

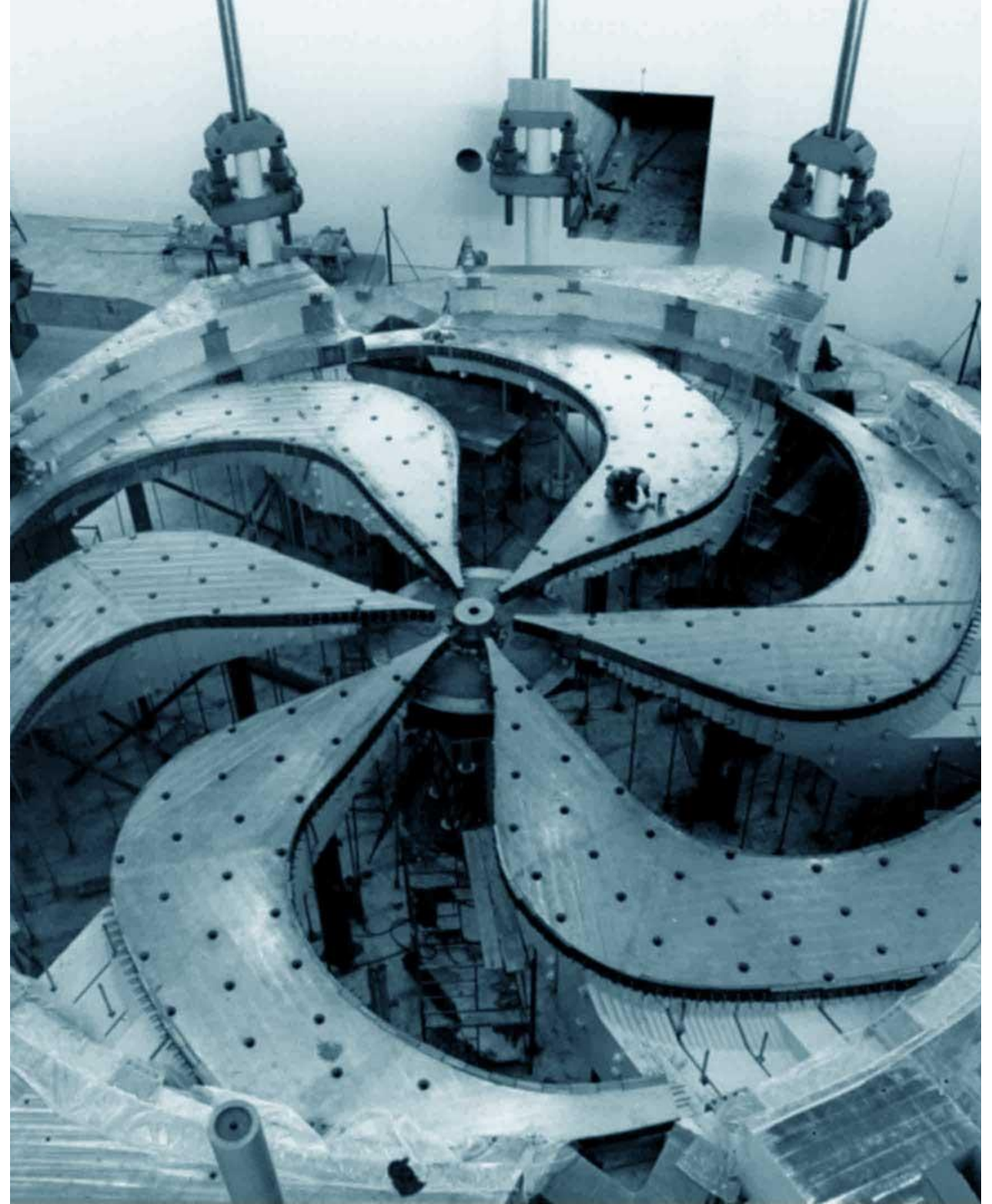
Scientific Computing

Status & Next 5YP

W. Fedorko, R. Tafirout

Scientific Computing Department

ACOT meeting, Fall 2024



Current Department Organization

- Common umbrella for existing activities:
 - Big data & Distributed Computing (ATLAS Tier-1) (R. Tafirout)
 - Machine Learning & Quantum Information Systems (W. Fedorko)
- Head / Deputy: R. Tafirout / W. Fedorko
 - Tier-1:

