SHARCNET™

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newsletter

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Mathematics and Computers Combined to Find Solutions

BY ASHLEY MCCARL, STUDENTS PROMOTING AWARENESS OF RESEARCH KNOWLEDGE (SPARK) PROGRAM AT THE UNIVERSITY OF GUELPH.

Ilias Kotsireas
Laurier Researcher

For centuries, people have used mathematics to solve problems – whether it's to determine the earth's rotation around the sun or the temperature required to make candy. With the computer's invention, math problems that would take years for a human to finish could be done in minutes. Now, a Wilfrid Laurier University researcher is capitalizing pairing math and computers to solve problems previously deemed impossible.

Prof. Ilias Kotsireas, Department of Physics and Computer Science, is developing mathematical models to solve problems in areas such as manufacturing and telecommunications. He's doing it by blending algebraic computation and computer science into a stream of mathematics called combinatorial design theory.

"The applications of combinatorial design theory are too numerous to enumerate", says Kotsireas. A key area where he sees lots of potential is in pharmaceutical design, to estimate which factors are important side-effects of a new treatment option.

Kotsireas began his study of mathematics by obtaining a degree in the field from the University of Athens in Greece. He paired this with a Master's and Ph.D in computer science from the Université Paris 6, in Paris, France, and claims this unique blend of education has given him the ability to use computer science principles with mathematical equations and theory.

While at a conference in 2003, Kotsireas connected the idea of using computational algebra and computer science to design a series of algorithms that lead to solutions of hard combinatorial problems.

Now he's bringing together resources from the network of researchers in SHARCNET to apply his models to other mathematical equations and theories, such as Hadamard and weighing matrices.

The SHARCNET network with its high performance computing capabilities provides the ability to exhaustively search for certain types of combinatorial designs which can then be applied to solve problems, says Kotsireas.

"The applications of combinatorial design theory are too numerous to enumerate."

Kotsireas actively involves students in his research work so they gain skills and become connected to the vast knowledge of SHARCNET researchers. He has also drawn from his education and research background editing many research publications and books and co-organizing scientific conferences.

His research funding is provided from SHARCNET, the Natural Sciences and Engineering Research Council, Wilfrid Laurier University and the European Union ENTER program.

in this issue:

Message from the Chair of the Board

Ted Hewitt,
Chair of the Board

"The continued growth of SHARCNET further strengthens our ability to provide a leading-edge collaborative research environment."

On behalf of the Board of Directors, it is my pleasure to announce a further expansion of the SHARCNET community by welcoming Nipissing University as our newest academic partner. With 17 academic partners, SHARCNET has emerged as the largest Canadian HPC consortium by number of institutions and, alongside WestGrid, supports the largest number of users and range of research in Canada. The continued growth of SHARCNET further strengthens our ability to provide a leading-edge collaborative research environment.

At the national level, the C3.ca Association, which was the central driver for HPC in Canada for the last decade, officially closed operations at the end of December. The work led by C3.ca culminated in the generation of the Long Range Plan for HPC in Canada, which included several recommendations, some of which have now been met. I would like to personally thank C3.ca for all of their efforts and paving the way for the creation of our new national voice for HPC, Compute Canada.

On the provincial side, the Ontario High Performance Computing Council has completed its provincial HPC research and development capacity plan and has now been reviewed by the Ministry of Research and Innovation. We expect that the final version of the plan will be released in the Fall of this year.

In addition, there are some changes to the SHARCNET Board to report. Last Fall, Dr. Ian Brindle, Acting Associate Vice-President Research, Brock University, assumed the role as Brock's representative, taking over for Dr. Michael Owen who is now the Vice-President, Research & Graduate Studies for OCAD. In addition, two new industrial representatives will be joining the Board in the next couple of months, namely Hans Tuenter, Senior Model Developer (Planning & Analysis), Ontario Power Generation and Robert Little, President of Altair Engineering Canada. As industrial representatives they will be ambassadors for HPC and SHARCNET, assist with the HPC knowledge transfer to the private sector and provide invaluable management experience. We are thrilled that they have agreed to serve on the Board and look forward to working with them in this capacity.

