ACENET ANNUAL REPORT 2022-23



Accelerating Innovation

ACENET HH-2037 Henrietta Harvey Memorial University St. John's NL, A1C 5S7 admin@ace-net.ca

A regional partner of the

Digital Research Alliance of Canada Partenaire régional de l'

Alliance de recherche numérique du Canada

Table of Contents

Message from our Chair and CEO	3
Our Community	6
Resource Demand	10
Skills Development	14
Serving Atlantic Canada	18
Financials	20
Acknowledgements	22
Partners	23

Research Spotlights

Sid Ahmed Selouani, l'Université de Moncton, L'Intelligence artificielle au service de l'interaction humain-système	4
Peter Lelievre, Mount Allison University, Preparing for Climate Change Effects with Geophysics	5
Shah Razul, St. Francis Xavier University, Preventing Freezer Burn and Saving Human Tissue	8
Josh MacFadyen, University of Prince Edward Island, Digitizing History	9
Erin Johnson, Dalhousie University, A Prize-Winning User	12
Xianta Jiang, Memorial University, Machine-learning: Making Connections Between the Brain and the Body	13
Tim Frasier, Saint Mary's University, From Megabytes to Megafauna: Driving Whale Conservation to new Depths with HPC	16
Chérif Matta and Lázaro Castanedo, Mount Saint Vincent University and Saint Mary's University, Quantum Chemistry of Molecular Evolution	17
Trishla Shah, Nova Scotia Community College, Making Data Meaningful	21

Message from Chair and CEO

On behalf of ACENET's staff and Board of Directors, we are pleased to provide you with our Annual Report. This report offers an overview of our activities over the past year, provides insight into our measures of success, and through our *Research Spotlights*, introduces you to some of the remarkable research we proudly support.

This past year was one of transition, evolution, and growth for ACENET.

We welcomed our new national organization and federal funder, the Digital Research Alliance of Canada, and made significant contributions to its successful Multi-Year Funding Proposal to ISED, providing the next two years of Digital Research Infrastructure operational and capital funding in Canada.

We were delighted to welcome Université de Moncton to our Atlantic consortium, and Dr. Francis LeBlanc, its Associate Vice President (Research), to our Board of Directors. Their expertise will undoubtedly enrich our governance and planning, especially as we strengthen our regional support of AI and Machine Learning (ML). In fact, ACENET will soon be hosting a new staff member at Université de Moncton, specializing in the support of these cutting-edge technologies.

ACENET's capacity grew substantially this past year as we welcomed six new staff members, adding new experience, skills, and perspectives to our team. Four of these roles were made possible through a new partnership with techNL. Through their *Find Your Future in Tech* initiative, ACENET will be developing and delivering a new Certificate in Advanced Computing, providing job-ready digital skills to learners in Newfoundland & Labrador. With this first experience under our belt, we aim to later expand availability to all of Atlantic Canada.

The techNL initiative gets underway just as we've completed our most successful training year ever. In 2022-23, ACENET delivered 256 hours of training across 65 separate training events. This resulted in nearly 7000 learner-hours of skills development in computing, programming, AI/ML, data management, and scientific visualization provided to learners coming from academia, industry, government, and the not-for-profit sector. This training not only fuels the research groups making discoveries in our colleges and universities, but contributes to the highly-skilled digital workforce driving our region's economy.

ACENET has continued to promote the power of advanced computing to industry R&D. This past year, we welcomed new industry clients, had our first graduate of our JumpStart for Start-ups initiative, collaborated with companies in the curriculum development for our advanced computing certificate, and worked with partners in the innovation ecosystem to encourage the adoption of advanced technologies in R&D.

None of this would be possible without the contributions of our funding partners and stakeholders. Your partnership, collaboration and advice have played a pivotal role in shaping our strategies, pushing our boundaries, and driving our success. We remain deeply grateful for your support and continued commitment to accelerating research and innovation in Atlantic Canada.

Sincerely,

Dr. Tana Allen Chair, ACENET Board of Directors **Greg Lukeman** Chief Executive Officer, ACENET







L'Intelligence Artificielle au service de l'interaction humain-système

Alors que les débats éthiques font rage sur le rôle de l'intelligence artificielle en art et dans l'aide aux devoirs pour les élèves, Sid Ahmed Selouani se concentre plutôt à développer des applications industrielles et améliorer la qualité de vie des gens.

Avec son Laboratoire de Recherche en Interaction Humain-Système (LARIHS), au campus de Shippagan de l'Université de Moncton, il utilise l'apprentissage automatique pour faire progresser l'interaction humain-système, avec des sujets aussi variés que la reconnaissance des émotions, de la parole pathologique et du langage, l'automatisation de la télépathologie et l'assistance intelligente aux robots industriels.

Sid Ahmed Selouani l'Université de Moncton L'intelligence artificielle L'apprentissage automatique dans les systèmes cyber-physiques, c'est-à-dire les systèmes qui intègrent des composants physiques et numériques, s'appuie sur des algorithmes complexes pour prendre des décisions et s'engager dans des actions dans le monde réel.

« Si je veux, par exemple, aider une personne qui a des difficultés à prononcer des mots, dit Selouani, suite à un accident vasculaire cérébral, par exemple, et elle ne peut prononcer que des bribes de mots, on intervient avec des algorithmes qui permettent de comprendre

comment la personne s'exprime et qui remplacent certains mots ou segments défectueux pour générer du texte ». Tel est l'objectif d'une entreprise fondée sur les recherches du LARIHS : commercialiser un logiciel qui fournit aux personnes souffrant de troubles d'élocution un interprète pour les aider à communiquer. Il pourra même générer un son dont la tonalité est proche de celle de la personne concernée. Le logiciel aidera également les médecins à suivre les patientes et patients, à voir leur évolution et à faire la rééducation.

Cependant, pour qu'un algorithme puisse discerner des paroles inintelligibles, il doit d'abord acquérir de l'expérience à écouter les humains parler. Cela nécessite énormément de données, d'analyses et de comparaisons, parfois même des millions de paramètres. Il faut alors des systèmes de superordinateurs de pointe, comme ceux fournis par ACENET et l'Alliance de recherche numérique du Canada, pour donner à l'algorithme la puissance de traitement et la capacité de stockage nécessaires pour effectuer les calculs requis. « Notre capacité de calcul a augmenté de 10 à 15 fois avec ACENET », précise-t-il.