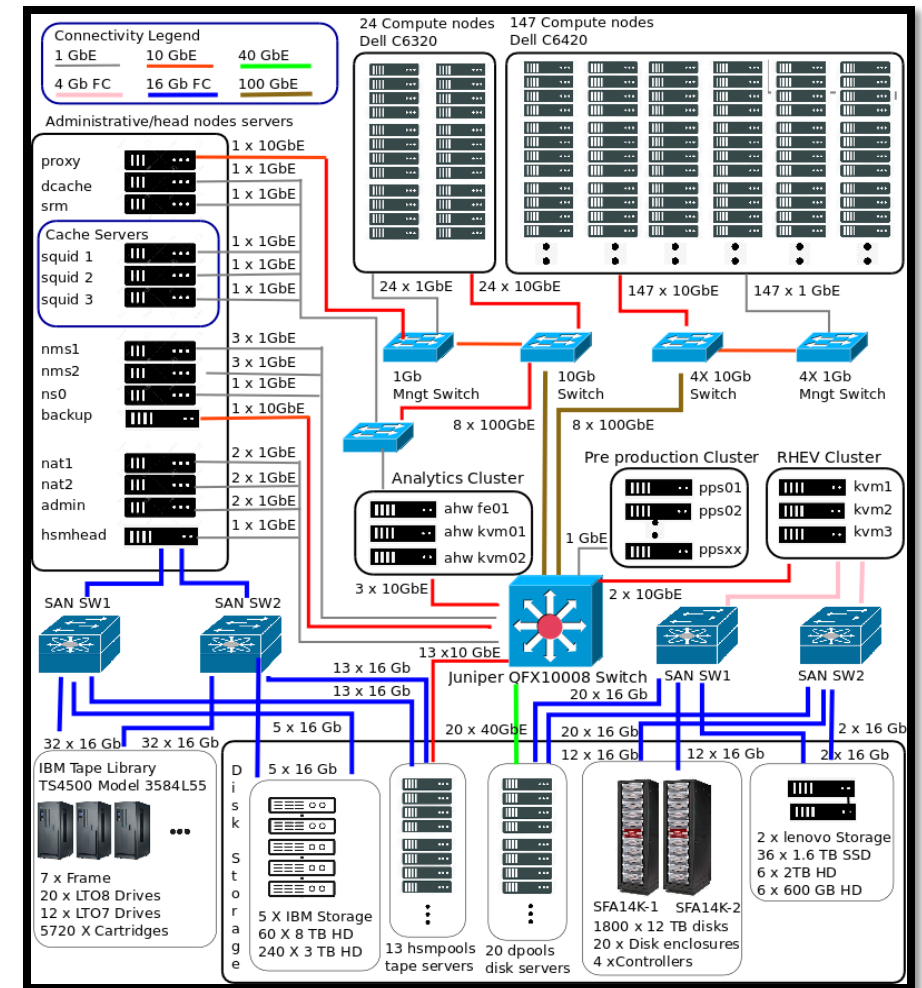
A. De Silva	X. Liu
R. Debhandari	D. Qing
F. Fernandez Galindo	Y. Shin
V. Kondratenko	A. Wong
 - QML: Javier Toledo (RA)

Affiliated Scientists:

C. Senko (Waterloo)
R. Islam (Waterloo)
P. Haljan (Simon Fraser)
J. Sirker (Manitoba)

ATLAS Tier-1 Centre & next 5YP

- Well established 24/7 distributed computing operations model with high availability & reliability:
 - data storage, data processing, simulations and user analysis in a highly secure environment
 - crucial user support for the entire collaboration
- Current capacity: ~9,000 cores ; 17 PB disk ; 45 PB tape
- Plan to continue Tier-1 operations in next 5YP with existing TRIUMF personnel complement
- New CFI IF 2025 funding proposal in preparation:
 - covers 2027-2031 period
 - \$5.3M from CFI (\$13.2M total project cost)
 - hardware expansion during LS3 & HL-LHC
 - personnel for computing R&D for HL-LHC
- Recently, secured crucial funding through special award of \$4.05M (from DRAC & BCKDF) to replace ageing equipment as bridging into next CFI:
 - active procurement process ongoing