I am also pleased to report that the SHARCNET Board and its HPC Strategic Council met in an all-day meeting on December 15th to get their input on SHARCNET's newly developed Strategic Plan. We were encouraged by their unanimous endorsement of the five-year plan. As recommended by the Council, key areas that we plan on focusing some of our efforts over the next few years include: embracing new uses of HPC including interactive use, computational steering and visualization; continuing our outreach efforts to non-traditional HPC users; pursuing fundamental research into HPC; working collaboratively with other consortia, both provincially and nationally; recruiting champions to help drive the use and development of the technology; and to make progress on the strategic front to ensure sustained funding for HPC. We plan to create a couple of working groups to address several of these issues.

The Strategic Plan will be released to the general community in the coming months through the SHARCNET website. I encourage you to read the document and pass along any feedback to the SHARCNET management team.

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

Over the last several months, there have been a number of important happenings, changes and new features at SHARCNET that I would like to bring to your attention.

Firstly, SHARCNET now requires that PIs renew their accounts. We initiated this process last Fall and plan to continue it on an annual basis. This is in addition to the process for PIs to renew their sponsored accounts that has been in place for some time now. The PI renewal allows us to clean up dormant accounts and to ensure that profiles are up-to-date for ongoing accounts. For an account to be renewed we ask that PIs ensure that their profile on the SHARCNET web portal correctly lists the area research, funding agencies that support the research and lists any relevant industry collaborations. This process also ensures that we have current publications and research data. All of this information is critical for demonstrating the value of SHARCNET to our funding agencies.

In addition, a user certification process has recently been instituted that classifies users into 3 levels. A user attains level 0 automatically on being granted an account; level I is granted after attendance at one of our bi-weekly AccessGrid New-User seminars followed by successfully answering a small quiz. Each level permits access to a defined level of system resources. The first level is intended to satisfy most users on an ongoing basis. For more demanding users/applications there is a second level that grants unrestricted access within the general scheduling policies. Level II requires a consultation with a SHARCNET HPC consultant; we may also approach users whom we think should have level II certification. The intent of certification is to ensure that users receive the proper orientation and training in the use of SHARCNET at the level they need without being in any way burdensome or onerous. Existing users will be grandfathered to level I. This process was described in the Summer, 2007 issue of SHARC Bytes and is also available online at: http://www.sharcnet.ca/Facilities/certification.php

A number of system enhancements have recently been introduced, including the addition of specialized software (Matlab, Fluent, FDTD), some of which requires a modest financial contribution by researchers who request access. A number of optional email lists are accessible through your SHARCNET web portal account that allow you to receive information about updates to the various software packages that we support. Improvements to job scheduling were implemented this past December. Over the next couple of months, we will evaluate the success of these changes.

I would also encourage users to review our draft policy governing disc usage at: http://www.sharcnet.ca/Documents/policies/storage.html. As usage of the systems increases we need to start implementing these policies. Some users will have already received automated email messages if their disc usage exceeds the limits described in the document. Although we have no intention, in the short term, to delete data, we may have to rethink our strategy if resources become scarce. I encourage users to consider using archive for storing older data. If you have particularly demanding data needs please contact us. These needs and solutions could range from temporary very large storage on our file systems to donating additional storage to be attached to SHARCNET. The Dedicated Resources Program that runs every six months can also allocate very large system resources, including disc space.

It is clear that the scheduling changes and enforcement of disc space limits will require, in some cases, more attention by users to their jobs. I hope that the modest additional work required to monitor your jobs will lead overall to a better user experience and, indeed, appreciation of the very capable systems at your disposal. For users who need to create a small database or access a database on SHARCNET (mySQL or postgres), we now have some capability to support this. For more information on these services, visit SHARCNET's online FAQ.

Hugh Couchman, Scientific Director

We now have AccessGrid rooms running at 14 of the SHARCNET partner sites, with another two expected to be operational very soon. The facilities have been used for the introductory seminars, training, graduate supervision, graduate courses, numerous SHARCNET management and technical meetings and have also

Continued on page 4

Scientific Director's Message, continued from page 3

allowed us to participate in the Coast-to-Coast seminar series that now runs among ACEnet, SHARCNET and WestGrid. If you are interested in using the system or joining these activities please contact Barb Autterson (barb@sharcnet.ca) for a booking and information. In addition to AccessGrid expansion, a number of smaller systems have recently come online, including:

- Grid Lab: This will allow, in a lab setting, experimentation on and investigation of various aspects of grid computing.
- SGI Altix: This system, "contributed" by Hermann Eberl at Guelph, is a 64 processor shared memory (NUMA) system with 128GB of RAM.
- FPGA system: This SGI hardware was donated to SHARCNET, via WLU. We have purchased a software environment and compiler that will allow users to experiment with development on FPGAs (Field Programmable Gate Arrays).
- SVA system: This scalable system, equivalent to an HPC cluster for visualization, allows for the visualization of very large datasets. Software is being installed that will allow for the turnkey display of common data formats (for example, Fluent, hdf5). The system also allows for the efficient remote display of rendered data anywhere across SHARCNET.

