TRIUMF

Scientific Computing Initiatives

Science Week 2022

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Discovery, accelerated

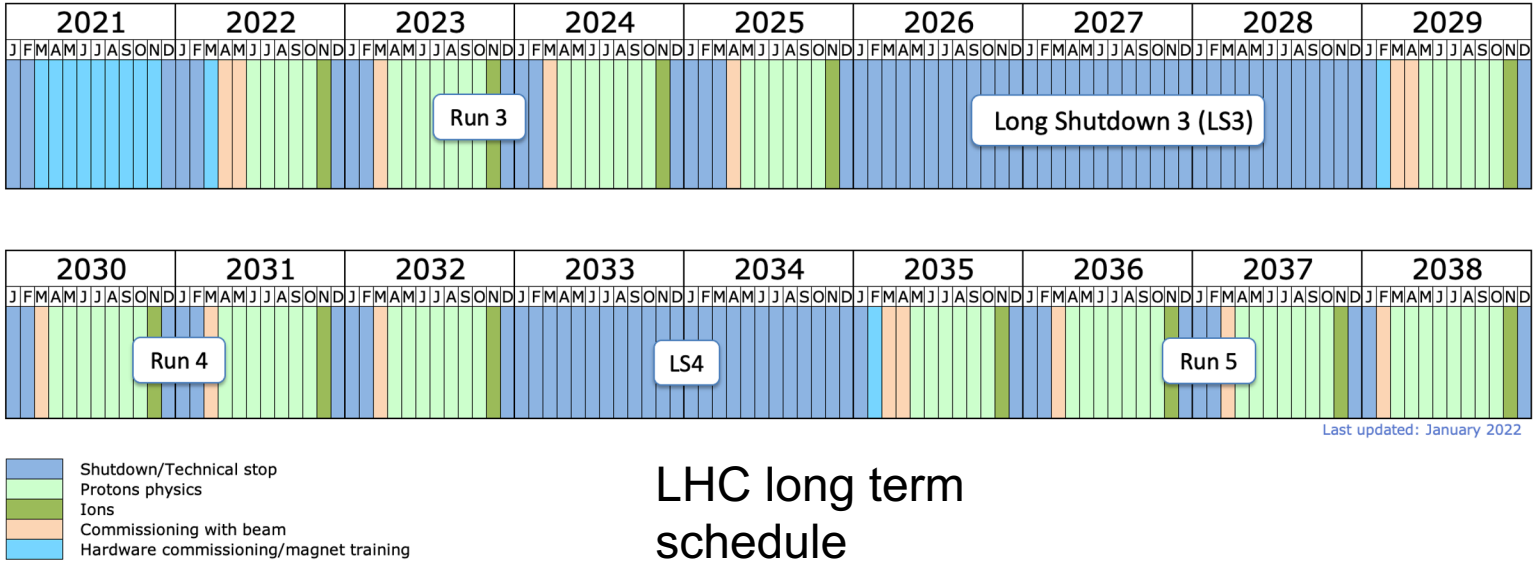
Scientific Computing Department Organization

- Recently created (fall of 2020), under Physical Sciences (formalized in spring of 2021)
- 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
  - A. De Silva
  - R. Debhandari
  - F. Fernandez Galindo
  - V. Kondratenko
  - X. Liu
  - D. Qing
  - Y. Shin
  - A. Wong

