CELEBRATING ATLANTIC CANADIAN RESEARCHERS

Annual Report
2015-2016

ACENET
accelerate discovery

computecanada
regional partner

CONTENTS

ACCELERATING DISCOVERY WITH ACENET

Accelerating discovery and innovation is the driving force behind ACENET. With a dedicated team of experts throughout the region, we provide advanced computing resources and expertise to researchers and industry throughout Atlantic Canada. Through our activities, we accelerate discovery and innovation, help attract and retain highly qualified people in the region and empower students with foundational skills in the high-demand field of advanced computing.

Initially founded to serve computationally-based research needs at five universities across Atlantic Canada, ACENET's membership has since grown to 12 post-secondary institutions and over 900 researchers. During the past 13 years, we've become an indispensable resource.

We are a regional partner with Compute Canada, the national organization responsible for advanced research computing in Canada. Through this partnership, we provide access to resources from across the country and represent our regional interests at the national table.

THE POWER OF TRANSFORMATION

The power of technology has truly transformed our lives. Advanced computing resources – which are at the core of ACENET – are making our world a better place. Healthcare professionals are diagnosing and treating more diseases; scientists are further examining the effects of climate change on our environment; and innovative start-ups are commercializing new products, transforming their ideas into reality.

As one of the most advanced computing networks in Canada, ACENET plays a vital role in our region. We accelerate discoveries and foster research that in turn provides important economic and social benefits to Atlantic Canadians.

Just as technology advances, ACENET is strategically evolving, growing our unique high-powered capabilities, adding new critical infrastructure and engaging with the broader community. This essential work is guided by our new CEO, Ann MacKenzie, who joined ACENET in November, bringing incredible strengths to our organization. Ann was appointed after the retirement of Ray Miller. During his tenure, Ray played a crucial role in ACENET's growth and success. I thank him for his stellar years of service and wish him well in his future endeavours.

Working with our partner institutions and researchers, ACENET is proud to provide valuable services throughout our region. I invite you to learn more about our research success in this report.

Sincerely,
Dr. Richard J. Marceau, P.Eng., PhD, FCAE
Chair, ACENET Board

HEARING OUR RESEARCHERS

During these past few months I've had the pleasure of meeting a number of our researchers and learning about the difference they are truly making through their work. In discussions with them, ACENET's team, institutional partners and our Research Directorate, I've gained a deeper understanding of the needs and concerns of Atlantic Canada's research community and the valuable contribution it makes to the region.

High on the list of research community priorities is having 'feet on the ground' researcher support. ACENET accomplishes this by the effective partnering of our Advanced Computing Systems Administrators with our Computational Research Consultants. It is critical that ACENET continue to host infrastructure, which requires these highly qualified people to support the equipment and community. In March, we submitted a proposal for a new data centre under the Canada Foundation for Innovation's infrastructure renewal process. While the results will not be announced until September, we continue to advocate for new infrastructure in our region.

Likewise, we must ensure that our skill sets develop in tandem with new technology and research needs. This past year ACENET added a big data and cloud specialist and is in the process of adding other new specialists, including one in bioinformatics.

I've been engaging extensively with our current funding partners and broader stakeholder groups, all of whom have expressed strong support for ACENET. I'm also exploring new ways of ensuring that we are well-positioned to continue serving the advanced computing needs of our community. Through the dedication, energy and passion of our team, we are committed to continuing to accelerate discovery in Atlantic Canada.

Sincerely,
Ann MacKenzie, CPA, CA, MEC
Chief Executive Officer, ACENET

HIGHLIGHTS FROM 2015-2016

ACENET supports 16 Canada Research Chairs

Training & Research Support

ACENET provides advanced research computing (ARC) training to students and researchers, and wherever possible, supports training initiatives by complementary organizations. In addition to one-on-one coaching, ACENET carried out 39 formal training sessions for 600 participants, supported Compute Canada's training partnership with Software Carpentry, and provided technical support to a Ladies Learning Code training day.

Two Atlantic Canadian students were among ten recipients across the country who received Compute Canada scholarships to the 2016 International Summer School on High Performance Computing Challenges in Computational Sciences. The winners were Neil Burke (PhD student, Computer & Information Sciences, Dalhousie University) and Lukas Spies (Graduate student, Scientific Computing, Memorial University). The summer school is taking place in Ljubljana, Slovenia.

Increasingly, ACENET is receiving requests for more specialized ARC training, and this year incorporated both Molecular Dynamics and Handling Big Data on the Cloud modules into our training catalogue.

This past year also saw ACENET acquiring new expertise in order to support demand in growing fields, with the hiring of a big data specialist and a software developer.

Supporting Research Excellence

ACENET is proud to support all of our researchers and recognizes the valuable contributions they make to the sciences, humanities, arts and society. Some researchers require more computing resources than are readily available with a default account. Others require a development environment to build portals or platforms. To accommodate these needs, Compute Canada holds annual competitions in which researchers from across the country submit proposals along with their computing requirements. Proposals are peer reviewed and additional resources are allocated according to research excellence and capacity. This year, a number of researchers received dedicated allocations.

Resource Allocation Competition
(computing cycles and storage)

Jahrul Alam, *Memorial University, Mathematics and Statistics*

Hossain Farid, *Dalhousie University, Agriculture*

Erin Johnson, *Dalhousie University, Chemistry*

Julie LaRoche, *Dalhousie University, Biology*

Randall Martin, *Dalhousie University, Physics and Atmospheric Science*

Erika Merschrod, *Memorial University, Chemistry*

David Pike, *Memorial University, Mathematics and Statistics*

Christopher Rowley, *Memorial University, Chemistry*

Mike Smit, *Dalhousie University, Information Management*

Josef Zwanziger, *Dalhousie University, Chemistry*

Research Platforms & Portals Competition
(developmental space and storage)

Mark Leggott, *University of Prince Edward Island, Library*

Randall Martin, *Dalhousie University, Physics and Atmospheric Science*

Jason Pearson, *University of Prince Edward Island, Chemistry*

Jon Saklofske, *Acadia University, English and Theatre Studies*

New Members

ACENET was pleased to welcome three new members this year - NSCAD University, the Nova Scotia Community College, and Mount Saint Vincent University.