Une telle puissance de traitement présente plusieurs avenues de recherche. Selouani et son équipe d'une vingtaine de personnes composée de post-doctorants, d'étudiantes et d'étudiants de tous les cycles et de personnel de recherche qui ont de nombreux projets en cours, chacun avec ses propres sous-projets.

LARIHS travaille, par exemple, sur un projet visant à apprendre aux robots industriels à trier les huîtres. Leurs algorithmes peuvent leur permettre de distinguer les huîtres vivantes des mortes et sélectionner les calibres désirés. Le laboratoire travaille également à l'optimisation des chaînes télépathologiques, c'est-à-dire la classification des tissus et des échantillons biologiques humains à distance. En traitant les images extraites d'analyses de biopsies, nous pourrons mieux détecter les anomalies dans les images numérisées, ce qui aiderait ainsi les médecins dans leurs évaluations.

Les possibilités d'application semblent innombrables. Alors, comment faire tenir tout cela dans un seul laboratoire ? « Notre savoir-faire, explique-t-il, que nous avons développé durant les 20 dernières années, est que nous sommes capables d'utiliser des algorithmes que nous avons développés pour une application afin de les adapter à une autre. »

Preparing for Climate Change Effects with Geophysics

As climate change causes ever increasing fears of flooding, Dr. Peter Lelievre's work in geophysical imaging becomes ever more important in the province of New Brunswick and beyond.

An assistant professor in Mount Allison University's department of mathematics and computer science, Dr. Lelievre is an applied geophysicist who images what's underground. Earlier in his career, that pursuit was tied to mineral exploration or "trying to help people find the materials such as metals that our society uses for basic building materials." More recently, he's become interested in imaging and understanding what happens with flood infrastructure.

"With climate change and rising sea levels, we need to understand more about how water moves through these flood barriers," Lelievre explains. "Geophysical imaging can help us better understand these things, and also to try and find any erosional issues that could cause a breach."



Peter Lelievre Mount Allison University Geophysics

Lelievre walks on the fields and marshes near Sackville, N.B. — which are the same places his research now takes place. Being at Mount Allison means he's surrounded by the dyke land and he, his wife, and his dog walk on it frequently.

"It's far more at the forefront of my mind in my daily life," he says. "It's been really nice to be able to shift and connect my research to that part of the local community and my daily life."

Lelievre uses tools that measure electrical and electromagnetic fields and then he uses heavy mathematical methods and computational power to process the data.

"We run the data through these algorithms that we develop and this creates an image of what's underground," he says of his use of the Digital Research Alliance of Canada's high performance computing tools. "That's where the heavy computational part fits in. These are tremendously large computational problems."

For his heavier research, an imaging task could require 600 CPUs, consume roughly two terabytes of memory and take over four days to finish. He and his research team use the modern Fortran programming language and create their own software to process their electrical and electromagnetic data and generate images of the Earth.

With the help of his students, postdocs and colleagues, he develops data processing methods that could be used in the field, and he collects field data to help test those methods.

"Eventually we'd like to be able to create data processing methods we can use in the field on a laptop, and so you'd just have a small, everyday laptop, where you get a result in effectively real time," he says, and adds that the history of computing tells us that could well happen in the near future.

A single imaging task could require 600 CPUs, consume roughly two terabytes of memory and take over four days to finish.

Our Community

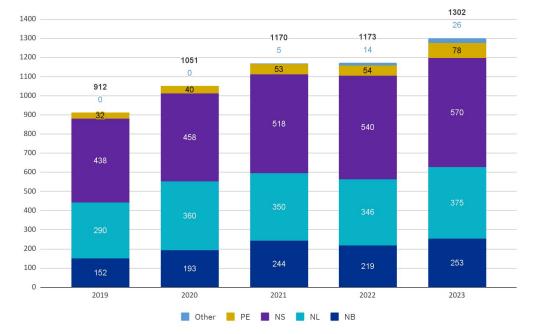
ACENET supports almost 400 research and innovation groups across the Atlantic region, with a total of 1300 users.

Over the past five years, ACENET's total client base has grown 43%, with the number of research groups growing 28%. The most significant five-year growth has been seen on PEI, which has more than doubled its number of users, followed by New Brunswick with 66% growth since 2019.

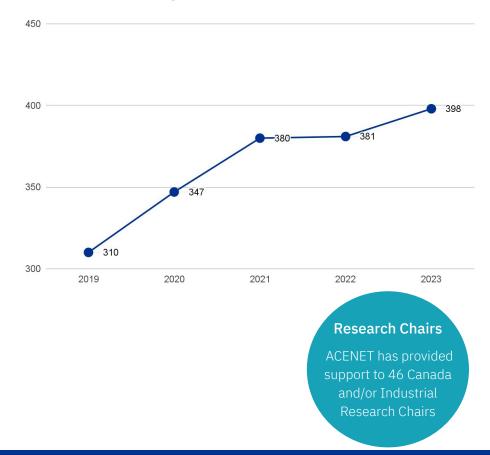
2022-23 User Growth

NB	16%
UNI 	1070
NL	8%
NS	6%
PE	44%
Other	86%
Total	11%

Number of Users in Atlantic Canada



Total Principal Investigators



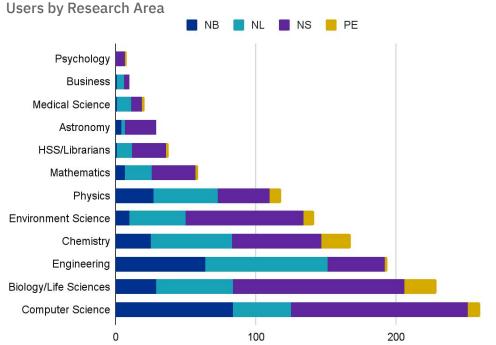
New Brunswick

64% of our NB clients are based at UNB, 29% at Université de Moncton, and 8% at Mount Allison University. No

Nova Scotia

72% of our NS clients are based at Dalhousie, 14% at St. FX and 8% at Saint Mary's.