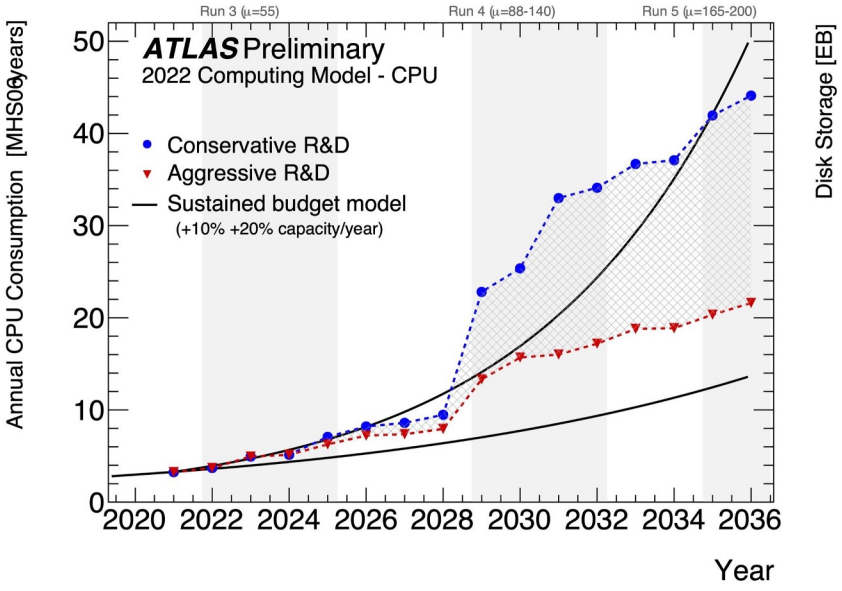
- Affiliated Scientists:
  - C. Senko (Waterloo)
  - R. Islam (Waterloo)
  - P. Haljan (Simon Fraser)
  - J. Sirker (Manitoba)

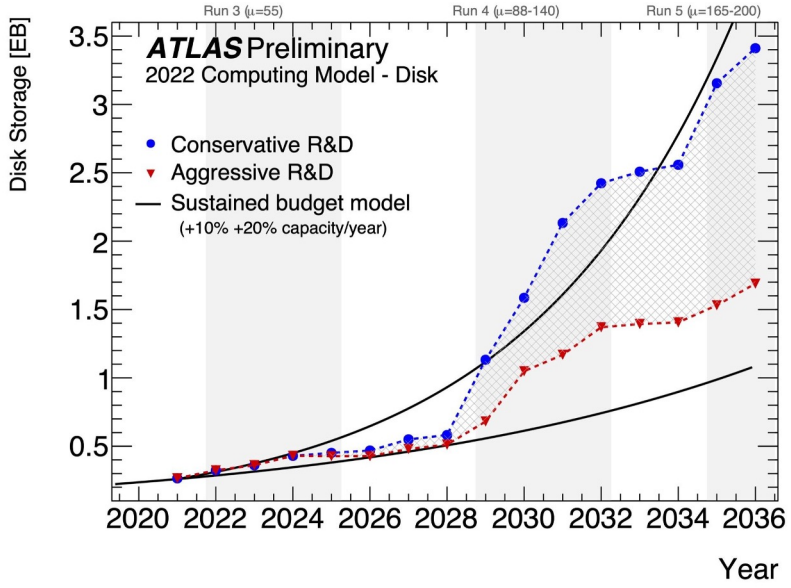
ATLAS Distributed Computing Needs

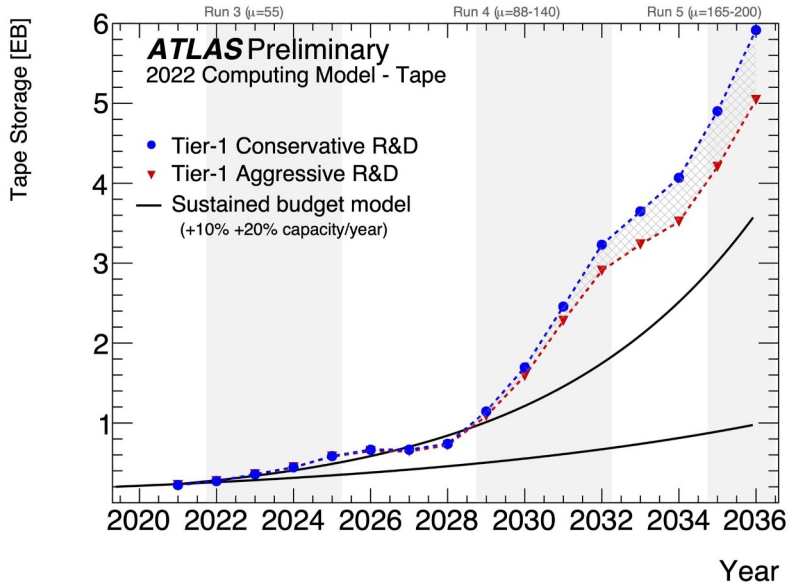
- Large-scale resources crucial to the LHC scientific program
- Tier-1 centres: providing 35-45% of required disk and CPU needs, and 100% of tape (computing model)
- HL-LHC Software & Computing Roadmap document (various needed developments to meet data challenge)