Growing our Digital Humanities Community

Compute Canada runs a national competition annually for two scholarships to the Digital Humanities Summer Institute, a two-week premier training event held at the University of Victoria each June. These scholarships are designed to not only support digital humanities research, but to enhance the skills of research consultants in this growing field. Each scholarship pairs a digital humanities researcher with a research consultant, and covers the registration for both team members, along with the travel costs for the consultant.

This year, ACENET was proud to have had both scholarships awarded to Atlantic Canadian researchers paired with members of our research support team. We congratulate Drs. Darren Abramson and Kate Scarth, both of Dalhousie University (Philosophy and English), along with ACENET research support staff Drs. Craig Squires and Chris Geroux.

New Atlantic Canada Data Centre

In March, ACENET submitted one of ten applications from across the country to host a new national data centre under the Canada Foundation for Innovation's Challenge 2 Stage 2 infrastructure renewal. If successful, the centre will be located at Dalhousie University. The site selection process is underway and a final decision by the CFI Board is expected in September.

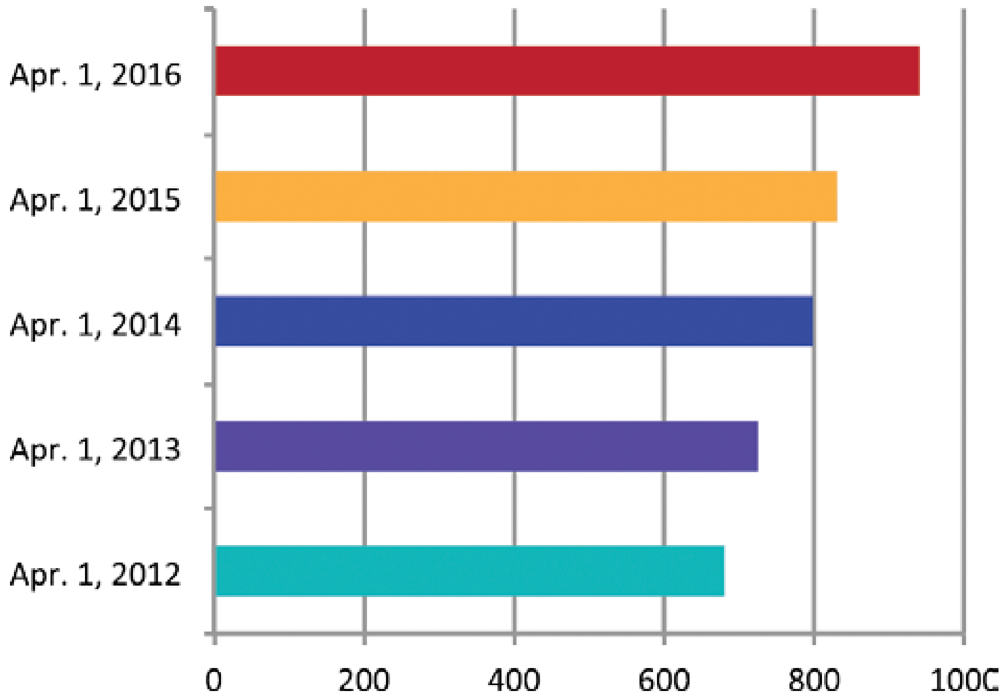
Advanced Research Computing Sponsorship Program

In the summer of 2015, ACENET launched its Advanced Research Computing (ARC) Sponsorship Program. This program aims to promote more use of ARC in Atlantic Canada, develop and retain highly qualified people, and cultivate new collaborations. The program supports researchers across all disciplines, with a total allocation of $60,000 for projects in amounts ranging from $1,000-$5,000. This year, $10,000 was committed to four projects, including a stage production through NSCAD University entitled Unconscious in the Sistine Chapel, which explores big data in both the story and the staging.

Recognizing Excellence

Ross Dickson, one of ACENET's Computational Research Consultants, received an Award of Excellence from Compute Canada during the 2015 High Performance Computing Symposium in Montreal. The award recognizes Ross for his exemplary client service and for his contributions to ACENET.

