Opening Galas celebrate HPCVL’s research successes

Deputy Prime Minister John Manley attended the opening ceremony for HPCVL’s virtual laboratory in Ottawa this past April, an event that built on the original opening gala for the high performance computing research facility last fall in Kingston. The events heralded North America’s newest premier facility for computational research, and provided scientists with the opportunity to showcase some of the results of accessing the lab’s facilities and technical support.

“These events are a significant milestone in the evolution of HPCVL as a leader in high performance computing facilities,” says HPCVL Board Chair Brad Ross. “They also provide an exciting glimpse into what can be achieved with these kinds of resources.” Since HPCVL was formed, over 200 researchers have used HPCVL’s facilities to conduct research. The central site, which now has 192 CPUs with 192GB of memory and 6.5TB of disk and is one of the largest HPC installations in Canada, achieved 93% utilization in March, showing both user acceptance and the pent up demand for these resources. The central site has been benchmarked at 195.9 GF, and HPCVL will appear in the June edition of the Top 500 list (www.Top500.org) of the world’s fastest HPC facilities. With new capacity being installed in June, it is expected that HPCVL will be well positioned in the top 200 of the Top 500 list.

Exciting research is happening with HPCVL resources, some of which we’ve highlighted within these pages. We’ve grown very quickly to become one of the premier high performance computing facilities in North America – and we’re dedicated to continuing those efforts in order to keep HPCVL members at the forefront of scientific achievements and research success.
FOUR YEARS AGO, HPCVL WAS FORMED WITH THE GOAL OF SUPPORTING RESEARCH AND EDUCATION. Researchers from Carleton University, the University of Ottawa, the Royal Military College of Canada, and Queen’s University gathered together to create a consortium with a goal to provide researchers with a leading edge virtual computing environment, thus driving innovation and contributing to the vision first developed by the federal and provincial agencies that are partners today. Now, that partnership is already a world-class platform for collaborative success.

More recently, the Sun/HPCVL partnership furthered this vision, positioning the virtual research lab as a reliable and secure computing environment that fosters innovation and allows scientists global access to one of the finest academic computing facilities world wide.

But this collaboration is about more than technology. The Sun/HPCVL partnership continues to grow and thrive - turning constant change into opportunity. Agreements that offer technical expertise and training, as well as research chairs and scholarships truly accelerate discovery and our collective ability to move intellectual property into the marketplace.

Partnerships drive innovation in research — but these important partnerships must be fuelled by supportive actions, such as technical capability, educational opportunities and appropriate funding. Together, these collaborative efforts work together towards helping to create opportunities for tomorrow’s brightest minds to fully utilize the power of a virtual computing environment.

HPCVL HAS BEEN SELECTED as a Sun Centre of Excellence in Secure Grid and Portal Computing for its efforts in building a secure grid environment and moving to secure portal-based interfaces to enable researchers from anywhere to access lab resources. The announcement, made in November 2001, is a strong endorsement of HPCVL’s leadership in the high performance computing field, and its ability to enable innovative global research through reliable, secure resources.

As a Sun Centre of Excellence, HPCVL will team with its partners to build a secure grid accessed by secure web interfaces to allow researchers in a wide variety of disciplines to access the resources they need no matter where they are located. The emphasis on security will enable researchers to pursue their research, confident that their intellectual property is protected.

“The commitment Sun is making to this effort brings international recognition to HPCVL and its partners,” said Dr. Ken Edgecombe, HPCVL’s Executive Director. “We intend to leverage this grant to build a seamless secure environment that is recognized as one of the best academic research environments in the world.”
Evolving research drives technical strategy

The rapid evolution of computer technology has been matched only by the imagination of the scientists who utilize these tools to expand the parameters of research. This symbiotic relationship leads to a challenge – one that Gary Braida, Stantive Solutions’ System Engineer for HPCVL, must effectively manage in order to continue to provide a leading edge environment for HPCVL members.

Gary works closely with HPCVL’s equipment, providing systems architecture support, implementation and maintenance. But he also acts as a resource for the group, providing vital expertise in the area of technical strategy for future applications, including hardware software and storage architectures.

“HPCVL members continue to ‘push the envelope’ in terms of pioneering research,” says Gary. “Part of my job is to anticipate their technical needs for the future by helping HPCVL develop technical strategies that include scalable and economical solutions for today and tomorrow.”

Gary says that HPCVL team members rely on technology’s ability to keep pace with research efforts. “HPCVL has a goal to create an environment that supports and stimulates new ideas and methods,” says Gary. “Technology’s role is to match that progression – and inspire new thresholds for research innovation.”