LHC long term schedule

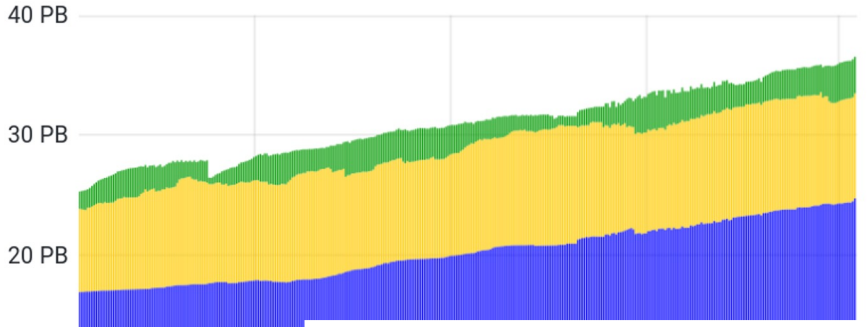


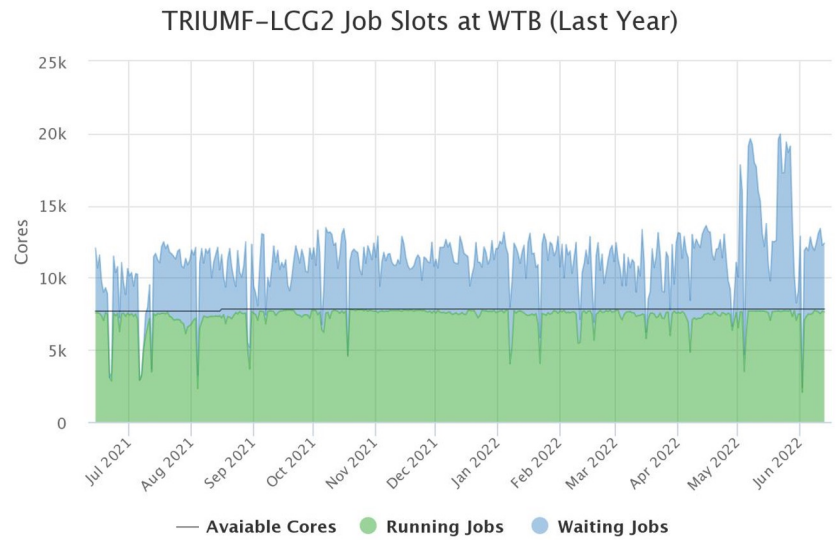


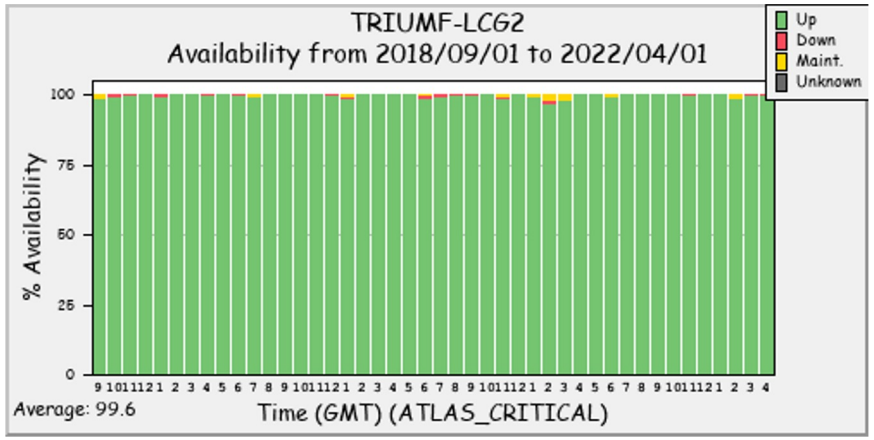


ATLAS Tier-1 plans

- Providing 10% of worldwide Tier-1 resources
- Relocated to SFU (since 2018), using CFI IF 2017
- CFI IF 2020 award (current): cover needs for Run-3
  - Capacity expansion
  - Capital for new personnel (R&D for HL-LHC)
- CFI IF 2023 proposal (cover LS3 and first two years of HL-LHC ($16.5M total project cost)
  - Submitted last Friday
  - Full refresh needed by end of 2025 / early 2026 (existing systems will be past 7 years) & capacity expansion
  - Expansion phases in 2027 and 2029
  - Need to follow closely technology developments / industry roadmap







