Executive Summary

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21st century computing involves a well-connected digital world where state-of-the-art computation enables research across all the sciences, including the health, environmental, applied, physical, life, social and human sciences. Canada needs sustained funding of computational infrastructure to build on the enormously successful investments made to date, to capitalize on Canadian researchers' proven ability to produce world-class research, and to take advantage of Canada's world-leading networking and telecommunications infrastructure.

Our vision is to create a sustained and internationally competitive high-impact, multi-institutional physical and human infrastructure for computationally based research that addresses the needs of industry and society for innovation, training and outreach.

This vision will be achieved through the sustained funding of high performance computing (HPC) infrastructure that builds upon the more than $250 million invested or committed over the past five years by the federal government, the provinces, the universities and industry. To increase Canada's competitiveness, and to gain new opportunities for research and development in support of our national economy and quality of life, the Long Range Plan Authors Panel makes the following overarching recommendations (where all recommendations are numbered according to the chapter in which they are presented and discussed, and hence the following recommendations appear in Chapter 1):

1.1 That a long-term funding envelope be developed (a) to provide sustained support for *mid-range advanced* computing facilities such as regional HPC consortia, and (b) to establish a pan-Canadian high-end computing facility that would have a sustained presence in the world's top 30 computing facilities.

1.2 That a national initiative be established to provide outreach, leadership, coordination, and oversight for HPC in Canada.

Impacts, Outcomes, Opportunities and Benefits of the Recommendations

Research has undergone a paradigm shift in which computational methods have assumed a pivotal role in driving the missions of the health, environmental, applied, physical, life and human sciences. In many fields, computation is now the primary driver of innovation. Our recommendations will ensure that Canadian research, industry, economic activity and society will, over a horizon of 15 years, be positioned to reap the internationally competitive benefits provided by HPC, benefits vital to our economic and social success.

There are no prizes or patents awarded for being second to solve a research problem. Our plan will have major impacts: it will establish a technology roadmap for computing-enabled research in Canada, it will provide the environment necessary for major new discoveries, and it will generate 21st century technological literacy via new research and training programmes. Having the best possible computing facilities and highly qualified personnel will significantly enhance research productivity, reduce time to manufacture and market, facilitate knowledge discovery and accelerate innovation.

Access to the best possible computing facilities leverages and maintains a pool of skilled personnel. Expertise is not an incremental benefit. These highly qualified people are the crucial resource needed to enable enhanced research and manufacturing productivity, accelerated discovery and industrial innovation. Canada's future opportunities are in the hands of these experts. Our country has many world-class researchers who now rely on HPC to make innovative discoveries at the international level. A sustained investment of public funds, growing from $76 million per year in 2006 to $97 million per year in 2012 and beyond, will allow Canada to remain competitive in this dramatically evolving technological future.

Competing in the Digital World

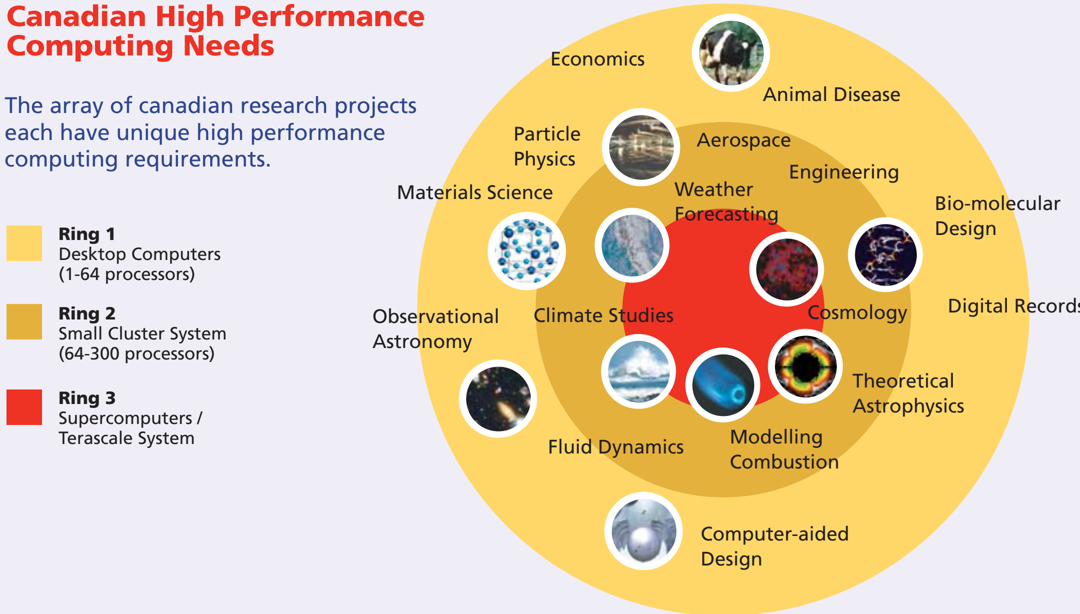
Recent progress in computing, information and communication technology has given rise to a revolution in computational research. With this technology, we can now do research on issues of national and global importance in new ways and with increased efficacy. Exemplary applications include understanding and protecting our natural environment, applying genomics, proteomics and medical imaging to human health, studying global climate change, developing nanotechnology, maintaining national security, finding cost-effective ways of dealing with the aging infrastructure of cities, and improving the efficiency of essential services, as well as predicting, protecting against, and recovering from natural and human disasters. We can also formulate innovative ways of answering such fudamental questions as how the universe was formed and what constitutes matter itself.

