OAK RIDGE National Laboratory

Quantum Computing in High Energy/Nuclear Physics

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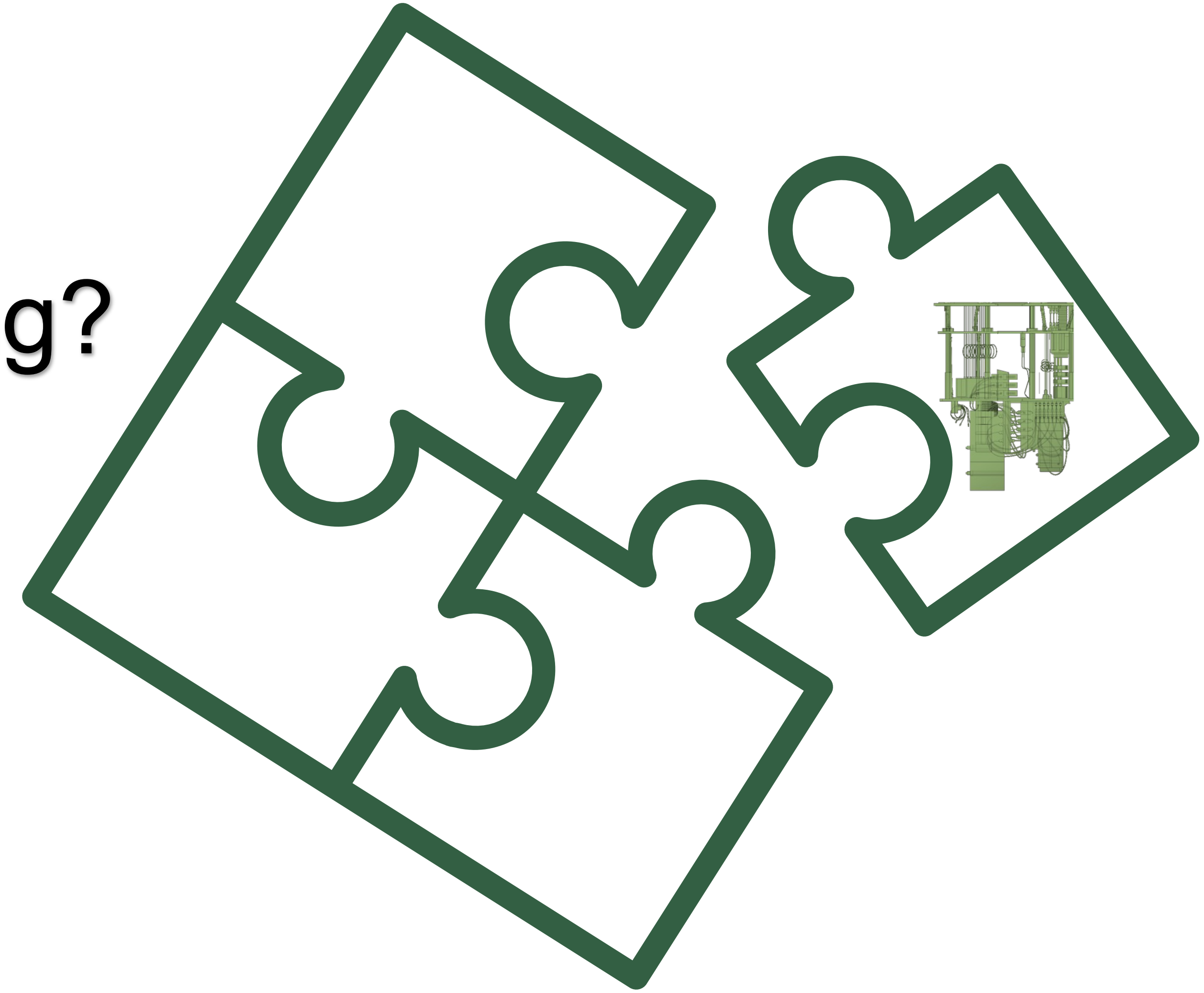
Physics Division, Oak Ridge National Laboratory

Why Quantum Computing?



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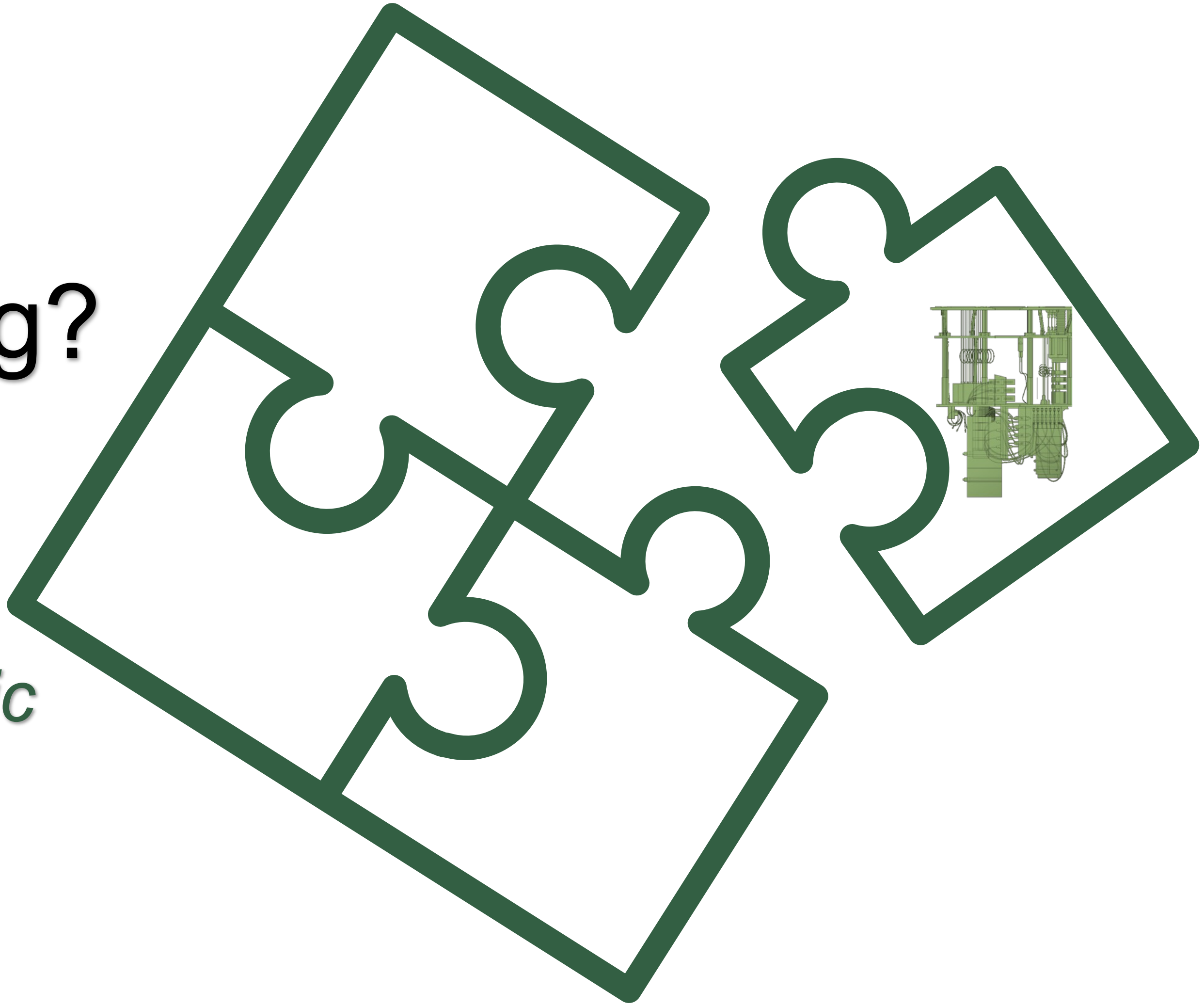
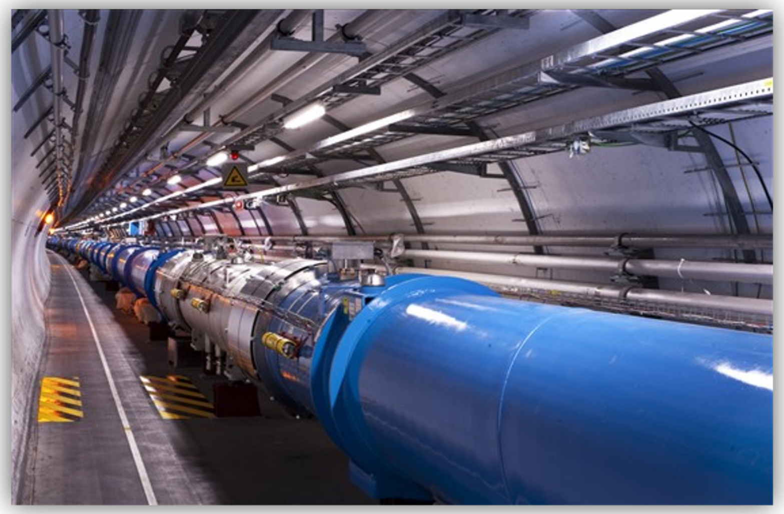