You may also recall that SHARCNET ran a comprehensive survey last Spring. I am pleased to report that several of the user suggestions made through the survey have been implemented and we are following up on several of the others. It is our intent to release the survey on an annual basis. Watch for the next survey in April, 2008!

We were thrilled to be able to re-introduce the SHARCNET Fellowships and Chairs Programs last year and recently announced a third call for proposals for SHARCNET Chairs. Another Dedicated Resources round is expected to be announced very soon, followed by a new Programming Competition to allocate programmer time to specific research projects. Announcements for competitions will be posted on the SHARCNET website and to our general mailing list.

As always, if you have any questions about these items or any other issues at SHARCNET please do not hesitate to contact me or SHARCNET staff.

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

At the Heart of the Source: The Molecular Level

RESEARCHER USES FUNDAMENTAL THEORIES TO UNDERSTAND MOLECULES

BY MARCEL NOOIJEN, UNIVERSITY OF WATERLOO

At a fundamental level the equations that describe molecules are amazingly simple and of universal validity, or so we think. To Prof. Nooijen, department of Chemistry at University of Waterloo, this mindboggling simplicity underlying a world of bewildering diverse and complex phenomena provides an irresistible sense of beauty, and potential.

The equations that govern the world of molecules which form the underlying microscopic basis for chemistry and biology have been known since ~1925 and fall under the heading of quantum and statistical mechanics. While the equations are known and simple, and fit on the back of an envelope, the solutions to these equations are extraordinarily complex. This should not come as a surprise, as after all, these solutions will have to describe 'all' phenomena in the world of the small.

The fields of computational chemistry and quantum chemistry aim to efficiently find solutions that describe the stability of molecules and their structures, investigates modes of chemical reaction and probes processes like the absorption of light and other types of interactions of molecules with radiation that provide most of our detailed knowledge at the molecular level. Using computational chemistry, new compounds, new materials and new pharmaceuticals can be created and studied on a computer ('in silico') and the most promising candidates are then developed further by experimentalists (in vitro and in vivo). Of course, the process more often runs in reverse and new compounds made by bench chemists are studied by computational chemists to obtain more insight in their workings and potential.

There is a remarkable synergy in the field of computational chemistry itself, in the sense that molecular simulations of large (say biologically active) molecules use models which are easier to solve, but which are based on molecular parameters which are obtained from more fundamental theories. There are a number of layers in computational chemistry, which go by the name of molecular mechanics, semi-empirical methods, density functional theory and first principles (or ab initio) theory, each one of which has its own community of researchers.

The field of research of Prof. Nooijen is at the fundamental quantum chemistry level of solving the most fundamental and most simple equations (but, which paradoxically are also the hardest to solve). The goal of his research is to find new methodologies and to create associated (user friendly) computer programs to push the boundaries of molecular realities that can be calculated at this most fundamental level. These programs can then push forward the boundaries of all the other layers that comprise computational chemistry as a whole.

In contrast to the simplicity of the laws of nature, the (efficient) computer programs and algorithms that can provide the most versatile description of molecules are very complex. Currently these programs are written by 'meta'-programs that interpret the underlying equations. So it is again a layered structure that enables progress. All of these layers: the design of basic new equations (approximations), the design of program synthesizers (i.e. meta-programs) and the optimization and implementation of the actual computer programs are part of the research activities in the Nooijen group. A prime focus is the development of methodology to describe transition metal chemistry, which shows a very rich and complex range of compounds, and is still poorly understood.