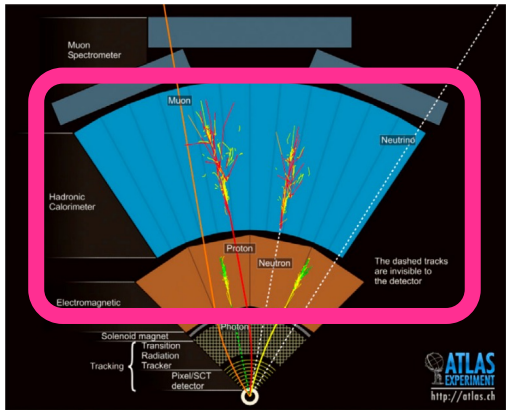
Machine Learning / Quantum Computing: Present Activities

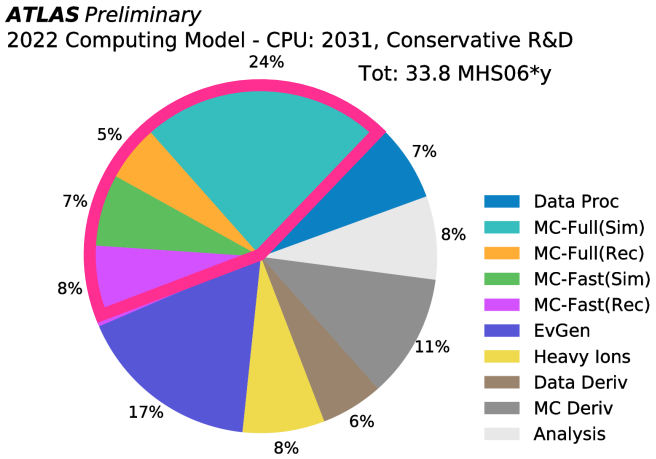
- Enchancing science outcomes through the application of ML and QC
- Technical and conceptual advisory on projects specified by TRIUMF PI's
  - Student / postdoc co-supervision
- Initiative in identifying opportunities for new projects
- Execution
- Maintaining SW / container stack
- Access to in-house ML computing – gateway to Digital Research Alliance of Canada (prev. Compute Canada)
- Currently active projects:
  - Particle physics: HyperK, NA62, ATLAS, Belle
  - AD/Beam physics
- HQP training:
  - COOP, Capstone Programs, UBC Master of Data Science, MITACS GRA …
  - Led organization of TSI "Cornerstone Models of Quantum Computing" 2020, 2021
- Local and International collaboration: Helmholtz Association, QAI, QuantumBC…
- New domain areas / will require expansion of manpower.

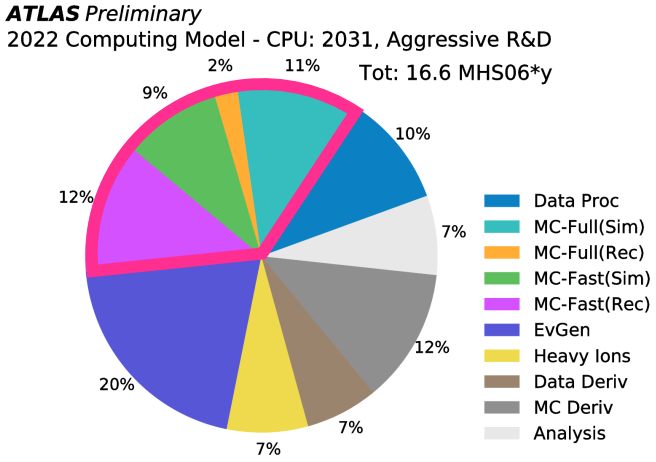
Examples of ML / QC projects I: Calorimetric Shower Generation for ATLAS