Our Community



Growing Humanities and Social Sciences Usage

Over the last number of years, we've seen a shift in research disciplines using digital research tools. Where advanced computing in Atlantic Canada was traditionally the domain of chemistry, environmental science and physics, we've more recently seen biology, engineering, and - driven by AI/ML - computer science increasingly leverage these resources in their research. (Check out computer science's usage of GPU on page 10!)

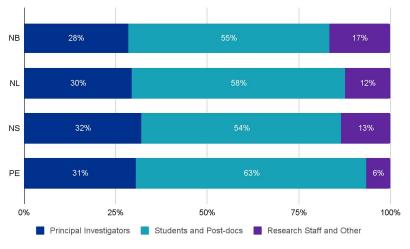
The humanities and social sciences (HSS) community is a newer user of advanced digital tools, and deserves a special mention. ACENET's support team has observed that demand for services from this group is growing substantially.

However, their needs frequently do not include HPC systems, and therefore researchers don't always become account holders on the national infrastructure and don't get included in our user numbers. HSS needs do, however, fall outside the technology platforms and assistance provided by most institutional IT services. Examples include the use of GIS analytical platforms, web scraping tools, other analytical software, and research data management. ACENET and its federation partners support these growing needs by hosting platforms, by teaching the needed skills to the HSS community and by providing consulting and guidance in technology aspects of projects.

Client Satisfaction

In the 2022 annual spring Alliance account renewal survey, Atlantic researchers rated the advanced computing resources available an average of 4.2 out of 5, the services provided 4 and their overall satisfaction 4.3.

Help desk ticket satisfaction surveys found that 89% of Atlantic researchers found the help desk excellent in the timeliness of its response, 86% rated the solution provided as excellent and 92% rated overall helpfulness as excellent (based on rating options of poor, adequate, good and excellent).



User Roles by Province

The majority of the users of our systems are students and postdocs, underscoring ACENET's important role in training Atlantic Canada's future labour force.



Shah Razul St. Francis Xavier University Chemistry

Preventing Freezer Burn and Saving Human Tissue

It sounds simple, but Shah Razul's work involves trying to understand what water molecules do when they get to below zero degrees Celsius because the possibilities that understanding offers could be life-changing.

When water crystallizes, its volume increases and it forms a regular structure that destroys, for example, cells, or, in the case of an organism, its delicate membranes and systems. As most of us will know, when food is frozen and we leave it too long, the ice separates out, leaving the food "freezer burned." A wasted chicken breast is one thing, but this problem also exists, for example, in cryopreservation of cells, tissues and organs.

"When water is in a close-to-frozen state, it exhibits some interesting behaviour," says Razul, an associate professor of chemistry at St. Francis Xavier University. "We're trying to understand what the water molecules are doing."

Razul's overarching goal is to find a way to keep water from forming crystals, and then apply that learning to real-world problems in areas such as food and health care.

"If we can, we can solve many problems related to freezing," he says, including, for example, potentially creating environmentally safer antifreeze products to replace or minimize the use of road salt.

He looks to creatures such as the wood frog, which uses glucose to stop the freezing process from destroying its tissues in winter. Razul therefore, is running simulations to look at the process of freezing and analyze what water molecules are doing in the fractions of a second just before they form crystals and freeze.

"A lot of my work now is involved with understanding how small biomolecules, such as different kinds of sugars and salts, stop water from freezing or slow down the process," he says, adding that he wants to figure out a biomolecular combination that would achieve this goal.

Over the past five years, he's been using computational principles to develop a cryoprotectant to preserve lobster meat. "We've tried it and it works," he says, adding that some companies from overseas are testing his system currently. "We had a taste test in Atlantic Canada, and we've published a couple of studies where the public indicated that it tastes as if it was cooked yesterday, preferring it to frozen lobster meat that is sold currently."

His next frontier is looking at the ways in which his process can preserve muscle cells and brain cells to see what kind of applications it might have in the healthcare field.

"No one has a definitive answer to how these cryoprotectants work at the molecular level," he says. "It's basically all trial and error. We try a little bit of this and a little bit of that and see whether it works."

To do his work, he's watching the behaviour of water in minute detail — fractions of seconds — and then he replicates the test multiple times. "Because of that, I generate a lot of data," he says, and that's why he couldn't do his work without ACENET's high performance computing.

"It's almost impossible to do this work without ACENET," he says. "I would need a year and a half to do it sequentially as opposed to one month with ACENET."

Digitizing History

Josh MacFadyen is the first MacFadyen in several centuries not to farm. And that, in a sense, is what's led to his life's work as an associate professor in the Applied Communication, Leadership and Culture (ACLC) program at the University of Prince Edward Island and a Canada Research Chair (Tier II) in geospatial humanities.

MacFadyen studies the environmental history of Canada, with a focus on Atlantic Canada. He's specifically interested in food systems and how humans, and even animals, have fed themselves over time and how they stayed warm in a world before fossil fuels.

"And that could have some applications for how we might right things going forward," he says, referring to perhaps novel ways to tackle climate change by learning from the past.

MacFadyen was trained as an historian, but over time, because he was using a lot of technology in his work, he became a digital historian.

"Digital historian is just a fancy way of saying we use spatial analysis, geographic information systems, and other digital tools related to large datasets such as historical Censuses to understand questions of how general land use and energy systems have changed, and how we've arrived at the modern world," he says.



Josh MacFadyen University of Prince Edward Island

> Applied Communication, Leadership and Culture

He says Atlantic Canada is the right place to be for his studies as it still has large areas that are predominantly agricultural, though that is gradually changing. For example, the move away from farming isn't limited to his family. In fact, it's long been a trend on the island, which has seen a 20 per cent decrease in farmland in the last 20 years. It's a fact he's considering in his field of study.

He uses Census data to get a granular look at such trends and he uses remote sensing — everything from aerial photos and satellite, to light detection and ranging (LiDAR) — to dig deeper.

"The sources I've been able to use most consistently are aerial photos — we've got the whole province covered right back to 1935," he says, and adds that he has used that data to develop products that would be useful to historians. His current is a portal for exploring maps, atlases, aerial photos and geospatial data related to the history of Prince Edward Island that resides at projects.upei.ca/geolab.