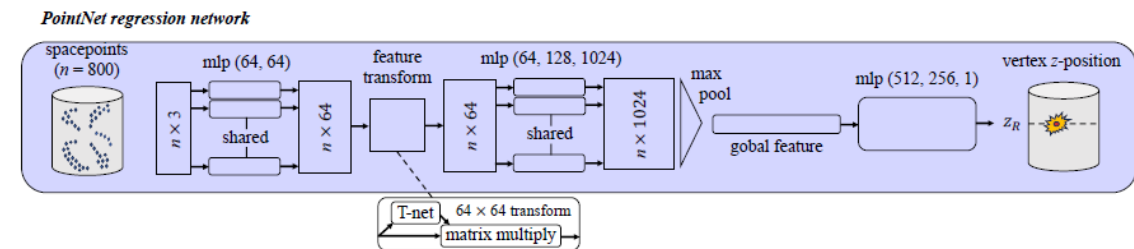
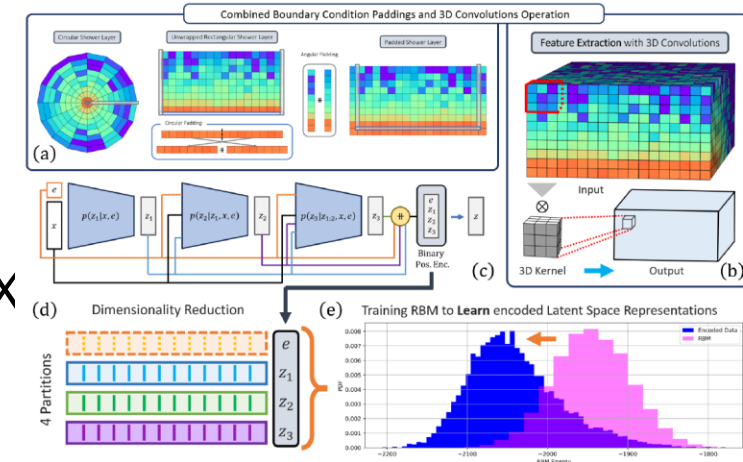


Digital Research
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Machine Learning and Quantum Computing Activities 1

- ML engagement recent since 2018
 - Part of the current TRIUMF strategic plan
- Supporting and driving multiple ML/QC aspects of projects:
 - ATLAS Quantum-Assisted ML
 - Accelerated calorimetric simulation: EPJC Letter accepted, PRX imminent, multiple conferences (IEEE, CHEP, NeurIPS)
 - Water Cherenkov HyperK/SuperK/WCTE/IWCD
 - Multiple threads centering on particle identification + reconstruction in Water Cherenkov detector
 - First look at real data with ML methods at SuperK
 - ATLAS Particle Flow
 - Improved calibration of calorimetric clusters
 - ATLAS Trigger/FPGA
 - Real time application of ML cluster calibration for Level 0 trigger for ATLAS @ HL-LHC
 - ALPHA
 - Reconstruction of annihilation vertex
 - Accepted at NeurIPS ML4PS, publication advanced draft
 - First look at data
 - NA62
 - CaloPID: Adopted, Published
 - RICHPID: In internal review



Machine Learning and Quantum Computing Activities 2

- Automated beam tuning with RIBs (ISAC I, B-NMR, DRAGON)
 - Aim automate beam steering with Bayesian Optimization in conjunction with Model Coupled Accelerator Tuning (MCAT) for optics.
 - On-going beam tests in ISAC MEBT HEBT and DRAGON
 - RSI in 2nd round of peer review. presented at IPAC
 - Plans to put tool in production before the long shutdown
- TIIGR w Life Sciences / SciTech
 - Aim to design detector for SPECT imaging for targeted alpha therapy with Ac^{225}
 - Initial detector design studies. Plans for ML image reconstruction and design optimization
 - Collaboration with Korean partners unfolding well.
- HQP support for all projects:
 - Postdocs, Grads, Coops/UG
 - MITACS
 - Capstone projects
 - Summer schools
 - Collaborations

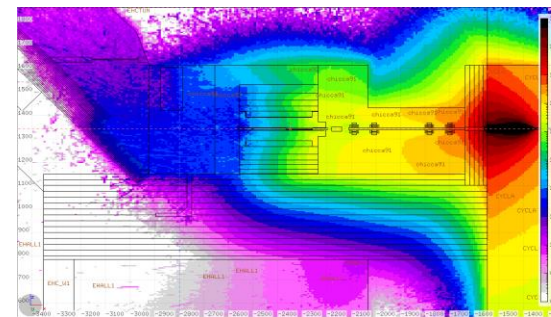
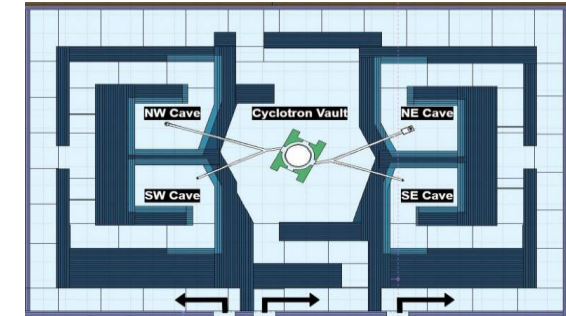
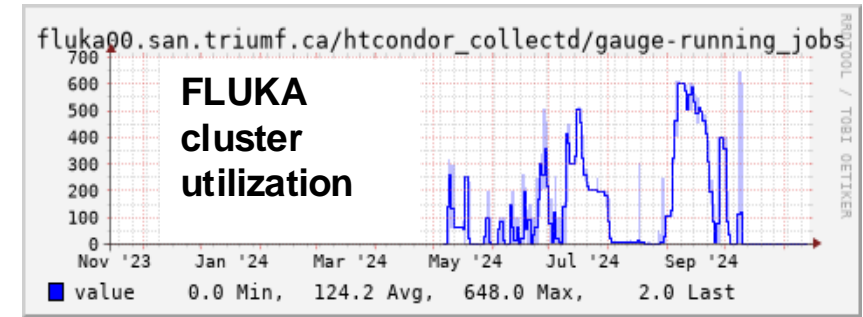