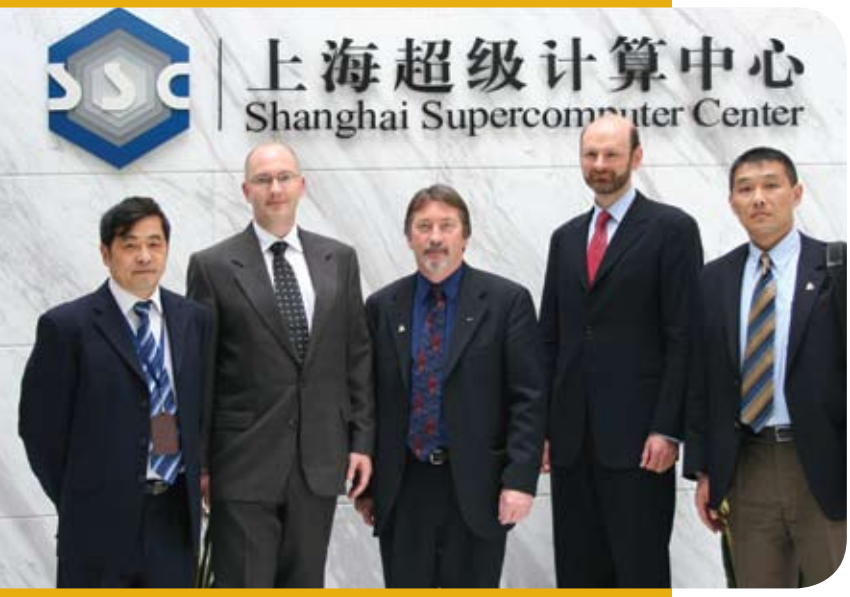
Very recently, the insight has emerged in the Nooijen group that one might push things a revolutionary step further. Theoreticians might tinker with the very laws of nature, such that solving the resulting equations by computer can be done extremely fast. Hence the physics is tailored to the most powerful computer algorithms, rather than the other way around. In this way a 'parallel' world can be created in silico, and if this world mimics the real word sufficiently well, this could in time become a very worthwhile tool for molecular design. Also, the prospects for computer games / virtual reality are tantalizing. We would be able to generate our own universes, showing immense complexity but designed such that they are calculable universes. If intelligence and evolution can become a part of such a calculable universe... there are no limits to where we can go as a human race.

Every summer Nooijen's research lab plays host to one or two of India's brightest student minds from the Indian Institute of Technology. The students work in collaboration with Nooijen on various research projects.

Nooijen has been a faculty member at the University of Waterloo since 2003. His studies are funded by the Natural Sciences and Engineering Research Council, the Canada Foundation for Innovation and the University of Waterloo. Also involved with this research are graduate students Dominika Zgid and Liguo Kong, and postdoctoral researchers Ondrej Demel and Bijoy Dey.

Marcel Nooijen
Waterloo
Researcher

SHARCNET and SSC Formalize Partnership



l-r, Xi Zili (Director of SSC), John Morton (SHARCNET), Ted Hewitt (VP-Research, UWO), Hugh Couchman (SHARCNET), Baolai Ge (SHARCNET)

BY BAOLAI GE, HPTC CONSULTANT, SHARCNET

Led by Ted Hewitt, Board Chair of SHARCNET, and Vice-President (Research and International Relations) for The University of Western Ontario, a delegation from SHARCNET visited the Shanghai Supercomputer Center (SSC) for a formal signing of a Memorandum of Agreement between the two HPC centres. The official ceremony, covered by the local and national media, was held at SSC on October 31, 2007, at which, Ted Hewitt and Xi Zili, Director of SSC, signed the document. SHARCNET's Scientific Director, Hugh Couchman, Technical Manager, John Morton, and HPTC Consultant, Baolai Ge, attended the ceremony.

Developing international relations is important to both organizations, and it is hoped that with the signing of the MOA, SHARCNET and SSC will benefit by working together and sharing each other's technical strengths and successes.

During the two day visit, SSC introduced its SHARCNET colleagues to the Center's operation. The SHARCNET delegation and SSC held meetings at the management and technical levels and discussed several future collaboration initiatives.

In order to kickstart collaborations, SSC and SHARCNET have agreed to work on a joint project – system verification after restart, which will include technical staff from both organizations. System verification and validation after system restart is a highly recommended function and is an issue that many HPC centers contend with. It is expected that hardware, software and services be set to normal operational mode before a restarted system can resume taking jobs. Currently there is no existing complete solution available for HPC system verification that will meet the various requirements. The goal of this project is to develop a toolkit for a set of specified common tasks.