Scholarship Winners...

Sun Microsystems of Canada and HPCVL are proud to congratulate the winners of the first Sun Microsystems of Canada scholarships, designed to attract new graduate students to our member institutions and to encourage research in the broad areas of computational science, computational medicine, computational social science, and computational humanities:

Fellows, Robert A. – Mechanical Engineering, Queen’s University
Franklin, Don – Psychology, Queen’s University
Gervais, Eric – Computer Science, Carleton University
Houde, Jean-Francois – Economics, Queen’s University
Jamieson, Randy – Psychology, Queen’s University
Jones, Michael – Psychology, Queen’s University
Kadantsev, Eugene – Physics, Queen’s University
Lee, Carrie – Economics, Queen’s University
Lepage, Ian – Physics, Queen’s University
Poppelwell, Peter – Electrical Engineering, Carleton University
Saligheh Rad, Hamidreza – Electrical Engineering, Queen’s University
Sayeed, Asad – Computer Science, Carleton University
Tasdoken, Sinan – Computer Engineering, Carleton University
HPCVL Student Internships

HPCVL is seeking 20 undergraduates from Canadian universities to use HPCVL resources in the coming 2002/2003 academic year.

This opportunity is available to undergraduates from any university who are working on Honours projects. One participant spot will be made available to each of the first 20 universities to send in an email request to HPCVL. Applications should be sent in by university faculty representing the students and projects beginning September 1, 2002.

We encourage applications from any discipline that would benefit from access to High Performance Computing (HPC) Virtual Laboratory resources. This is an exciting opportunity for Honours students to have access to one of North America’s leading HPC facilities.

All participants would be subject to HPCVL’s standard policies and procedures, which can be found at www.hpcvl.org. Professors who are interested in giving an Honours student access to HPCVL facilities should send an email to hpcvl@post.queensu.ca starting September 1, 2002.

HPCVL symposium highlights:

To celebrate the formal opening of HPCVL last fall, a symposium was held at Queen’s University and included the following topics:

- **Dr. Chris Ferrall**, Department of Economics, Queen’s University: The Computational Approach to Economic Policy Analysis
- **Dr. Gary Slater**, Department of Physics, University of Ottawa: Single molecule microfluidics: From the lab to the supercomputer
- **Dr. Jörg-Rüdiger Sack**, Department of Computing Science, Carleton University: High Performance Spatial Modelling
- **Dr. Alain St-Amant**, Department of Chemistry, University of Ottawa: Recent Advances in Computational Chemistry: Trying to Model the Real Thing
- **Dr. Douglas Mewhort**, Department of Psychology, Queen’s University: Human memory and the supercomputer

“Our success to date demonstrates both the need for this type of facility and the range of our achievements,” says HPCVL board member and Principal Investigator Andrew Pollard. “I am confident that our scientific impact will continue to grow and our institutions will individually and collectively reap tremendous benefits.”

Mark S. Staveley

MARK STAVELEY JOINED HPCVL as a Scientific Computing Specialist in February 2002, and is the technical lead for the development of our web-portal environment. He holds an M.Sc. in Computer Science from the University of Waikato in Hamilton, NZ, as well as a B.Sc. in Computing and Information Science from Queen’s University.

Mark is an Adjunct Lecturer with the School of Computing at Queen’s University, as well as the Director of Research and Development for Geomatic Solutions, a company that provides geocoding services to businesses that rely on GIS information.

BARBARA SCHURMAN

BARBARA SCHURMAN JOINED HPCVL as Associate Director in March 2002. A graduate of the University of Guelph with a B.Sc. in Agriculture, Ms. Schurman has extensive experience in the private sector, and was responsible for the creation and implementation of a business development program for Bell Canada, building private/public partnerships with Ontario communities.

For the past 15 years, Ms. Schurman has devoted much of her time to management and communication of technology and environmental issues, and has been responsible in various roles for government and stakeholder relations.
Opening Galas continued from page 1...

David Bogart, Executive Director, Ontario Innovation Trust spoke at HPCVL’s Kingston opening in November 2001.

Ken Edgecombe, Executive Director of HPCVL, Everett Anstey, President, CEO and Chairman of the Board of Sun Microsystems of Canada Inc., David Bogart, Executive Director of the Ontario Innovation Trust, Carmen Charette, Senior Vice President, the Canada Foundation for Innovation and Bill Leggett, Principal of Queen’s University at Kingston proudly display their HPCVL T-shirts at HPCVL’s Kingston opening in November 2001.

the facilities to achieve significant results, using powerful technology that delivers secure and remote access to laboratory resources from around the world.