Talented Canadian researchers and technicians were able to understand the SARS virus quickly because they had access to state-of-the-art computational infrastructure.

(For more details, see sidebar on page 14)

Canadian High Performance Computing Needs

The array of canadian research projects each have unique high performance computing requirements.



Canada can be a world leader in computationally based research in the 21st century, but this will require sustained, generation-long investments that enable it to compete on a global basis. In the United States, Europe and Asia, annual investments are orders of magnitude greater than those in Canada. For example, the U.S already spends about \$2 billion (US) per year in support of HPC, and the recent passage by Congress of H.R. 4516, the Department of Energy High-End Computing Revitalization Act of 2004, will establish supercomputer user facilities that will provide U.S. researchers access to some of the world's most advanced computers. In addition, a Blue Ribbon Advisory Panel recently recommended that the U.S. National Science Foundation (NSF) invest a similar annual amount in Advanced Cyberinfrastructure - distributed computing, information technology, and communication technology. Canada has an enviable computer network (established by the federal and provincial governments through CANARIE Inc. and the associated regional networks), but it does not have a long-term strategy to support these networks and the HPC resources that they host. Without such a plan, known HPC initiatives in other countries pose a significant threat to Canada's future economic competitiveness.

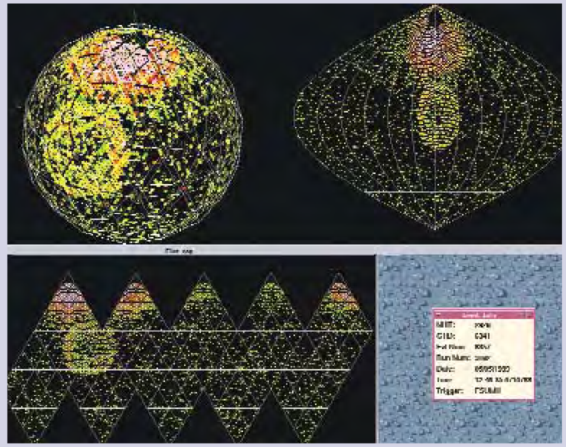
Partnerships between Canadian industry, universities and research institutes are growing, and will continue to grow as the investment in HPC hardware and expertise (people) continues. Industry must have the assurance that it can hire the talented people needed for both long and short term product development and that it will continue to benefit from a substantial pool of innovative research and researchers. To educate and retain these experts, Canada needs advanced HPC infrastructure.

HPC Needs

Computer-based simulations of our physical world open up new vistas. Traditional laboratory experimentation and the theoretical analysis of many complex problems in isolation are often no longer adequate. Computational modelling of very complex, multi-scale phenomena is becoming the key tool for answering difficult questions. For example, the design cycle and thus time-to-market of an aircraft engine or even a whole airplane can be reduced by HPC (see the sidebar on page 11). Computer-aided design is now considered essential to the development of the products of tomorrow.

In our Long Range Plan (LRP), we represent the range of computing capability as a series of concentric rings. The outermost ring represents the enormous aggregated capacity of *desktop machines* and *workstations* each capable of billions of calculations per second.

Sudbury Neutrino Observatory



Different projections of the Sudbury Neutrino Detector (SNO) photomultiplier array with two rings clearly present. This event is the result of a high energy neutrino produced from a cosmic ray interaction in the atmosphere on the opposite side of the earth. After passing through the earth, the neutrino interacted in SNO, scattering an electron, which can be seen as the less intense secondary ring. The colour and density are proportional to the energy of the event.

Where are the missing neutrinos? This question had for decades been puzzling scientists trying to understand the Universe. Canada gained considerable international recognition for leading the team to answer the question and hence better understand the world around us.