A fresh approach to scientific computing in HEP/NP

Experimental High Energy/Nuclear Physics

TRIUMF
Canada

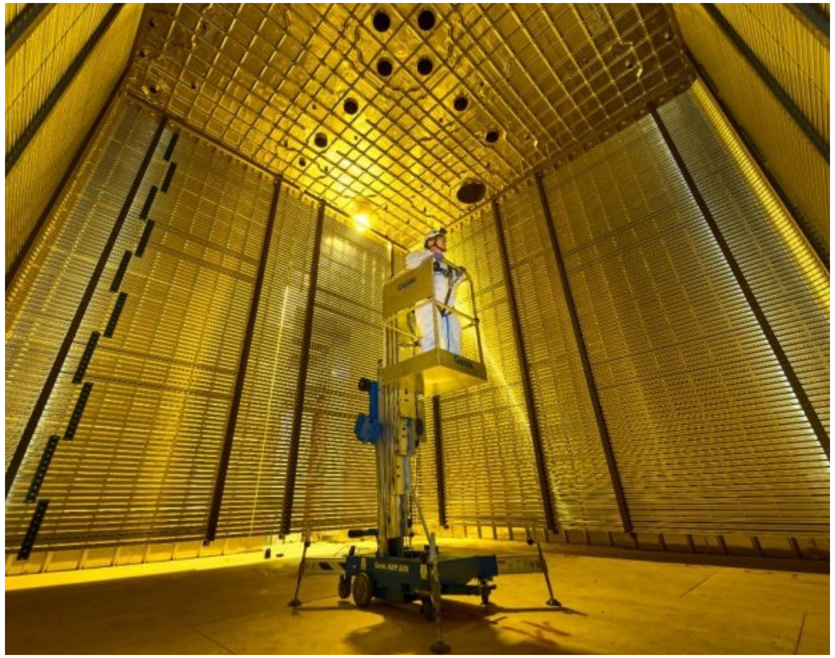
DUNE (Neutrino Experiment)
USA



Large Hadron Collider
(Particle Accelerator)
Switzerland

Experimental High Energy/Nuclear Physics

TRIUMF
Canada



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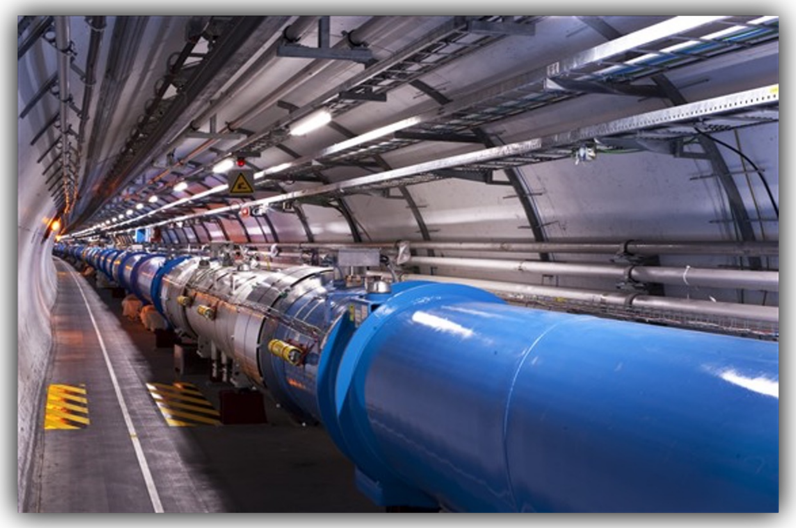


Large Hadron Collider (Particle Accelerator)
Switzerland

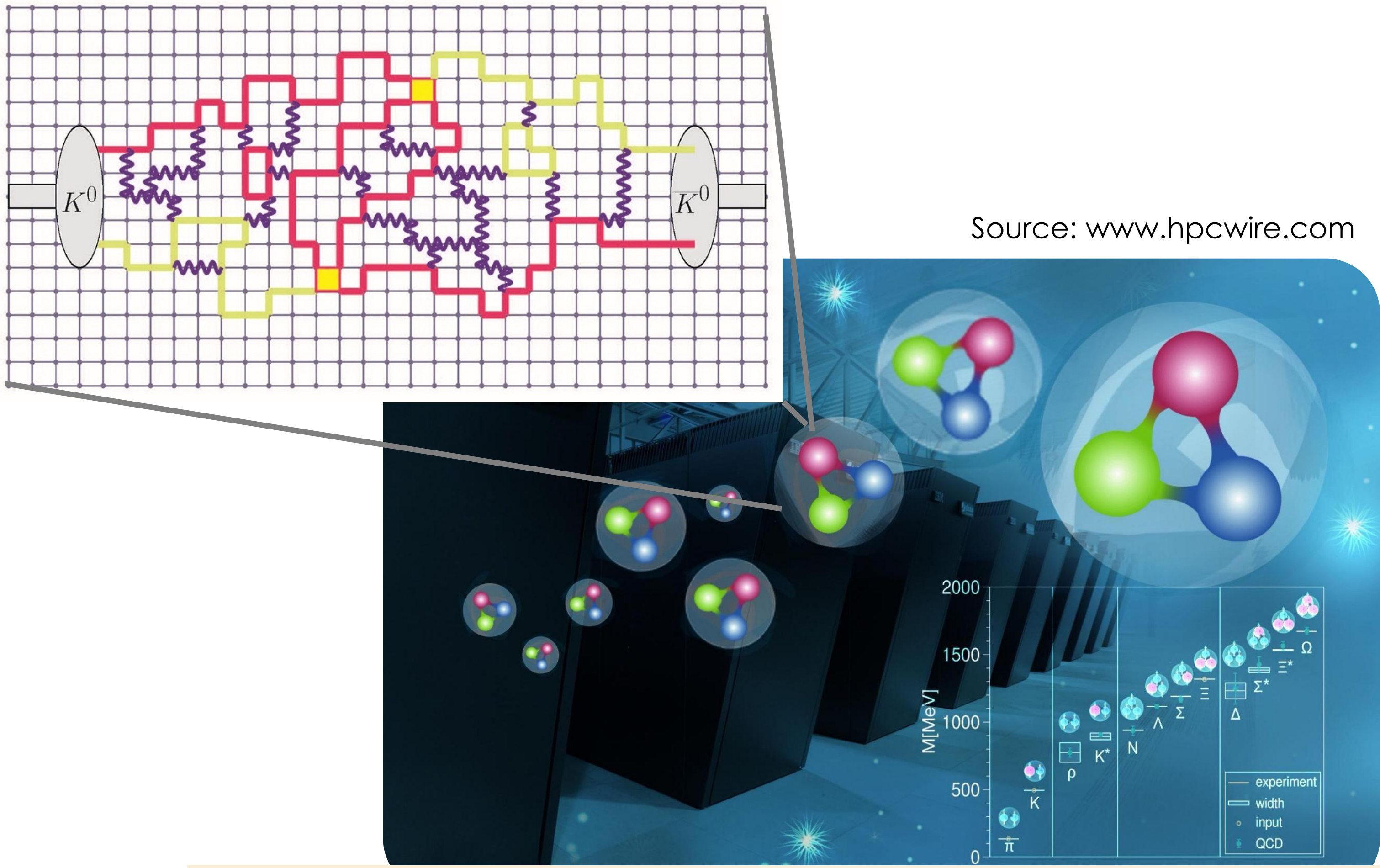
Large, complex datasets that pose a challenge to conventional information processing systems

but also…

In lattice QCD computations, continuous space-time is replaced with a four-dimensional lattice, each site corresponding to a specific point in space and time.

- We study quantum objects that possess some interesting properties - **such as entanglement and superposition**.
- Features that make it difficult to study – **even with current information processing techniques!**
- Lattice QCD calculation require thousands of node-hours at supercomputing facilities to simulate the building blocks of an atom at the scale of ~0.01 fm.

Source: www.hpcwire.com



If the spacing between lattice points is reduced by a factor of two, the computational time required to solve this new problem will be a hundred times greater!

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So what about using quantum computers to study quantum systems?

" Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy"

– Richard Feynman

A simple, yet powerful idea.

The Power of Quantum Computing

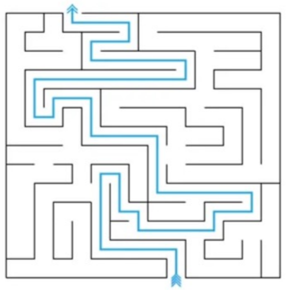
$$|\psi\rangle^{(3)} = \alpha|000\rangle + \beta|001\rangle + \gamma|010\rangle + \delta|011\rangle + \cdots$$

2^3 simultaneously!

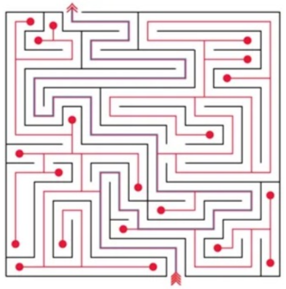
$$\{000, 001, 010, 011, 100, 101, 110, 111\}$$

One at a time!

Cancel out the wrong paths!



Brute-force searc



Quantum Computing

- **Exponentially large Hilbert space**
- **Entanglement**
- **Superposition**
- **Interference**

With only 273 qubits, we can represent more basis states than the number of atoms in the universe!

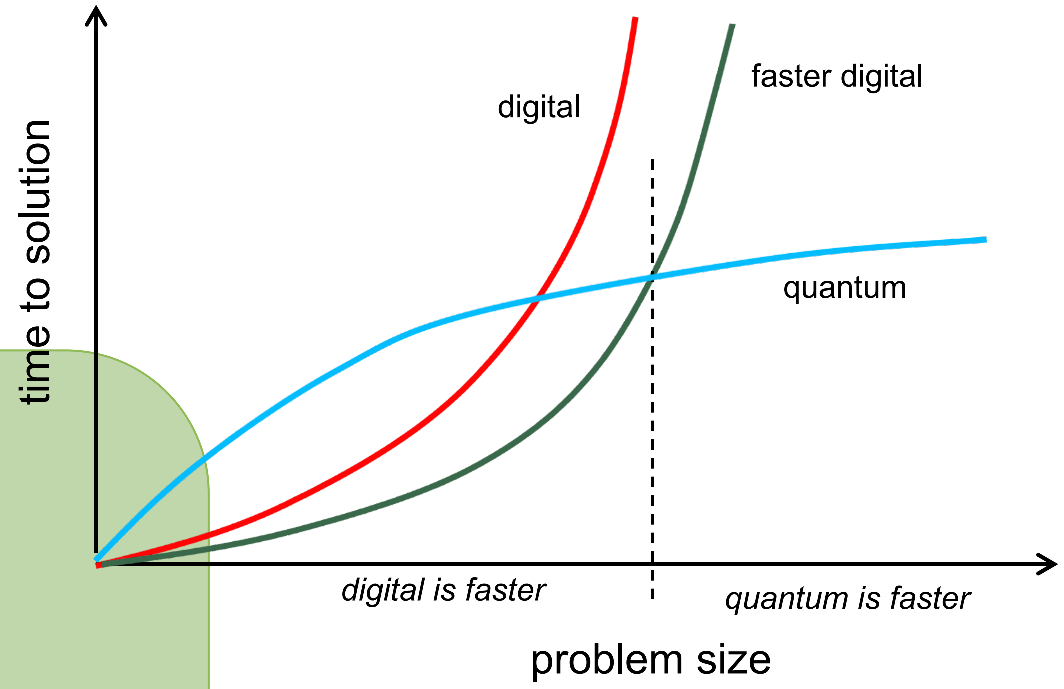
But the true power of quantum computing comes from entangling qubits together…

Allowing us to evaluate multiple configurations in parallel

To manipulate accessible states and cancel out outcomes that are not relevant to our problem.