To develop these tools, MacFadyen has used the services of the Digital Research Alliance of Canada through ACENET by participating in workshops and training modules for the humanities and social sciences.

"They're just tremendous," he says of the workshops and networking. "I just thought 'Wow, what a great way to join this regional, highly skilled and very active group of people who are trying to create resources for the humanities and social sciences in Atlantic Canadian universities.' They're offering these regular training modules, and some are specifically for us."

"I just thought 'Wow, what a great way to join this regional, highly skilled and very active group of people who are trying to create resources for the humanities and social sciences in Atlantic Canadian universities.' They're offering these regular training modules, and some are specifically for us."

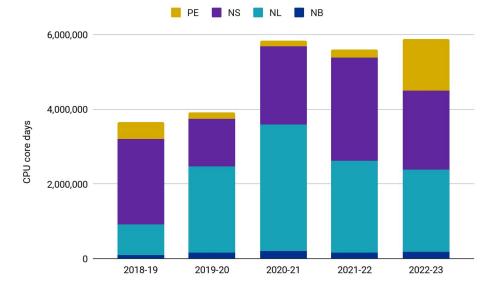
Resource Demand

ACENET supported over 1300 users in Atlantic Canada use 5,894,868 CPU days and 38,965 GPU days in 2022-23. The combined value of these resources is over **\$9.4 million** based on commercial pricing for ACENET's Siku system.

Usage has grown over the last 5 years but is constrained by the amount of resources available. No new national systems have been added since 2021.

Province	CPU core-days	GPU-days	Value
NB	174,033	12,920	\$ 772,380
NL	2,221,487	13,693	\$ 3,507,477
NS	2,124,767	10,251	\$ 3,235,251
PE	1,374,581	2,100	\$ 1,902,655
TOTAL	5,894,868	38,965	\$ 9,417,764

Annual CPU Usage by Province



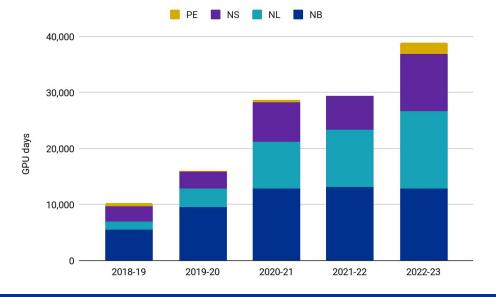
PEI Growing

This past year, PEI used almost 40% more CPU compute cycles than the previous four years combined, and in June through September, almost as much as the other Atlantic provinces combined.

Usage by Research Area

Researchers in Physics and Chemistry continue to be the largest consumers of compute resources, together using 64% of Atlantic CPU time and 26% of GPU time. Thanks to increasing AI/ML research, we see the most GPU demand coming from Computer Science researchers, who used 63% of the Atlantic GPU time consumed in 2022-23. Due to AI/ML, Computer Science researchers represent our largest user growth over the last 5 years.

Annual GPU Usage by Province



Resource Demand

Annual National Resource Allocation Competition (RAC)

Annually, the Digital Research Alliance of Canada runs a peer-reviewed competition for researchers requiring resources beyond the default they're allotted with an account. With demand for resources continuing to exceed capacity, nationally RAC 2023 was able to meet 47% of all of the CPU requested (7% less than 2022) and 20% of the GPU requested (4% less that 2022).

The competition received 28 applications from Atlantic Canada, and awarded 42% of the CPU requested and 8% of the GPU requested.

	NB	NL	NS	PE	Total	% of Request Approved
Number of applications	1	9	18	0	28	
Compute Years	0	3468	6510	0	9978	42%
Graphical Processing Units Year (GPUs)	70	10	30	0	110	8%
Cloud (vCPU) Years	0	16	762	0	778	100%
Storage (TBs)	40	825	2907	0	3772	75%
Cloud Storage (TBs)	0	8.3	106	0	114	100%

Integrated Infrastructure

ACENET continues to offer its well-received infrastructure integration services, where researchers receiving funding from the Canada Foundation for Innovation (CFI) and other sources intending to buy advanced computing infrastructure, can have these resources integrated into ACENET's Siku system.

Through this service, ACENET provides the researcher with architecture advice, procurement support, professional system management, and access to a larger system than if their resources were hosted in isolation.

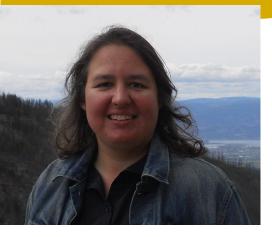
Researcher's contributed infrastructure is provided to them on a top-priority basis, but is able to be used by the rest of Siku users when not in use by the project, maximizing the value of public investments. Through these integrations across Atlantic Canada, our Siku system has grown from 2000 cores in 2019 to over 8000 cores in 2023. This represents an additional investment of **\$2.5 million** in Atlantic Canadian digital research infrastructure.

Commercial Cloud

There is growing recognition that commercial cloud has advantages for certain workloads and researcher needs. ACENET is working with major cloud providers (AWS and Google Cloud Platform) to identify suitable pilot projects to better understand the capabilities and limitations of the public cloud in an Atlantic DRI landscape.

	NB	NL	NS	PE	Total
Integrated projects	2	1	7	2	12
Total value integrated	\$ 91,298	\$ 431,276	\$1,764,948	\$172,198	\$2,459,720

Installed in late 2019, ACENET's Siku (meaning "sea ice" in Inuktitut) cluster was funded in large part by the Atlantic Canada Opportunities Agency (ACOA) with the intention of generating regional economic benefits through industry engagement, while recognizing the important work that ACENET does for academic research in the region.



Erin Johnson Dalhousie University Chemistry

A Prize-Winning User

Erin Johnson wouldn't have won the prestigious Steacie Prize, awarded to early-career scientists, in 2021, without the Digital Research Alliance of Canada's high performance computing and the services of ACENET.

"That's a completely fair statement," says Johnson, who was an early adopter of high performance computing, dating back to her student days at Carleton University, Queen's University and Dalhousie University, as well as her postdoctoral work at Duke University. She's now a professor and Herzberg-Becke Chair in Theoretical Chemistry at Dalhousie University.