ML + QC projects 2025-30

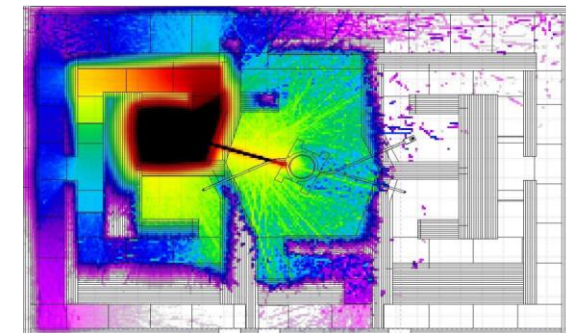
- Continued support and leadership of existing ML & QC projects
- 5YP ARIEL Support:
 - Automatic beam tuning will support accepting beam from ARIEL into ISAC
 - Methods can be transferred to different beamline section
 - Relieve operators to manage x3 simultaneous beamlines
- Infrastructure:
 - In house rapid ML development machine(s) need periodic upgrades/replacement
 - Risk to program
 - 'Behind' state of the art
- 5YP alignment and risks
 - Extra personnel difficult under 5YP constraints
 - Additional 1 FTE ML-dedicated personnel would be needed for sustaining existing program + modest expansion
 - Nuclear Physics, Material Science, Life Sciences
 - Small likelihood of TIIGR getting delayed dependent on what personnel gets re-allocated

ARIEL & IAMI support / FLUKA cluster

- Since 2020, a significant portion of the old ATLAS Tier-1 centre capacity is being utilized for large FLUKA simulations campaigns:
 - 336 physical cores added to existing IS&T cluster via special network configuration (for security); jointly managed
 - crucial for ARIEL shielding design (time sensitive)
 - recent large simulation campaign for IAMI
- Cluster also used by PIF/NIF and other projects, like FLASH
- Additional features implemented since early 2024:
 - HTCondor batch system for efficient access
 - enhanced monitoring for cluster utilization
- CNSC approval received in May 2024 to operate the 500 MeV cyclotron with current BL4N shielding configuration.



ARIEL Proton Cave



IAMI TR24

Extra Material

CAM Initiative

- Project Driven by the Digital Research Alliance of Canada / Aim and scope:
 - The Controlled Access Management (CAM) for Research Data Initiative aims to enable collaboration between Canadian data repositories and research institutions to enhance research data management and research security.
- TRIUMF selected as partner organization along with other institutions (application made in 2023)
- There are monthly meetings with partner organization representatives
- TRIUMF is participating in two working groups:
 - Technology & Services
 - Data Governance & Data Stewardship
- Involvement from Scientific Computing and IS&T departments



**Digital Research
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ATLAS Software & Computing Roadmap for the HL-LHC

- Roadmap has many components dealing with various topics & challenges:
 - Network infrastructure ready for Run 4
 - Detector Description, Simulation and Digitization projects
 - HL-LHC datasets replicas and versions management
 - Core Software and Heterogeneous Computing / Accelerators
 - etc.
- ATLAS Heterogeneous Computing & Accelerators Forum established recently
- To tackle the combinatorics in a high luminosity environment, investigate tracking on GPU. For this to succeed:
 - define a suitable Event Data Model,
 - develop a toolchain that supports e.g. CUDA kernels
 - provide GPU friendly implementations of the geometry and magnetic field.
- ATLAS Tier-1 CFI proposal (IF 2025) has capital provisions to hire additional personnel to work on software R&D for HL-LHC era.

ACTS - A Common Tracking Software

