IN 1965, INTEL CO-FOUNDER GORDON E. MOORE THEORIZED THAT THE number of transistors that could cost effectively be built on a single chip was doubling approximately every year.

That statement, dubbed “Moore's Law”, was revised by Moore and others over time, but the expectation that each new chip version would result in greater speed persisted in the minds of users. Now, as chip temperatures approach that of rocket engines, it’s clear that this expectation cannot be achieved – and that technology must develop new ways in order to meet the demands of our modern times.

The evolution of technology inevitably brings with it a necessary paradigm shift, always coupled with the uncomfortable but necessary requirement of change. HPCVL has long been dedicated to providing its users with the technology to match the pace of discovery – and to providing the vital support required to ensure that researchers have the training they need to adapt to the changes that help them optimize their use of the lab.

In order to solve the problems associated with chip heat and performance, producers are moving to multiple CPU cores per chip, keeping the cycle speed down by using multiple...
change, it may also require an investment in time for researchers transitioning to the new hardware. HPCVL has long been committed to a high level of user support, offering free workshops throughout the year, as well as hands-on support from our professional team members who can provide help with porting codes and gaining access to hardware and software.

More and more, high performance computing is playing an indispensable role in the cultivation of scientific knowledge and technological development. As one of Canada’s leading secure high performance computing environments, HPCVL is dedicated to anticipating the needs of users for today and tomorrow – employing not only the latest technology to address the complex requirements of today’s researcher, but the support team necessary to help our users adapt to our ever-changing technical world.

The result for researchers is the ability to do more work faster at an energy cost of less than two watts of electricity per thread. That’s also good for the environment – as is the fact that the new units, which are approximately 17 kg, take up a small portion of a rack while performing the same way as an older unit that took up an entire rack and weighed 1,122 kg. Cooling costs for these units are significantly decreased, as is the energy to power them and the space to host them.

This new technology offers tremendous benefits to HPCVL users – but, like most change, it may also require an investment in time for researchers transitioning to the new hardware. HPCVL has long been committed to a high level of user support, offering free workshops throughout the year, as well as hands-on support from our professional team members who can provide help with porting codes and gaining access to hardware and software.

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 threads - or processes - per core. Using multiple threads per core also helps keep the CPUs operating at optimum efficiency, giving users the opportunity to get more done in the same amount of time.

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New Technology: 10,000 thread Sun T5140 cluster

Chip Multi Threading (CMT) is a technology that allows multiple threads (processes) to simultaneously share a single computing resource, such as a core. This greatly increases the efficiency of usage of the core. At the same time, multiple cores share chip resources, such as memory controllers and caches, thereby improving their utilization. The result is unprecedented per-chip performance.

For an introduction to CMT, see http://www.cs.sfu.ca/~fedorova/Teaching/CMPT886/Spring2007/schedule.htm.
For more background, see http://www.hpcaconf.org/hpca11/papers/23_x_spracklen-chipmultithreading-1.pdf.
Meet HPCVL team members....

Baohua Zhang is a graduate of Carleton University, where he received his M.Sc. in Information and System Science Degree in 2005. His research focused on network traffic management and performance optimization.

Before joining HPCVL as a System Engineer in October 2007, Baohua worked as a Technical Support Specialist at Nortel Networks, and as a system engineer for a network company in China. He also has experience in system integration and testing for a medical warehouse system, and worked as a software developer in the telecommunications industry. As a system engineer at HPCVL, Baohua provides computer system support, upgrades, maintenance, and system/network administration.

Ashley Wightman received her degree from York University in 2002 and joined Innova Corp shortly after graduation as part of the customer support team to handle all American and United Kingdom accounts. She moved to Kingston in 2005 and joined Educational Testing Services Inc. as the project coordinator, organizing conferences used to develop standardized testing in Ontario.

Ashley has been working at HPCVL since August 2007. She provides administrative support, handles related projects such as the HPCVL-Sun scholarships and outreach program, and liaises with consortia institutions to manage finances and other issues.

CMT machines are ideally suited for applications that require “a good mix” of operations, and that scale well in parallel mode.