The Power of Quantum Computing

Quantum computers have the potential to accelerate some difficult tasks



Quantum Computing

- **Simulation of atoms, molecules, materials and quantum fields.**
- **Find hidden subgroups/periodicity.**
- **Function inversion/search.**
- **Combinatorial optimization.**
- **Sampling complex distributions.**
- **Linear systems, eigenvalues/vectors.**

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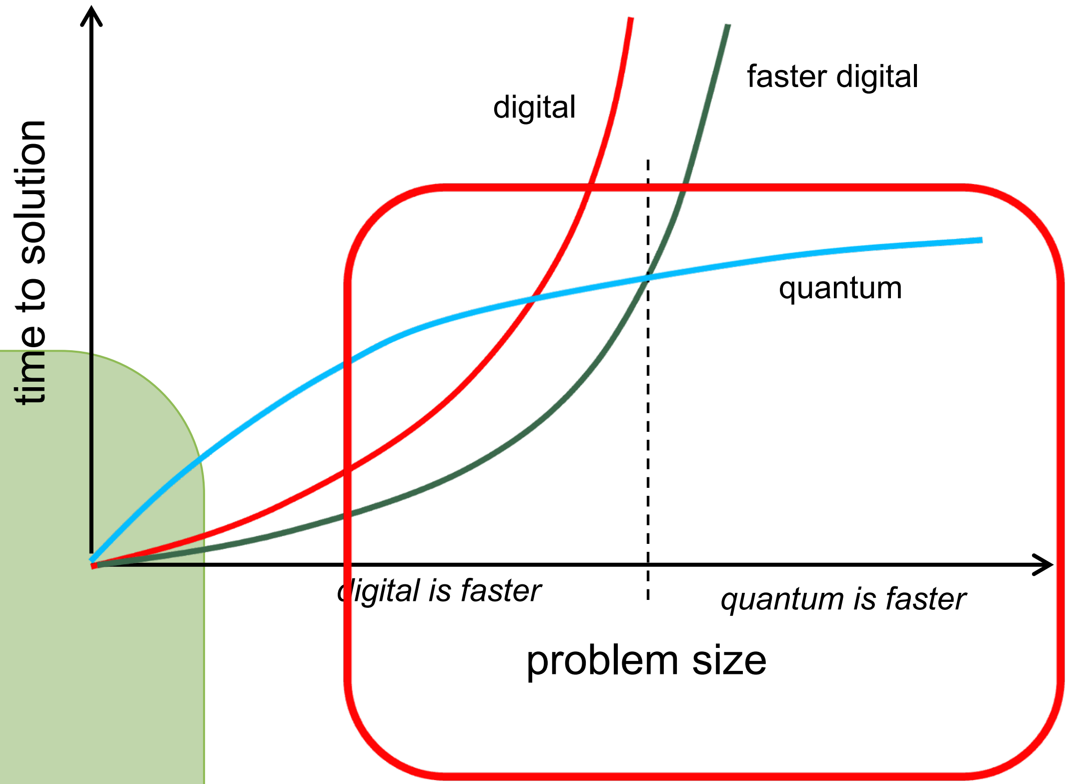
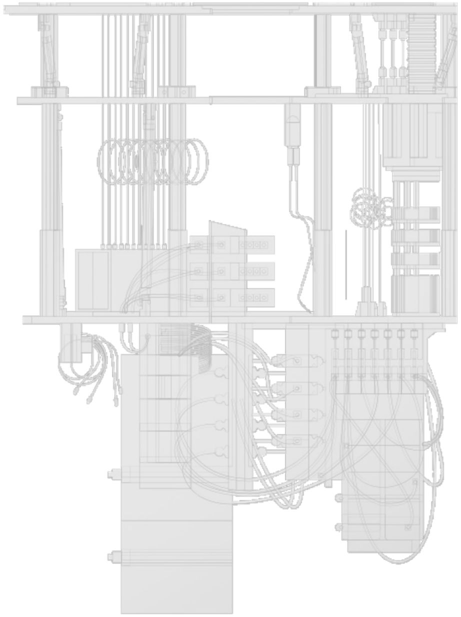


Expected advantage with increasing problem size/complexity.

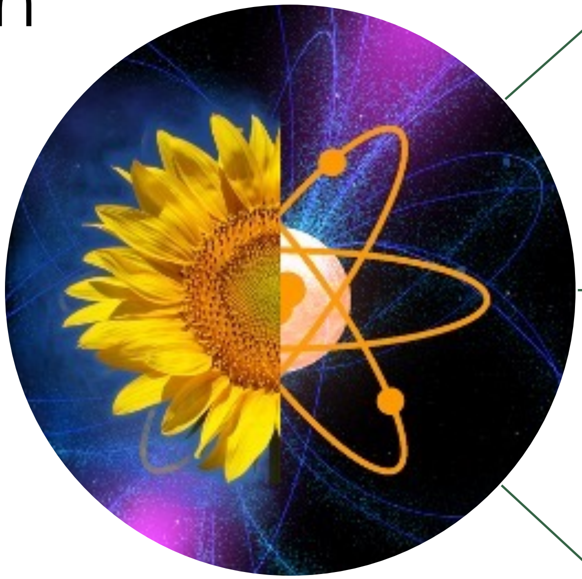
Quantum Computing in the NISQ Era: Is it true? Are we there yet?

- Developed for deployment on **Noisy Intermediate-Scale Quantum (NISQ)** devices.
  - Few qubits (couple hundreds),
  - Noisy,
  - Low gate fidelity – limits the number of operations that can be executed.
- Applications spurred by the release of Qiskit, Xanadu's PennyLane / Google's Tensorflow.
- **Co-design**:
  - *Algorithmic development/research is adapting to match the pace of hardware development.*
- Motivated by access to **cloud-based** NISQ processors and commercial applications.
- Hybrid frameworks to leverage benefits of both classical and quantum computing - ***variational quantum circuits***.



Quantum Information Science: Beyond Quantum Computing

Quantum Information Science



Networks

- Develop enabling science & technology for a future continental-scale quantum internet.

Sensors

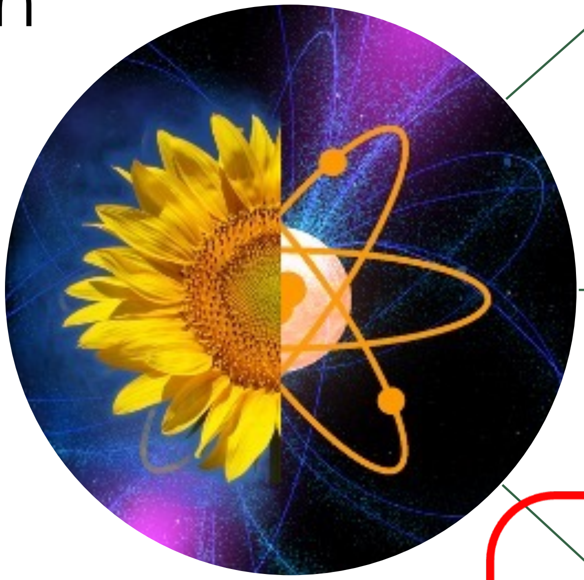
- Develop quantum sensors that perform better than any classical equivalent to deliver new scientific discoveries and technical breakthroughs.

Computing

- Development of platforms and algorithms to simulate quantum physical processes.
- Accelerating quantum information processing (including QML).

Quantum Information Science: Beyond Quantum Computing

Quantum Information Science



Networks

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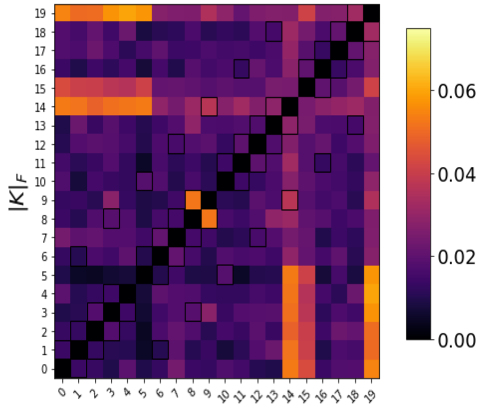
The topic of this talk!

Quantum Computing at ORNL

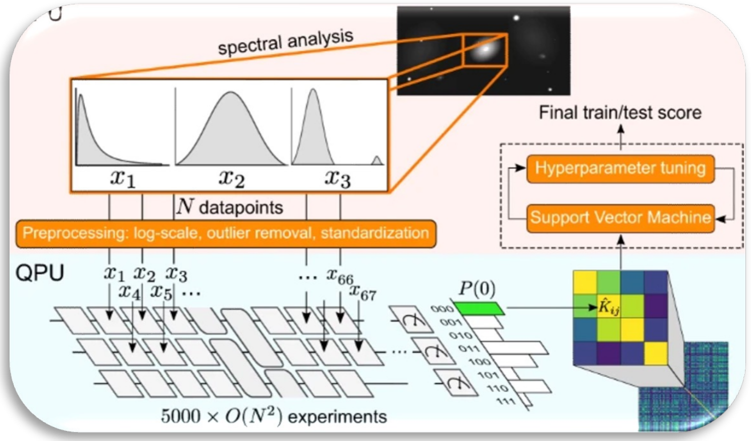
- Broad range of research areas:
  - Quantum physics simulation, machine learning, combinatorial optimization.
  - Software libraries, compilers, simulators.
  - Hardware characterization and error mitigation.
- Simulations for first demonstration of quantum supremacy. **Nature 574, 505-510 (2019) DOI: 10.1038/s41586-019-1666-5**
- First simulation of nuclear physics over cloud computer. **PRL 120, 210501 (2018) DOI: 10.1103/PhysRevLett.120.210501**
- First single source, hardware-agnostic HPC + Q programming framework.

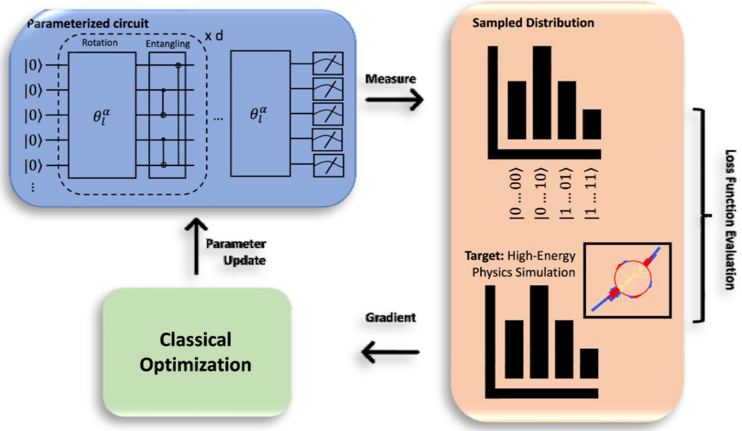


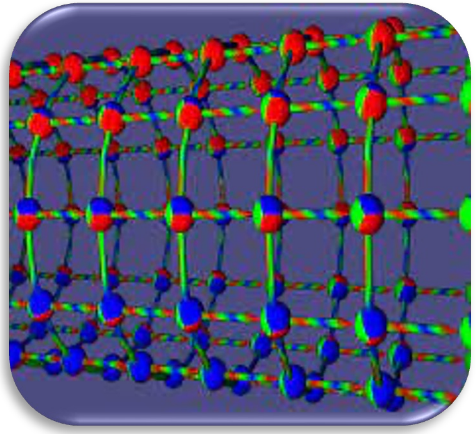
Readout error correlations in a 10-qubit device

Slide borrowed from Ryan Bennink ☺

Quantum Computing Applications to HEP/NP







Supervised Learning

- Classification based on kernel methods, optimization.

