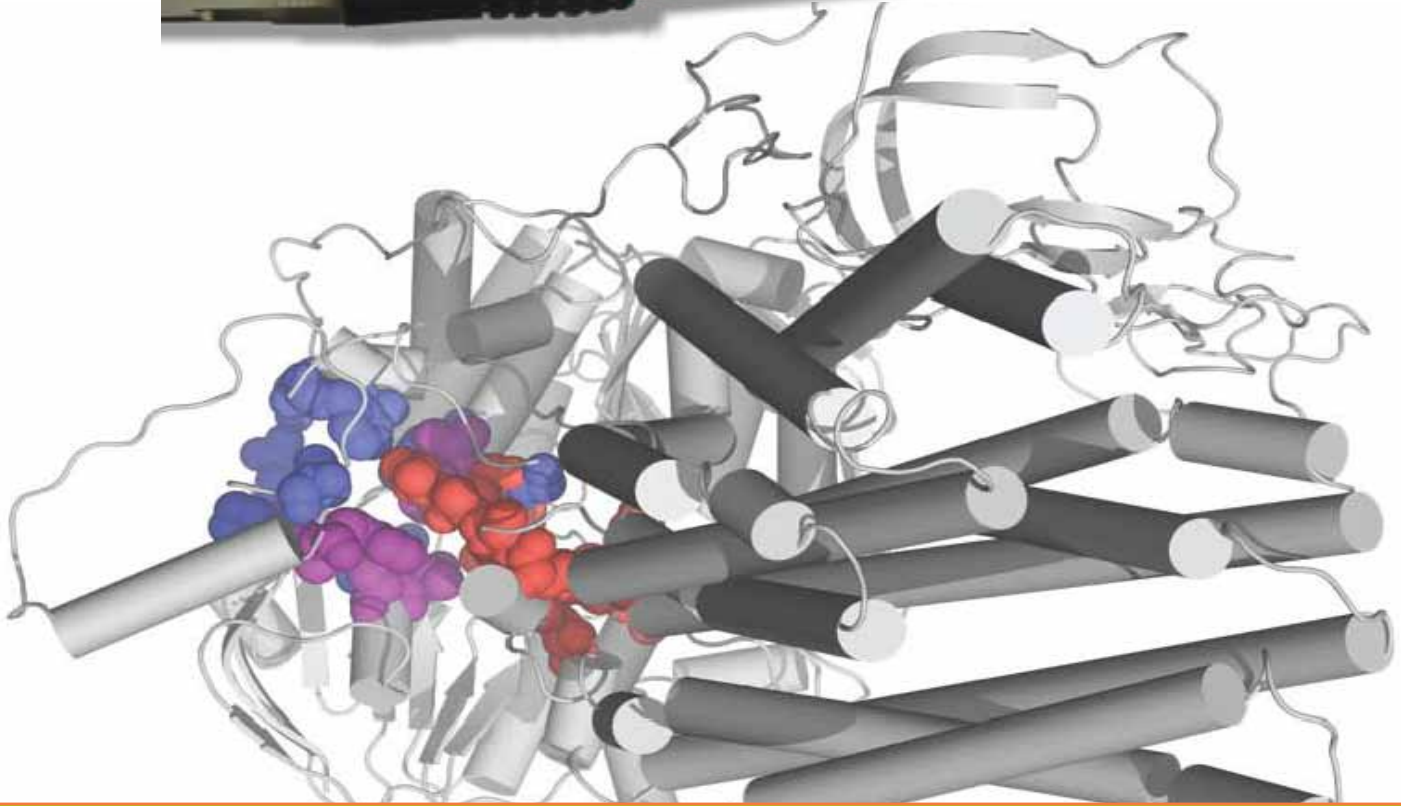


SciNet

PORTAL



vol.2

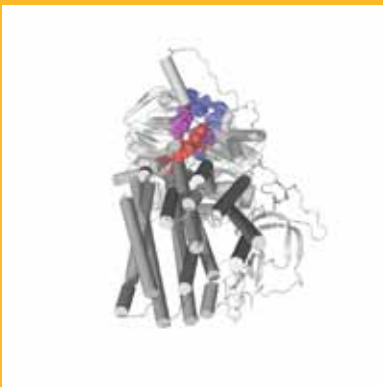


CANADIAN SCIENCE AT SCALE

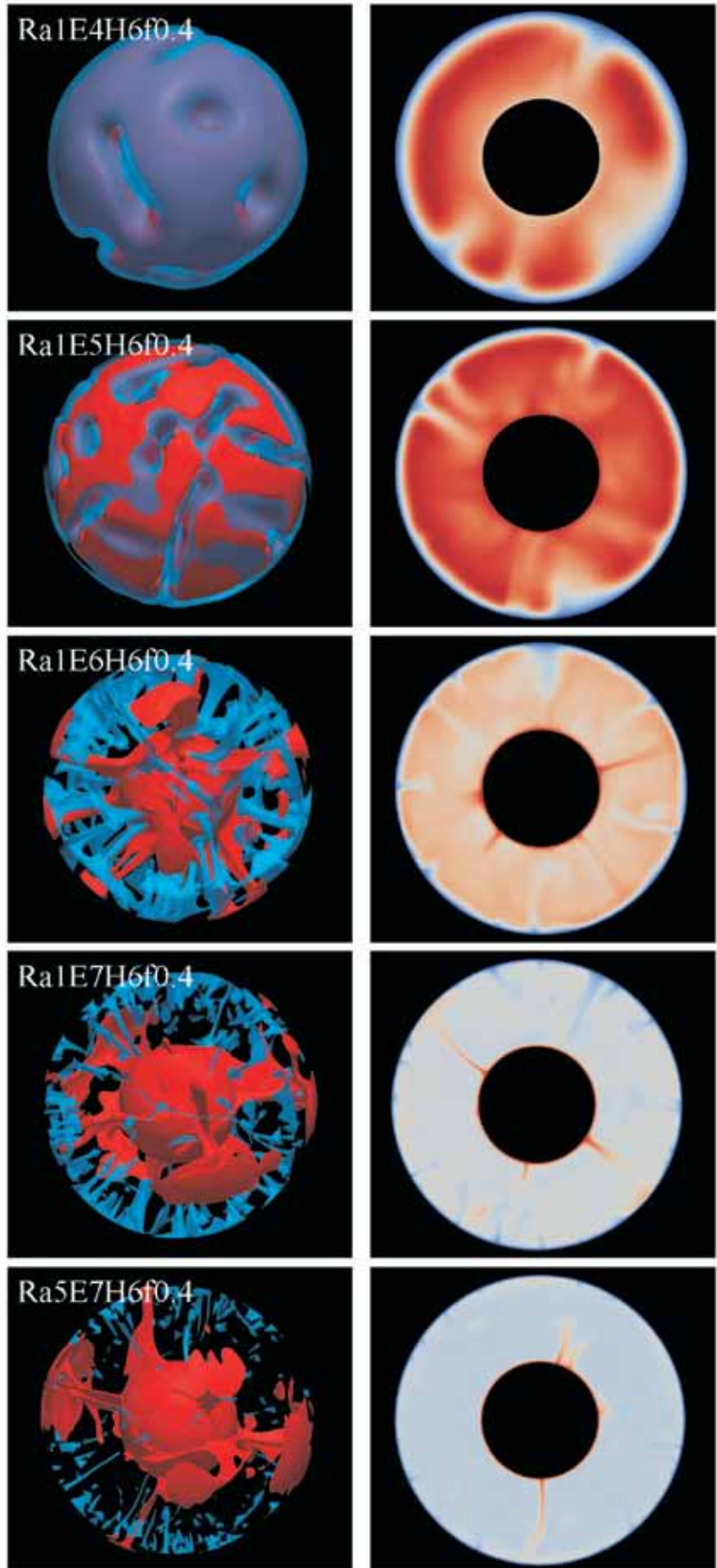
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CANADA

IN THE P RTAL

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Cover: Marshal Zheng; a close-up of individual binding sites of the two compounds on a protein (see page 8 for more details)



DIRECTOR'S MESSAGE

The past year at SciNet, the second during which our systems have been fully operational, has been exceptionally rewarding, with our two machines being fully subscribed and highly productive of new research results. Operations have not been without incident, however, the most amusing (and unsettling) of which involved an attack on the data centre by a raccoon which managed to fry itself on a transformer! Although this did lead to a brief reduction of service on the TCS system, this was fully restored in a reasonably timely manner. We have since been obliged to raccoon-proof the facility! Our hope is that we will not have run afoul of the animal rights lobby.

As an example of an area of research that has benefited immensely from SciNet, I hope that the reader will not mind my focusing on one of the subjects in which my students and I are active, namely that of global climate change. In this field one of the most urgent needs is to provide high spatial resolution projections of the global warming process for the next century or more so that appropriate environmental policy may be designed in order to mitigate and adapt to the expected changes. The methodology that has been developed internationally to provide the needed projections involves the local “dynamical downscaling” of the results that are produced using global scale models which cannot yet be run at the high spatial resolution required for policy development purposes. The computational load required is simply too onerous given available resources at all of the laboratories in which such work is ongoing. Dynamical downscaling involves the “nesting” of a high resolution regional climate model (or models) within the global scale model, with the nested models being driven by the global scale parent.

Here in Ontario, the availability of SciNet has made it possible to begin to develop high resolution climate change projections for the province and for the Great Lakes Basin as a whole. This work has been strongly supported by the Ontario Ministry of the Environment and has led to the recent completion of a series of very detailed papers describing what is expected to occur in this region of the North American continent over the next century. The impact of the presence of the lakes turns out to be of first order importance and has required significant improvements in the climate models themselves as these generally have not included explicit treatments of the physical processes associated with the exchange of momentum, heat and moisture that have such a significant impact on local climate state.

This is only one of the many areas of scientific and engineering research which are being strongly impacted by the existence of SciNet. This edition SciNet PORTAL features several others.