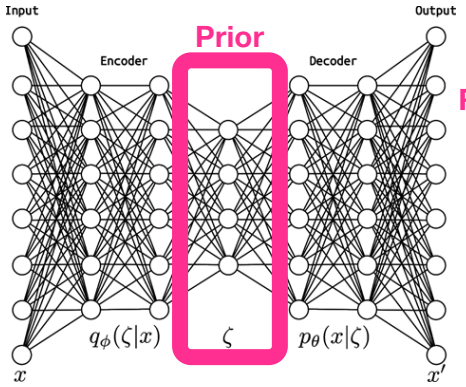
- Aim to replace First-principles (GEANT) or parametrized calorimeter simulation with a Quantum-Assisted Deep Learning Model

Cross-section ATLAS Detector



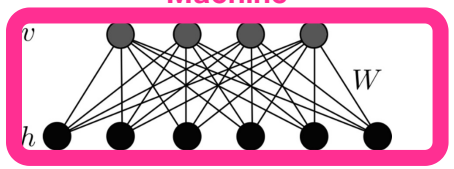




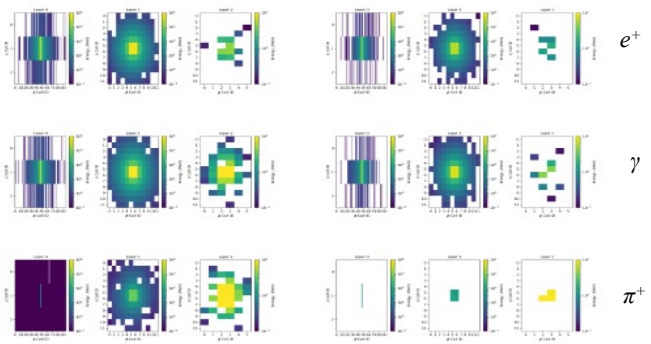


Variational Autoencoder

Prior:
Restricted / Quantum Boltzmann Machine



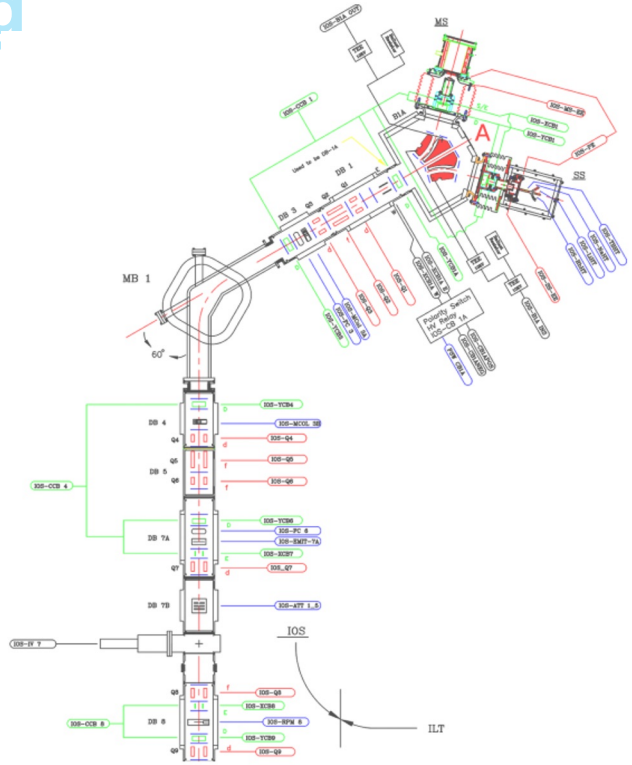
Showers generated by the model



- Using open GEANT4 particle-gun dataset resembling ATLAS LAr EM calo $\gamma/e^+/\pi^+$
- Performance demonstrated with classical analog of a quantum model
- Paper + poster ML4PS@NeurIPS2021; Talk at Helmholtz Association Physics at the Terascale; Poster at Quantum Days
- Development on-going aiming for sampling from D-Wave QPU:
- Intend to move to ATLAS datasets

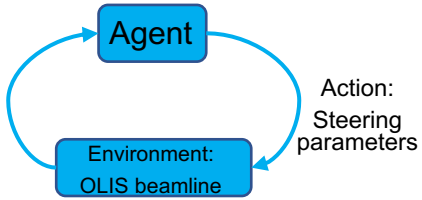
Examples of ML / QC projects II: Beamline tuning