Following the opening gala in Kingston last fall, a research symposium highlighted some of the leading edge work being undertaken through the initiative. Researchers reported on activities that ranged from economic policy and fluid dynamics to studies involving the human mind.

“High Performance Computing resources have a significant international impact, both in terms of research results and attracting top talent,” says Mr. Ross. “HPCVL is proud of its achievements as a virtual computing facility, and continues to develop innovative resources that attract and support scientists in their quest to address the most challenging of research problems.”

10 reasons to join:
We’re more than a powerful computing environment – at HPCVL, you’ll access a vast range of valuable benefits designed to fully support your research efforts:

1. **SECURE RESEARCH ENVIRONMENT**
   Protect your intellectual property with leading-edge security solutions.
   www.hpcvl.org/security/index.html

2. **ADVANCED SUPPORT**
   Take advantage of the hardware and software support as well as methodology expertise offered by HPCVL team members.
   www.hpcvl.org/support/index.html

3. **GRADUATE SCHOLARSHIPS**
   Entice top talent to your team with attractive graduate student scholarships offered annually by HPCVL and Sun Microsystems of Canada Inc.
   www.hpcvl.org/scholarships/index.html

4. **PROFESSIONAL TECHNICAL DEVELOPMENT**
   Improve the quality and extent of your research tools with HPCVL’s workshops and educational programs.
   www.hpcvl.org/support/index.html

5. **HASSLE FREE WORK ENVIRONMENT**
   Eliminate the need to seek specialized equipment or deal with hardware and software.
   www.hpcvl.org/support/index.html

6. **GLOBAL VISIBILITY**
   Raise the profile of your research and institution through HPCVL publications, news stories and media events.
   www.hpcvl.org/press_news.html

7. **IN-DEPTH SYMPOSIA**
   Use HPCVL’s annual members’ symposia to share information, gain knowledge, and collaborate on research challenges.
   www.hpcvl.org/upcoming.html

8. **SOFTWARE**
   Enjoy access to standardized and specialized software, upgrades and licensing, along with comprehensive technical support and advice.
   www.hpcvl.org/software/index.html

9. **REDUCED GRANT WRITING**
   Benefit from the combined efforts of members to obtain resources, programs and specialized hardware for advanced research projects.
   www.hpcvl.org/research.html

10. **ACADEMIC OPPORTUNITIES**
    Benefit from our educational opportunities, including Chairs in the Computational Sciences established by HPCVL and Sun Microsystems of Canada Inc.
    www.hpcvl.org/research.html
Advanced calculations for molecular systems

COMPLEX CALCULATIONS THAT ALLOW THE MODELLING OF CHEMICAL REACTIONS HAVE REACHED NEW LEVELS AT THE UNIVERSITY OF OTTAWA. By accessing HPCVL resources and using a specific density functional software package (DeFT), computational chemistry professor Alain St. Amant and his group have been working on extending the ability to allow users to perform accurate first principles calculations on molecular systems containing up to 200 atoms. These calculations facilitate the modelling of enzymatic reactions, using computational methods that can provide “snapshots” or “movies” at the atomic level to give us new insights into how to build a better drug or how to accelerate (or impede) an enzyme’s activity.

Work within the group includes:

Fast Multipole Methods - Previously, long-range electrostatics were the only part of DeFT that did not scale linearly (CPU time being directly proportional to system size); a fully linear scaling program allows the group to tackle much larger systems. This work is essential to the proper modelling of very large and aqueous systems.

QM/MM Methods: Work previously produced using quantum mechanical (QM) software is now being examined with molecular mechanical (MM) software. This QM/MM approach allows one to model very large molecular systems: the few atoms essential to a system’s reactivity are treated by QM means while all other atoms are handled at the simple MM level.

Solvation Models - A modified version of the popular COSMO solvation model has been implemented, approximating the effects of a solvent without actually using explicit solvent molecules by replacing them with a continuum possessing the same dielectric constant.

Divide-and-Conquer Methods - DeFT’s efficiency is largely due to its divide-and-conquer (DAC) schemes, where the molecule is divided into smaller subsystems and these subsystems are independently worked upon in sequence, then appropriately pieced together. Group members have exploited DAC’s subsystem aspect to create a coupled QM/MM scheme where truly important atoms are treated at a high QM level while the others are treated by a lower level QM theory.