Asked how she would explain her job to a guest at a cocktail party, Johnson says she studies intermolecular interactions within the materials all around us.

"These are the weaker interactions between molecules as opposed to the stronger bonds within a molecule," Johnson explains. "So, we would, for example, at a cocktail party look at the interactions in beer or wine in a glass — those types of interactions within a liquid or a gas or within a molecular crystal."

She does this to predict such properties as reactivity, hardness, and conductivity, among others.

"Any chemical observable is something that we can predict through this type of modelling," she says.

Johnson's lab, however, might surprise those who envision her working in a chemistry lab full of beakers and bunsen burners. Rather, it's a computer lab from which she's developed methods for modelling that are some of the most accurate and efficient available. It was those methods that won her the Steacie Prize.

"We then take those methods and apply them to problems in chemistry," she explains. "One of the particular problems we're focusing on is the problem of molecular crystal structure prediction or how molecules would come together to form a 3D solid."

She likened the ways molecules come together to the ways in which Lego bricks do. "There are many ways you could conceive of molecules coming and packing together, but not all of those are going to be stable," she says. "So the challenge is trying to predict how they will actually pack in a solid."

Once you solve that puzzle, there are applications across several industries, one of the most recognizable being pharmaceuticals.

"If you are producing a drug and you want it in pill form, you want a solid but soluble state," Johnson says. "When you try to formulate new drugs, you want to screen for all the possible polymorphs (transformations to another form) and find out which ones are the most stable. What you don't want is for it to easily form a particular polymorph that's not a very stable one and then change over time so that it's no longer soluble."

These methods also have applications for electronics, but instead of looking at solubility, the property of interest would be conductivity.

"Like the solubility, the ability of charge to flow through a material is also dependent on the particular polymorph" Johnson explains. "You can think of many applications where the different solid state properties between polymorphs would affect whether a material was promising or not."

Johnson says her work would be "completely impossible" without ACENET's services.

Machine Learning: Connecting the Brain to the Body

Xianta Jiang uses machine learning and wearable-sensor technology to study how the brain works in telling the body what to do and how to move. Currently, he's using these techniques to solve a healthcare problem for those who have prosthetic hands. But he doesn't work in a hospital setting; rather, he works in a computer lab.

A professor of computer science at Memorial University, Jiang works with a team of students to study all of the different ways humans use their hands. With that information, they'll use machine learning to help those who wear prosthetics control them.

"Controlling the prosthetic hand is a super difficult problem to solve, because when a human's hand is amputated, the brain has a harder time communicating to the arm about how to maneuver the prosthetic limb," Jiang says. "We are trying to help people control them as naturally as possible, and without surgery. To try to solve the problem, we use muscular sensors attached to a part of the arm to infer movement intentions from the area of the brain used to control the hand."

However, it's difficult to make the connections that allows the brain to send the right signals to the hand.

"For that, we attach a camera to the prosthetic and when the camera can identity the target, the hand can configure correspondingly – just like self-driving," he says.

That's the hands-on part of the research, but, in the end, much of the work is done by his students in a computer lab using the high performance computing resources of the Digital Research Alliance of Canada and ACENET. They identify the grasp types the prosthesis user will need and use computer modelling to fine-tune the fit.

"It's quite a basic question, but we need a lot of computing resources for it," he says. "We are working to cover 95 percent of daily life grasps with a total of 16 movements and need a lot of data to train this model, so we use high performance computing."

He said he couldn't do his work without ACENET's services. "It's not affordable to purchase the computing power we'd need," he says. "We need a lot of memory."

Another of Jiang's projects involves monitoring human activity using wearable devices such as smartwatches. The goal is to find a way to allow rehabilitation staff or sports coaches to monitor their patients' progress digitally.

This work is still in the early collaboration stage and not yet commercialized. "For this one, we'll collaborate with industry over the next few years," he says.



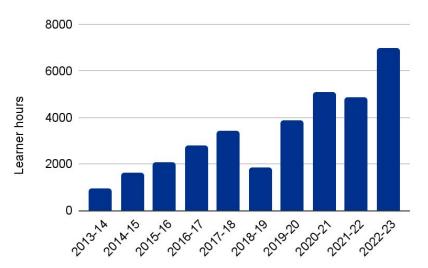


Xianta Jiang Memorial University Computer Science

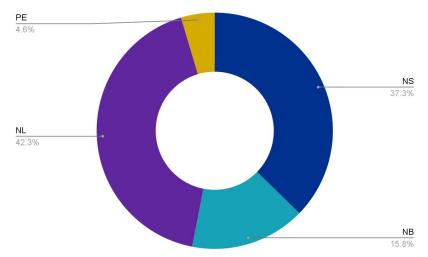
Skills Development

During the past year, ACENET delivered 256 hours of training through 65 events with almost 1800 participants for a total of **6957** learner hours*.

Training Delivered by Year



2022-23 Learner Hours by Province



"Meghan Landry, one of the two instructors, helped me realize what perplexed me because of her crystal-clear instruction and amazing presentation."

Post-graduate Student

ACENET offers advanced computing skills development to faculty, research staff and students across all our post-secondary institutions, as well as to private industry, not-for-profits and government in Atlantic Canada. Topics range from introducing the concept of high performance computing, the skills needed to use the national systems, various programming languages, techniques such as version control, scientific visualization and machine learning, and advanced sessions in parallel computing. Our training fills a gap for most participants, teaching transferable skills not typically covered in regular curriculums.

In 2022-23, ACENET staff provided our regional community with 256 hours of training via 65 unique training events. Almost all training sessions were online and promoted region-wide.

Almost 1800 Atlantic Canadian researchers, students and industry attended regional and nationally coordinated training sessions this past year. Through these events ACENET delivered almost 7000 learner hours, our highest impact over the last 10 years. This training is highly valued, with 95% of workshop participants considering ACENET training sessions to be relevant and beneficial in our post-event surveys.

Additionally, 495 researchers, students and industry participants attended ACENET outreach sessions explaining our services.

* A 'learner hour' is one learner in training for one hour.