- Augment/Automate beamline tuning
- OLIS: Starting point for AI-tuning
  - Low current
  - Non-radioactive
  - Manual tuning by operators takes many hours, taking away from research beam time
- Goals for learning agent:
  - Optimize beam transmission
  - Mitigate unknown misalignments
  - Improve speed and accuracy of tuning

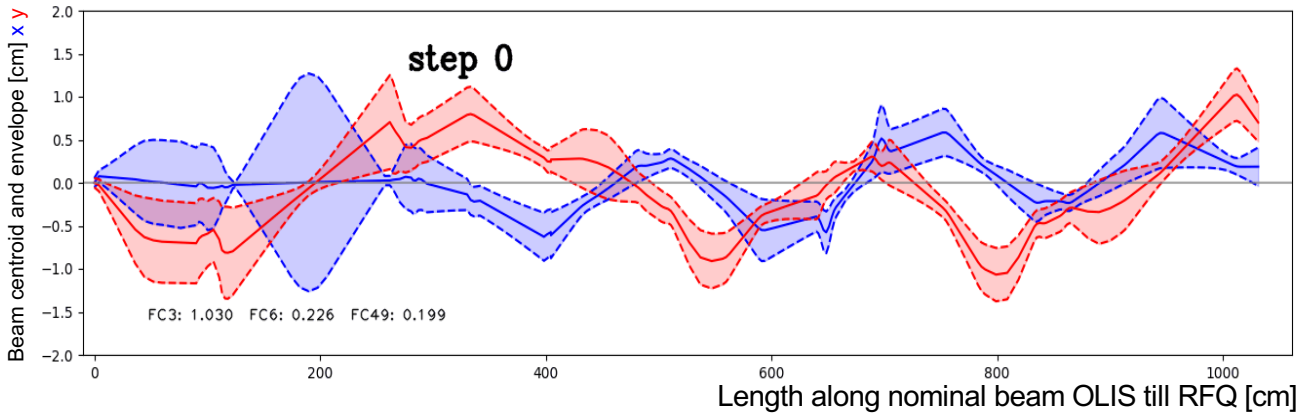


Source: Beam Physics Note TRI-BN-20-13R, Olivier Shelbaya

- Reinforcement Learning:



- Actor-Critic method with state memory (Recurrent Deep Deterministic Policy Gradients -RDPG)



Scientific Computing: 20-Year vision and the 5-Year Plan

- Scientific Computing Topical Group identified and discussed three themes:
  - Scientific Computing Infrastructure: *"Establish a focused and coherent approach to research computing"*
  - ➢ need to find suitable space/solution on-site to host additional ML platforms (currently at UBC with Theory)
  - **Research Software & Applications**
    - *"Enhance science output through the application of modern scientific computing and Machine Learning technologies"*
    - ➢ ongoing discussions with PSD departments and across divisions needed to assess and justify additional manpower
  - Quantum Computing User Facility
    - *"Establishment of Trapped Ion Quantum Computing user facility"*
    - ➢ review triggered by the director; panel formed in March; report delivered.
- Ambition to take advantage of AI and QC articulated in individual topical group 20-year vision documents
- 20-year vision Advance Copy:
  - *"The ever-increasing amount of data produced in these experiments will require advances in high-performance computing, artificial intelligence, and quantum computing."*
  - *"TRIUMF will be seen as a strategic asset in the implementation of the National Quantum Strategy, specifically in the areas of quantum sensors, materials, and computing"*
  - *"…we will support the Canadian quantum computing community in its ambitions by enabling access to relevant TRIUMF's expertise and capabilities"*

Translating vision into a plan

- Are there more opportunities within Physical Sciences for ML/QC applications worth attacking in 2025-30?
  - Initiated consultations with the PSD departments
- Are there opportunities and need for support for ML and general Scientific computing applications in Life Sciences and Accelerator Division
  - Automated beamline tuning
  - Predictive maintenance
  - Cyclotron simulation ↔ massively parallel GPU SW development
- Are there opportunities to exploit synergies and consolidate SW development / model building in SW modeling passage of particles through matter (GEANT/FLUKA)
  - target design (LS/AD)
  - treatment design (LS)
  - detector design (SciTech)
- Are we not thinking about an aspect of Scientific Computing we should be?
- What would it take to make it happen?
- Let's talk!