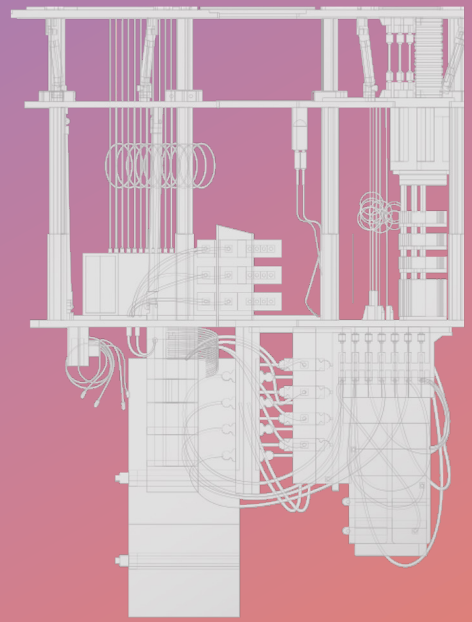
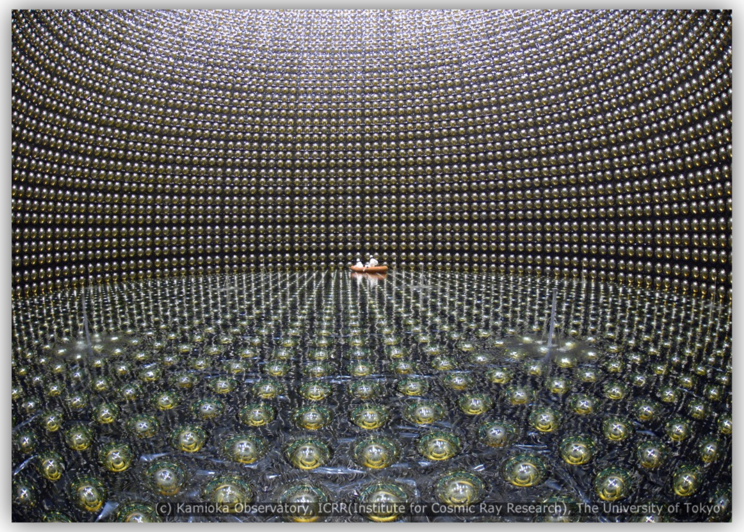
Opportunities in Quantum Information Science and High Energy Physics



Andrea Delgado (she/her/ella)

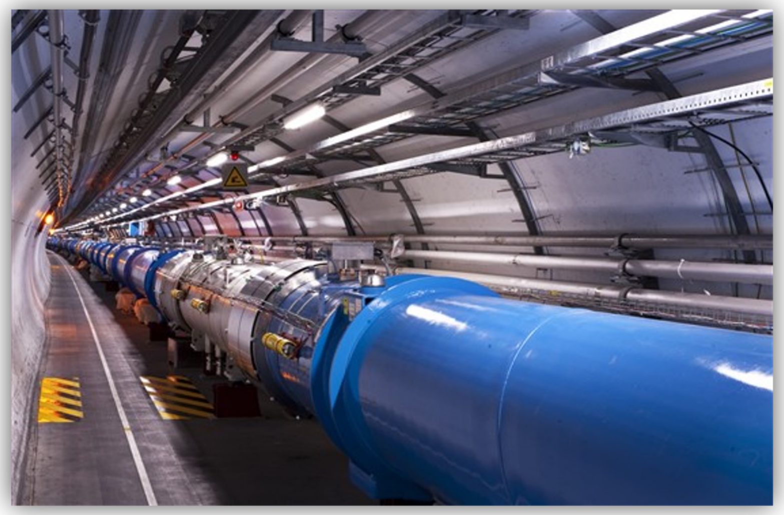
Oak Ridge National Laboratory

Highlights of last couple of decade's experimental HEP Program



Super-Kamiokande (Neutrino Observatory))
Japan, underneath mount Ikeno
First evidence of neutrino oscillation