Atlantic Canadian Researchers Using ACENET/Compute Canada Resources

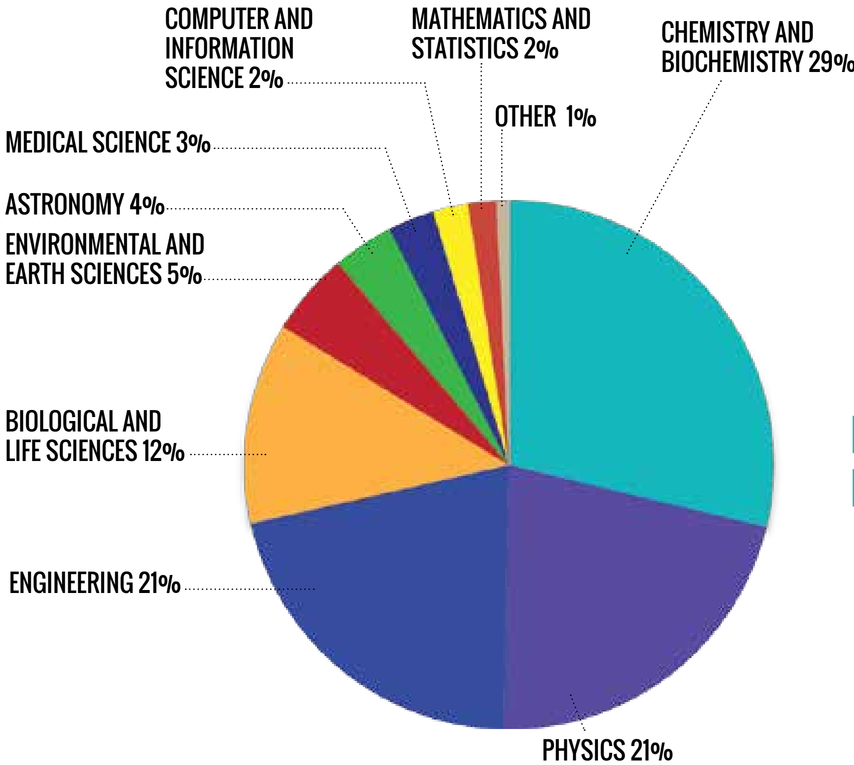


1,444

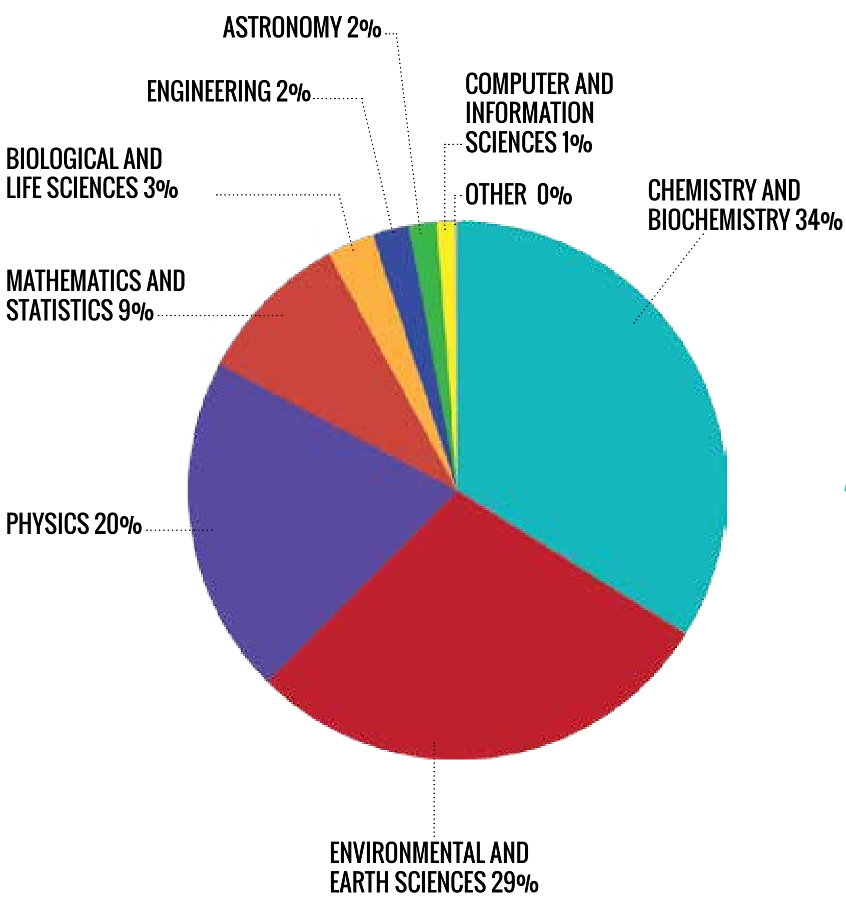
1444 Atlantic Canadian researcher publications have been enabled by ACENET and Compute Canada over the past four years.

870

This past year, ACENET responded to **870** help requests through **support@ace-net.ca**, varying from quick and easy to lengthy and complex.

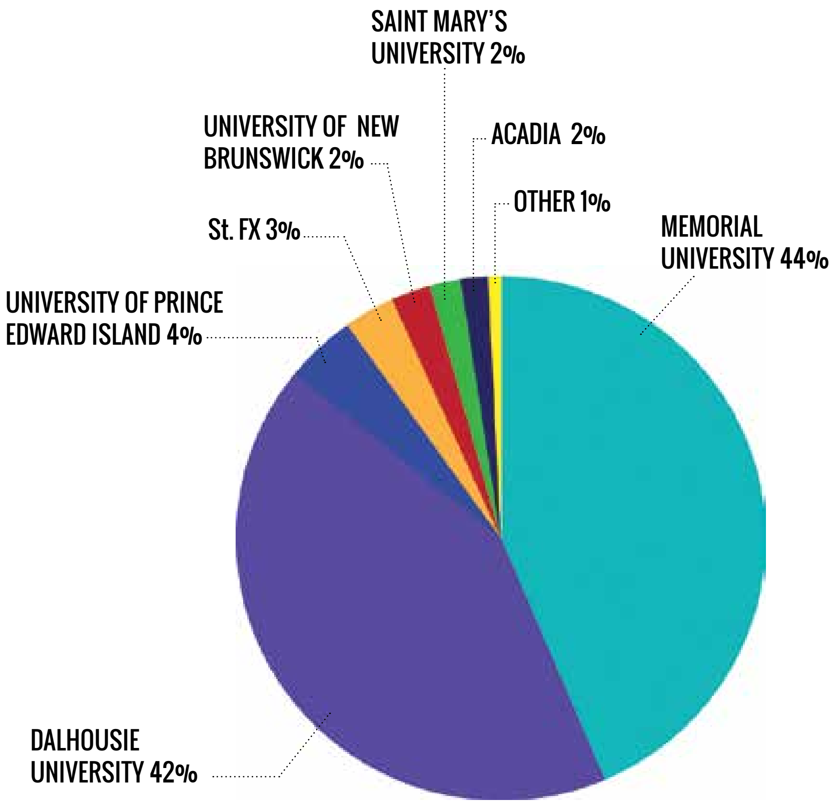


National Usage By Disipline



Atlantic Canadian Usage By Discipline

Atlantic Canadian Usage by Institution



Research Fellowship Program

Through a generous corporate donation, ACENET was excited to be able to support 23 undergraduate and 14 graduate students this year through our Research Fellowship Program. Research projects were varied and included modelling currents for tidal power in the Bay of Fundy, nanoparticle-based targeted drug therapy in cancer, improving the frailty index used with aging populations, and projects with applications for biofuels, DNA sequencing and brain tumours. Atlantic Canadian post-secondary institutions have a very talented pool of students and ACENET is proud to play a role in their development.

Some of these students are continuing on with their fellowships this coming year, along with a new group of recipients. We hope to be able to continue our fellowship program in the years to come.

"The ACENET fellowship for undergraduate students is a wonderful resource for students like myself. I learned an immense amount this summer; everything from specific physics concepts to programming skills to a researcher's mindset. I found it very beneficial to have a chance to do research now rather than having to wait until my honours project. Having this opportunity will leave me better prepared for my honours and as a result I will learn so much more."