*Dick Peltier
SciNet and Department of Physics*



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Left: a research image from a study on mantle convection and surface motion. There are feedbacks to the climate from the changes happening in the interior of the planet which create variations on the surface of Earth such as the location of the continents and elevations. Temperature field variation as a function of the Rayleigh number Ra and internal heating rate for a number of models with curvature parameter $f = R_{CMB} / R_{surf} = 0.4$ and non-dimensional rate of internal heating of 16.2 for the single pale planets (rigid surface). The left panel at each snapshot demonstrates two cold and hot isosurfaces with temperatures $0.8\theta_{ave}$ and $1.2\theta_{ave}$ respectively where θ_{ave} is the mantle mean temperature. The right panel shows a cross-section of the mantle convection. This figure displays a subset of a large number of benchmark models obtained at different curvature parameters. The model results are used to establish a general power law relation of the mean mantle temperature to the Rayleigh number, internal rate of heating and curvature parameter. (C) Hosein Shahnas and Prof. W.R. Peltier

@ SCINET

SciNet News & Events

November 2011 to February 2012

SciNet will be offering a Scientific Computing Course to be held weekly for 13 weeks. The content is split into three parts:

1. Scientific Software Development
Python, C and C++, git, make, shell, modular programming, testing and debugging
2. Numerical Tools for Physical Scientists
Modelling, floating point computations, validation+verification, visualization, ODEs, Monte Carlo, linear algebra, FFT
3. High Performance Scientific Computing
Profiling, optimization, openmp, mpi and hybrid programming

Second Wednesday of each Month

SNUG + TechTalk

TechTalks are 1/2 hour mini tutorials held as part of the SNUG meetings.

Next meeting dates: Nov. 10th, Dec. 14th

November 23rd

Visualizing Data with Paraview

December 12th

Introduction to GPGPU with CUDA

Jamaican Canadian Association Youth come for a Tour

November 26th

SciNet was pleased to host the youth of the Jamaican Canadian Association for a tour of our facilities. A group of 30 children from grades 1 to 12 came to hear about the research being done, see the machines, do a few hands on simulations for themselves and enjoy a pizza lunch.

Both staff and visitors seemed to have a great time.

The JCA wrote: "The presentation was very informative and engaging for all of us - the tour accomplished our goal for the program: to expose the students to broader applications of computer technology. Thank you for allowing us to come!"



SCINET UPDATES

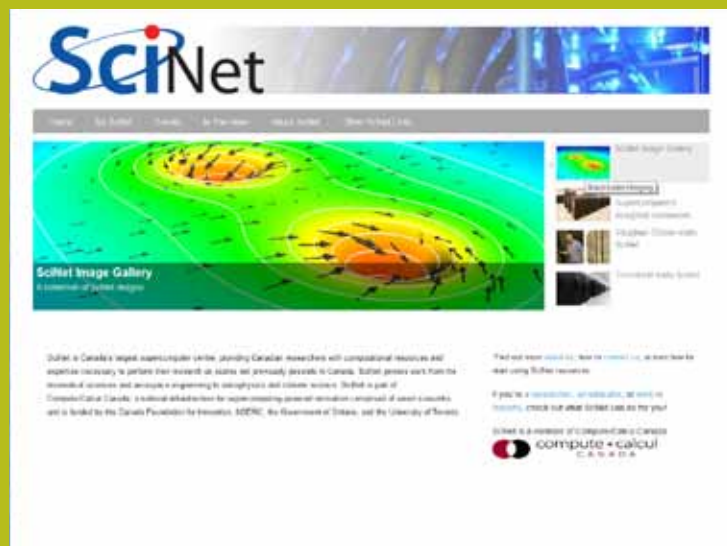
NEW SITE

SciNet is happy to announce that the new website has finally gone live! You can find the freshly redesigned site at

www.scinethpc.ca.

Improved features include an integrated courses page, easier navigation, and sections specifically for educators, industry professionals, media, academics, and, of course, our very valued users.

Take a tour and let us know what you think!



STAFF PROFILES



Parallel Programming Analyst

RAMSES van ZON

Ramses van Zon is a parallel programmer analyst at SciNet. His primary responsibility is to provide advice and support to users on topics such as code optimization, application porting, workflow, improving efficiency, and parallel programming. For example, he has worked with computational biologists to improve their workflow and storage access patterns, leading to a fourfold increase in throughput. Ramses is very interested in new developments in computational science and software development, and in new parallel programming languages and computing environments that can improve the performance and scalability of applications.

He is also involved in the training of users through SciNet's workshops, courses, user group meetings, and SciNet's first for-credit graduate course on scientific computing that started this year. He wrote and maintains the SciNet User Tutorial and contributes to the SciNet wiki.

Ramses has a undergraduate degree and PhD in theoretical physics from Utrecht University in The Netherlands. He has worked as a researcher at the Rockefeller University in New York and at the Chemical Physics Theory Group of the University of Toronto, where he has also taught Physical Chemistry. In addition to theoretical work on fluctuations in non-equilibrium systems, he has developed computational techniques for molecular dynamics simulations and path integral calculations and has over 20 year of coding experience in several programming languages and 5 years of non-embarrassingly parallel programming experience.

DANIEL GRUNER

Daniel Gruner is CTO-Software at SciNet. Together with the team of application software parallel programmer analysts he supervises, they provide most of the user support at Scinet, particularly as relates to code implementation, parallelization, optimization, workflow, and general scientific programming. In addition, the support team provides instruction to users in the form of specialized courses on programming languages, parallel programming techniques, and general scientific computing.