Without the availability of advanced computing facilities to interpret data collected deep in a mine in Sudbury, important aspects of solar neutrino production would have remained an enigma. These and other visionary studies would not have been possible without the significant direct and indirect investments in HPC. (For more details, see case study on page 41)

"Canada has emerged as a world leader in the field of particle astrophysics. Several exciting new international projects which probe the structure of the universe and the properties of the particles within it are currently being launched. The characterization and analysis of data from these extremely large and complex detectors requires enormous computing resources. A high performance computing facility is essential for Canada to remain at the forefront of this rapidly developing field."

Dr. Tony Noble
Director, Sudbury Neutrino Observatory Institute
Canada Research Chair in Particle Astrophysics
Queen's University

They provide essential "foundational" computing and visualization tools. The two inner rings represent smaller numbers of progressively more powerful computers: these are systems capable of running applications on much larger numbers of processors. The middle ring - *the mid-range computing facilities* - are those computers that have the power of many hundreds to thousands of workstations. At the centre are the *high-end* or *tera-scale computers* with the capability of tens of thousands of workstations.

Many general research problems can be solved with desktop computers. This plan recommends that the granting councils (NSERC, SSHRC and CIHR) continue to provide comprehensive funding for this outer ring. However, access to mid-range computing facilities is essential for an increasing number of key research areas as illustrated by the majority of the case studies contained in this Long Range Plan. These facilities are also enabling interdisciplinary research, such as the marriage between nanotechnology and biology, engineering and medicine, and materials science and chemistry. At the centre of the plan, access to high-end computers will allow Canadian scientists to tackle the "grand-challenge" problems, whose solutions will have a fundamental impact on the evolution of high-end technology and, by extension, on Canada's position as a world leader in health care, science and culture

We recognize two critical needs. The first and greatest need is for sustained, generational support for the mid-range computing facilities so that Canada can derive maximum benefit from the funds already invested. This will address the needs of most of the HPC-dependent research community.

A pivotal component of sustaining credible HPC capability at the mid-range and higher is the requirement that we develop and sustain the pool of HPC support personnel. HPC researchers rely on the expertise of the talented individuals who operate the systems and provide computational support. There is neither a current sustainable funding mechanism nor an established process for developing this human infrastructure. Retention of the research base that has been increasingly attracted to our Canadian university/hospital complexes is directly related to our HPC support personnel capacity. Current international practice - which is not yet followed by Canada - is to allocate about 25% of total expenditures to HPC support personnel. Canada must move towards this level of investment if it is to maximize the capabilities or potential of its computational scientists, its HPC infrastructure and its overall research capacity.

The second critical need is for a sustained pan-Canadian high-end computational facility that has a sustained presence in the world's top 30 most powerful computing facilities. This facility must also include the crucial corresponding support personnel to maximize the research potential of the computational hardware. We anticipate that an expert national procurement group, which represents the needs of the various scientific communities, will determine the acquisition, evolution, location (which may change over time) and precise form of this high-end facility. This group would likely be composed of members of key funding agencies and client groups.

These needs lead us to the following recommendations (in Chapters 2 and 5):

2.1 In addition to the continued funding of foundational research computing infrastructure (desktop, workstation and small system) by the granting councils, we strongly recommend that the research computing infrastructure in Canada moves towards a model that supports regional mid-range computing facilities and a world-class high-end facility. By 2012, this will require the following (in order of priority and including in each case capital infrastructure, human infrastructure and operational costs):

   a. $76 million/year in sustained funding and ongoing support for mid-range computing facilities. This support will (i) build on the present HPC regional consortium model (where universities in a region cooperate to provide shared multi-purpose HPC resources, as well as the human infrastructure to operate the system and to train and support the researchers), (ii) support major special-purpose in-house computational facilities for exceptional cases where it is impossible or inefficient to use a shared multi-purpose facility, and (iii) promote collaboration and create synergies that extend beyond computation.

b. $19 million/year to establish and sustain a multi-purpose pan-Canadian high-end computing facility and to fund appropriate support personnel. We anticipate only one such facility in Canada.

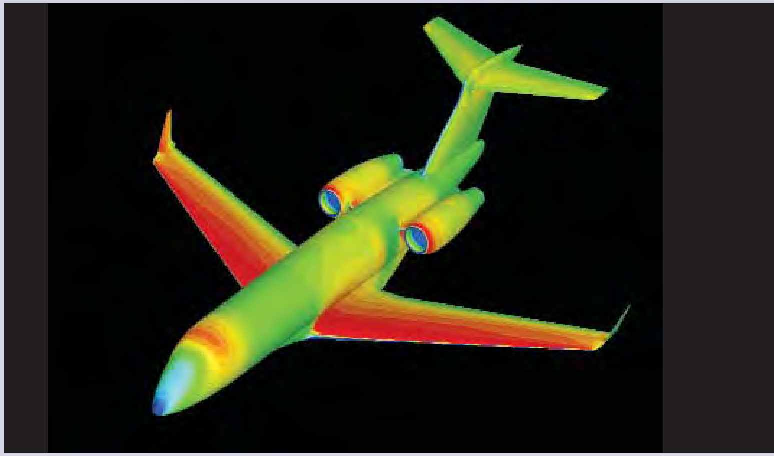
In addition $2 million per year will be needed to fund IMPACT Canada to be discussed below.

