the talk itself. We look forward to continuing and expanding this outreach effort in the coming year.

The SHARCNET Supercomputer-in-a-Box is a portable cluster comprised of eight dual-core Apple Mac Minis, with an Ethernet interconnect and a MacBook Pro serving as the head node. Apple computers ship with software that simplifies the process of bringing up a working cluster through peer-based configuration, and the included Xgrid clustering software is well-suited to illustrating the load on the compute nodes dynamically. SHARCNET is currently employing a graduate student to develop a more comprehensive demonstration framework for the SiB, so the future looks promising for the humble Supercomputer-in-a-Box!

Class of '09

2009 SHARCNET Summer School

BY BAOLAI GE, HPTC CONSULTANT, SHARCNET

The 3rd annual SHARCNET Summer School on high performance and technical computing was held at the Sheridan Institute of Technology and Advanced Learning Oakville campus, June 1-5, 2009. The week-long workshop was attended by nearly 60 attendees, many of them graduate and undergraduate students. Among the attendees were several post-doctoral fellows, faculty and staff members from across the consortium. Most attendees were new to high performance computing and are planning on doing research using SHARCNET's facilities.

Summer School 2009 offered intensive courses on various subjects, including programming distributed and shared memory systems, cell systems and GPGPUs, as well as general programming in C++, Matlab and debugging. Courses were taught in both lecture and hands-on formats. The attendees showed great interest in learning and practicing the skills necessary for parallel and high performance computing. Among the courses, participants had an overwhelming interest in message passing interface (MPI) for programming distributed systems (clusters) and OpenMP, the industrial standard API for multithreaded programming on shared memory systems.

Besides traditional lecture and lab sessions, a new session on problem-solving was introduced this year. The problem-solving session provided a forum for the participants to present and discuss the numerical and high performance computing related problems originating from their research. During the problem-solving session, two problems arising from research projects were presented and analyzed in class. Sample code was shown to demonstrate the design and implementation.

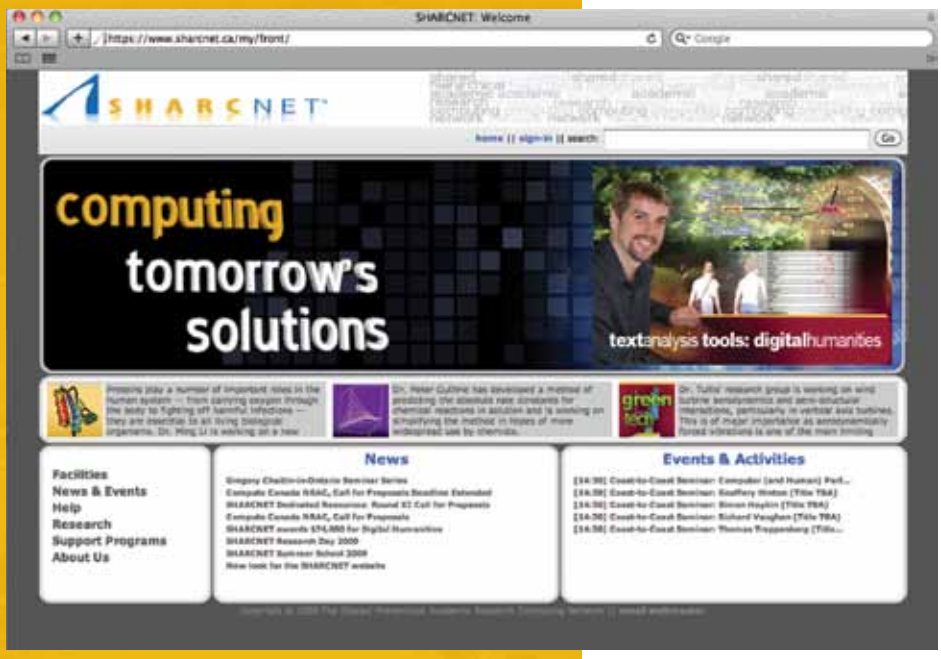
Beyond in-class learning and practice, social events in the evenings were planned by the workshop organizers, including dinner and drinks at local restaurants and pubs.

As part of its commitment to training highly qualified personnel (HQP), SHARCNET provides financial support along with travel and lodging subsidies to ensure that students from across SHARCNET are able to participate. This year, accommodations were in the student residence where the workshop sessions were held, providing additional convenience for those who stayed overnight.

SHARCNET Summer School is an annual workshop providing attendees with the opportunity to learn and share knowledge in high performance and technical computing on platforms with the latest technologies. Prior to 2007, the event was called the Fall Workshop. In order to provide more in-depth material and enhanced hands-on training, the annual workshop was extended to a full week of lectures and lab activities. To accommodate a week-long set of activities, the event was moved to the June timeframe, hence the name change.