The analyst group is also heavily involved in community outreach activities, helping to bring the excitement of scientific research and computing to a wide-ranging audience. In particular we are involved with high-school students (SATEC @ W.A. Porter C.I.) and community groups (Girl Guides, Jamaican Students Association), who will likely have a new outlook on their professional lives as a result of engaging "real, live" scientists.

Daniel has more than twenty-five years' experience working with a variety of programming languages, parallel computing, scientific modelling, artificial intelligence, software architecture, windowing system GUI programming, administration of large Beowulf clusters and large shared-memory parallel computers, system administration, and networking. He earned a bachelor's degree in chemistry and physics from the Hebrew University of Jerusalem, and a Ph.D. in chemical physics from the University of Toronto.



Chief Technical Officer-Software

NEUROSCIENCE



High Performance Computing in Population Neuroscience

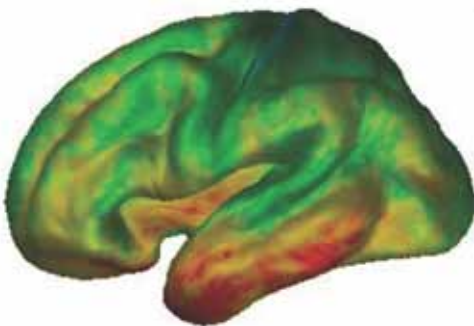
~ Dr. Tomáš Paus, M. Mallar Charkravarty & Rosanne Aleong;
Rotman Research Institute, Baycrest

The advent of in vivo brain imaging lifted limitations inherent in post mortem studies. We can ask now what shapes the brains both from within (genes) and without (social and physical environment) in large samples of individuals drawn from the general population. What are the main reasons for pursuing this endeavor? First, we believe that by understanding inter-individual variability in the (healthy) human brain vis-à-vis variations across individuals in their genes and environments, we gain knowledge about a process leading to a particular state of brain structure and function. Second, by gaining insights into the process, we are taking the first step towards enabling prediction: individuals with a particular constellation of distal causes and ensuing developmental cascades will likely differ in the state of their brains at a particular time in their life and, in turn, in their risk for developing brain disorders, such as depression or dementia. Thus, in the long run, understanding distal causes and associated processes will lay down the foundations for personalized and preventive medicine. In our work, we rely on magnetic resonance imaging (MRI) to quantify subtle variations in the structure of the human brain, particularly during the adolescent period. Over the last 25 years, MRI has had a tremendous impact on neuroscience; it offers high-resolution snapshots of individuals' brain anatomy at a single time point and allows researchers to resolve the shape and volume of grey matter (clusters of neurons that reside on the outer cortical ribbon of the brain and in clusters deep within the brain) and white matter (the axonal "wiring" that connects disparate grey matter regions). Structural MRIs have become one of the main data types in our laboratory. In fact, various flexible parameters may be derived from MRI for the analysis of brain structure. There are several fully automated software packages that allow for the quantification of the volume of different grey-matter and white-matter structures. More advanced algorithms are also available to quantify local variations in brain shape (i.e., thickness of the cortical ribbon) and volume. By coupling these metrics with genetic markers (over 500,000 single nucleotide polymorphisms/study volunteer) and behavioral, dietary, and lifestyle metrics obtained during a 15-hour assessment, our research allows for a better understanding of the relationships between the body, an individual's environment, and brain function

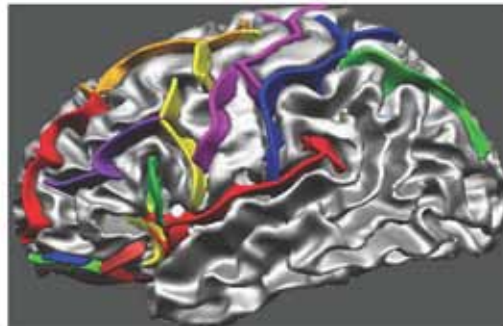
and dysfunction. In order to address the complexity inherent in such relationships, we require thousands of datasets. We have been involved in several studies acquiring these types of data. These include the Saguenay Youth Study (n=1,000; a study of adolescents in northern Quebec aged 12-18 years; 500 were born to mothers who smoked during pregnancy), the IMAGEN study (n=2,000; a European study of 14-year old adolescents), and the ALSPAC study (n=500; a cohort of male adolescents studied from birth). High-performance computing is absolutely necessary to manage the complexity of analyzing such data. Scinet allows us to pre-process an entire dataset of several thousand images in a single day; under normal laboratory settings, this pre-processing would take weeks (even with the use of a regular cluster). Access to the general-purpose cluster (GPC) allows us to analyze the variables and permutations within these variables as never before. Typically, estimation of cortical thickness and regional brain volumes for a single individual can require up to 18 hours and 6 hours, respectively, on a single CPU. This year, we used 84,000 hours of processor time alone for data pre-processing. Next year, we anticipate data collection from 900 additional subjects from the Saguenay region (parents of the adolescents who volunteered in the original study) and 3,000 additional young individuals and their parents from Finland (using a similar recruiting paradigm as the Saguenay Youth Study). We project that we will require an addition 93,600 hours of processing time for these new datasets. In the past 12 months, our utilization of Scinet resources has allowed us to identify a specific genotype that is associated with lower brain volume among female adolescents, develop novel methods for coupling craniofacial and brain development, create novel paradigms for the understanding of face perception, and analyze the brain response to faces in a probabilistic fashion.