Recognising that computationally based research and training are essential, implicit, components to the long-range strategic research plans of most universities in Canada, we have several strong recommendations relating to human infrastructure (in Chapter 3):

3.1 That the granting councils, in consultation with the universities, develop funding opportunities which strengthen research programs both in the foundational technologies of HPC and in HPC application development;

Bombardier

"Engineers designing and developing a high performance aircraft are faced with several competing issues, such as how to achieve optimal cruise performance, how to design flaps and slats for optimum performance at take-off and landing, how to optimize the wing's structural integrity and how to best install engines for minimum interference. At Bombardier, CFD aerodynamic computations are significantly enhanced with access to HPC and provide reliable answers to many of these questions. The judicious use of CFD methods, ranging from panel methods to 3D Navier-Stokes solvers for complete aircraft configurations, allows the aerodynamicist to cost-effectively reach optimal configurations, of highest safety. This more thorough aircraft design optimization focuses wind tunnel testing and considerably reduces the costly and time-consuming number of experimental iterations. At Bombardier, we firmly believe our competitive edge is critically dependent upon use of, and access to, HPC. HPC was crucial to design our first Regional jet, and it will continue keeping us flying."



Computational fluid dynamics (CFD) simulation used in the design of Bombardier Challenger 300 at Mach 0.70 [REF 10]

Fassi Kafyeke
Manager, Advanced Aerodynamics
Bombardier Aerospace, Montreal

3.2 That universities develop training opportunities at the fundamental and advanced levels to enhance HPC skills in the research and development environment; and

3.3 That an amount equivalent to at least 25% of the annualized HPC hardware expenditures be allocated annually to fund HPC support personnel (adopted when establishing the funds required for recommendations 2.1 and 5.1).

Present Organization for Delivering HPC

There is currently no single organization responsible for delivering HPC, although multiple agencies are investing in its development, the recruitment of its researchers, and in the training of its personnel. It is essential that one coordinating mechanism be identified: HPC expenditures are enormous and cost-efficient HPC development will require the development of effective national strategies.

The result of existing investments has been six geographically distributed regional HPC consortia (WestGrid in western Canada, SHARCNET and HPCVL in Ontario, CLUMEQ and RQCHP in Quebec, and ACEnet in the Atlantic Provinces). These facilities knit together researchers, technical analysts and computational infrastructure at more than thirty universities. In addition to these consortia, some university/hospital complexes (such as the University of Toronto and its associated hospitals) and single universities (such as the University of Victoria) have developed significant in-house HPC facilities.

Centralized HPC resources, in the form of general-purpose consortia or domain-specific HPC facilities, have grown across Canada because the benefits of large shared resources are greater than those of several smaller, single-user dedicated systems. The consortium installations provide a wide range of researchers from across Canada with access to a range of different computing platforms, since each facility reserves on average up to 20% of its resources for suitable research projects by scientists from other regions. Domain-specific facilities are appropriate where large communities of scientists within a particular discipline require extensive HPC support for common computational problems. In either setting, the use of a shared facility allows increased aggregate throughput and can satisfy a larger user community, while still meeting the needs of the individual user. The sharing model provides clear economies of scale in personnel, space utilization, power consumption, back-up support, system administration, technical support, system up-time, software licensing, and hardware support. This leads us to recommend the following (in Chapter 5):

5.2 We recommend that funding requests for HPC computer resources be evaluated in the context of what can be provided by existing HPC facilities, either general-purpose consortia or domain-specific facilities, so that the most cost-effective use can be made of investments in HPC. Requests that genuinely cannot be reasonably satisfied using this existing infrastructure should compete on their merits for existing sources of funds such as conventional CFI envelopes or equipment funds from the granting councils.

The physical network for an umbrella HPC organization already exists. High-speed, high-bandwidth networking permits researchers to share large volumes of data, creating "communities of practice" among geographically dispersed experts. They can access resources and data thousands of kilometres away as if they were located next door. This is the basis for what is known as "grid-based computing". Its impact on the scientific community is comparable to that of the Internet on society at large. GRID Canada, which is a partnership between CANARIE Inc., the National Research Council of Canada and the C3.ca Association Inc., is leading the effort to move Canada in this direction. These advanced networks provide the essential connectivity between the HPC computing rings, but they do not have long term funding (for example, the funding for CANARIE lasts only until 2007).