Unsupervised Learning

- Generative modeling, data augmentation.

Field Theory Simulation

- Mapping fields into quantum systems.

Delgado, A., Hamilton, K. E., *et al.* **Quantum computing for data analysis in high energy physics**. arXiv: e-Print: 2203.08805 [hep-ex]

Bauer, C. W., et al **Quantum Simulation for High Energy Physics**, arXiv: e-Print: 2204.03381 [quant-ph]

For a more recent overview from the QC for HEP group + IBM: Di Meglio, Jansen, et al arXiv:2307.03236 [quant-ph]

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Accelerating information processing with quantum machine learning

Quantum Machine Learning?

The main goal of Quantum Machine Learning (QML) is to speed things up by applying what we know from quantum computing to machine learning

Quantum Computing

- Exponentially large Hilbert space
- Entanglement
- Superposition
- Interference

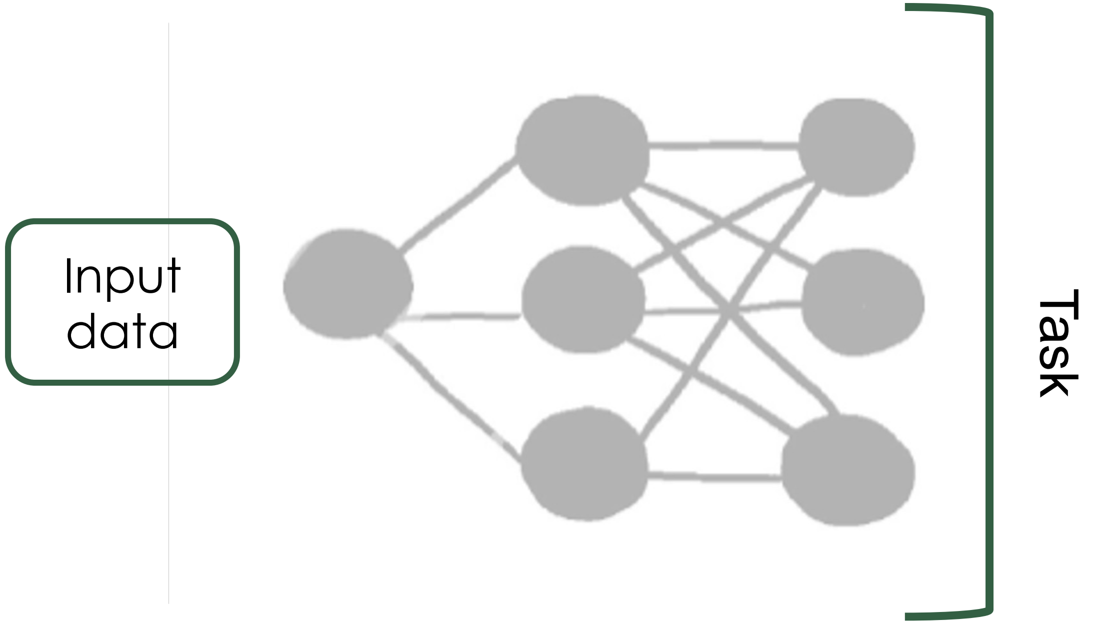
- Linear algebraic problems
- Kernel methods
- Optimization
- Deep quantum learning

Machine Learning

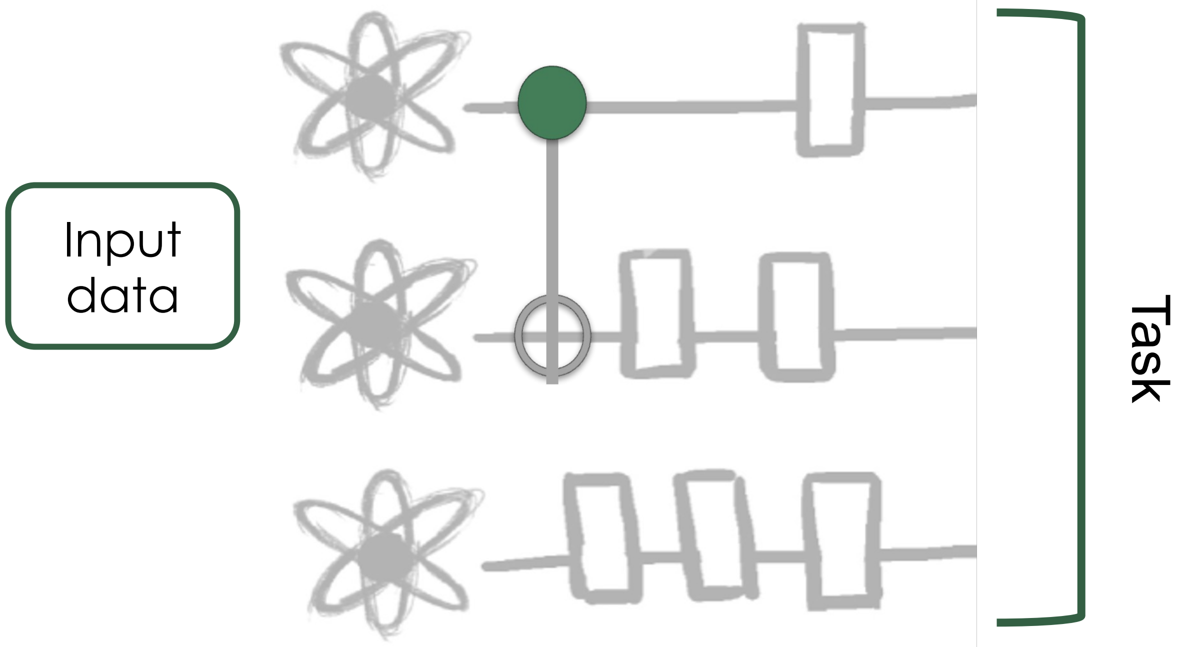
- Inference
- Optimization
- Fitting over a large feature/hyperparameter space

QML takes elements from classical machine learning theory, and views quantum computing from that lens

Quantum Neural Networks



A quantum circuit with quantum gates that rotate or entangle qubits



Benedetti, arXiv:1906.07682

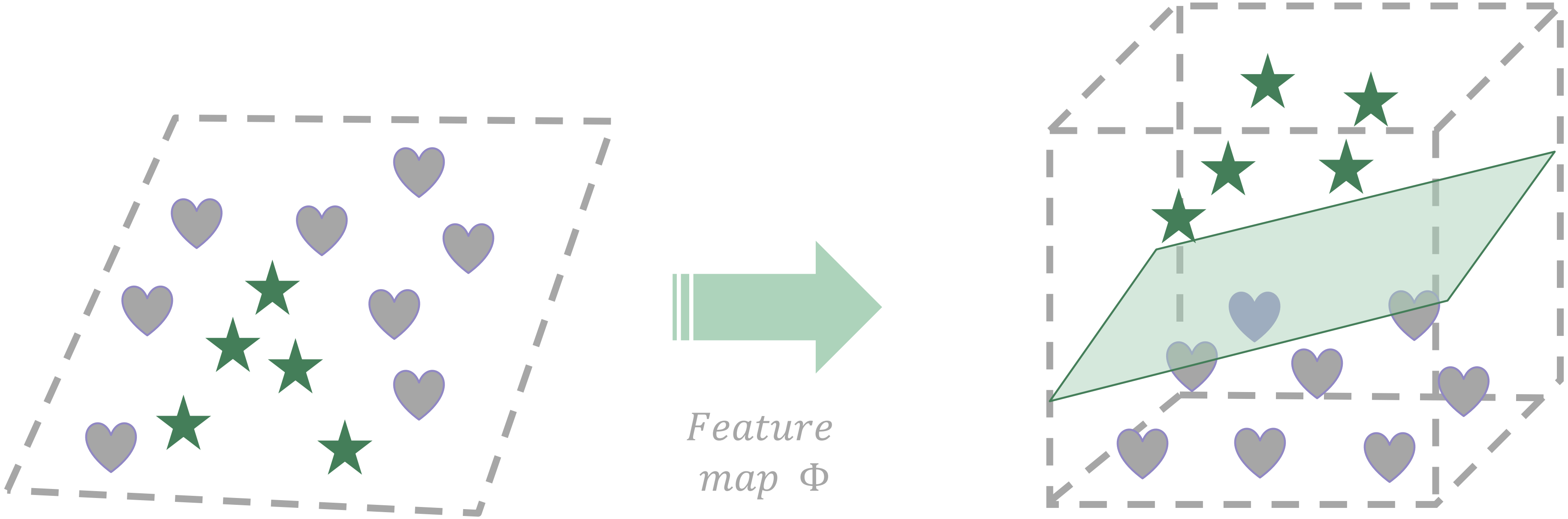
In both cases, learning describes the process of iteratively updating the model's parameters towards a goal

Why QML?

Quantum machine learning models for supervised learning and kernel methods are based on a similar principle.

A high-level overview, for more details check references: *arXiv:2101.11020, Phys. Rev. Lett. 122, 040504 (2019), Nature. vol. 567, pp. 209-212 (2019)*

Kernel Trick



Input Space

Feature Space

Supervised Learning with Kernel-based Quantum Models

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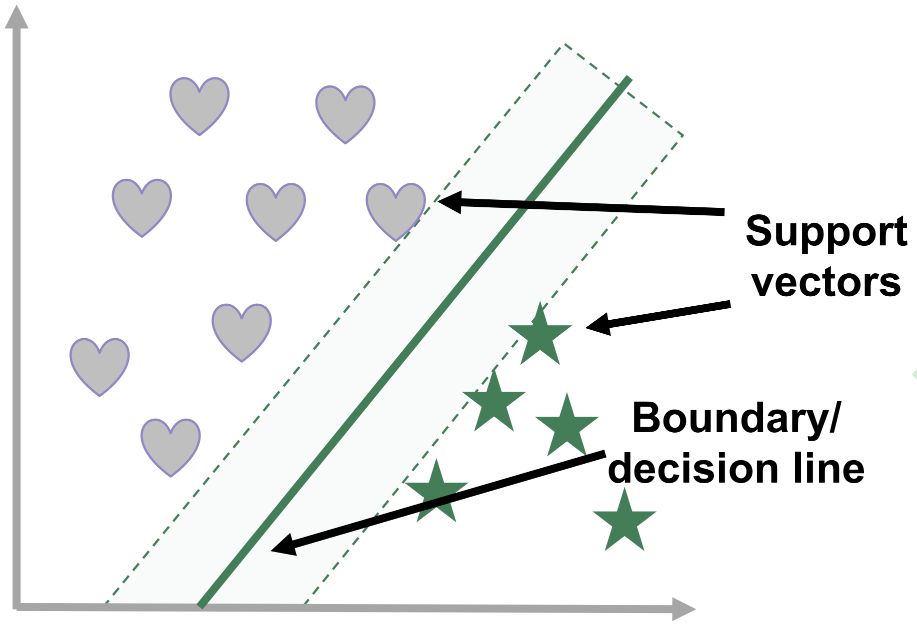
Support Vector Machine

$$\tilde{m}(\vec{s}) = sign\left(\sum_{i=1}^{t} y_i {\alpha_i}^* K(\vec{x}_i, \vec{s}) + b\right)$$



$$L_D(\alpha) = \sum_{i=1}^{t} \alpha_i - \frac{1}{2}\sum_{i,j=1}^{t} y_i y_j \alpha_i \alpha_j K(\vec{x}_i, \vec{x}_j)$$