Tomáš Paus M.D., Ph.D.
Tanenbaum Chair in Population
Neuroscience; Professor of Psychology and
Psychiatry, University of Toronto

M. Mallar Charkravarty; Scientist, Centre for
Addiction and Mental Health



Cortical thickness



Cerebral sulci

BLACK HOLES



Magnetic Fields Keep Milky Way's Central Black Holes Hungry- For Now

~ Ue-Li Pen, Bijia Pang; CITA, University of Toronto

~ Christopher D. Matzner, University of Toronto

~ Stephen R. Green, University of Chicago

~ Matthias Liebendörfer, University of Basel

Two researchers in the University of Toronto, Bijia Pang and Ue-Li Pen, have run the largest three-dimensional (3D) magnetohydrodynamics (MHD) simulation ever performed in Canada. 17,576 cores on the GPC supercomputer at SciNet were used concurrently to run $(4,680)^3$ grid cells on an adaptive grid with an effective resolution of 64000:1 in the 3D MHD simulation of non-radiative accretion onto the supermassive black hole at the Galactic centre.

Telescopes can see light from distant galaxies; but it takes a supercomputer to see why the centre of our own is so dark.

The intense gravity near black holes makes for a violent, active region of space. Gas or stars that wander too near are torn apart, their energy released as X-rays. In the centre of the Milky Way, 26,000 light years away, is a black hole over four million times heavier than our Sun, but only modestly brighter. It's eerily quiet -- too quiet.

This dark object, with 4.3 million times the mass of the Sun, is located near the compact radio source Sagittarius A*. Being massive and relatively close, it is the largest apparent event horizon in the sky; in fact both the hole and its surrounding gas flow are marginally resolved (using radio and x-ray

observations, respectively).

A curious feature of this black hole, and others like it, is its very low luminosity given its intense gravity and the ready supply of hot gas in its surroundings. Indeed, it emits only one solar luminosity in x-rays (a few hundred solar luminosities over all bands), whereas a naive estimate is over a million times brighter!

Pang and Pen, along with co-workers Christopher D. Matzner of the University of Toronto, Stephen R. Green from University of Chicago, and Matthias Liebendörfer from the University of Basel, have argued that magnetic fields play a critical role in resolving this discrepancy. In a suite of smaller simulations, these authors have uncovered a phenomenon in which magnetic fields choke the accretion flow and slow convective motions. Their simulations are distinguished by very large dynamical range, outer boundary conditions causally disconnected from the flow regions of interest, and very long runs which are capable of approaching true steady state. An observational prediction of their model is a very slow variation of the Faraday rotation measure, which can be tested by observations with new telescopes like ALMA. If confirmed, it will bring us

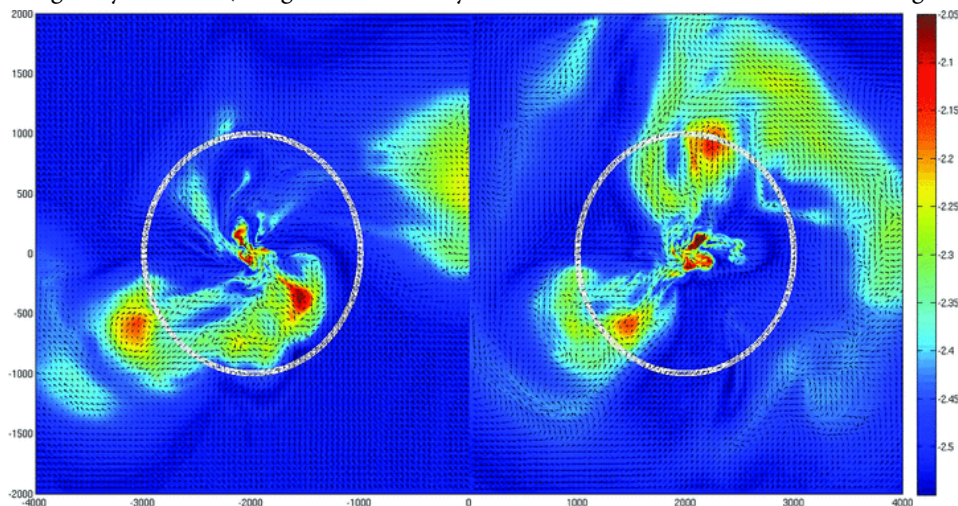
to a new level of understanding for this mysterious black hole.

The team used supercomputers at SciNet, in the University of Toronto, performing the largest computer simulations ever done in Canada, to test out their new theory.

"We've long thought that magnetic fields can choke off the flow of material into the black hole" says Prof. Ue-Li Pen of CITA. "Our earlier work suggested this, but then, it just wasn't possible for a simulation to look at the huge range of lengths - from light years to light minutes - needed to track the hot gas as it falls all the way towards the black hole."

"But our new methods, and SciNet, let us do just that," added Dr. Bijia Pang. "We broke up the region of space near the black hole into 100 billion zones, and spread them over almost 18 thousands processors on SciNet's largest cluster. This finally gave us the resolution we needed to test our model - we could see, with unprecedented accuracy, the fields halting the turbulence and keeping the gas from falling in."

Their work was published in the September edition of Monthly Notices of the Royal Astronomical Society.