Tevatron (Particle Accelerator)
Illinois, USA
Top quark discovery



Large Hadron Collider (Particle Accelerator)
Switzerland
Higgs boson discovery

Large, complex datasets that pose a challenge to conventional information processing systems – can Quantum Computing **speed up some computational tasks?**

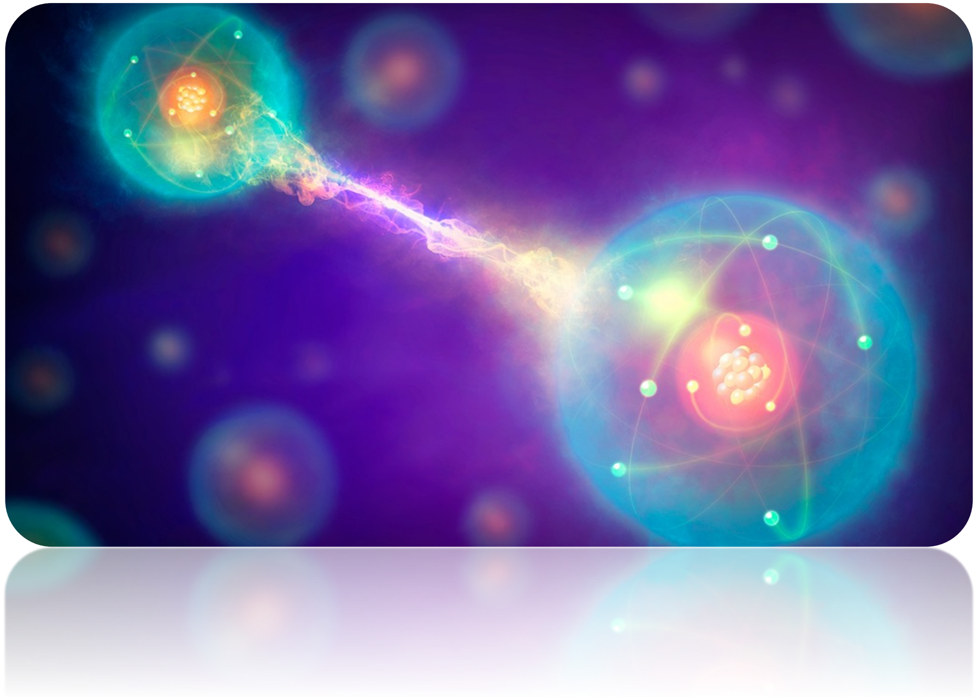
Why Quantum?

“ **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.

... our subject of study is quantum mechanical objects with some interesting behavior ...

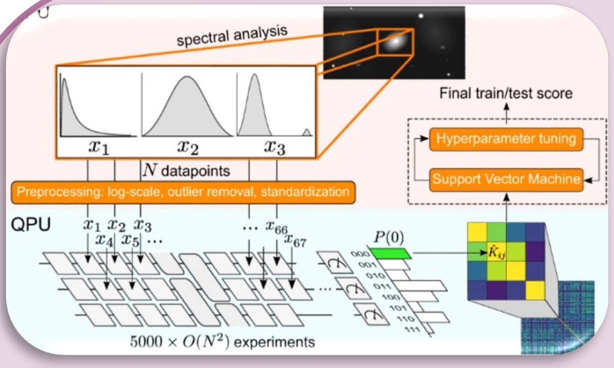


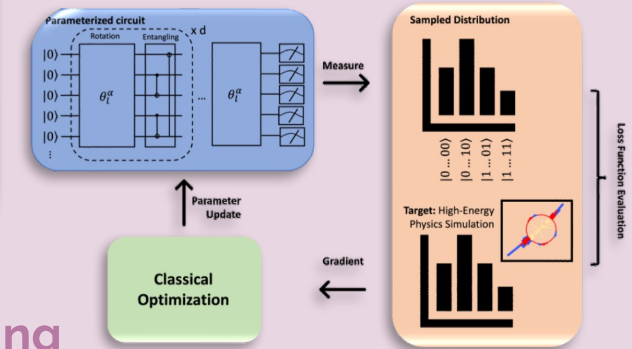
such as entanglement,

superposition, interference

features that make it difficult to simulate with current information processing techniques (lattice QCD, many-body problems).