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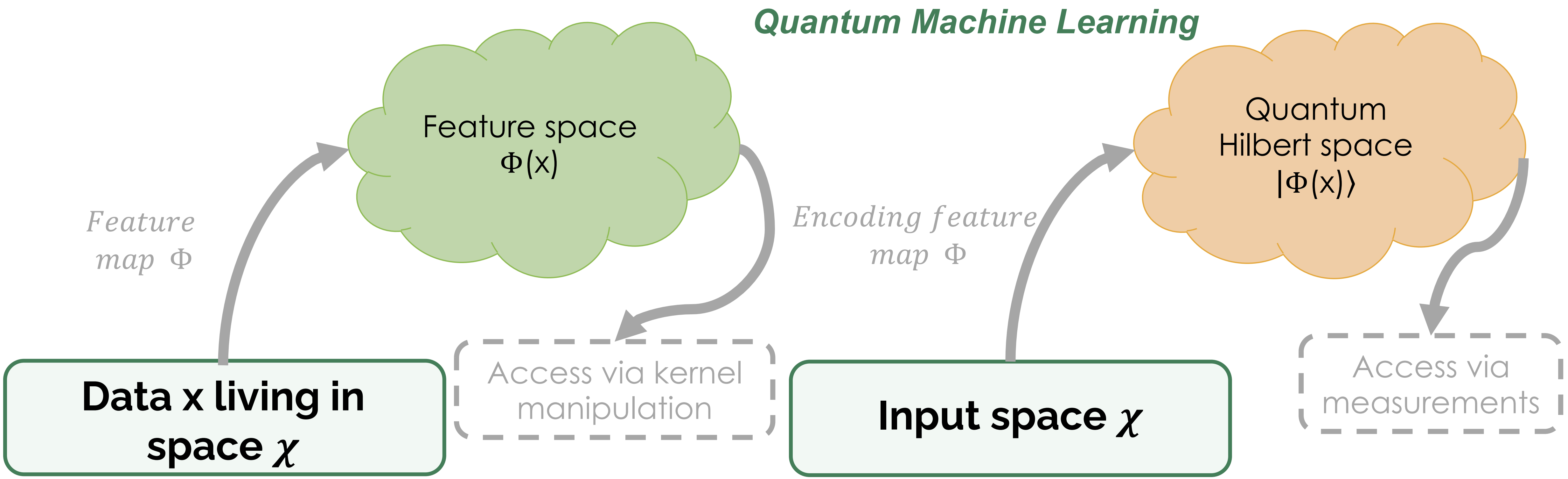
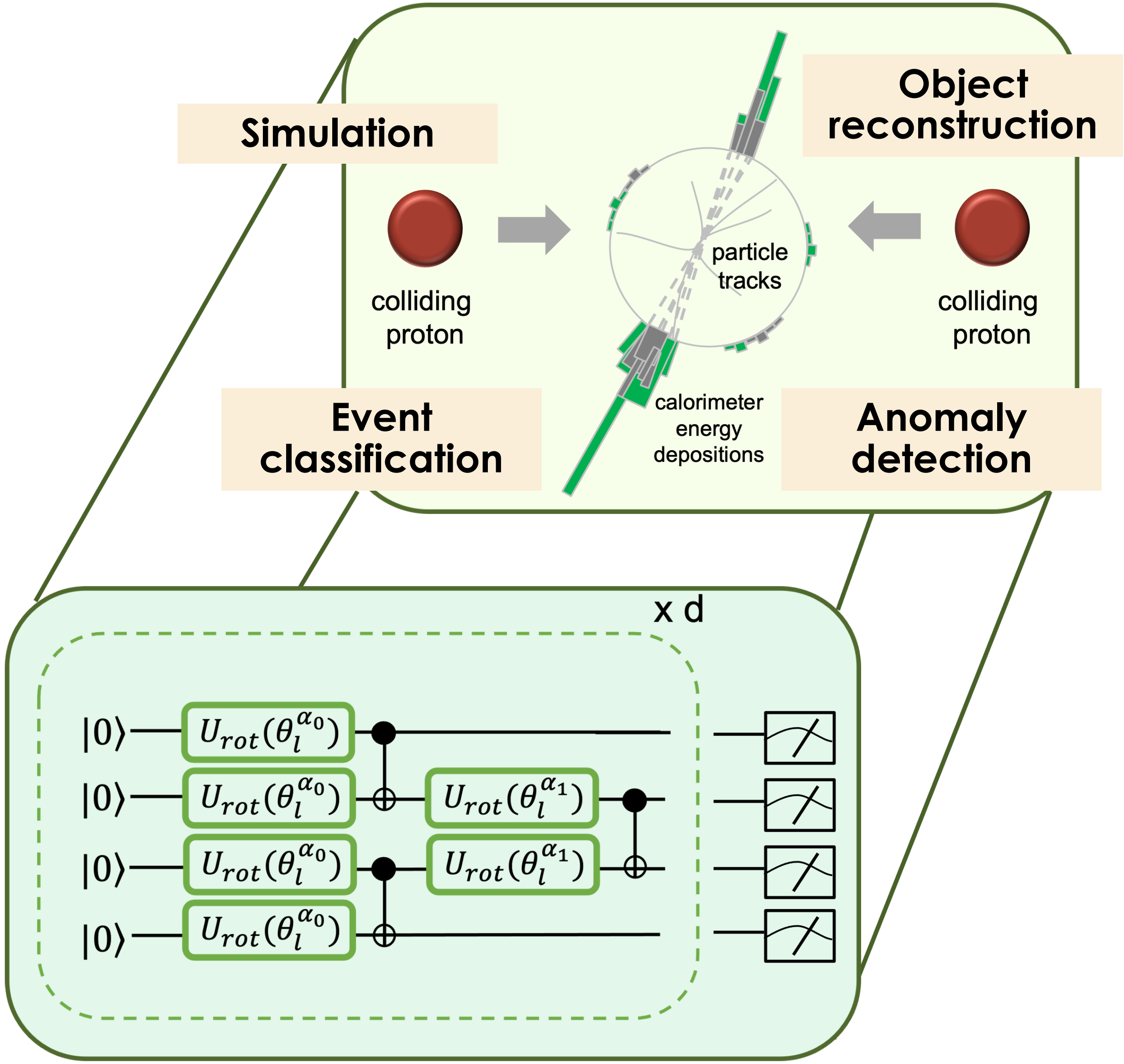


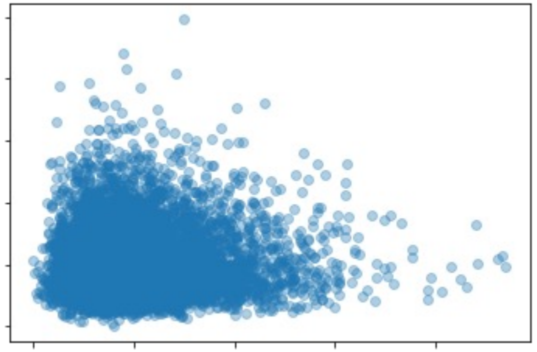
Distribution Modeling with Quantum Circuits

- The PQC model is a quantum unitary with trainable components
  - From a fixed initial state, a PQC prepares a new quantum state
  - The choice of measurements determines what information is extracted
- Generative models aim to learn the underlying distribution of data to generate new points
  - The **Quantum Circuit Born Machine (QCBM)** is built from a PQC
  - It can be trained using non-adversarial methods
  - Can be highly expressive depending on ansatz design
  - The prepared state is projected onto a fixed basis, generating and sampling from a discrete distribution

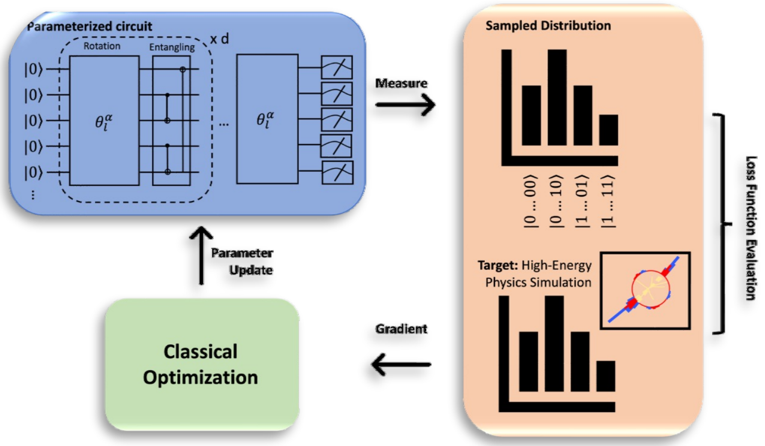


Application: QCBMs in High Energy Physics

- QCBMs can be used to model posterior distributions—they are trained with the objective of preparing a target distribution with high-fidelity
- The target is not encoded in the PQC
- It is defined over a discrete set of bitstrings and can be constructed from multi-dimensional datasets of observations

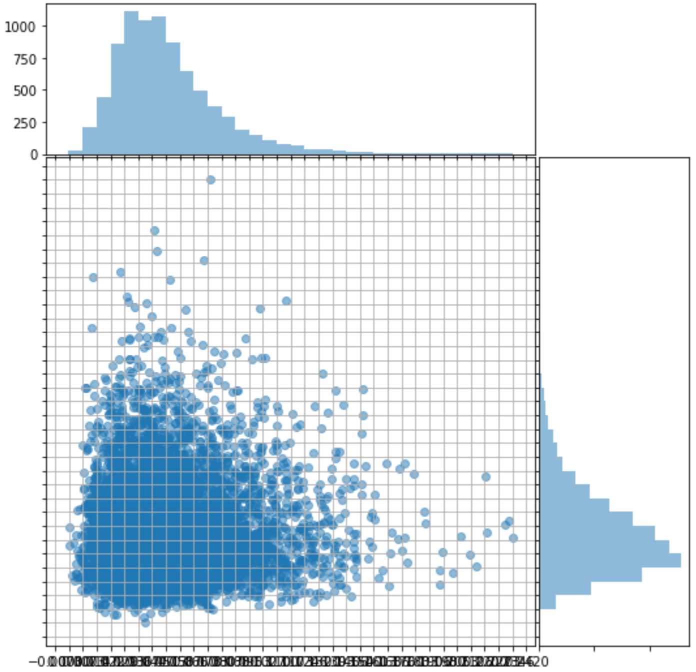


Given a distribution defined on several correlated variables



Construct a target distribution by "pixelating" the continuous space

Concatenate coordinates and normalize intensities



Delgado, Hamilton: arXiv:2203.03578 [quant-ph]

