"Future Directions In Scientific Computing"

TRIUMF's 20-year Vision
Scientific Computing
Topical Group summary

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Topic covered & Group Members

- **Scientific Computing**:

Covers big data, advanced research computing infrastructure, machine learning and artificial intelligence as well as quantum computing

- Broad range of activities across the laboratory's domains and research portfolio
- Plays a crucial role in facilitating TRIUMF's mission of discovery and innovation

- **Group members:**

Wojciech Fedorko (TRIUMF)

Paul Haljan (Simon Fraser U.)

J.J. Kavelaars (U. of Victoria & NRC Herzberg)

Anna McCoy (U. of Washington)

Petr Navratil (TRIUMF)

Crystal Senko (U. of Waterloo)

Reda Tafirout, chair (TRIUMF)

Isabel Trigger (TRIUMF)

Community Engagement Process

Various strategies used to gather information and inputs from the community:

- Solicitation via SurveyMonkey, and the ThoughtExchange platform (rather insubstantial)
- Several one-on-one consultations conducted by the topical group members with various experts and key stakeholders
  - Representatives of TRIUMF's nuclear physics program
  - Members of the Core Computing & Networking, and DAQ groups; as well as Life Sciences, and Accelerator divisions.
  - Key researchers from U. of Waterloo with expertise in quantum information science
  - Other national laboratories: Individuals in a leadership position from FNAL, BNL, JLAB, and CERN
  - Representatives of HEPNET, NDRIO and NRC.
- Reviewed relevant White Paper submissions to NDRIO as part of the Canadian DRI ecos.
- The particle physics community needs are largely encapsulated in the IPP brief submitted to the NSERC LRP committee.
- Reviewed DOE labs strategies regarding AI and quantum computing initiatives

Outcome of the process & High-level Themes

The topical group has identified three distinct, although not completely orthogonal, generic areas of activities that TRIUMF should continue to be engaged into and expand upon, as well as new initiatives to remain relevant and competitive for the coming decades:

- **Scientific Computing Infrastructure**
- **Research Software & Applications**
- **Quantum Computing User Facility**

"These areas have been identified as those where TRIUMF would play a unique and distinct role, as a national laboratory, with most benefit to its community, while maximizing synergies with other entities, including Universities, NDRIO, CANARIE, industry partners, other national and international laboratories, and virtual organizations."

Full summary document available online

Vision

for Scientific Computing

"I do not fear computers. I fear lack of them."

- I. Asimov

"A classical computation is like a solo voice—one line of pure tones succeeding each other. A quantum computation is like a symphony—many lines of tones interfering with one another."

- S. Lloyd.

Our Vision for Scientific Computing

TRIUMF will establish state-of-the-art scientific computing infrastructure and services

A coherent and focused approach to scientific computing will add tremendous value to the on-site experiments, and local research groups across the laboratory

TRIUMF will enhance its science output through the application of modern scientific computing and Machine Learning technologies

TRIUMF will train highly qualified personnel in AI, heterogenous hardware utilization and physics simulations

TRIUMF will operate a quantum computing user facility, providing quantum computing access to academic and industry users across Canada and internationally

Research performed at the center will have transformative societal impact

	Now	Action	2042
Theme 1	• Current scientific computing activities at the laboratory are somewhat fragmented • Overall support structure not well defined • Not keeping up with technological advances	Establish a focused and coherent approach to research computing	TRIUMF will establish state-of-the-art scientific computing infrastructure and services
Theme 2	• Modelling of the passage of particles through matter is critical to particle and nuclear physics, detector development, life sciences. Synergies currently not realized • ML is starting to get traction in some areas of research at TRIUMF and research supported at TRIUMF but it's adoption is not widespread among the represented fields. • Massively parallel software utilizing heterogeneous computing infrastructure is important for several core science topics at TRIUMF – however efforts in this area are not centrally supported	The establishment of a scientific computing center of excellence.	TRIUMF will enhance its science output through the application of modern scientific computing and Machine Learning technologies
Theme 3	• No publicly available academic quantum computer is currently available. Free and for-fee offerings exist from commercial vendors. • User center providing reliable no-red-tape access to state-of-the art trapped ion quantum computer will spur research in fundamental quantum computing and quantum computing applications, including in the fields core to TRIUMF's mission.	Establishment of Trapped Ion Quantum Computing user facility	TRIUMF will operate a quantum computing user facility, providing access to academic and industry users across Canada and internationally

TRIUMF will establish state-of-the-art scientific computing infrastructure and services

A coherent and focused approach to scientific computing will add tremendous value to the on-site experiments, and local research groups across the laboratory

- Organizational changes so IT services and functions only focus on the business end of TRIUMF's operations (e.g., Mail, Web applications, documents, collaborative tools, etc.)
- Establish an on-premises advanced computing infrastructure dedicated solely to research computing, with minimal total cost of ownership and with varying capabilities to serve also the local theory group for parallel code developments
- Establish a service layer, similar to cloud computing, so users can deploy their own services within a trusted and secure framework
- Keep abreast of technological advances in the computing industry. Establish collaborative agreements with industry to gain competitive edge.
- Enhance DAQ capabilities with co-processors (such as FPGAs and GPUs) in online processing chains
- Support Tier-1 like facility operations and work in concert with NDRIO
- Continue to collaborate on international projects, such as the Worldwide LHC Computing Grid and the European Grid Infrastructure, through which key developments and innovative technologies emerge regarding advanced networks, distributed computing, workload management, and data management.

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- Modest increase in personnel dedicated to modelling and software creation for codes used for modelling passage of particles through matter and other physical simulations.
- Gradual increase in personnel supporting AI effort. Hiring will follow a pattern where each expert has appreciation for at least one of the fields (Life Sciences, Nuclear Physics, Particle Physics, Accelerator Physics) in addition to ML expertise. Focus will be on breadth of fields represented.
- Establishment of formal model of funding the personnel via a combination of research grants and operating funds.
- Establishment of a succession of pilot projects in AI focusing on breadth of projects.
- Establishment of managed project workflow for detector or target modeling.
- Incorporation of the personnel into an excellence center.

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Research performed at the center will have transformative societal impact

- Initial establishment of a prototype center through CFI funding with close collaboration from University partners
  - Technical and Scientific team growth
- Establishment of custom pilot projects performed using the developed infrastructure
- Maturation of the infrastructure into initial user center; Establishment of merit-based open access scheme
- Partial or full transition of the personnel into permanent positions
- Continued growth and update of the infrastructure with the feedback to the University partners developing new quantum computing machines and quantum computing methodologies.
- Continued operationalization of new quantum computers into a supported user center