< 2D slice of the simulation for 6003 box at 15 Bondi times. Colour represents the entropy, and arrows represent the magnetic field vector. The right-hand panel is the equatorial plane (yz), while the left-hand panel a perpendicular slice (xy). White circles represent the Bondi radius ($r_B=1000$). The fluid is slowly moving, in a state of magnetically frustrated convection.

CYSTIC FIBROSIS

Cystic fibrosis is the most common fatal genetic disease among Caucasians. In healthy individuals, the CFTR protein maintains a thin layer of fluid on the surface of epithelial cells. However, in patients with CF, a genetic defect causes the protein to be misfolded and retained within the cell, unable to reach the surface to perform its function. Thick, sticky mucus builds up in the lungs of affected individuals, inhibiting their ability to breathe and creating an inviting environment for deadly bacterial infections. In the past, progress has been made in clinical care, by controlling infection and enhancing nutrition, but most researchers currently believe the next major increase in lifespan for patients with CF will be brought about by targeting the disease at a molecular level. Small molecules that interact directly with the mutant protein to rescue it to the cell surface have been previously identified, but their precise mechanisms of action are currently unknown.

Marshall Zhang, a grade 11 student at Bayview Secondary School, under the supervision and support of Dr. Christine Bear and Steven Molinski at The Hospital for Sick Children, used the SciNet HPC Consortium at the University of Toronto to define the binding sites of these compounds with the mutant protein, and thus identify potential molecular targets for future therapeutics. These computational studies involve finding the lowest energy conformation of the ligand on the surface of the protein. In-silico modeling of the interactions of two small molecules with the mutant CFTR protein implied different mechanisms of action, with one compound intervening later in the biosynthetic processing pathway than the other. This suggested the feasibility of a combination treatment, and in-vitro studies demonstrated a synergistic effect between the CFTR modulators in combination in their correction of the disease-causing molecular defect. Not only do computational methods allow researchers to understand the mechanisms of action of individual small molecules, they also pave the way for new approaches to therapies for disease, such as the cocktail treatment developed in Marshall's study.

Grade 11 student uses SciNet in search for cure to Cystic Fibrosis

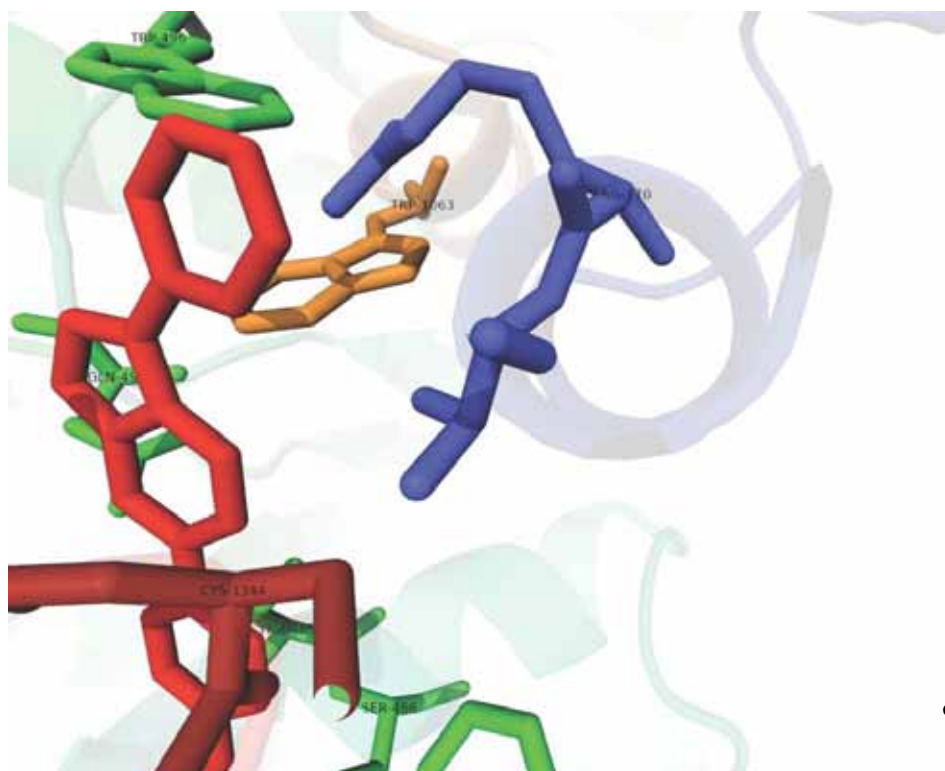
~ Marshal Zhang, Bayview Secondary School;
~ Dr. Christine Bear, Hospital for Sick Children



Beyond looking at molecules individually, high-performance computing also allows scientists to examine thousands of compounds for potential drug candidates. Virtual screening, enabled by the computational power of SciNet, allowed Marshall to identify certain structures that may play a role in the efficacy of these modulator compounds. Screening a diverse chemical library of thousands of drug-like molecules and comparing their binding affinities to the protein quickly revealed chemical motifs among the top hits. In combination with the molecular targets identified through the individual small molecule simulations, computational methods have provided a potential foundation for future rational structure-based drug design. Virtual drug discovery is quickly emerging as a complement to traditional high-throughput screening, improving "hit rates" and allowing for analysis even before biochemical assays are established.