Phoenix McCloud,
Undergraduate Student - Physics,
University of Prince Edward Island

Fellowship Recipients in 2015-16:

Amin Akbari, *Graduate Student, Engineering, Dalhousie University*

Seyedabdolrasoul Asaee, *Graduate Student, Engineering, Dalhousie University*

Ernest Awoonor-Williams, *Graduate Student, Chemistry, Memorial University*

Thomas Bennett, *Graduate Student, Mathematics & Statistics, Acadia University*

Amanda Cameron, *Undergraduate Student, Chemistry, Cape Breton University*

Kody Crowell, *Undergraduate Student, Physics, Acadia University*

Tait Du, *Undergraduate Student, Physics, Mount Allison University*

Thomas Faour, *Undergraduate Student, Physics, St. Francis Xavier University*

Spencer Farrell, *Undergraduate Student, Physics, Dalhousie University*

Tiffany Fields, *Undergraduate Student, Astrophysics, Saint Mary's University*

Maria Flynn, *Undergraduate Student, Pharmacy, Memorial University*

Jonathan Garry, *Undergraduate Student, Physics, Dalhousie University*

Cole (Matthew) Grbavac, *Undergraduate Student, Economics, St. Francis Xavier University*

Anna Haley, *Undergraduate Student, Engineering, Dalhousie University*

Sean Hartery, *Undergraduate Student, Physics, Dalhousie University*

Trent Hilliard, *Graduate Student, Engineering, Dalhousie University*

Shane M. Holden, *Undergraduate Student, Physics and Physical Oceanography, Memorial University*

Mahdi Hosseinali, *Graduate Student, Engineering, University of New Brunswick*

Ricarda Konder, *Undergraduate Student, Medicinal Chemistry, University of New Brunswick*

Chi Li, *Graduate Student, Physics, Dalhousie University*

Alexander MacKenzie, *Undergraduate Student, Computer Science, Saint Mary's University*

Shahrazad Malek, *Graduate Student, Physics and Physical Oceanography, Memorial University*

Ifenna Mbaezue, *Undergraduate Student, Chemistry/Biology, Saint Mary's University*

Phoenix McCloud, *Undergraduate Student, Physics, University of Prince Edward Island*

Bonita McCuaig, *Graduate Student, Biology, Memorial University*

Siobhan Morris, *Undergraduate Student, Physics, St. Francis Xavier University*

Garrett Muir, *Undergraduate Student, Chemistry, Mount Allison University*

Devin O'Malley, *Graduate Student, Engineering, Dalhousie University*

Adam Proud, *Graduate Student, Molecular & Macromolecular Science, University of Prince Edward Island*

Emma Shouldice, *Undergraduate Student, Physics, Dalhousie University*

Jonathan Smith, *Undergraduate Student, Mathematics & Statistics, Acadia University*

Patrick Strongman, *Undergraduate Student, Physics, University of Prince Edward Island*

Yi Sui, *Gratuate Student, Oceanography, Dalhousie University*

Erin Wetter, *Undergraduate Student, Engineering, Dalhousie University*

Islay Wright, *Undergraduate Student, Mathematics, Dalhousie University*

Semra Yalcin, *Graduate Student, Biology, Memorial University*

MINING WILLIAM BLAKE

"If he were alive today William Blake would have been a multimedia artist"

says Acadia University English professor Jon Saklofske. After all, the great British poet and visual artist left a complex and vast body of work ranging from the romantic to the surreal. "Blake was an inventor," says Saklofske. "He would have realized that computers are important tools and I think he would have made good use of them."

Saklofske certainly is making good use of the technology. He is an active participant in the emerging field of digital humanities – the practice of applying computer technology in various ways to the study of the humanities. He's using it for his ongoing research into the works of Blake, but he's gone much further than that, creating a digital online tool called NewRadial that helps scholars conduct and share online research.

"People have been digitizing works of literature and art like crazy for the last 15 years," says Saklofske. "Now it's time for us to start doing something with these vast digital collections."

Saklofske's interest in online research began when he started using the William Blake Archive, a web-based multimedia source featuring the works of Blake. "It's a great site, but there are limitations," he says. "The interface didn't allow me to do everything I wanted to do." He began working on an alternative interface, a modified way of accessing and participating in the Blake Archive - one that would allow more detailed search parameters and user participation. He dubbed the online platform "NewRadial" and immediately extended it beyond the study of Blake to work with other online multimedia collections.

NewRadial has proved to be a huge boon to Saklofske's research. For example, he's used it to study Blake's artistic representations of the Biblical Leviathan. "Blake drew Leviathan as a coiled serpent," he says. "NewRadial allows me to collect other representations of Leviathan during Blake's time and compare them with Blake's work."

The platform also promotes open social scholarship as other researchers are able to create their own collections, leave marginal comments or start a comment stream. "By integrating diverse and often isolated online resources through something like NewRadial, we can look at 500 years of written culture and understand how the way we tell stories, use language and express our worldview has changed and evolved over the centuries. It's a very effective tool."
By getting involved with ACENET, Saklofske was able to move NewRadial off of the small Macintosh server that it originally resided on and make it faster and more powerful. ACENET also opened his eyes to new possibilities for the technology and for the field of digital humanities.

DIGITAL HUMANITIES

Digital humanities is a broad field and one that a lot of traditional humanities scholars still have a hard time taking to, according to Saklofske. "There is still a noticeable divide between computer science and the arts. A lot of the time the efforts of Compute Canada tend to be directed toward science, but there is really a lot that can be done in the study of the arts as well. Computers are changing the way we do research and communicate that research with each other and a broader public. William Blake was very much about thinking beyond the box, in the same way that computers are allowing us to think beyond the page."

EXPLORING THE WORLD OF NANOPARTICLES

The world that Martin Mkandawire studies is very, very small, but his work could have a massive impact on human health and the treatment of diseases, including cancer. He's also playing a significant role in helping to clean up the environment, particularly around mining and industrial sites.

Mkandawire is a chemistry professor and scientist at Cape Breton University (CBU) who uses spectroscopy and photochemistry to study the properties of nanoparticles – microscopic objects less than 100 nanometres in diameter. He studies organometallic compounds and interactions between molecules and nanoparticles that have at least one bond between an atom of an organic compound and a metal. He's also working to develop devices using natural biological processes as the model, including developing and improving efficiency of organic solar cells based on cyanobacterial photosynthesis.