This leads us to the following recommendation (in Chapter 2):

2.2 We recommend the continued support of CANARIE Inc., the optical regional advanced networks, and Canadian grid initiatives, and that these networks be maintained and enhanced in concert with new HPC investments.

Proposed National Initiative: IMPACT Canada

In recognition of the need to coordinate HPC facilities across Canada, to advise Canadian research funding agencies on HPC issues, and to develop and implement outreach and training programs, we make the following recommendation (in Chapter 4):

4.1 We strongly recommend the establishment of a body, IMPACT Canada, to provide national leadership, coordination, and oversight for HPC in Canada.

The name IMPACT Canada captures the essential elements of a well-connected, highly competitive digital world: **I**nnovation, **M**anagement, **P**eople, **A**pplications, **C**ommunication and **T**echnologies. IMPACT Canada will foster innovation. By providing management and coordination, it will enable people to reach their research potential. It will also assist in the development of the computer applications that will lead to scientific breakthroughs; it will foster the movement of ideas and interaction through broad communication strategies, and it will oversee and coordinate the acquisition and operation of the enabling technologies.

This initiative will provide an ongoing assessment of the rapidly changing field of HPC to identify emerging areas of strategic importance to Canada. It will create strategies for enhancing HPC research in the health, environmental, applied, physical, life, social and human sciences. It will also coordinate existing HPC resources across the country and help allocate new HPC resources to maximize the competitiveness of Canadian research. It will have full-time staff to facilitate program development, training, and co-ordination of symposia. This team will also provide advice and specialized assistance to HPC centres across the country.

It is envisaged that IMPACT Canada will play a key role in outreach and training. For example, it will work closely with universities, hospitals, colleges and consortia to deliver an early introduction to computational science to young Canadians via the World Wide Web. This medium is now recognized as a vital tool for promoting awareness of science. The innovative outreach programs of IMPACT Canada will be designed to demonstrate to our next generation of young researchers the central role that high performance computing can play in both learning and research.

An excellent example of a spin-off that would not have been possible without HPC is the Montreal-based biotechnology company Neurochem Inc., which grew out of research conducted at Queen's University. The company is publicly listed (TSX: NRM) and now has a market capitalization of over $1 billion.

(For more details, see case study on page 29).

IMPACT Canada will also develop training strategies in HPC foundational technologies (such as data-mining tools, meta-computing, performance evaluation tools, advanced visualization and automatic parallelization) to help balance Canada's acknowledged strengths in computationally based research.

The Prime Minister's response to the 2004 Throne Speech called for a Canada at the leading edge of the 21st century economy. We offer an HPC strategy that can make Canada ***the*** country that most fully realizes the potential of HPC. Initial HPC investments within our universities and hospitals have sown the seeds for new and exciting economic gains for Canada. Momentum has been created over the last several years by the establishment of excellent mid-range computing infrastructure. Much more action will follow once Canadian small- and medium-sized enterprises (SMEs) gain access to the resources that will be available through IMPACT Canada. While SMEs are recognized as Canada's economic engine, they do not have the resources to invest in HPC based pre-competitive research. Funding of IMPACT Canada will be one step towards closing this gap.

We envisage IMPACT Canada working with groups such as the National Research Council (NRC) / Industrial Research Assistance Programme (IRAP) to facilitate access of the SME base in Canada to HPC, to highly qualified personnel, and to advanced research outcomes and equipment. This includes linking SMEs with researchers and research opportunities.

Funding

Sustained funding will be a prerequisite for meeting the burgeoning needs of current and future computationally based research, and for ensuring that the present Canadian investment is fully exploited. As a result of the past four CFI competitions (1999, 2000, 2002 and 2004), the public (CFI and Provinces) has invested over $250 million in computational infrastructure and this has been supplemented with funding from industry and the universities. The total capital investment currently averages more than $40 million per year. NSERC now provides over $1 million annually in operating funds for these facilities. CFI currently provides a portion of the operating funds for *some* of these systems (about $6 million per year), but this funding may not be available for CFI competitions after 2004. There is no other system in place to maintain the funding of the existing infrastructure after CFI operating support runs out.

Unlike most other types of infrastructure, HPC becomes outdated very quickly: Moore's Law (see the sidebar on page 32) dictates that HPC equipment be upgraded about every three years if Canadian facilities and research are to be sustained at an internationally competitive level. To sustain the current infrastructure, our community must submit multiple applications to multiple agencies with multiple reporting and assessment mechanisms (and the timings of these are highly variable). The uncertainties engendered in the current Canadian funding environment — in contrast to the firm commitments to HPC made by our major international competitors — place Canadian research and development at a significant competitive disadvantage; this results in failures to capitalize on many opportunities.