Every year, the hosting institution for Summer School is rotated amongst SHARCNET's 17 partner institutions. "I was thrilled to have Summer School at Sheridan College this year," said Ed Sykes, SHARCNET Site Leader. "This is the first time a major SHARCNET event has been hosted by one of its College members – and Sheridan was very excited about it. Summer School was one of Sheridan's significant events for 2009. The instructors were great and I heard from many students how much they liked the training and the hands-on experience. I hope we can host Summer School again in the future."

For additional information and pictures from this year's event, please visit: http://www.sharcnet.ca/events/ss2009/



New look for the SHARCNET website

Earlier this summer, SHARCNET launched an updated version of the www.sharcnet.ca website. Along with the new look, we've also enhanced functionality, navigation and content within the site. The SHARCNET website is one of our primary communications tools and we also make extensive use of the web portal and wiki for account management, information exchange, and interactions among staff and users. The website, along with our RSS feed, provides comprehensive and up-to-date information to the broader HPC community. Users are encouraged to check out the new format!

Pawel Pomorski,
University of Waterloo

Swimming with SHARCS: New Staff

SHARCNET is pleased to announce Pawel Pomorski as our newest HPC Programming Specialist based out of the University of Waterloo, commencing earlier this summer. Pawel has a research background in theoretical condensed matter physics and biophysics, with a particular interest in modeling nanoscale systems relevant to quantum electronics, as well as in studying problems relevant to biological systems of current interest, such as protein and DNA translocation through cell membrane pores. He received his Ph.D. from McGill University in 2002, then worked as a postdoctoral fellow at the North Carolina State University in Raleigh, and afterwards at the University of Western Ontario.

BY PAWEL POMORSKI, HPC PROGRAMMING SPECIALIST, SHARCNET

Modules on SHARCNET

One of the challenges for the users of any Unix-based system is correctly configuring their environment variables in order to compile and run their programs. These variables contain essential information, such as the directory paths where the required executable and library files are located. This information also determines which version of a software package will be run by default. Configuring and managing these variables can be a complicated process on a supercomputing consortium such as SHARCNET, with its assembly of various clusters, each typically deploying different hardware, with its own associated versions of software. For those users of SHARCNET who use packages installed and maintained by its staff, it is likely that the default environment variables are perfectly adequate. These default configurations have been customized for each system with great care and should be appropriate for most situations. However, for users who need to set up a special environment configuration, there will now be an easier way to do this, through the use of modules, a new mechanism for easy configuration of the environment variables that will be gradually implemented on SHARCNET clusters in the early fall of 2009. As with the current setup, the concept of the default environment will continue to be implemented, so users who see no need to use modules, or who already use custom configuration scripts to initialize their environment, should be able to continue using SHARCNET clusters with minimal or no changes on their part.

Modules are a well-established Linux tool and should not be confused with modules used in Fortran programming. In a nutshell, they provide a simple way for the user to carry out the necessary change of the environment variables required to run any installed version of a program with a single, straightforward command. As a result, it will no longer be necessary to edit any shell initialization scripts. The need to provide the location of required libraries will also be eliminated, as the modules mechanism will do that automatically.

To illustrate the usage of modules with a simple example, let's consider gcc, the GNU C compiler installed on all SHARCNET clusters. It should be noted that it is not a high performance compiler and should not be used for compiling programs that will consume large amounts of computational resources. Still, it is a very well known compiler useful in certain situations. It comes in multiple versions, and while usually it makes sense to use the most recent version available, there may be instances where using an older version is preferred, mainly to compile older code. The use of modules to select which version is invoked by the gcc command will now be illustrated.

After logging into any cluster, executing "**gcc -v**" will give the current version of the compiler invoked by the gcc command. To see which other versions are available, the user will now execute: "**module avail gcc**" to list the available versions of gcc (to see all available modules execute "**module avail**"). The output will typically look like this: "**gcc/3.4.6 gcc/4.2.4 gcc/4.3.4**". To select the latest version, the user would now execute: "**module load gcc/4.3.4**". After doing this, executing "**gcc -v**" will now report that the version of the compiler invoked by the gcc command is 4.3.4. To unload this module and go back to previous configuration the user would execute "**module unload gcc/4.3.4**". To switch to a different version of gcc (i.e. to disable the current default version and enable another) the command would be "**module switch gcc/3.4.6**", for example. Each of these commands automatically changes all the necessary environment variables to ensure that the new compiler version can find all the resources it needs in order to work.

To see which software packages are available through modules, please check the SHARCNET web portal pages describing our software, where a special column in the software package information table will indicate whether that mechanism has been implemented for that package. Much more extensive documentation on the use of modules will be available on our web portal as well. In particular, the documentation will describe how to select modules to be loaded automatically at the start of each session. We hope to carry out the transition to using modules as smoothly as possible, but if users encounter any difficulties due to the change, SHARNET staff will be happy to assist. Overall, modules should make using SHARCNET much more convenient and every user should familiarize themselves with the advantages they offer.

SHARCNET™

Shared Hierarchical Academic Research Computing Network

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