One of the largest cities in the world, a mega city with a population of 19 million and a modern city with science fiction skyline, Shanghai is a mirror reflecting the dynamics of the fast growing economy in China and is leading new trends in the 21st century. Located in Zhangjiang, Pudong – the vast, hi-tech zone of Shanghai – along with neighboring research and manufacturing giants such as HP, Intel and AMD, Shanghai Supercomputer Center is a large R&D service center for HPC. Publicly funded and established in 2000 as a public platform for high performance computing, SSC serves research institutions and companies in Shanghai and the

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SHARCNET Awards $400k in Fellowships

SHARCNET is pleased to announce the results of the Round VII competition for Fellowships and Dedicated Resources. With $1.75m in funding requests from 85 applications, this was another competitive round.

SHARCNET is awarding $436,939 over two years for 26 new Fellowships for visitors, graduate, undergraduate and post doctoral students. With matching contributions of $384,099 provided by the researchers, the total investment to increasing the number and quality of research personnel using high performance computing totals over $800,000.

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

About the Fellowships Program

One of SHARCNET's key objectives is to recruit and support research personnel who utilize HPC. This objective is accomplished through the Fellowships Program, which provides funding for postdocs, students, and distinguished visitors. Fellowships are awarded via a grant competition process administered by SHARCNET.

Since 2001, a total of 182 Fellowships have been awarded through seven funding rounds. Supporting these individuals allows SHARCNET to increase the number and quality of research personnel involved in HPC, leading to significant scientific discoveries. We anticipate announcing the next Fellowship competition in the coming months, with a deadline in September, 2008.

SHARCNET Awards $700k in Research Chairs

SHARCNET is also pleased to announce the results of the Round III competition for SHARCNET Research Chairs, targeted at non-traditional HPC disciplines and those that will build expertise in HPC tools and techniques. The Board of Directors approved the allocation of five new SHARCNET Research Chairs as follows:

Institution	Research Area
Brock University	High Performance Symbolic Computing
McMaster University	Computational Epidemiology
Lakehead University	Biorefining
Laurentian University	Mathematical and Computational Materials Science
University of Waterloo	Systems Design Engineering

This allocation allows the institutions to begin recruitment efforts for a suitable Chair candidate. Each award is conditional on final approval of the Chair candidate by the SHARCNET Chairs Selection Committee and the Board of Directors.

About the Chairs Program

The Chairs Program is a cornerstone of SHARCNET's mission. Its goals are to enhance research requiring high performance computing (HPC), to build a community of expertise in HPC amongst its partners and to attract world-class researchers. The program provides bridge salary funding for tenure-track faculty positions for up to two years. SHARCNET Research Chairs are expected to enhance research using HPC and to promote interdisciplinary studies and interactions among departments and universities. The program is intended to attract new recruits to a department or faculty.

Since July 2001, SHARCNET has provided bridge funding for 13 SHARCNET Research Chairs, and has recently allocated funding for an additional eight positions, five of which are currently in the recruitment stage. A call for proposals for a fourth round was issued in February, 2008.

Applications are evaluated by the SHARCNET Chairs Selection Committee, which includes representatives from across disciplines from the SHARCNET partner institutions.

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

"International collaboration is very important to SHARCNET. We are excited about this partnership with SSC and hope that we can learn a great deal by working together."

-Ted Hewitt

SSC Formalize Partnership, continued from page 6

surrounding Yangtze Delta area. With over 70 regular employees, SSC is actively involved in the city and national projects. SSC plays a significant role in building the city's infrastructure of digitization and plays a leading role in the China Grid project.

This is the second time the SHARCNET executive team has visited SSC. In October 2005, Scientific Director, Hugh Couchman, and the Site Leader for the University of Waterloo, Jeff Chen, visited SSC while attending an international HPC conference hosted by SSC. Dr. Couchman was invited by SSC, along with a number of international HPC centre directors to attend a round table meeting.

SSC has international linkages to HPC research centres around the world. Since 2005, SSC has established relationships with the Finnish IT Center for Science (CSC), the Korea Institute of Science and Technology and, most recently, SHARCNET.