**We suggest you consider using the new compute cluster if:**
- Your application is explicitly or automatically multi-threaded (for instance, using OpenMP) and scales reasonably well.
- Your application is explicitly parallel (for instance, using MPI) and not too communication intensive. Ideally, your application combines MPI-type parallelism with multi-threading on the processes.
- You need to execute a large number of relatively short jobs, i.e. throughput computing.
Beyond the periodic table

Nuclear magnetic resonance unlocks the potential for chemical compounds

NUCLEIC ACID ISN’T EXACTLY A FAMILIAR TERM in the average household – but for Dr. David Bryce, it’s an organic substance that he hopes to understand better in a quest to develop treatments for a virus with a much more recognizable name: HIV.

Dr. Bryce and his team in the Department of Chemistry at the University of Ottawa conduct research primarily in the area of experimental nuclear magnetic resonance (NMR) technology, a close relative of the magnetic resonance imaging (MRI) technology common in health care settings. Unlike MRIs, which examine living tissue, NMR allows scientists to study the structure and properties of molecules and materials, as well as molecular dynamics. Using NMR spectroscopy, Dr. Bryce and other researchers can examine chemical compounds in many forms – as gases, liquids, solutions or solids.

“Although much of the research in our lab is very fundamental rather than applied, it has the potential for some very interesting applications,” says Dr. Bryce. “In the end, the more we understand the structure and dynamics of molecules, the more equipped we are to design ‘better’ molecules for particular applications.” One aspect of NMR research in Dr. Bryce’s lab is the determination of the structures of nucleic acid complexes, with potential applications for HIV drug development. This research is done in close collaboration with a team of researchers at the Institut de Biologie Structurale in Grenoble, headed by Dr. Jerome Boisbouvier. “We are working on solving the solution structure of an RNA-RNA complex to understand how retroviral RNA interacts with a viral protein in HIV,” says Dr. Bryce. “We’re hoping that this work may help in the development of aptamers which could block or interrupt the interaction – and perhaps eventually lead to the development of anti-HIV drugs.”

All of this study produces a large amount of data that must be pieced together to provide an overall picture of the RNA complexes – a monumental task that is best handled by supercomputers. In the case of molecular dynamics, HPCVL resources perform the computations required, while quantum chemically-calculated values tell researchers where to best begin simulating their experimental spectra with NMR spectroscopy. HPCVL resources are also used to validate experimental results.

A member of HPCVL since 2005, Dr. Bryce says the high performance computing resources at the virtual lab allow his team to focus on the science of the studies, and to be able to rely on accurate computations for three-dimensional study. “Much of our important work relies on the computation of complex data to interpret the results of NMR,” he says. “HPCVL is key to that interpretation, giving us the information we need to keep moving forward.”
THE JULES VERNE SCIENCE fiction novel *Journey to the Centre of the Earth* documents the adventures of a professor who travels through a volcano in Iceland to discover the composition of the Earth's core. This fictional feat is not an option for today's scientist – but Dr. John Tse, the Canada Research Chair in Theoretical Materials Science at the University of Saskatchewan, is working on ways that we can virtually experience that journey, using technology to understand what lies beneath our feet.

Dr. Tse studies the fundamental behaviour of materials and then tries to manipulate them, with the goal of designing energy efficient materials that have novel applications. His theoretical studies of the nature of chemical bonding in solids and their relationship with physical properties can aid in the design of new materials with specific functions – such as the design of superhard alloys that could help Canada maintain a leading edge in the manufacturing industry.

In order to do this, Dr. Tse and his colleagues work to understand the relationship between a material's structure and its properties, using different models and conditions, such as high pressure or temperature changes. By using sophisticated equipment such as the Canadian Light Source Synchrotron (CLS) in Saskatchewan, Dr. Tse and his team study properties that are then tested by solving complex mathematical equations using high performance computing. "High performance computing provides the ability to extrapolate and better understand experiment data," he says.

These theoretical methods also allow him to mimic the conditions normally only found deep inside the earth, so that he can extrapolate and predict what is happening and provide a better understanding of the structure of materials underneath the earth and in other giant planets.

Dr. Tse notes that high performance computing is vital to his work. "Computational science is the new paradigm for the rational design of new materials," he says. "Through numerical modeling using resources like HPCVL, we can study phenomena not typically amenable to experimentation because of extreme conditions such as high pressure and high temperature. High performance computing opens up a whole new world of experimentation."