The dozens of atoms in the substrate, the thousands of atoms of an enzyme, and the tens of thousands of atoms in the surrounding water make for a truly daunting system to simulate. The methods on which we are working will allow this to be a possibility, helping us discover a receptor’s affinity for a new drug or the rate of an enzyme catalyzed reaction essential (or deleterious) to our well-being.

Materials simulations produce important results

A GROUP WITHIN QUEEN’S UNIVERSITY’S PHYSICS DEPARTMENT is using the support of HPCVL and international collaborators to produce important results on materials problems. The group’s work, led by Queen’s University Physics professor Malcolm Stott, is using materials simulation methods based on density functional theory which circumvents the need to treat directly the interaction of each of the many electrons in the system.

Stott’s team applies density functional theory in the simulation of the electronic and structural properties of materials, treating quantum mechanical behaviour of electrons on an equal footing with the motions of ions. He notes that having access to HPCVL facilities is vital to this work. “HPCVL not only provides powerful computational facilities, but also professional technical support,” he says. “This support includes helping tune and test computer code, organizing helpful workshops and providing extensive on-line resources.”

Work at a glance...

Calcium Phosphates – A material which incorporates Si stabilized alpha-tricalcium phosphate (Si-TCP) has been developed by Queen’s University Physics professor Michael Sayer and Kingston-based Millenium Biologix Inc. This material has been found to actively participate in naturally occurring bone replacement processes in the body.

The group is engaged in a major study of calcium...
Technology helps unlock the mysteries of neutrinos

SIGNIFICANT RESULTS FROM THE SUDBURY NEUTRINO OBSERVATORY (SNO) are being realized more rapidly, thanks to the resources of HPCVL. The observatory, which conducts experiments 6,800 feet below the Earth's surface, uses the large disk space available through HPCVL's supercomputers to run large amounts of data that can be accessed by an extensive collaboration of scientists working to understand the role of neutrinos in relation to the sun and the future evolution of our universe.

Queen's University Physics professor Dr. Aksell Hallin, who started working with the SNO project in 1991, says that membership in HPCVL has allowed the group to realize data results more quickly. “Previously, calibration data took two to three weeks to process,” says Dr. Hallin. “Now, those same results can be achieved in a couple of days.”

The Sudbury Neutrino Observatory is built inside Canada's Creighton Nickel Mine, with a lab equivalent to the size of a 10-story building. Planned and operated by a 100-member team of scientists from Canada, the United States and the United Kingdom, the observatory uses a spherical tank filled with 1,000 metrics tons of heavy water to detect and measure the properties of neutrinos, elementary particles of matter with no electric charge and very little mass emitted by the sun.

Because neutrinos interact so weakly that almost all of them pass through the entire Earth without interacting, SNO scientists use heavy water underground to stop a tiny fraction of them and to restrict radioactivity, which can affect results.

Previous experiments had found fewer electron neutrinos than suggested by calculations based on how the sun burns, a mystery that had puzzled scientists for years. Now, SNO experiments have been able to determine that electron neutrinos change their type on the way from the sun, explaining the deficit. More recent experiments have resulted in a method for measuring the total number of all neutrinos, which is then compared with calculations of the nuclear reactions powering the sun.

The ability for scientists to access super-computing facilities is vital to this type of work, says Dr. Hallin. “Parallel processing gives us a very straightforward way of analyzing the data,” he says. “Without HPCVL resources, we would have to be much more ingenious in devising methods for analysis.”

Equally important, Dr. Hallin notes, is the ability for collaboration through portal-based interfaces for remote access. “SNO succeeds because of the combined efforts of our international team. Technology is the vital tool that helps us work together to unlock the mysteries of neutrinos.”

Materials Simulations cont’d...

phosphate based materials, investigating the role of Si doping in the stabilization of Si-TCP, the possibility of using other dopants, and the origin of the bioactivity.

Cluster Solids – A large amount of work has been done to investigate the possibility that robust clusters of a small number of atoms have some existence in liquid alloys at elevated temperatures.

Real Space Tdft – Work has begun on projects in which the electronic structure - wave functions and density - are calculated directly on a real space grid of points rather than using one of the traditional basis sets such as localized orbitals or large sets of plane waves. Unlike plane wave based methods, this scheme naturally allows the computational task to be shared efficiently among many processors, enabling the simulation of larger and more realistic systems.
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HPCVL web site at a glance:

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- HPCVL Contacts
- Training Info
- Setup FAQ's
- Software FAQ's
- Documentation
- Policy Documents
- Sign-up Forms
- Fee Schedule
- Member Forms
- Notices

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www.hpcvl.org