Industry Ready Skills

ACENET developed and delivered a customized series of workshops in Python and AI/ML to participants in MUN's Drilling Data Analytics initiative, a partnership with Exxon.

Skills Development

ACENET continued to deliver advanced digital skills training across a wide range of topics and difficulty levels. During the last year we offered:

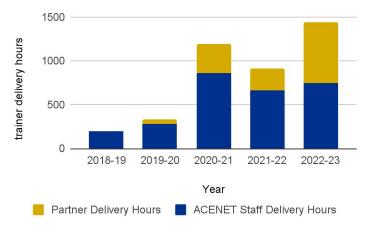
- Basics: Introduction to HPC
- Basics: Introduction to Linux
- Basics: Introduction to Shell Scripting
- Basics: Job Scheduling with Slurm
- Molecular Dynamics
- Introduction to Natural Language Processing
- Introduction to Genomics Data Organization & Analysis
- Introduction to Neural Network Architecture
- Basics of Computers
- Introduction to Spreadsheets
- Introductory Programming with Unix Shell, Git and R
- Introductory Programming with Unix Shell, Git and Python
- Modern Fortran for Scientific Programming
- Parallel Computing School 2022
- Introductory Programming with R
- Cloud from A to Z
- Introduction to Deep Learning
- ACENET HSS Series (4 sessions)
- Visualization with R
- Introductory Python for Ecologists
- National HSS Winter Series (15 sessions)
- Big Data Analysis with Spark
- C as a Second Language
- R for Ecologists
- C++ as a Second Language
- R for Social Scientists

The range of training topics ACENET routinely delivers can be found on our <u>website</u>, with new topics and initiatives continuously under development.

Initiatives

An area of success in recent years has been the development of training collaborations with other organizations in an effort to leverage resources and broaden our participant base. We have worked with partners such as the Ocean Tracking Network, Mathworks, Dalhousie's Institute for Comparative Genomics and our federation colleagues. ACENET staff spent a collective 750 hours delivering training this past year, but through these relationships, leveraged an additional 690 hours of outside effort to deliver training to Atlantic Canadians.

ACENET Staff and Partner Training Hours



Coming Fall 2023

ACENET is creating a comprehensive e-learning course for the REDCap secure data collection tool

"You really have a good grasp on how to handle online meetings. Your use of the features of the online software, and being wary of the limitations of digital meeting spaces served to make this presentation very valuable. It did not feel like a diminished experience compared to an in-person event as a result."

Industry participant



From Megabytes to Megafauna: Driving Whale Conservation to New Depths with HPC

"I think whales are kind of like dinosaurs," says Tim Frasier. "Almost everyone is interested in them at some point in their childhood, but some of us don't grow out of it."

Frasier, now a biology professor at Saint Mary's University in Halifax, Nova Scotia, is following his dream. His lab studies genetic variations in whale populations to fuel conservation efforts using high performance computing (HPC). Their present focus is on the North Atlantic right whale and Saint-Lawrence beluga.

By observing the variability of an individual's genome over its lifetime, Frasier and his students determine how inbreeding and traumatic events, such as ship strikes or entanglement in fishing gear, make individuals and populations less able to recover and reproduce.

The Frasier Lab sequences whale genomes from minuscule pieces of skin collected humanely by field teams. They then compare the variation in gene expression in healthy and injured whales, the life histories of which they know thanks to data collected by researchers through photo-identification over the last several decades. All these data

provide the basis to understand how the cumulative effects of inbreeding and multiple stress factors can cause individuals to not reproduce or live as long.

Frasier specifies, however, that these analyses involve millions of DNA fragments, which take up huge amounts of both storage space and computing power. "You just can't do it on a normal computer." Access to ACENET and the Alliance's supercomputing facilities are instrumental in enabling his lab to tackle complex genetic analyses that would otherwise be impossible.

Frasier gets asked a lot how this kind of information translates into helping conservation. One way is by influencing policy. Existing legislation imposes limits on different industries according to their impact on whales. For example, a North American right whale hit by a ship or entangled in a fishery somewhere along the east coast of the US and Canada could trigger either a ship slowdown in the area or completely shut down that fishery for the season. He explains that these triggers might only be quantified based on whether the whale died or not, "like a yes-no question." But if Frasier's research can show that these incidents change their reproductive success for years afterward, then it would also demonstrate that current measures are vastly insufficient to help populations recover and thrive in the long term.

These analyses involve millions of DNA fragments, which take up huge amounts of both storage space and computing power. Access to ACENET and the Alliance's supercomputing facilities are instrumental in enabling his lab to tackle complex genetic analyses that would otherwise be impossible. Frasier's work both advances our understanding of whales and provides a framework for devising more appropriate measures to encourage population recovery. It also highlights the importance of computing resources in modern biology research and conservation. "Without ACENET, we wouldn't be able to do this work," he says. "It's just such a great resource that we have, and many of the geneticists in Canada that I know feel that way."

Tim Frasier Saint Mary's University Biology

Quantum Chemistry of Molecular Evolution

PhD candidate Lázaro A. M. Castanedo and his adviser Chérif F. Matta are trying to answer one of the fundamental questions of molecular evolution: Why did nature pick the particular DNA structure humans have now as a carrier of our genetic information instead of other equally plausible choices?

"In the absence of constraints, nature's chemical reactions always choose the path that is the least costly in terms of Gibbs (free) energy," explains Matta, who is a professor at the Department of Chemistry and Physics at Mount Saint Vincent University. Gibbs (free) energy balances the tendency of nature to increase randomness as time progresses and its tendency to seek the lowest possible energy. "Could nature have made less costly choices than those that led to today's DNA? If so, why didn't it?"

Describing the project, Castanedo, who is pursuing his PhD at Saint Mary's University in collaboration with Mount Saint Vincent, says he compares the energies of different combinations of building blocks of nucleic acids (that is to say DNA and RNA). In addition, chemistry textbooks provide ample descriptions of the structural and chemical differences between DNA and RNA, but Castanedo and Matta want to know why that is, and if the observed forms are somehow energetically advantageous.

As an extension of this work, they are also investigating whether some of the nucleotides nature hasn't chosen have applications in drug development.