As Industrial Research Chair for Mine Water Management at the Verschuren Centre for Sustainability in Energy and the Environment at CBU, Mkandawire devotes much of his research to mine water remediation and management, developing cost-effective cleanup and treatment strategies, mostly based on principles of nanotechnology. One of those strategies involves using sensors that contain protein bound to nanoparticles that change colour, or fluoresce, when they come in contact with certain pollutants – acting as chemical canaries in coal mines. "We're using nanoparticles for biosensor development," he says.

Mkandawire and his team are also using nanotechnology to make cancer radiation treatments safer and more effective. Amanda Cameron is an undergraduate chemistry student at CBU and the recipient of a 2015 ACENET Research Fellowship. She is also one of the authors of a landmark paper on gold nanoparticle absorption rates published in the Royal Chemical Society journal Nanoscale. Under Mkandawire's direction she is studying the interaction of nanoparticles with certain cancer drugs. "Right now there are a lot of negative side effects associated with some cancer drugs," says Cameron. "If we attach those drugs to a nanoparticle that targets the cancer cells we can better target the tumour without affecting the healthy cells around it."

By injecting metallic nanoparticles directly inside cancer cells, small doses of radiation can be highly targeted to kill cancer cells without harming the healthy cells around it. "With this technique, a small amount of radiation has a strong effect," says Mkandawire.

His team also worked on targeting nanoparticles at the mitochondria in cancer cells – a study they published in the Royal Chemical Society journal, Nanoscale.

Nanotechnology research may also lead to major improvements in one of the world's oldest medical treatments: wound dressings. Mkandawire is testing smart wound dressings that contain magnetic nanoparticles incorporated in wound dressing fibres capable of detecting bacteria and increasing conditions during wound healing such as temperature or pH – conditions that can kill the bacteria without the need for antibiotics or other drugs. "Right now you have to keep undressing the wound and checking for infections," says Mkandawire. "Smart dressings would allow you to keep the dressing on without disturbing the wound and still be well protected from the possibility of infection."

To carry out his studies Mkandawire uses the ACENET computer network to run complex algorithms before he puts his theories to laboratory testing. "We can enter in parameters like thermodynamic properties, reaction rates, the energy of interaction, type of interaction, and strength of the molecular bonding. It allows us to analyze what will occur over time. They are extremely complex calculations and they take a long time to run on the computer. ACENET speeds up the process and allows us to do a lot more in the limited time we have. It's a great resource."

MAKING A DIFFERENCE

CHARTING THE MECHANICS OF HUMAN AGING

Andrew Rutenberg has always had a keen interest in biology. The Dalhousie University physics professor says that he chose the field of physics because he loves the simple way that the discipline explains the world around us. But he is also applying his physics training to the study of biological systems.

Rutenberg began his exploration of biological systems by building computational models of bacteria – one celled organisms that he describes as "functional nanomachines." He spent years studying the mechanics of cell division, how bacteria moved proteins from inside to outside, and how parasitic phages kill their bacterial hosts. All are complicated processes that require spatial and time awareness, something that seemed difficult for such simple organisms to accomplish. "A bacterium doesn't have a brain", says Rutenberg. "A single cell doesn't have simple rulers or watches. We developed mathematical models for how those physical processes could work within a bacterial cell."

Today Rutenberg is concentrating his research on human biology. He's working with Ken Rockwood and Arnold Mitnitski, professors at the Dalhousie Faculty of Medicine, to develop a computational model of aging. Using the Frailty Index that was developed by Rockwood and Mitnitski, they try to better understand the mechanics of aging over a large statistical population by modelling conditions that affect the health and well-being of an aging population. Rutenberg and his ACENET Research Fellowship student Spencer Farrell have built their computational model using ACENET systems.

"WE USE MODELS TO TRY AND UNDERSTAND CAUSE AND EFFECT"

says Rutenburg "by adjusting the parameters we can understand how the parameters in the model change how the model behaves."

Farrell developed the algorithm that allows the model to run. He says computational power is the key to seamless operation of the model – something that the ACENET network is able to provide. "The model uses a lot of CPU time and storage space," he says. "We typically run 10 million samples for each set of parameters. It takes about an hour and generates about 50 gigabytes of information." That scale is the key to accuracy, according to Rutenberg.

"Biological systems are noisy, nonlinear and typically far from equilibrium. They're living systems and they're complex. While from our background in physics our impulse is to simplify them, you can only simplify so far before you lose all the interesting science. We simply can't make headway with complex mathematical models with pen and paper; we have to solve them computationally."

"*ACENET facilities provide what scientists need*," Rutenberg says. "*It's what almost everyone uses now*."

THE MATHEMATICS OF A BUMPY RIDE

Everyone who flies has experienced turbulence – that uncomfortable sensation of dropping and shaking that happens as an airplane flies through a mass of unstable air. It's always unpleasant, and can even be dangerous in some cases.

Scientists have struggled for a long time to understand and predict turbulence and its effect on aircraft, automobiles, buildings and other common objects, but its causes have largely remained a mystery. Now St. John's-based scientist Jahrul Alam is making inroads in the study of turbulence and he's using a lot of computational muscle to conduct his research. Alam is an associate professor of mathematics at Memorial University of Newfoundland and an expert in the field of atmospheric turbulence. "I try to characterize atmospheric turbulence mathematically," he says. To do that he's harnessing the computing power of ACENET, using a mathematical simulation model called adaptive wavelet large eddy simulation.

Turbulence is a complex process involving millions of tiny variables. To try and understand how it works Alam cuts his data down into atmospheric samples that measure 500 cubic meters in volume. "The smaller the sample the more accurately we can study the process, but turbulence has such huge degrees of freedom that we have to filter the data into manageable portions," he says. "We could never measure it if we broke it down into something like cubic centimetres, for example. The calculations would be too large."

One of the great enigmas about turbulence is the fact that there is so much of it in places like Atlantic Canada where the ground is often cold. It's one of the questions that Alam seeks to answer with his calculations. "We know that turbulence is created by heat rising from warm ground, but we don't really understand why it would be so intense in places where the ground is cold," he says. "Or at night." In regions with a cool ground, episodes of wind gusting often manifest as short turbulence bursts, making it even more complicated to measure and predict.

Varying ground conditions also add complexity to the study, says Alam. "When wind hits mountains, trees or buildings, turbulence is sometimes enhanced by the interaction."