For his work, Marshall won first place at the National Sanofi-Aventis BioTalent Challenge, and will be traveling to Washington to compete internationally. He was also awarded a gold medal at the Canada-Wide Science Fair and will be a member of Team Canada at the Expo-Sciences International this summer in Slovakia.

▼ below: proposed binding site of one of the compounds investigated, at a key interdomain interface of CFTR



ATLAS EXPERIMENT



ATLAS @ SciNet

~ Leslie Groer, Neil Knecht; SciNet,
University of Toronto

As the Large Hadron Collider (LHC) at CERN in Geneva, Switzerland concludes an extremely successful year of running, high-energy particle (HEP) physicists, postdocs and students at the University of Toronto along with about 130 Canadian colleagues and about 3,000 international colleagues from thirty-eight countries continue to eagerly analyze the debris from the proton-proton collisions recorded at the heart of the giant 100-million electronic channel digital “camera” known as the ATLAS detector. The LHC successfully delivered 5.61 inverse femtobarns of proton-proton collisions, a measure of the number of collisions (about 400 hundred trillion), at the highest centre-of-mass energy ever produced in a particle collider, 7 trillion electron-Volts (7 TeV). The ultimate goal of smashing these protons together at ever higher energies is to probe the most fundamental building blocks of matter and the forces that govern the universe. In particular, the LHC and the two large general purpose detectors ATLAS and CMS, were designed to explore the energy regime where electroweak symmetry breaking occurs and where new phenomena such as supersymmetry or extra dimensions may be lurking. The holy grail for the experiments is the discovery of the Higgs boson which in the standard model of particle physics is the embodiment of the Higgs field, interactions with which impart mass to all the other fundamental particles (and ultimately us!), but there is every expectation that surprising new phenomena will appear too, as has happened over the last few decades whenever the energy scale is increased.

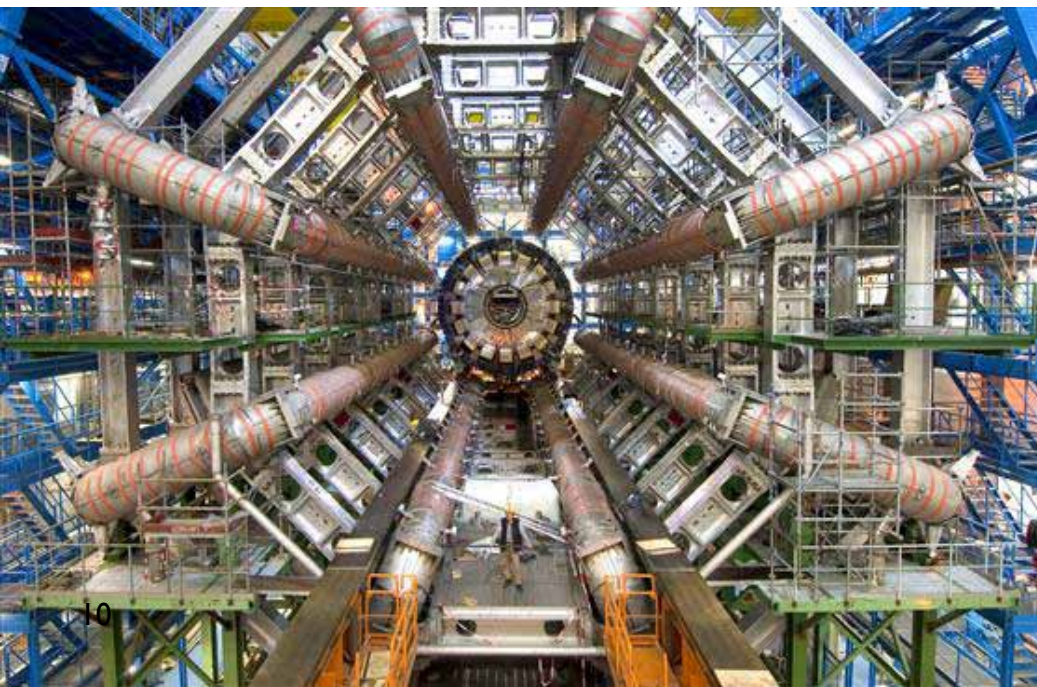
The University of Toronto HEP group has been intimately involved in the ATLAS project for over a decade and constructed some of the main calorimeter detector components in the basement of the Physics building before shipping the completed detector off to CERN in 2004 to be installed in the collision hall, 100 metres underground. UofT has also

provided computing platforms for storage and analysis of the data, going back to the CERN test beams in 2003 and for running large numbers of simulations of the proton-proton collisions. The Physics department had a dedicated cluster that joined the Worldwide LHC Computing Grid (WLCG) in 2004, under the guidance of Dr. Leslie Groer, and provided what is known as an ATLAS Tier-2 Analysis facility until the SciNet computing systems came online. In fact, that same year, Dr. Groer, now a Technical Analyst with SciNet dedicated to ATLAS computing support, and Dr. Chris Loken, then at the Canadian Institute for Theoretical Astrophysics but who is now the Chief Technical Officer for SciNet, met to discuss the idea of a single much larger cluster that could simultaneously meet the computing demands of theoretical astrophysics and experimental particle physics and mapped out a design that is not very different from the SciNet GPC, although with computing core counts doubling almost every new CPU generation the final GPC cluster has twice the capacity than was originally envisioned.