“Computational science is the new paradigm for the rational design of new materials.”
IN THE FAMOUS scene from *2001: A Space Odyssey*, renegade supercomputer HAL perceives the humans aboard its spaceship to be a threat, and kills a number of them before having its ‘higher brain functions’ removed by Dave, the remaining astronaut on board. In the real world, supercomputers lack HAL’s ability to think like a human – but they are becoming increasingly important scientific tools for modelling how the human brain functions. At Queen’s University, Dr. Stephen Scott and Ph.D. student Tim Lillicrap are studying ways to develop large scale artificial neural networks designed to replicate the complex processes of the brain – not, of course, to replicate HAL, but to help us better understand the inner workings of the human mind.

Human brains are goal oriented. We don’t actively think about how we are going to pick up a cup; we simply perform the action. But deep inside our brains, a number of processes contribute to that action, sending messages and signals to guide us towards our ultimate goal. And learning from experience plays an important role – for example, it doesn’t take us long to learn to pick up a hot cup by the handle. Computers can pick up the cup, but they don’t yet know to use the handle unless specifically told to each time.

By introducing an artificial neural network to data in the form of photographs, Lillicrap and Dr. Scott are teaching the computer to retain that knowledge for future reference – and to apply that knowledge in creative ways to novel situations. “As children, humans tend to be able to extract statistical regularities from audio and visual data in order to learn about the world around them,” says Dr. Scott. “We’re hoping to help computer networks to do the same thing.”

The visual data encountered by a person in the course of just a single day amounts to many gigabytes of data. Lillicrap, who is also collaborating on the computer code with Ph.D. student Blake Richards at the University of Oxford, notes that HPCVL is a critical resource for their research. “We need the size and speed of high performance computing to handle the data sets similar to those encountered by the brain,” he says. “With the support of supercomputing, we can teach artificial networks to learn on the realistically large amounts of data required to truly work towards unlocking the mysteries of the human thought process.”
ONCE SIMPLY A TERM for scientific measurement, “nano” has evolved into a buzz word vital to the arsenal of science fiction writers and marketing executives, embodying everything from fictional weapons and personal music devices to cars. But this diminutive word (derived from the Greek for “dwarf”) is more than marketing hype – according to scientist, Dr. Bill Atkinson, it has a huge role to play in the future of materials physics research.

Dr. Atkinson, an Associate Professor at Trent University in Peterborough, Ontario, models clusters of atoms arranged to simulate various kinds of disorder, with a goal to better understand the science behind new material design. One area of interest is high temperature superconductors, a family of materials discovered in the late 1980s that have remarkable electronic and magnetic properties at low temperatures.

“High temperature superconductors can carry huge amounts of current with little or no energy loss,” says Dr. Atkinson. “But it’s become clear that the electronic properties of these materials really depend on the amount and kind of disorder present in the samples – an understanding that takes place at the level of atoms.” By learning more about the fundamental physics of new materials like superconductors, Atkinson and his group can help others develop technology for vital tools, such as better cable for energy efficiency or the next generation of nanotechnology within computers.

High temperature superconductors may also someday have a large impact on the transistor. “This device has probably had a bigger impact than any other discovery made in the 20th century,” says Dr. Atkinson, “and it continues to grow smaller and smaller. Now, we have the opportunity to understand how we can grow transistor-like devices from new materials, such as high temperature superconductors.”

Dr. Atkinson is currently working with a German group creating nano-devices from high temperature superconductors and other related compounds – devices that may eventually replace the current silicon-based technology used in computing.

A member of HPCVL since 2003, Dr. Atkinson returned to Canada from the United States partially to take advantage of the high performance computing clusters available in the country. “A typical problem involves modeling structures consisting of a few thousand atoms,” he says. “My research would simply not be possible without high performance computing facilities.”
IMAGINE THAT YOU COULD choose between one powerful car – say, a Ferrari – and a fleet of smaller but more efficient cars – perhaps a Toyota Prius. You also have many places to go and a number of people to take with you. Which car would you choose?

The multi-car Prius option is a great example of HPCVL’s new technology – multiple thread chips that allow researchers to get a number of jobs done at once rather than having to perform one task at a time. Always ahead of the curve, HPCVL Director Ken Edgecombe and his team have made the technology available for researchers so that they can maximize their time as well as the potential of high performance computing. Plus, there’s an added bonus: the opportunity to conduct research in an eco-responsible way.

The old saying “many hands make light work” is an apt descriptor of multi-threading technology. Just as moving from serial to parallel computing offered significant benefits to researchers, multi-threads allow scientists to get more work done in the same period of time, while addressing the very real issues of computer chip heat and performance that have precipitated this evolution.