Nonetheless, CFI made significant investments in HPC in 2004 that will roll out in 2005, and support is in

Year	2006	2009	2012
	(Funding in $ millions[1])		
HPC capital infrastructure:			
Consortia	44+13*	49+14.5*	54+16*
High-end (tera-scale) facility	10+3*	12+3.5*	14+4*
HPC operations:			
Human infrastructure	13+4*	15+4.5*	17+5*
Facilities	8	9	10
IMPACT Canada	1	2	2
Total public contribution:	**76**	**87**	**97**
Total industrial contribution*	20	22.5	25

[1] In 2004$ * Industrial contribution

place for a period of time through CFI; therefore, this plan sees the need for a phased build-up of funding to maintain the consortia and initiate the development of a high-end computing facility that will have a sustained presence in the world's top 30 most powerful computing facilities. We recognize an initial need for $76 million per annum from public funding in 2006 and this will grow to $97 million in 2012. It is anticipated that there will be an additional contribution from industry ranging from $20 million in 2006 to $25 million in 2012. The total annual budget (2012) required to provide and to maintain a nationwide world-class HPC infrastructure will be $97 million from public sources.

This leads us to the following recommendation for funding (in Chapter 5):

5.1 We strongly recommend that a long-term funding envelope be developed to support HPC in Canada. We anticipate that this funding could be phased in over a period of six years as follows:

Funding beyond 2012 will be based on future planning. The numbers are difficult to predict considering the changes in technology costs, increases in human resource costs, and other factors outside of our control or not yet known.

Based on this steady-state annual budget requiring public funding by 2012, of $97 million required annually:

- $76 million annually is for ongoing support for mid-range advanced HPC, including capital infrastructure ($54 million), human infrastructure ($14 million), and facility costs ($8 million);

- $19 million annually is for the high-end facility ($14 million for capital, $3 million for human resources and $2 million for facility costs); and

- $2 million annually is for IMPACT Canada (including people and operating expenses).

This budget presupposes that the granting councils continue to fund research projects made possible by access to the HPC infrastructure.

This long-term funding initiative will need to be re-evaluated every five years, perhaps as part of a national review of Canada's international research competitiveness. We suggest that the following performance evaluation criteria should be reviewed:

- Academic excellence (publications, awards, retention and recruitment of faculty);

- Qualified personnel produced (graduate students, postdoctoral fellows, technicians and research associates);

- Societal/economic impacts (patents, spin-offs, industrial partnerships, technology transfers, improved infrastructure, health outcomes, outreach activities); and

- Effect of the investments in HPC on Canada's international competitiveness.

For Canada to remain competitive with the rest of the world, HPC demands ongoing investment. Today's computational infrastructure supports an increasing number of researchers (almost 2000 in 2004) who are sowing the seeds for explosive growth in future computational needs. A stable HPC environment supports the activities of many of Canada's key technology clusters as well as of all the federal National Centres of Excellence (NCEs). These activities will continue to grow.

As well, the next large generation of computationally literate scientists is in the second or third year of their undergraduate studies. Their entrepreneurial and intellectual aspirations are being forged in an environment of expanding infrastructure, and their eventual research infrastructure needs will be well beyond the current HPC environment. On average, a student currently in an undergraduate program will require 15 years to become established in one of our many research professions. Their expectations are that the requisite infrastructure will be available to them as they move on to graduate degrees and then establish themselves between now and 2020.

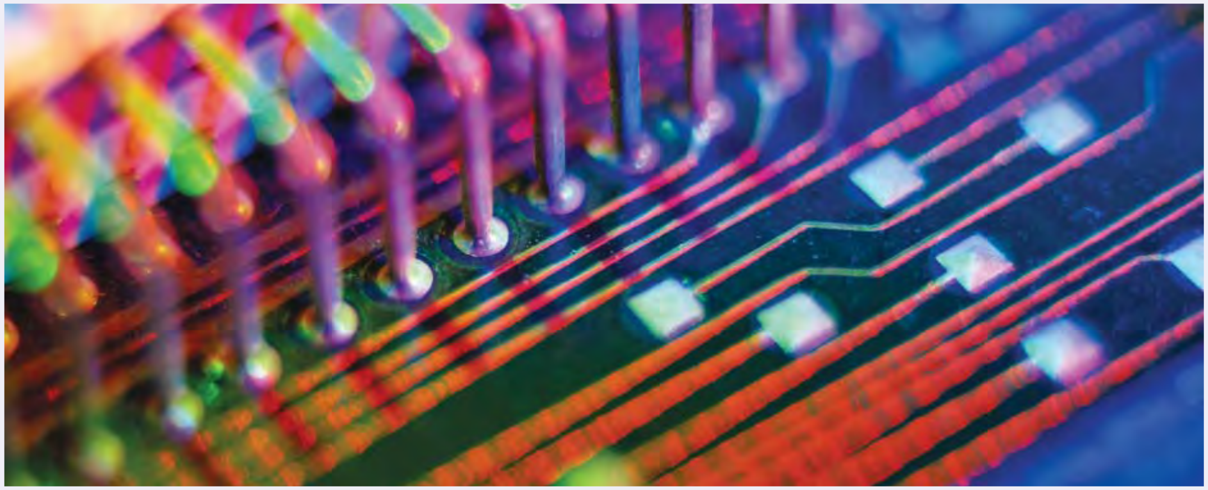
It often takes a decade or more to build strong research teams and to have their technology evolve from ideas to commercial products. It takes at least as long to train the next generation of people with advanced research capabilities. The creative sparks ignited in today's graduate students using the current CFI-funded infrastructure will not realize full potential for Canada unless these students have access to appropriate resources throughout their studies and on into their academic, public sector, or industrial careers. Failure to invest now will seriously damage Canada's innovation agenda. Long-term support for HPC will allow Canada to derive maximum benefit from its current funding initiatives.