Alam's research will ultimately have huge practical applications in fields such as airline safety, structural design and environmental science. With climate change, incidences of serious turbulence will increase, he says – particularly the headline-grabbing incidents that involve injured passengers, aircraft damage and emergency landings. "If we can understand turbulence, maybe we can learn to predict it more accurately so that aircraft can avoid it," says Alam.

ALAM'S RESEARCH WILL HAVE HUGE APPLICATIONS FOR AIRLINE SAFETY, STRUCTURAL DESIGN & ENVIRONMENTAL SCIENCE.

Alam says his study using wavelets and the ACENET computer network is unique and is producing some significant results. "These are techniques that very few people in the world are using," he says.

Climate change is also making Alam's work more pressing. "If we continue global warming, the incidences of atmospheric turbulence will increase," he says. At the same time, humans are constantly changing the surface of the planet by cutting down forests, building tall buildings and reengineering the ground. All of it has an impact on turbulence. "We need to understand it so that we can predict it and design better structures, and better aircraft and automobiles to deal with it."

MAKING MOLECULES DANCE

It's a revolutionary idea – a technique that could change the design of nuclear power plants. Mount Allison University scientist Khashayar Ghandi is experimenting with the possibility of converting nuclear radiation directly into electricity using gold nanoparticles that act as a sponge to soak up electrons. Currently nuclear reactors create electricity by heating steam to drive large dynamos. The conversion process Ghandi envisions would eliminate the steps required to convert the energy to thermal and then mechanical energy – increasing efficiency and decreasing costs.

Ghandi is an associate professor in chemistry & biochemistry and an associate of the physics department at Mount Allison. His research focuses on sustainable and environmentally friendly energy production methods, and chemical processes for industry. He is working with Atomic Energy of Canada Limited to study radiation produced in nuclear reactors, and with the Atomic Energy of France (a country that produces 75% of its electricity from nuclear power) to understand more about the safe storage of nuclear waste.

Ghandi and his team are also working on other green energy solutions, including the development of a process to use sunlight to create hydrogen – a potential storage system for solar energy that would make solar a practical main energy source even when the sun isn't shining.

Other projects include the development of nuclear shields that could lead to more effective radiation treatments for cancer. Ghandi is also experimenting with using specialized clay materials to compress atoms and molecules from three dimensions down to two – a process that has the potential of changing the properties of substances at a molecular level. "If you think about carbon atoms, a diamond is made of carbon atoms spread out into three dimensions," he says. "Graphite has the same atom in two dimensions." Because of the complexity of his work, Ghandi and his team often travel to facilities such as TRIUMF national laboratory in Vancouver, ISIS at the Rutherford Appleton Laboratory in the UK and JPARC in Japan to use particle accelerators, pulsed muon sources and other advanced technology. But much of his experimental work is conducted at Mount Allison, often requiring elaborate computer simulations, scientific mechanical design that also need computer design and simulations, spectroscopic and quantum mechanical simulations. Ghandi was one of the first users of the ACENET computer network, joining it shortly after it began. "ACENET is a very important resource for us and provides my research students with great opportunities," he says.

The computational power of the ACENET system allows Ghandi to construct elaborate chemical reaction models and test them mathematically before subjecting his ideas to real world testing in the lab. "We're dealing with lots of data and we have to do some heavy data crunching," he says. "By doing it this way it helps us to understand the chemistry that's at work and allows us to make predictions of how reactions are going to behave. That way we can design new materials to perform certain functions before we go to the lab. I always like to have some intuition and a mathematical model before I start."

Ghandi says his work is motivated by the need to develop cost-effective green energy systems, but another passion drives him as well. "The other works we do don't have a practical application at all," he says. "We do it for pure imagination. To increase our fundamental understanding of the way atoms and molecules behave. To watch them dance and to understand how this dance led to new physics and chemistry."

FREUD, JOYCE AND THE POWER OF BIG DATA

It doesn't take long for the audience to sense that "Unconscious in the Sistine Chapel" isn't a typical stage play. For one thing there are no props or scenery pieces. Instead, the backgrounds, including the elaborate artwork of the Sistine Chapel, are created using interactive projected lighting technology. A hologram of sorts.

As the play unfolds, the audience realizes that this is a conversation about the power and influence of big data, using big data processes to create the action.

David Clark, an Associate Professor of Media Arts at NSCAD University, is one of the creative minds behind the landmark play. "The play is an exploration of big data," he says. "It asks the question whether we can extract physical data from artifacts in history.

Clark is no stranger to this kind of production. His award-winning multimedia projects have appeared at venues including Sundance, the SIGGRAPH Computer Conference, Transmediale in Berlin, and the Museum of Moving Images in New York. But he admits that Unconscious in the Sistine Chapel is unlike anything he's worked on before. "There are a few things we're inventing," he says. "We're doing things like using interactive props. For example, when an actor picks up a pair of binoculars and starts scanning the horizon with them, the projection of what he is seeing can be seen by the audience."

At the core of the technology is the "holodeck" of the Sistine Chapel, an effect created using a networked eight projector array. The new technology also lights the actors with body position tracking technology. Daniel Oulton is the creative technologist and programmer who is designing the body position tracking technology.

The play is a piece of speculative fiction about a chance encounter in 1905 between psychoanalyst Sigmund Freud, author James Joyce and their companions in the Sistine Chapel.

The action is interspersed with scenes of two modern characters; Phoebe, an archivist with a romantic view of history, and Phil, an investor working on a project that uses virtual reality environments reconstructed by data mining to re-animate history. Through the course of the play, it becomes clear that the interaction between Freud and Joyce is a manifestation of Phil's project.

Michael MacKenzie is the author of Unconscious in the Sistine Chapel. "He's an early innovator of virtual technology in theater," says Clark. "My involvement began two summers ago when Michael workshopped the play. We started talking about using a large amount of technology to convey ideas about big data and history."

THE NEW TECHNOLOGY LIGHTS THE ACTORS WITH BODY POSITION TRACKING TECHNOLOGY.

ACENET is providing support for the project by sponsoring Unconscious in the Sistine Chapel through its Advanced Research Computing Sponsorship Program. The organization is also providing technical consultation to the project. "We were able to connect with the ACENET Data Cave at Saint Mary's," says Clark. "They provided a lot of technical advice."