But the new technology isn’t just great for science. It’s also a way to address the fact that in three or four years, information technology will be the largest contributor to greenhouse gas emissions – far greater than the Ferrari we mentioned earlier. By moving towards multi-threading technology, HPCVL has already reduced its footprint, along with the costs to both cool and power the units. HPCVL’s partnership with SUN, which is leading the industry in the move toward chip multi-threading and eco-responsible computing – offers a powerful future for researchers and the earth.

HPCVL exists to forward the work of its researchers, and so the main focus for upgrading resources has always kept this goal foremost in mind. But it’s great to know that we can provide technology that blends the sleek styling of a Ferrari with the footprint of a Toyota Prius. With multi-thread computing, we can count a win for the lab, for the researchers – and for our planet.

Doug Girvin
President,
Stantive Technologies Group
Where are they now?

HPCVL/Sun Scholarships, awarded at $5,000 per year, are intended to attract new graduate students to HPCVL member institutions and to encourage research in a broad range of study – from engineering and computational sciences to humanities and medicine. More than 400 graduate students and post-doctoral fellows have access or have received high performance computing training using HPCVL’s facilities.

**Delphine Courmier**

Originally from France, Dr. Delphine Courmier studied under HPCVL member Alain St. Amant at the University of Ottawa, where she studied comets and ice structures, working on theoretical models to mimic ice and better understand its reaction in various environments.

Today Dr. Courmier works at Odotech, a Montreal-based specialized environmental company focused on measuring and monitoring odours and predicting their impact. There, she is engaged in the preliminary phases of assessing the sensor material requirements of the company’s automated odour monitoring systems, and will soon be working on the development stage of new materials that will be more specific and also work at lower temperatures.

**Michael Jones**

Dr. Jones completed his Ph.D. on an HPCVL scholarship in 2004 at Queen’s, where he studied under HPCVL member Doug Mewhort. His dissertation proposed a new computational model of how humans learn and represent information about the meanings of words from statistical experience with natural language, and it was subsequently published as the lead article in Psychological Review, the premier theoretical journal in the field of psychology.

Following his Ph.D., Dr. Jones was an NSERC-funded postdoctoral fellow at the Institute of Cognitive Science, University of Colorado at Boulder, where he continued his work simulating the human brain and incorporated his models into applied computational systems for educational assessment. In 2006, he took a tenure-track position as Assistant Professor of Psychology, Informatics, and Cognitive Science at Indiana University in Bloomington.

As Director of the Computational Language and Cognition Laboratory at IU, Dr. Jones continues to use large-scale computing to explore simulation models of human language and memory, and incorporates these models into artificial intelligence systems.
Interested in applying for a scholarship?

Eligible applicants must be enrolled in an accredited graduate degree program in Computational Sciences and Engineering at one of HPCVL's member institutions.

Scholarship Winners...

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For more information, please visit the HPCVL website at: www.hpcvl.org
Secure access and help desk support – no matter where you work

TODAY’S global work environment can require researchers to access work at varying times of day – from home, secondary offices, or even from other countries. HPCVL offers a secure and convenient way for users to take advantage of the lab’s tools and resources anytime, anywhere, with a secure portal that can be accessed using Java and a web browser.

The HPCVL portal is easy to use and a great way to access user support specialists on coding or programming issues. Once users have set up an account through the HPCVL office, a connection to the lab is available through a web browser. “The portal allows researchers to work at home or abroad without having to install specialty software or go through a complicated process,” says HPCVL Research Computing Security Officer Costa Dafnas. “It provides a secure global desktop with all the data and resources at your fingertips.” Because the data is located on HPCVL servers, users can see the information they need without requiring the hardware to house it.

The portal also allows users to customize and organize their front page, so that applications can easily be accessed from one area. Discipline-related programs can be grouped and placed alongside other administrative or computing resources for convenient use during sessions.

One of the key benefits of the portal is the ability to connect in real time with lab staff for help with coding or programming. HPCVL staff create a shadow system with the user to view the current session and provide input. “The shared session is completely secure, and lets us work through any problems together,” says Scientific Computing Specialist Hartmut Schmider. “It gives users immediate answers, no matter where they are located.” Currently, the lab has four computing specialists who work with researchers to improve, install and run their codes on the HPCVL facilities.

For more information about the portal and remote help desk capabilities, contact HPCVL at help@hpcvl.org
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