"One of the applications of discovering new nucleotides is that they can be used to produce similar molecular structures for drug discovery," says Castanedo, who received the 2020 Abe Leventhal Research Bursary from the Alzheimer Society of Nova Scotia for his work in developing molecules to prevent and detect dementias. "They could be used to develop new treatments for Alzheimer's, cancer, and other diseases."

Castanedo says he could do this research in a lab by synthesizing and comparing the components, which would take decades worth of human labour, or, he could approach it theoretically using computers, taking a fraction of the time.

"We predict what happens in the 'real world' using the computational infrastructure of the Digital Research Alliance of Canada and ACENET, which has thousands of cores and a panoply of state-of-the-art computational quantum chemistry software," he says. "So, you can actually create a model of this molecule on the computer and obtain, among many other properties, its Gibbs energy."

Castanedo is one of Saint Mary's University's heavier users — with 416,000 CPU hours in the last year (about 47 years of CPU time) — because he's been analyzing a total of 2,530 molecules for this project.

"For each of these molecules, a CPU needs to run continuously anywhere from, say, 20 to 200 CPU hours. These calculations are computationally intense, as we use high levels of quantum chemical theory, such as density functional theory (DFT), to obtain accurate predictions," he says.



Chérif Matta Mount Saint Vincent University Chemistry



Lázaro A. M. Castanedo Saint Mary's University Biochemistry

Castanedo is one of Saint Mary's University's heavier users with 416,000 CPU hours in 2022-23 (about 47 years of CPU time.) He's been analyzing 2,530 molecules.

Serving Atlantic Canada

We Have Specialists! Bioinformatics Computational Fluid Dynamics Cybersecurity Data management Humanities and Social Sciences Machine learning Molecular Dynamics Visualization

Accelerating Discovery

The expertise of our research consultants and advanced computing systems administrators is at the heart of ACENET's success, and often makes a pivotal contribution to the success of a research or innovation project. Still, a number of clients encounter barriers to realizing the full benefits of advanced computing due to a lack of internal expertise with technical challenges, and require more in-depth support than is provided within our normal services.

Recognizing the potential for capacity-building and research acceleration through more in-depth and focused support engagements, ACENET has been developing and just launched a new initiative to target dedicated support to projects with a high potential to benefit. The **Embedded Technical Support** program pairs our technical experts with innovative projects that have high potential for success and impact, and that require advanced computing resources, programming support and/or in-depth technical expertise. Some examples of areas we can help are: code parallelization, profiling and optimization for HPC systems; scientific or data visualization; data analytics; workflow migration from the desktop to a cluster; research portal creation on a cloud platform; and, incorporation of advanced computing into research programs.

Talent Development

ACENET was selected as one of 10 <u>techNL</u> partners to deliver its \$27 million *Find Your Future in Tech* digital skills program. Through our Certificate in Advanced Computing, 25 to 40 participants in Newfoundland & Labrador will receive training in high-demand advanced computing skills. The program has enabled us to engage four additional staff members to help develop and deliver the curriculum. Once developed, we plan to roll out the program Atlantic-wide and transition it to a micro-credential.

Local Support

We have 17 technical support people located at six of our member institutions across the region.

Artificial Intelligence

ACENET has been working hard over the past year to support the explosion of demand for AI support and services.

- We partnered with Springboard Atlantic to commission an Atlantic Canada AI asset map, identifying research expertise, infrastructure, and industry active in AI.
- We established a new research consultant position at Université de Moncton to support AI in all of Atlantic Canada.
- ACENET supported NBIF's Artificial Intelligence Fund by undertaking technical reviews of proposals, providing research support to funded projects, and offering hosting services for any infrastructure resulting from this funding. The <u>three projects</u> announced in the inaugural 2022 competition are all ACENET clients.

A Bioinformatics Win-Win

Over a six month period, one of our research consultants, Dr. Serguei Vassiliev, dove deep into a research project with Dr. Om Rajora's group in the department of Forestry and Environmental Management at UNB. With no high performance computing or computational bioinformatics experience, the group needed some help. Along with many hours of discussion, Serguei educated himself in computational bioinformatics, installed software, developed parallelization schemes, wrote submission scripts and analyzed data. He also trained the group in computational techniques such as genome assembly and annotation, transcriptome construction, differential gene expression analysis, and identification of protein-protein interaction networks. The results:

- 1. Reduced computational analysis time from weeks on a workstation to hours on a supercomputer;
- 2. The group has gained advanced computational skills critical to their work;
- 3. One publication in the International Journal of Molecular Science, with a second publication underway both co-authored by Serguei; and
- 4. We now have a bioinformatics specialist on our research consulting team!

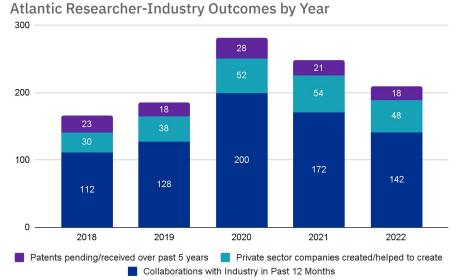
Serving Atlantic Canada

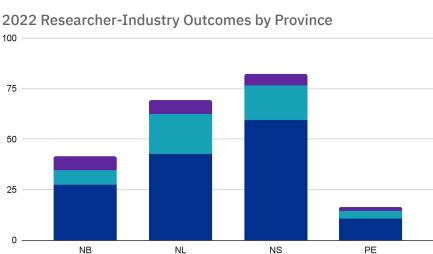
Industry

During the Alliance annual spring account renewal, Principal Investigators (PIs) are asked to indicate any industry outcomes of their research that relied on the infrastructure and services provided by ACENET and the national platforms. The latest data we have is for the 2022 renewal.

In looking at the numbers from 2019 to 2022, there was significant growth in 2020, which then dropped back in 2021, and again in 2022. The sudden increase in 2020 could be attributed to pandemic lock-downs with a shift in researcher focus to areas such as Covid-related research. Interestingly, despite the variation in total volume, the number of unique researchers region-wide involved in commercial activity remained relatively constant over the three years at 139, 135 and 133 respectively. This could be a result of an increase in focus required for teaching, as most institutions adopted virtual learning post-lockdown.