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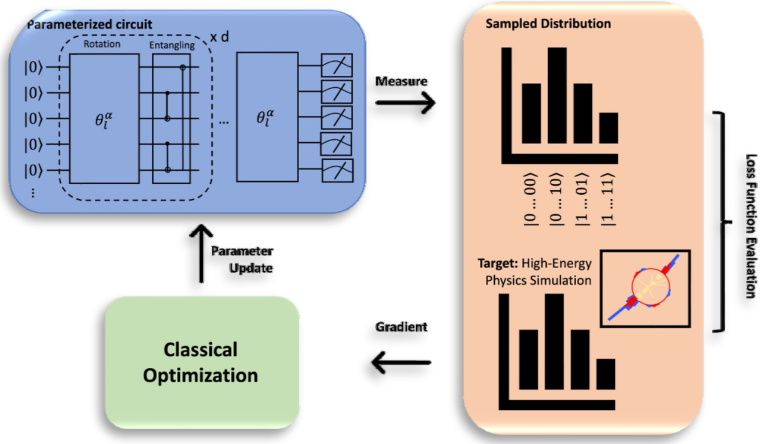
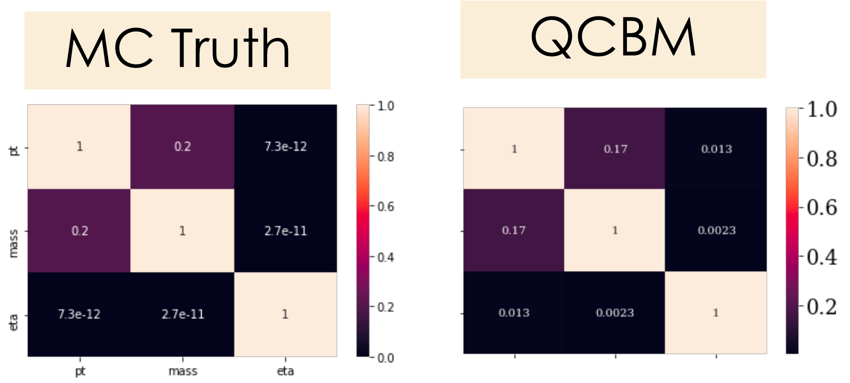
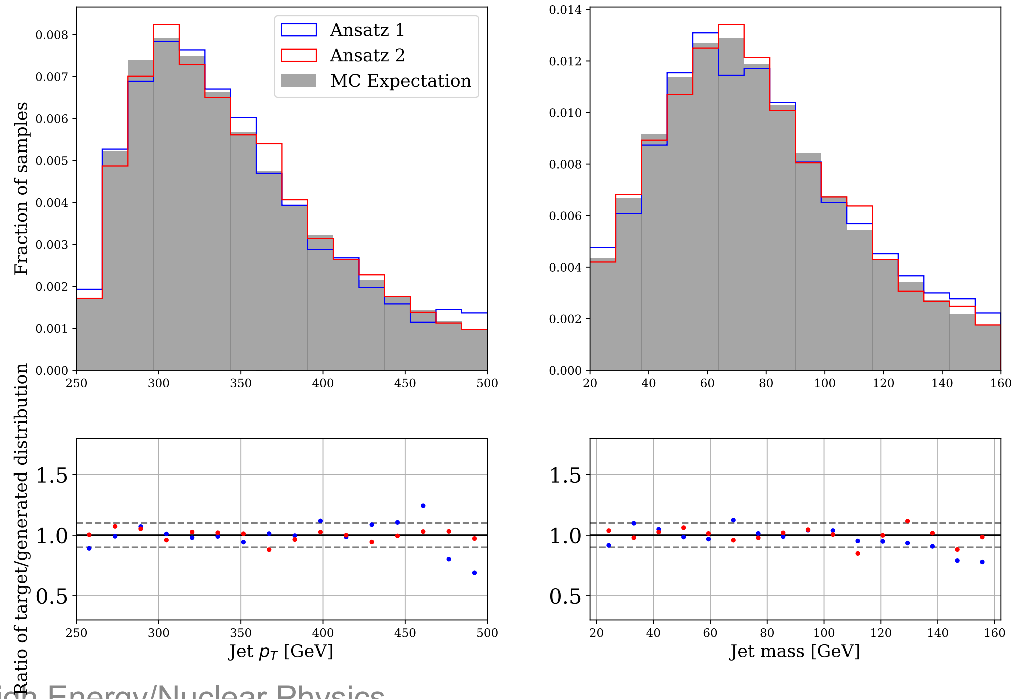


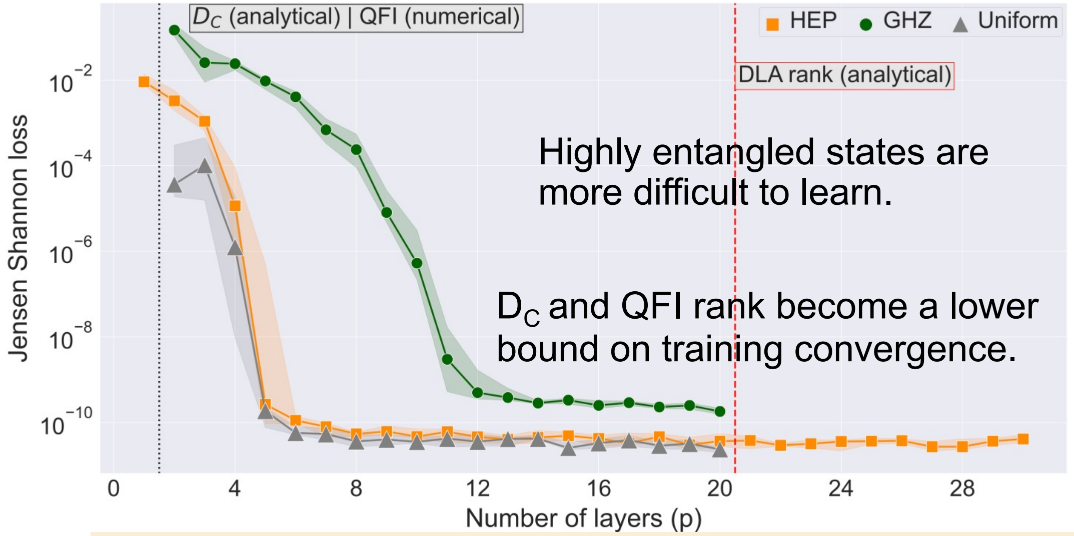




Delgado, Hamilton: arXiv:2203.03578 [quant-ph]

Some comments on QML, with no particular emphasis in HEP/NEP applications

- QNNs are models that are yet to be characterized, i.e., what is the model capacity, what are some good bounds for overparameterization? How do these affect overfitting and generalization?
  - Can we borrow tools from classical ML?
  - What metrics/parameters can we leverage from quantum information theory?
- Current QML paradigm favors QPUs for inference and classical systems for training.
  - Quantum inference presents fewer technical challenges compared to quantum training.
  - Quantum training is resource-intensive and anticipated to necessitate the power of HPC.
- Quantum data is a prerequisite for leveraging the advantages of quantum inference.



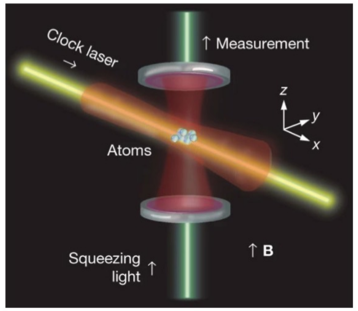
Delgado, Rios, Hamilton: arXiV:2307.03292 [quant-ph]

Our goal: Place ORNL at the forefront of HPC/Quantum applications (from the algorithmic/software perspective)

Can we re-evaluate our current experiments in BSM searches/precision measurements?

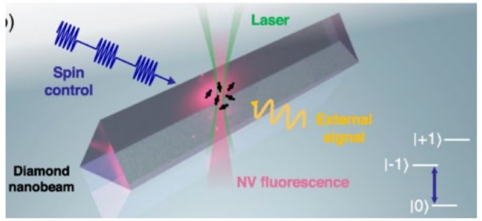
- Recent developments in quantum sensing have inspired novel ideas for dark matter detection through quantum enhanced techniques.
  - Quantum sensors are able to detect very small changes in motion, electric and magnetic fields.
- Open questions:
  - Could QS complement BSM searchers at large-scale facilities such as the LHC?
  - Can we couple quantum algorithms to quantum devices?

entanglement-enhanced atomic sensors



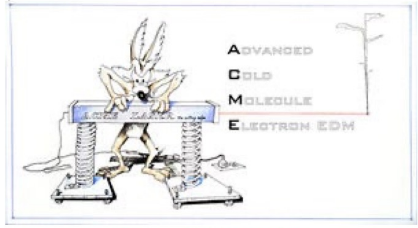
[Nature **588**, 414 (2020)]
[arXiv:2106.03754 (2021)]

NV centers in diamond



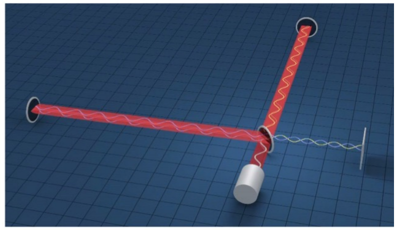
[PRX **10**, 031003 (2020)]

precisions measurements with molecules



[*Science* **343**, 269 (2013)]
[*Nature* **562**, 355 (2018)]

interferometry



[Phys. Rev. Lett. **123**, 231107 (2019)]
[Phys. Rev. Lett. **124**, 171102 (2020)]

quantum sensing review:
[*Rev. Mod. Phys.* **89**, 035002 (2017)]