The SHARCNET delegation also visited the Shanghai Municipal Informatization Commission (SMIC), the governing organization for SSC. SMIC Vice-Director, Liu Jian, met the delegation and introduced Shanghai's IT infrastructure and the roadmap for communication and digitization. An ambitious goal of the city is to have Internet access via WiFi anywhere and anytime by 2010. According to Liu, by the end of 2006 the IT industry amounted to 13% of the total GDP of Shanghai. This year it is expected to reach 13.8%. Information technology is the top industry in Shanghai. For instance, currently, of the 19 million people, over 90% of households have computers, 50% of them have Internet access and over half of them are using broadband.

Aside from the official visit to SSC, Ted Hewitt also visited Shanghai Jiaotong University, one of the leading universities in China, and the Zhangjiang Hi-Tech Research Park. SHARCNET is looking forward to hosting a reciprocal visit of SSC personnel this Summer.

For more information about the Shanghai Supercomputer Center, visit their website at: www.ssc.net.cn/en/

SC'07 Canadian Presence – A Success Story

MARIE-CLAUDE DUQUETTE, EVENT COORDINATOR, SC'07

"Enabling Canadian Research Excellence & Innovation through HPC" was the moniker for the Canadian HPC booth at the annual Supercomputing'07 conference, held this past November in Reno, Nevada. Across Canada, seven major consortia of universities, colleges and research institutes provide HPC, collaboration and visualization facilities for the benefit of Canadian researchers. In the HPC arena, Canada is known for developing the world's best national, trans-consortia, interoperable non-homogeneous HPC environment and is gaining international recognition as a major player in HPC.

No successful journey can be achieved without a great team effort along with individual commitment, and this is certainly true of the SC'07 Canadian Coordinating Committee whose efforts and contributions helped to make the Canadian booth a huge success. It is my great pleasure to thank the members of the Committee (namely Susanne Baldwin (CANARIE), Cindy Munro (SHARCNET), Ken Edgecombe (HPCVL), Jill Kowalchuk (WestGrid), and Graham Mowbray (ACEnet)), along with Mike Totten from CANARIE who contributed his design and graphic talents. With funds provided by our industry sponsors, we were able to create a new, high quality and professional Canadian HPC display for the 2007 conference. A special thanks to CANARIE, our one and only gold sponsor, along with silver sponsors, IBM, HP and SUN, and bronze sponsors, Cray, Liquid Computing and SGI.

In addition to attracting the many conference attendees, the booth was also a gathering place for the Canadians who were in attendance and was a great opportunity to meet and link with other Canadian researchers and colleagues. I also wish to thank the various consortia personnel who managed the booth through the conference period. They always did their job with a smile with the utmost professionalism.

Next year's SC'08 conference will be held at the Austin Convention Center in Texas, November 15-21 2008. Visit http://sc08.supercomputing.org/ for more information.

l-r, Doug Roberts (SHARCNET), Dave McCaughan (SHARCNET), Adam Munro (SHARCNET), John Morton (SHARCNET), Marie-Claude Duquette (C3.ca), Mike Bauer (SHARCNET), Brian Corrie (WestGrid)

SHARCNET Outreach

SHARCNET has continued its outreach activities along several fronts. The first "super-computer-in-a-box" (SIB) prototype was completed. The prototype SIB was built from 8 Mac-minis which were networked together using gigabit Ethernet to form the small "cluster". The main node was a Mac laptop. The cluster was encased in a single unit that enclosed the Mac-minis and their individual power supplies.

Mike Bauer gave a presentation at the Educational Computing Organization of Ontario on November 9th, 2007 on SHARCNET, high performance and parallel computing. He demonstrated several simple parallel applications using the SIB for a small audience of teachers. The teachers found the examples interesting and were positive about SHARCNET's efforts to reach the high school community and encouraged SHARCNET to continue its efforts.

As a result of using the SIB for demonstrations, we decided to refit the prototype to simplify its transportation and setup. The revamped SIB has been completed with a new enclosure, simplified networking and a new carrying case. We are now working on adding new examples. If you have any ideas for good examples or even some of your own code that could be adapted for a simple example, please contact Mike Bauer (bauer@csd.uwo.ca).

SHARCNET was also asked to participate in a research showcase, held on January 25th, 2008, at the London Convention Centre, which saw more than 1,000 attendees from industry and academia gathered together to review the work being done at Western. SHARCNET provided a poster that presented SHARCNET and showcased some of the work being done by SHARCNET researchers.