In 2022, ACENET supported 142 industry collaborations involving 85 researchers during the previous 12 months. During the previous five years, 34 researchers enabled by ACENET created or helped to create 48 companies, and 14 researchers had 18 patents received or pending.





Patents pending/received over past 5 years Number of Collaborations with Industry in Past 12 Months

ACENET supports industry directly system Siku, our consultants for support, and our training. We offer

- A free trial program on our Siku
- Jump Start for Start-ups, compute hours and 20 hours of months - a value of \$5000.
- up to \$5000 of our in a Government of Canada

Siku clients enjoy **monthly usage** reports, no data transit fees, and the ability for clients to **set usage** caps in order to control their

Financials

On 1 April, 2022, the Digital Research Alliance replaced the Canada Foundation for Innovation as federal funder and Compute Canada as national coordinator of Advanced Research Computing in Canada.

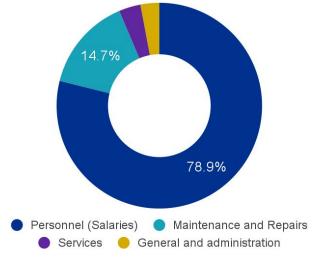
Financial Summary

1 April, 2022 to 31 March, 2023

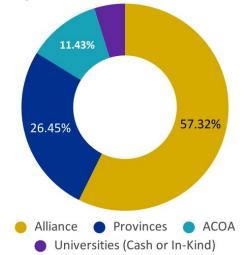
Expenses

Personnel (Salaries)	\$ 1,796,130
Infrastructure (maintenance & upgrades)	335,847
Services	77,914
General and Administration	67,433
	\$ 2,277,324
Funding	
Alliance	\$ 1,305,255
Provinces	602,450
ACOA	260,243
Universities (Cash or In-Kind)	109,376
	\$ 2,277,324

Expenses 2022-23



Funding 2022-23



ACENET was created in 2003 as a consortium of five universities and received its first funding in 2004. We now serve almost all post-secondary institutions in the region, and will celebrate our 20th anniversary in 2024.

Making Data Meaningful

Whether it be for a community project to determine which water is safe for drinking, or a hospital-based project to determine the most efficient and effective ways to treat mental illness, Trishla Shah is an expert in taking the data we collect so easily today, and making them meaningful.

As the IT research scientist at the Nova Scotia Community College and a PhD candidate in computer science at Dalhousie University, Shah focuses on designing solutions by analyzing massive amounts of data. For example, Nova Scotia's water comes from various places, including freshwater lakes, but also possibly from contaminated lakes, she says.

"We want to educate the organizations taking care of our water resources so we can see how we can preserve the well water and how we can make sure the water from the fresh lakes is not contaminated," Shah says, adding that many of her projects come to her after receiving funding from a national social innovation fund.

Private IT companies that want to design and test a product from scratch also often approach the research scientist.

"We are being approached by startups, by midsize companies and by large-scale companies," Shah says. "We are being approached by organizations that take care of Indigenous communities. One project we're working on involves artificial intelligence, Indigenous communities and Halifax's storied Bluenose ship."

For another project, Shah is helping small and medium-sized enterprises identify the right clean technology investments for their business. Her lab is building a data repository to provide solutions to scale access to low-carbon emissions for businesses in the agri-food, construction and manufacturing industries. The repository is integrated from various sources using web-scraping and text-mining techniques. The parameters of the data repository will be set to allow an algorithm to forecast carbon emission reductions and analyze the return-on-investment of various interventions.

Shah and her team get involved from the beginning, first collecting the data, then building a database, preprocessing, storing and managing the data in a way that ensures they're secure and making sure there's no breach. From there, they can make models of the data so they don't have to analyze them manually.

Shah hasn't used the services of ACENET directly, but she has circulated its many training programs among the information technology students at the college.

"We have a lot of academic programs that have IT in them," she says. "And students might want extra practice, or students might need to have something like a prerequisite. With ACENET, the courses are really applicable and I like to circulate them among students who need additional practice on that topic. So that's my interest with ACENET. I'm a fan."

In addition, Shah is in the process of designing her own student training module that has an online portal where students can enrol themselves in training that is focused on real-time projects.

"I have proposed to the committee that's approving my student training module and funding that ACENET's courses be prerequisites."



Trishla Shah Nova Scotia Community College Data Science

Acknowledgements

Board of Directors

Tana Allan	Board Chair, Acting VP (Research)	Memorial University
Jennifer Bain	Associate VP Research	Dalhousie University
Adam J. Sarty	Associate VP Research	Saint Mary's University
Richard Isnor	AVP Research & Graduate Studies	St. Francis Xavier University
Laura Estill	Associate Professor, Tier 2 Canada Research Chair in Digital Humanities, ACENET Research Directorate member	St. Francis Xavier University
Francis Leblanc	Vice-recteur adjoint à la recherche et Doyen	Université de Moncton
David Magee	VP Research	University of New Brunswick
Greg Naterer	VP Academic & Research	University of Prince Edward Island

Research Directorate

Erin Johnson	Professor, Department of Chemistry	Dalhousie University
Samuel Stewart	Assistant Professor, Medical Informatics; Director, Health Data Nova Scotia	Dalhousie University
Alison Farrell	Research Data Management and Public Services Librarian Health Sciences Library	Memorial University
Alison Malcolm	Associate Professor, Department of Earth Sciences	Memorial University
Vincent Hénault-Brunet	Assistant Professor, Department of Astronomy and Physics	Saint Mary's University
Laura Estill	Associate Professor, Tier 2 Canada Research Chair in Digital Humanities	St. Francis Xavier University
Shah Razul	Associate Professor, Department of Chemistry	St. Francis Xavier University
Ian Church	Associate Professor, Principal Investigator Ocean Mapping Group	University of New Brunswick
Xander Wang	Assistant Professor, School of Climate Change & Adaptation	University of Prince Edward Island

Digital Research Alliance of Canada Research Council Atlantic Canada Members

Catherine Lovekin	Associate Professor, Department of Physics	Mount Allison University
Laura Estill	Associate Professor, Tier 2 Canada Research Chair in Digital	St. Francis Xavier University
	Humanities	

Partners

Member Institutions