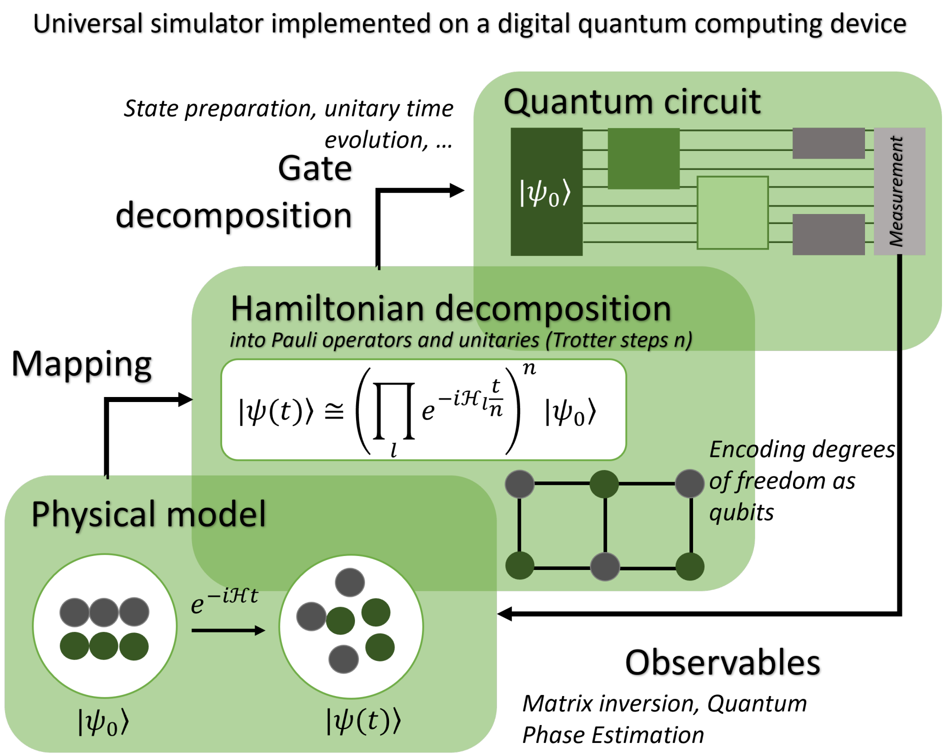
Simulating Quantum Physical Processes

Hamiltonian Simulation in Digital QC

1. State Preparation
   - Ground state or excited state of the Hamiltonian being simulated.
   - Mapping the degrees of freedom of the Hamiltonian to those of the quantum processor, i.e., Jordan-Wigner transformation, etc.

2. Dynamic evolution
   - Usually involves a process called Trotterization.

3. Measurement and post-processing
   - By taking the expectation value of an operator, etc.

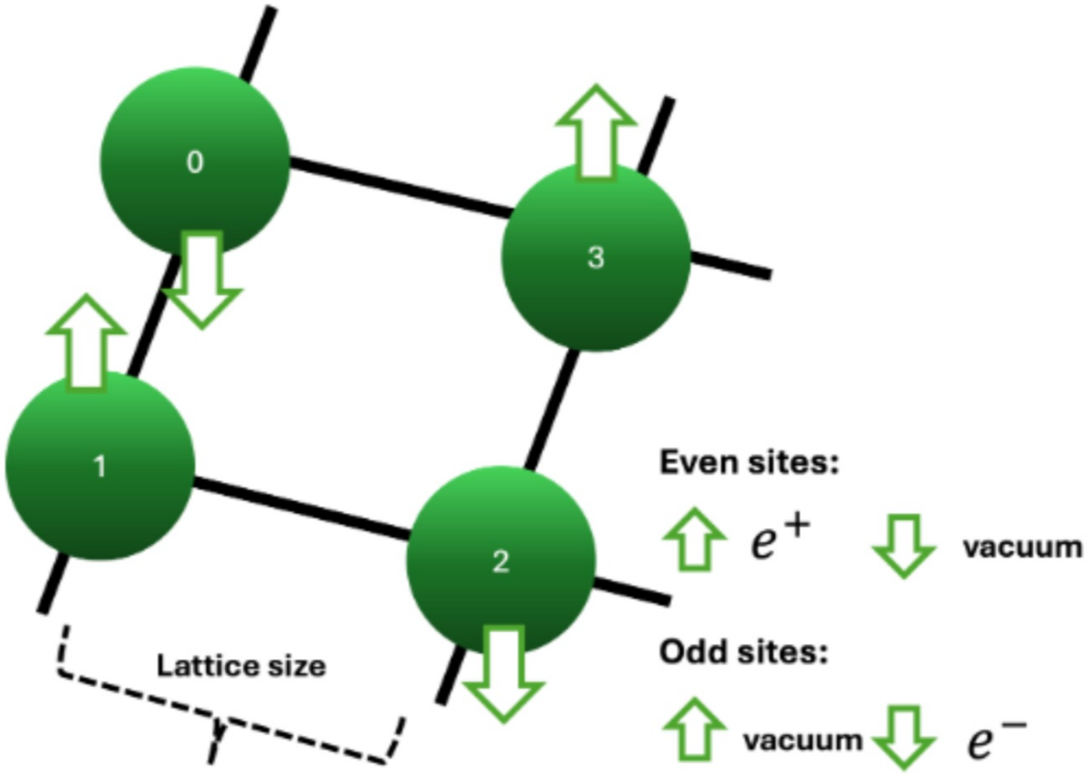


An example: The Schwinger model – Vacuum State Preparation

- 1+1D quantum field theory of QED.
- Used extensively in QC applications due to several features of interest:

  mass gap, charge screening, a chiral condensate, and a topological theta term can be incorporated

1. We start by discretizing the Hamiltonian on a lattice, and using the staggered fermion formulation.
2. Mapping to qubits – Fermionic and gauge field operators.
3. Construct a quantum circuit to evolve the initial state (known) towards the desired state of the H.



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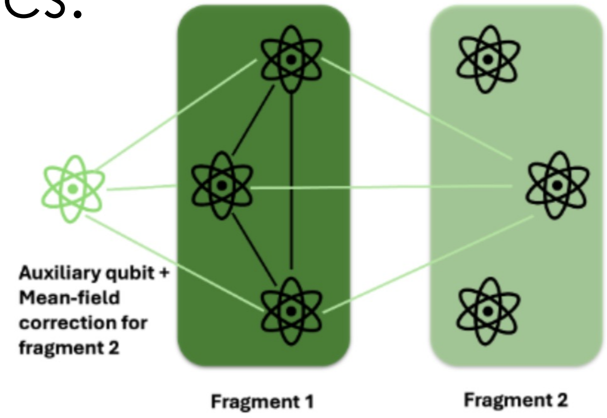
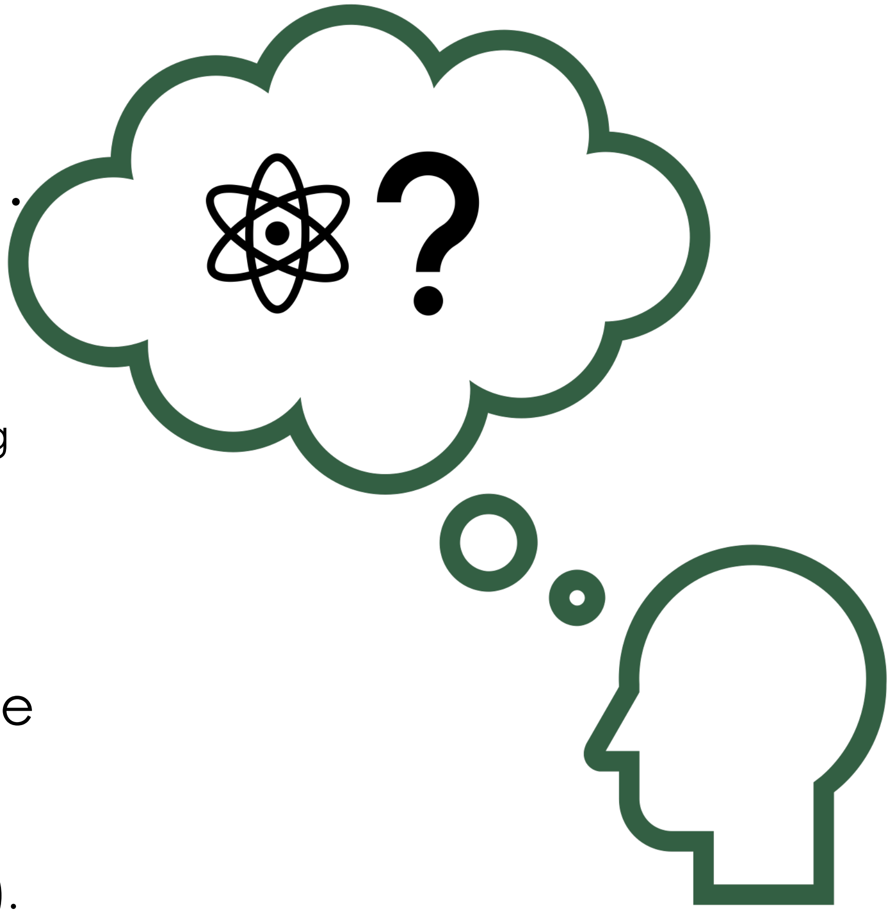
Are we there yet? Can we simulate an interesting system?

- Not quite… lots of resources needed
  - Jordan-Wigner transformation:
    - For a small lattice, with N = 4 sites, we require 4 qubits for fermionic operators + 1 qubit per link (8 qubits total). Not scalable!
  - Relies on "*Trotterization*" for dynamics, necessitating deep and wide quantum circuits.
  - *For state preparation:*
    - *Adiabatic state preparation: Require deep circuits due to slow evolution (the Hamiltonian changes sufficiently slow compared to the energy gap between the ground state and the first excited state),*
    - *VQE: High measurement overhead* to interpret quantum state information.

- But… we can apply many techniques from nuclear physics:
  - Smart ansatz design: Unitary Coupled Cluster (arXiv:2109.15176)
  - Mean-field approximation (arXiv:2309.05693)



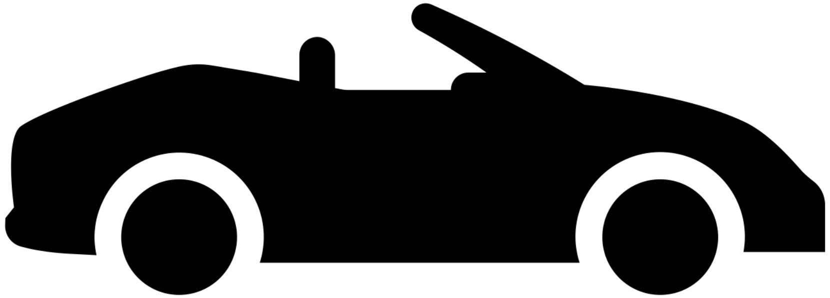
Lessons Learned



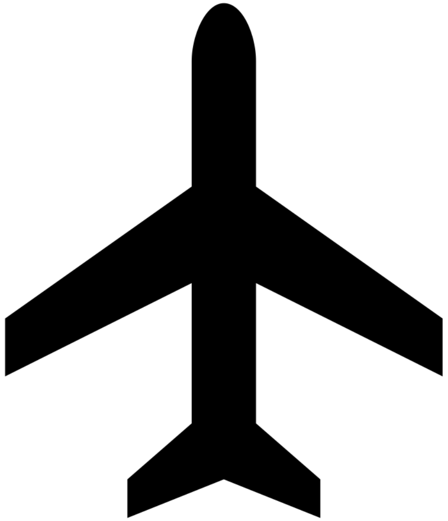
- We've come a long way from one-qubit classifiers and simulating the Deuteron (~5 years).
- Benefited from collaborating with other disciplines:
  - Chemists are leading efforts for Hamiltonian simulation, incorporating domain knowledge (UCC, mean-field approximations, etc.)
  - Trotterization is all about operator algebra (Math!)
  - Computer science for complexity theory and writing pretty code.
- We have to move away from thinking about "what can we do with QC" to "what kind of applications will actually benefit from QC"?
  - Hybrid on the near-term, fault-tolerant in the future (not so far away!).
  - Think about workflows, what computational primitives can be outsourced to quantum processors?
- What tools can we borrow from HEP/Nuclear physics?
  - HPC computing tools,
  - Theoretical tricks.