The sheer demands of the experiments at the LHC both for computation and data storage necessitated the construction of tiered computing facilities around the world with the Tier-0 facility being at CERN, and ten Tier-1 facilities for ATLAS, one of which is hosted at the dedicated centre at TRIUMF in Vancouver, and about seventy Tier-2 facilities, five of which are at the shared consortia facilities in Canada. The SciNet infrastructure provides the largest ATLAS Tier-2 Analysis Centre in Canada and equals the resources provided by WestGrid, which has its Tier-2 centres distributed across the University of Victoria, Simon Fraser University, and the University of Alberta. In the last few months, the CLUMEQ facility at McGill has also come online. Grid computing tools, based on the Globus toolkit, provide the middleware

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The eight toroidal magnets can be seen on the huge ATLAS detector with the calorimeter before it is moved into the middle of the detector. This calorimeter will measure the energies of particles produced when protons collide in the centre of the detector. ATLAS Experiment © 2011 CERN



to tie all these facilities together and to provide access to the users across the globe. There are many layers of software support from the LHC experiments and projects such as the European Grid Initiative and Open Science Grid to provide the WLCG platforms.

ATLAS was a key player in the original SciNet consortium discussions and system specifications, especially for data storage. As a large shared facility though, certain design choices could not be dictated solely by the ATLAS requirements and therefore there were some challenges to install the grid middleware and in particular the ATLAS software on the GPC and the large General Parallel File System (GPFS). Testing of the software and experience with running thousands of jobs on the shared GPFS file-system took some tuning, some of which is detailed more extensively in [1]. In particular, real ATLAS analysis and simulation jobs were run by UofT postdocs and students in the early days of SciNet to stress-test the system and improve on the final layout and tuning for GPFS, software provisioning and batch job distribution. The ATLAS software components are continually being monitored, tweaked and improved by Dr. Groer and Dr. Neil Knecht, who joined SciNet in early 2010 to also provide ATLAS support.

The SciNet facility routinely runs about 5,000 jobs a day for the ATLAS experiment, about a quarter of the total jobs run across Canada. SciNet is also the first Tier-2

production site in North America to be connected via a ten gigabits per second network to the prototype LHC Open Network Exchange, a facility that is being developed to allow rapid large volume data movement between the LHC sites to occur on dedicated optical links across the world, rather than competing with the regular research and education traffic that occurs between campuses and research institutions. These links will allow tens of terabytes to be moved to or from SciNet per day.

The resources provided to the ATLAS experiment also contain a “Canadian-only” component at each site, namely access to privileged queues and data storage under Canadian control, which allows the over 150 physicists in Canada to remain competitive with their international colleagues in analyzing the complicated datasets coming from the collider and making new discoveries. Of particular note, the Toronto group played a key role in publishing some of the very first proton-collision results from the ATLAS experiment in 2010. Just a few months after the LHC turned on, a search for di-jet resonances allowed the world’s best limit to be placed on excited quark states (jets are the observed narrow collimated spray of particles that result from the hadronization of quarks and gluons). This work was spearheaded by UofT’s Prof. Pierre Savard, co-convenor of the ATLAS Exotics Group, and his Ph.D. student, Sing-Leung Cheung. This result

relied heavily on a series of special Monte Carlo simulation runs that were done at SciNet in the spring of 2010 in support of the Jet-Energy Scale group which is co-convened by UofT’s Prof. Richard Teuscher. Over a few intense weeks, the SciNet ATLAS Tier-2 facility was used to run over 72,000 grid jobs, corresponding to over 0.5 million cpu-hours, by using up to four times the steady-state cpu allocation, resulting in 3.6 million simulated events and 28 TB of data. This simulation campaign, which would not have been possible using the standard ATLAS resources, provided crucial input to the determination of the systematic error, which was already at the 7-9% level after only a couple of months of data-taking. This impressive early precision fed into the very first physics papers with collisions from the LHC, which was of particular importance for the resonance search and standard model di-jets papers, where the jet energy scale is the largest uncertainty.

On December 13th, tantalizing new results from ATLAS and CMS were presented at CERN from the 2011 data that hint that the Higgs boson may have been discovered at approximately 125 GeV. The LHC will resume proton-proton collisions early in 2012 and will deliver at least four times the number of proton-proton collisions than in 2011, which should lead to conclusive evidence of the existence or non-existence of the Higgs boson. If found, the larger datasets will allow detailed exploration of the Higgs boson properties. In addition, other favoured physical theoretical predictions beyond the standard model such as supersymmetry or extra-dimensions should start yielding observable results or theorists may have to scramble back to the chalk board.

Analyzing all this data will keep the SciNet ATLAS Tier-2 facility extremely busy over the next few years. This is indeed an exciting time in particle physics.

[1] SciNet: Lessons Learned from Building a Power-efficient Top-20 System and Data Centre, 2010 J. Phys.: Conf. Ser. 256 012026, <http://iopscience.iop.org/1742-6596/256/1/012026>

< Model of ATLAS created entirely of LEGO blocks by Sascha Mehlhase. ATLAS Experiment © 2011 CERN