At present, the CFI is structured to fund new infrastructure for innovative research. The CFI has played a pivotal role in establishing Canada's strong position in HPC. However, the CFI's present mandate and future funding to 2010 is not well adapted to ensuring the long-term viability of major multi-institutional infrastructure such as the regional HPC consortia. Once infrastructure is established, however, it is vitally important that - subject to review - it is kept up-to-date and that the researchers using the infrastructure are supported on a predictable long-term basis.

There are various ways that this new program could be implemented using existing mechanisms, including designated new funds within the CFI or through a special tri-council initiative (as for the Canada Research Chairs directorate). Alternatively, it could be implemented through a separate funding mechanism employing the review criteria outlined above. The implementation of the Long Range Plan will require leadership and substantial financing from the federal government. However, it would be desirable for provincial governments also to participate in this strategy. This would allow them to augment the national HPC infrastructure in ways that address specific provincial HPC priorities. Addressing these individual perspectives was beyond the scope of this plan and will require discussions between the two levels of government.

Conclusion

Over the past 5 years, Canada has established a strong international position with respect to mid-range HPC facilities. This has attracted many outstanding researchers to Canadian universities and helped Canadian industry to grow. However, if we are to keep these people and gain the full benefits of the investment, this HPC infrastructure must be sustained at a competitive level. If we are also to address the grand-challenge problems, it will also be necessary to establish a high-end computing facility. At present, Canada currently ranks 14th in the world in terms of HPC capacity relative to GDP (Chapter 5); below all countries with whom we regularly compare ourselves. The adoption of the recommendations in this plan would move us to 6th place (between Germany and Mexico). With this investment and these facilities, Canadian researchers can be leaders in discovery and innovation, and Canadian industry can be internationally competitive in a new and lucrative range of fields.



Neurochem and a Treatment for Alzheimer's Disease

By supporting spin-off companies, Canada is not only supporting the sustainability and self-sufficiency of leading-edge Canadian research, it is investing in home-grown economic success.

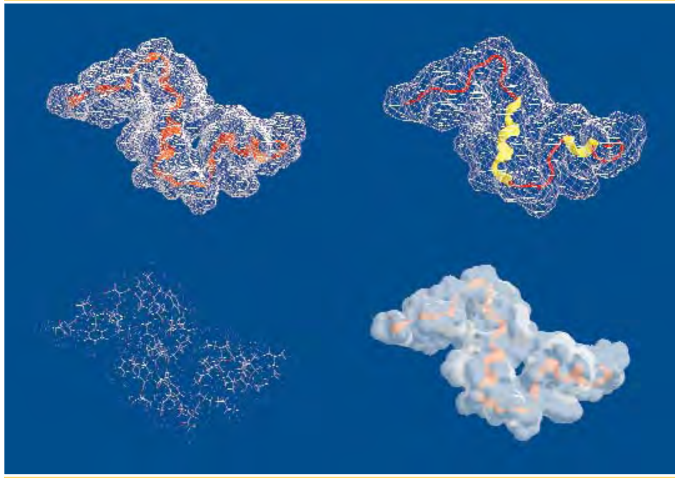
Neurochem has been heavily involved with HPC developments, and was initially spun out of Queen's University. Having grown into a mid-sized Canadian drug company with about 100 employees, it is now a Canadian success story. HPC played a leading role in this success, acting as the central tool during the commercialization of university-developed technologies.

The pharmaceutical sector is an important component of the economies of developed countries. As the world's population increases and confronts the ever-expanding health problems of the modern world, the discovery of new chemical entities (NCEs) as therapeutics for human disease will become one of the major achievements of the 21st century.