The play will debut at the new Halifax Central Library's O'Regan Hall. The production has been designed specifically for the library space. "We've scaled O'Regan Hall to the dimensions of the Sistine Chapel," says Clark. "The challenge will be to develop the production for other theatre companies."

TAKING THE EARTH'S TEMPERATURE

The greenhouse effect is nothing new. In fact the phenomenon has been influencing the temperature of Earth for billions of years. The existence of carbon dioxide molecules in the atmosphere acts as a blanket, trapping heat and allowing Earth's temperature to remain warmer than it would be otherwise. But in the last 200 years, human activity has been adding greenhouse gases into the atmosphere at rates exceeding any natural process, making the carbon dioxide blanket thicker and warming Earth even more.

As the planet warms up, most of the additional energy from the enhanced greenhouse effect is stored in the ocean – about 93% in total. The rest is distributed among the continents, in the frozen ices known as the cryosphere, and in the atmosphere.

Dr. Hugo Beltrami is a professor at the Climate & Atmospheric Sciences Institute, the Environmental Sciences Program at St. Francis Xavier University and a new Canada Research Chair in Climate Dynamics. He and his graduate students conduct research in the area of global-scale climate change. They are using geothermal data obtained from mining exploration boreholes, reaching deep into the ground to study the changes of the temperature at the continental surface during the last millennium. It's a complicated process. "We have to go down about 500 metres just to measure the remnants of past ground surface temperature changes that occurred in the last millennium," he says. "If we want to estimate changes further in the past, we have to go much deeper."

Beltrami's research is attempting to measure how much energy is stored in the ground and also how energy is distributed between the ground and the atmosphere. It's critical information for environmentalists, policy makers, planners and scientists. As the ground becomes warmer, more carbon dioxide is released from soils, increasing the atmospheric concentration of greenhouse gases.

WE ARE STUDYING TEMPERATURES AT THE CONTINENTAL SURFACE OF THE EARTH OVER THE LAST MILLENNIUM

Another aspect of Beltrami's work relates to regional climate modelling. For example, he and his graduate students have conducted extensive research to project the potential effects of climate change on the propagation of the tick that carries Lyme disease in Nova Scotia and Ontario. He is also developing a climate services centre that will translate global climate model predictions into information that is useful at a local level. The information would allow individual municipalities to access local climate projections, increasing awareness of the potential consequences of climate change on things like infrastructure and public health. The service may also help to support the development of policies to build resilience and mitigate the societal impacts of a changing regional climate.

Every part of Beltrami's research requires his team to use intensive numerical modelling. The numbers are huge and the calculations would be impossible to run on a regular computer. He's been a user of ACENET since the program started. "ACENET is an essential resource for us," he says.

SOFTWARE TOOLS FOR SCIENTIFIC RESEARCHERS

Paul Muir's research has focused on developing software

to help scientists accomplish their goals. Muir is a professor in the Department of Mathematics and Computing Science at Saint Mary's University. He is the co-author of a number of software packages including MIRKDC, BVP_SOLVER, EPDCOL, BACOL, BACOLR, and the new BACOLI – software that can be applied in analyzing complex systems in a variety of scientific fields. Over his career he has worked with researchers on computer based projects in fields such as fibre optics, genetics, computational finance, and on applications such as blast dynamics, epidemiology and pharmacokinetics.

"Computational work is now a major part of what is being done by people in the sciences," he says. "At the same time they're collecting a lot of data. My research involves the development of software tools to help scientists solve complex mathematical models that arise in their research. I am also interested in efforts to help scientists better manage computer based workflow in their research."

One of Muir's most recent investigations involved simulating the growth of brain tumours. The project started out as a test challenge for Muir and his ACENET summer student Alex MacKenzie and the BACOLI solver. "We didn't develop the model, but we were interested to see how well our software would work in solving the model," says Muir. One of the challenges is that a brain tumour grows at a different rate in the white and grey matter regions of the brain. "We developed a different representation for the rate of diffusion of the tumour that allowed for a sharp but continuous transition between the regions, and successfully applied our software to this modified model."

Muir says that while some people have the perception that computer simulations are highly accurate, this is not necessarily the case. There are always computational errors and it is important to deal with them using software that provides adaptive error control. It's a perception that Muir works hard to try to change. "It's my mantra – for accurate and efficient computations you have to use software that adapts the computation on-the-fly to attempt to control some estimate of the error. This improves both the accuracy and efficiency of the computation."

Muir and MacKenzie also worked with the Saint Mary's ACENET Data Cave – a powerful three dimensional immersive environment designed for visualizing data. The goal was to make the cave more accessible to scientists who might not be comfortable using complex software. "Alex developed new software tools that sit on top of the cave software already available – software that can make the facility more accessible to scientists who do not have a strong programming background," says Muir.

Muir is enthusiastic about the efforts of Software Carpentry (http://software-carpentry.org), an organization that teaches computing skills to help researchers in science, engineering, medicine, and related disciplines. He has recently organized two Software Carpentry boot camps at Saint Mary's; ACENET co-hosted the sessions and also provided resource support to help with the workshops. The boot camps teach researchers how to better manage the computer-based workflow in their lives. "There are great computational tools out there." he says. "But if scientists don't know how to use these tools, they're missing out on a lot of potential scientific advancement."

PREDICTING THE INFLUENCE OF THE OCEAN ON MACHINES AND STRUCTURES

Understanding how machines and structures perform in the ocean has important implications for everything from the way ships manoeuver to how tidal power turbines respond to massive hydraulic forces. One University of New Brunswick scientist is working hard to increase that understanding and he's employing some powerful computational tools.

Andrew Gerber is a professor of mechanical engineering at UNB. He's an expert in the field of computational fluid dynamics (CFD) and high performance computing, a discipline that focuses on solving the equations that govern fluid movement using supercomputers. Supercomputers are needed to study in detail how ocean turbulent fluid motion interacts with machines and structures situated within it. Oceans are extremely demanding environments. For man-made systems to survive requires detailed understanding, something that supercomputer simulations can provide.

Gerber is involved with a number of important projects including a tidal power study in the Bay of Fundy and a project with Defence Research and Development Canada to study the performance of Canadian naval submarines.

"We do a lot of work with submarines," says Gerber. "We simulate extreme manoeuvers on the computer to see what's happening to the forces and moments acting on the body of the submarine as it moves through the water. It's very expensive for the navy to do experiments of this type so our simulations allow them to make predictions without the need for extensive experimentation".