Will QC ever replace our classical computers?

Think about:

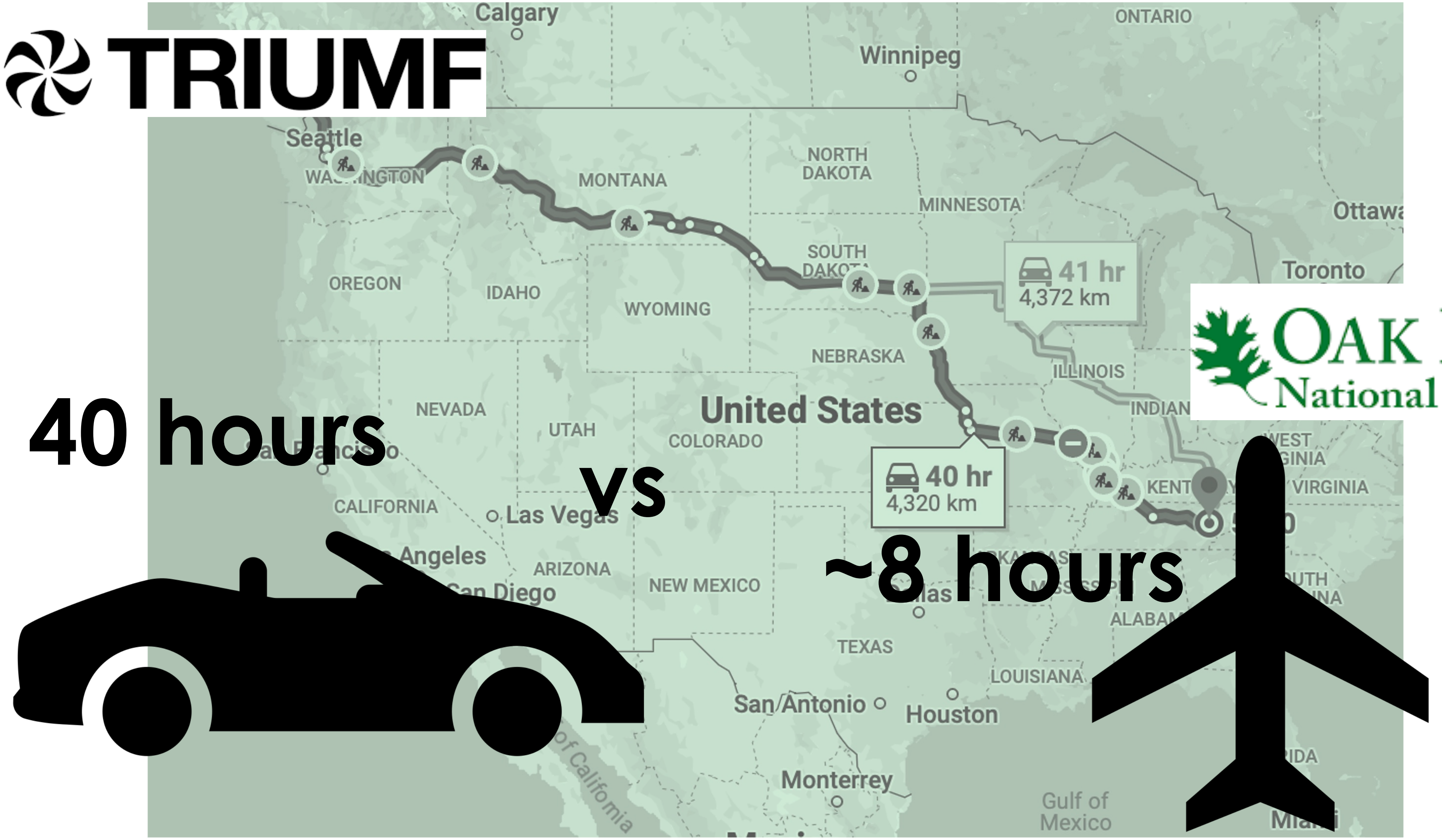


vs



Would you rather drive than flying from TRIUMF to ORNL?

TRIUMF



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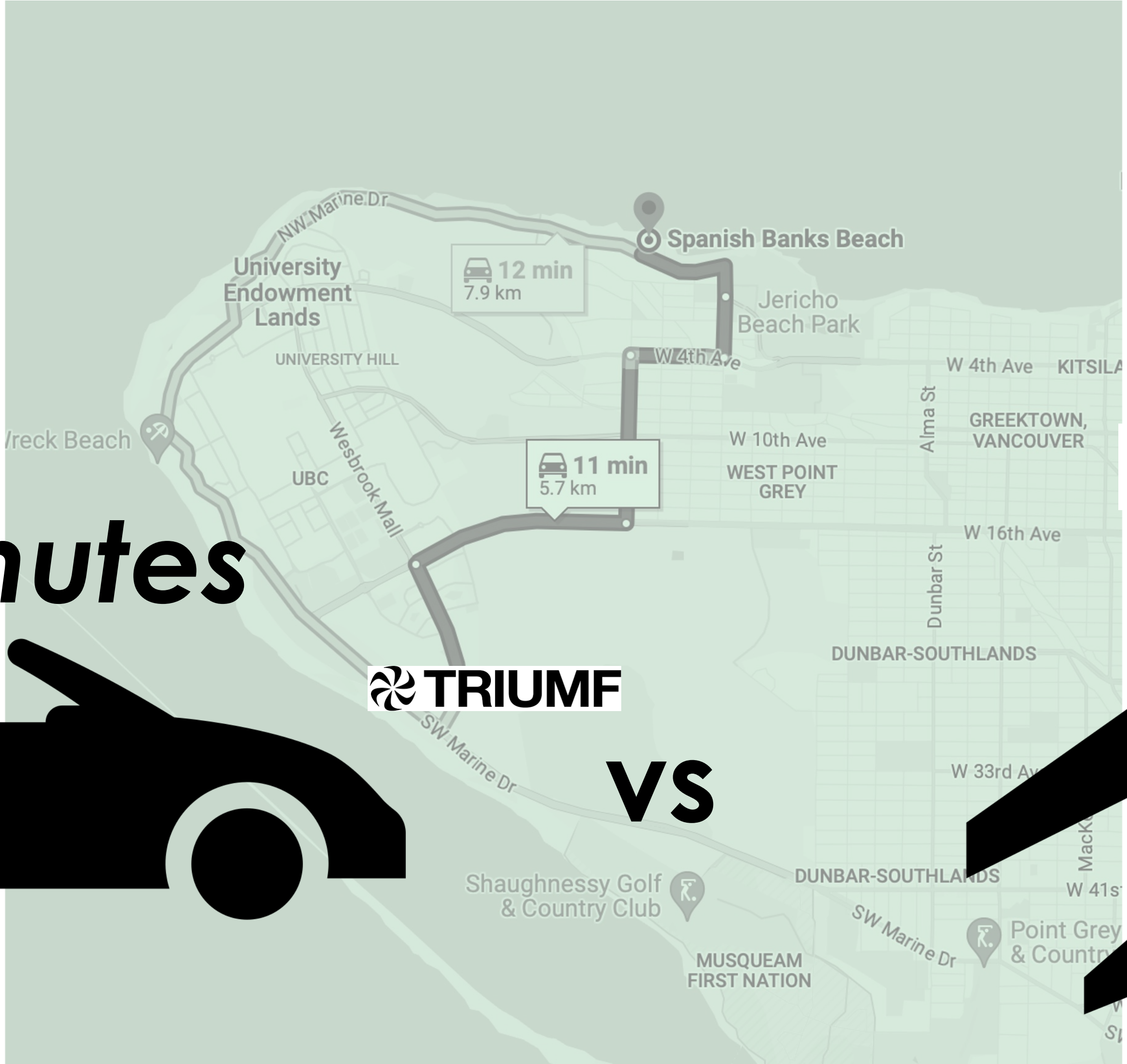
40 hours

vs

~8 hours

Source: maps.google.com

Would you rather drive than flying from TRIUMF to Spanish banks beach?



11 minutes

vs

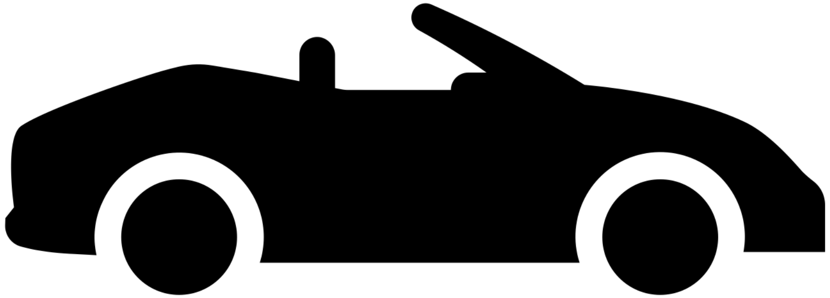
$$\text{Time} = \frac{\text{Distance}}{\text{Speed}} = \frac{5\text{ km}}{800\text{ km/h}} = 0.00625\text{ hours} \approx 0.375\text{ minutes}$$

Source: maps.google.com

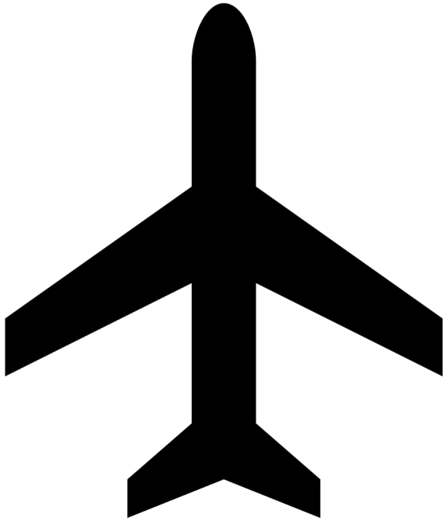
Will QC ever replace our classical computers?

We can think about classical computers as the car and quantum computers as the plane in this analogy…

It depends on where you want to go!



vs



Thank you!

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