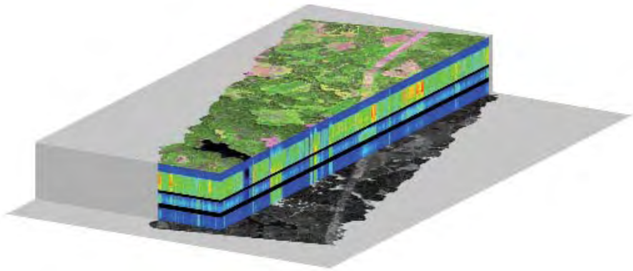
The ability of HPC resources to produce and analyze data in a timely manner helps to push research forward. There are numerous examples of the importance of HPC to drug discovery. One critical discovery used calculations within an HPC environment to enable the design of novel molecules for binding to beta-amyloid, a peptide involved in Alzheimer's disease. Scientists estimate that up to four and a half million people in North America currently suffer from Alzheimer's disease. This Canadian discovery may lead the way to prevention of the disease, which currently has an incidence rate of approximately 360,000 new cases each year. The resulting compounds have now entered phase III human clinical trials in Canada, with a potential cure only a few years away.

"Canada needs more Neurochem success stories. The availability of HPC will be important to this goal. Moreover, the pay-offs will be just as great: an effective drug for Alzheimer's disease or a single new antibiotic drug with widespread usefulness will be a "billion-dollar molecule"."

Dr. Donald Weaver
Canada Research Chair in Clinical Neuroscience
Professor of Chemistry
Dalhousie University



One of the leading approaches to drug design for Alzheimer's disease is to engineer molecules that can bind to the beta-amyloid peptide (shown here). Since this peptide has never been effectively crystallized, such structural studies are totally dependent upon molecular modelling and simulation studies within a high performance computing environment. These computer-aided studies are crucial in enabling the design of drug molecules that interact selectively with discrete disease-causing molecules.



The data cube above was created from a hyperspectral image, which was taken by AVIRIS (Airborne Visible/Infrared Imaging Spectrometer) in 2002 over the Greater Victoria Watershed District. The image is 1988 pixels long by 1331 pixels wide, each pixel covering 4 metres on the ground.

Hyperspectral images typically contain hundreds of narrow spectral bands, whereas digital camera images only contain three: Red, Green and Blue. Each band covers 10 nanometres in the electromagnetic spectrum. This image contains 204 spectral bands in the visible and infrared wavelengths. Each layer in the cube cut-out is one band.

The top layer shows a false colour composite, which consists of two bands in the infrared and one band in the visible wavelengths. Pink represents areas with no vegetation, light green represents areas with young forest, dark green represents areas with more mature forest and black represents areas containing water.

The greyscale part of the cube shows the image at a single band, 2400 nm, the largest wavelength detected by AVIRIS.

Maintaining Canada's Environmental Beauty

Canada has over 418 million hectares of forests, representing 10% of the forested land in the world! With this 10%, Canada is a global leader in some of the areas of forestry research such as remote sensing research in forestry and forest monitoring and carbon accounting.

The Canadian Forest Service (CFS), a branch of Natural Resources Canada (NRCan), is a leader in remote sensing research related to forestry and forest monitoring. CFS use large volumes of remotely sensed data to create products for forest inventory, forest carbon accounting, sustainable development monitoring, and landscape management. With a remote imaging library of over 2200 images the size of remote sensing data is getting larger and larger. In order to provide high spectral and spatial resolution imagery for accurate analysis HPC is critical to process and transport these images from remote sites nationally to be housed in a fully accessible repository. For example, a typical AVIRIS image can be about 4 Gigabytes. Multiply this by 2200 times and you can begin to appreciate the significant impact that HPC and high-speed networks have on processing these high quality remote sensory images.

CFS not only relies on high performance computing to gather, process and store remote sensory images; it needs HPC to facilitate its collaborative research and product distribution across Canada and allow the public to access the research results in a timely fashion. Without HPC the Pan-Canadian network of forest research centres would not be able to process remotely sensed data collected from the field every day. HPC also significantly reduces the computational time required for time-consuming applications and modeling.

The impact of this research not only plays a pivotal role in the timely analysis of results for forest management, forest inventory, forest industry, and public information, it provides next generation forest measuring and monitoring systems that respond to key issues related to climate change and to report upon sustainable forest development of Canada's forests both nationally and internationally.

"Economically, HPC not only facilitates this new method of research in remote sensing and forestry, it provides a return on investment that could generate a 1% improvement in forest product sales, which would amount to a benefit of $700 million annually in Canada alone."

Dr. David Goodenough
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Natural Resources Canada
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