Tyson Whitehead

Swimming with SHARCS: New Staff

SHARCNET is pleased to announce the appointment of Tyson Whitehead as one of SHARCNET's new HPC Programming Specialists commencing January 2, 2008. Based out of Western, Tyson is a PhD candidate in Applied Mathematics. His current work, which he will be defending shortly, involves a novel application of asymptotics to aid in HPC (and other) Monte Carlo solutions to Bellman's equations. Prior to taking up graduate studies at Western, he worked on robotic seed sorting, specifically computer imaging, at AgriVision Inc. He is an open source enthusiast, and is looking forward to being involved in the various projects going on at SHARCNET.

BY HUGH MERZ, HPTC CONSULTANT, SHARCNET

HPC Accelerators

There is a clear trend of leveraging parallelism to improve application performance in HPC. Two types of devices based on highly parallel architectures that have been successful in specialized applications but have seen limited use in HPC are graphics processing units (GPU) and field programmable gate arrays (FPGA). With recent design improvements targeted at general purpose computing and the emergence of high-level programming toolkits they are becoming increasingly attractive for use as HPC accelerators. In order to stay abreast of these new developments, a number of systems containing these devices are nearing production status and will be available within SHARCNET.

SHARCNET currently has two GPU-based clusters on the road map. The first, which fills a traditional role for GPUs in HPC, is an HP SVA (scalable visualization array) cluster named "rainbow", which is nearing production status at McMaster. The SVA is comprised of 21 nodes, each of which contains an NVIDIA Quadro GPU, and will be targeted towards parallel rendering and visualization tasks. Users can expect a 10x speedup by using the GPUs for rendering over the host CPUs, with performance scaling to multiple nodes depending on the dataset.

The second GPU system will be located at Waterloo and intended for general purpose computing. Traditionally programming GPUs involved mapping algorithms to graphical APIs, but with the advent of the NVIDIA CUDA toolkit it is now possible to program the GPU using an extension to the C programming language, including mathematical libraries that provide BLAS and FFT functionality. Coupled with excellent performance gains in recent GPU architecture generations (Figure 1), speedups in excess of 100x that of the host CPU have been obtained with amenable codes. The current accelerator candidate for this system is the HPC-oriented NVIDIA Tesla GPU, with a peak single precision performance of 500 GFLOPS per card.

On the FPGA front, a new SGI Altix RASC (reconfigurable application specific computing) system, including 2 Virtex-4 FPGAs, is nearing production status at Wilfred Laurier. Named "school", the system is installed with the Mitrion-C programming language, an implicitly parallel high-level language that is similar to C or Fortran. A high-profile example of acceleration on this system is the Mitrion-C Open Bio Project, which provides a BLAST-N implementation that runs 20x faster than on the host CPU.

The degree to which a code will benefit from these accelerators depends on how well the algorithm will map to the underlying hardware. GPUs and FPGAs obtain significant performance gains by operating on multiple data elements simultaneously, much like a SIMD instruction or a vector processor. As such, applications that exhibit a high degree of data parallelism are the best candidates for speedup, and programs that are sequential in nature will not see any speedup. Another important consideration is the lack of double precision arithmetic units in contemporary GPUs. Using double precision also limits the size of code that can be run on an FPGA, so these accelerators are primarily targeted at single precision or fixed point arithmetic.

SHARCNET is currently looking to assist researchers in porting appropriate codes to these platforms, please contact us if you are interested.

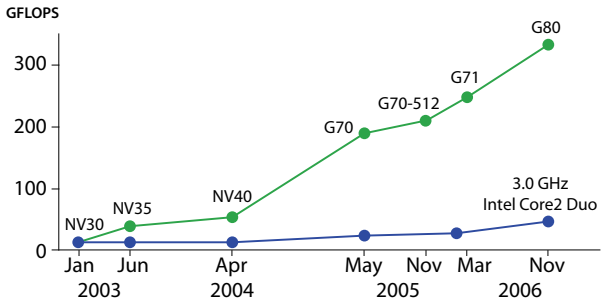

Figure 1: Comparison of peak single precision GFLOPS between generations of NVIDIA GPU and Intel CPU architectures

Shared Hierarchical Academic Research Computing Network

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