Gerber's work with tidal power focuses on making detailed fluid flow predictions to support tidal power turbine deployments in the Bay of Fundy. He and his colleagues at UNB are working with the Fundy Ocean Research Centre for Energy (FORCE), and with researchers at Acadia University and Dalhousie University, to measure tidal flow and energy potential in the Minas Passage near Parrsboro and in Grand Passage at Brier Island, Nova Scotia. This work will have a huge impact on where turbine arrays are deployed considering issues such as survivability and maximizing power output.

The tidal study involves huge volumes of water requiring complex calculations. Twice each day 10 cubic kilometers of seawater are forced through the Minas Passage – 10 billion tons of water that represent an outflow more than 40 times the amount that flows from the Saint Lawrence River over the same period of time. With technical support from ACENET and funding from the Canada Foundation for Innovation, Gerber set up a "contributed system," a computer cluster operated by Gerber's UNB laboratory and managed by ACENET. Under the system, any unused cycles are turned over to ACENET for other researchers to use. The system is powered by the latest Graphical Processing Unit (GPU) hardware, and combined with a CFD simulation software (EXN/Aero) that can efficiently utilize the new hardware, the complex tidal simulations can be completed much more rapidly with high-resolution.

In addition to his work at UNB, Gerber is also a partner in a spinoff company called Envenio Inc., a Fredericton-based firm that provides computational fluid mechanics services and engineering software development to engineers and companies. Its flagship product is EXN/Aero, which is specifically designed for next generation hardware.

Gerber says that as climate change becomes more prevalent, understanding the movements of fluids in the oceans and atmosphere and their impact on infrastructure will become crucial. "One of the goals of Envenio is to help engineers build better designs for extreme weather events in the ocean or atmosphere and to provide the computational tools to do so."

THE PHYSICS OF FOX MOVEMENT IN COMPLEX LANDSCAPES

Sheldon Opps recalls watching a large silver fox from the window of his Prince Edward Island home last winter. The fox in question was navigating the urban sidewalk, maneuvering around high snowbanks, even pausing to check for traffic before crossing the street. "He was tracing a path just like a human would," Opps says. "He was very comfortable in his urban environment."

Opps spends a lot of time thinking about urban foxes. The University of Prince Edward Island physics professor has been conducting an ongoing study of fox movement patterns within highly fragmented habitats such as urban Charlottetown. But Opps is not a biologist. He's an expert in the field of soft condensed matter physics, where he applies the tools of statistical physics to study a variety of biologically relevant physical systems, including liquids, colloids, foams, gels and biological tissues. The interest in fox behaviour came via his wife Marina Silva-Opps, a biologist at UPEI, and from his interest in applying the methods of computational and statistical physics to study other complex systems – such as animal movement.

The life of a fox in Charlottetown is fraught with challenges. Along with the typical dangers that a city presents – traffic, hostile dogs and homeowners, a lack of natural food sources – the animals must deal with ever increasing habitat fragmentation that breaks up their traditional hunting grounds. Opps is studying what that fragmentation means for both foxes and humans.

Habitat fragmentation is having some unusual effects on the highly adaptive fox population. For one thing, the animals are quickly becoming semi-domesticated as homeowners feed them and even give them names in many cases. "We're seeing the same patterns happening that we believe led to the domestication of dogs thousands of years ago," says Opps. According to the current theory, wild wolves began living in close proximity to humans in the Palaeolithic age to take advantage of their hunting leftovers, eventually becoming domesticated by the process. "The conjecture is that in 50 or 100 years, if this continues, foxes could become domesticated here in Charlottetown as they have in other areas in the world, such as Russia".

Patrick Strongman is a physics undergraduate student at UPEI and an ACENET fellowship holder who is working with Opps on the fox project. As part of his research project, Strongman developed the algorithm used to track fox movements and identify cluster points where animals gathered.

The algorithm compiled hundreds of data points including individual fox movements, distances travelled, velocity and GPS information, and used the data to run simulations of fox movements based on changing urban conditions. Strongman says the ACENET computer network was key to the project. "It cut down to a few hours what would have normally taken weeks to complete," he says.

THE LIFE OF A FOX IN CHARLOTTETOWN IS FRAUGHT WITH CHALLENGES.

Opps admits that fox habitat is an unusual subject for a physicist to be studying – particularly one trained in theoretical disciplines such as quantum mechanics and statistical physics. But he says it's not really such a big stretch. "Like any physicist I'm a problem solver," he says. "Physicists are usually busy looking across time and space or peering down into the realm of quantum mechanics. But just as a telescope looks back into time to study the beginnings of the universe, a study like this can unlock the secrets of how life evolved over time. Everything is interconnected. Humans and foxes are all a part of an evolving universe."

FINANCIALS

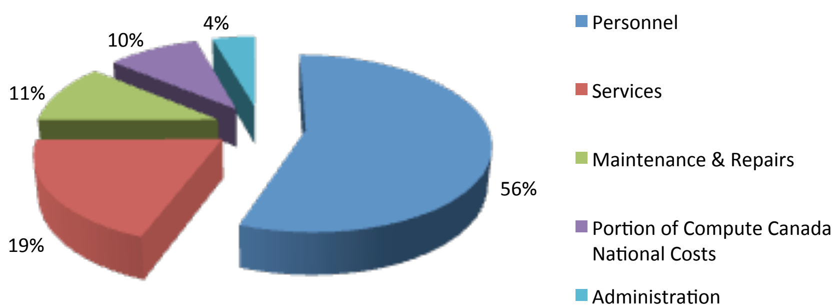
Financial Summary Report

April 1, 2015 - March 31, 2016

Revenue	Amounts
Provincial Agencies (NSRIT-NS, RDC-NL, NBIF-NB)	$1,143,234
CFI	$1,018,917
Institutions	$385,143
Total Revenue	**$2,547,294**

Expenses	Amounts
Personnel	$1,416,934
Services	$491,029
Maintenance	$281,642
Portion of Compute Canada National Costs	$244,283
Administration	$113,406
Total Expenses	**$2,547,294**

Expenses 2015 - 2016



Fellowship and Sponsorship Awards Committed

Research Fellowships 2015-2016	$250,000
Sponsorship 2015-2016	$10,000

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