Quantum Computing Applications in High Energy Physics



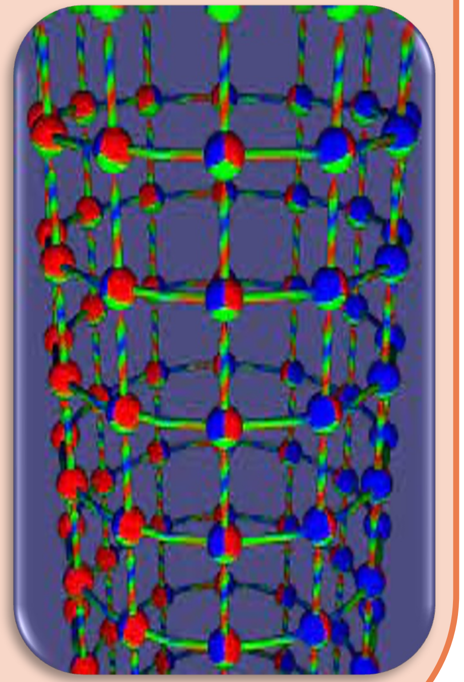


Quantum Machine Learning

- Supervised learning: Classification based on kernel methods, optimization.
- Unsupervised learning: Generative modeling, data augmentation.

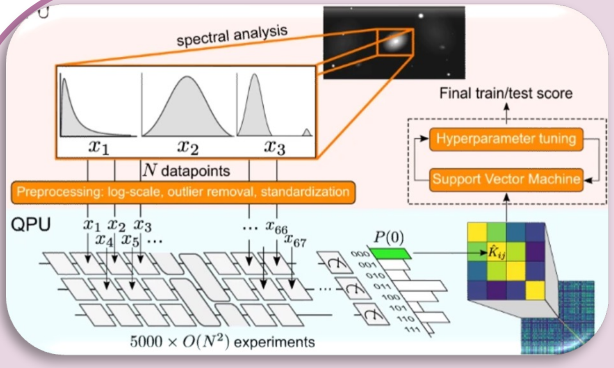
Field theory simulation

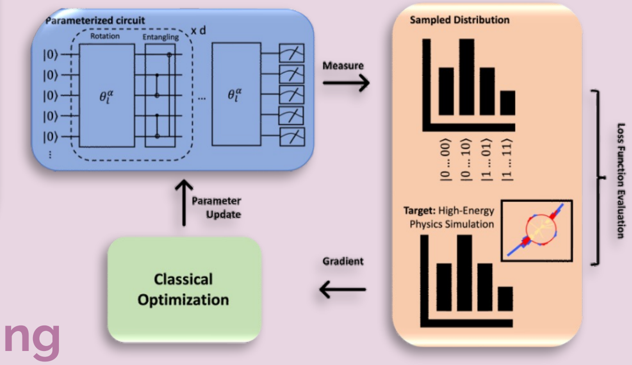
- Mapping fermionic/bosonic degrees of freedom into quantum system.
- Significant overlap with condensed matter.



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

Quantum Computing Applications in High-Energy Physics





Quantum Machine Learning

- Supervised learning: Classification based on kernel methods, optimization.
- Unsupervised learning: Generative modeling, data augmentation.

The focus of this talk

Quantum Machine Learning

The main goal of Quantum Machine Learning (QML) is to apply what we know from quantum computing to machine learning

Quantum Computing

- Exponentially large Hilbert space
- Entanglement
- Superposition
- Interference

Quantum Computing ∩ Machine Learning

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

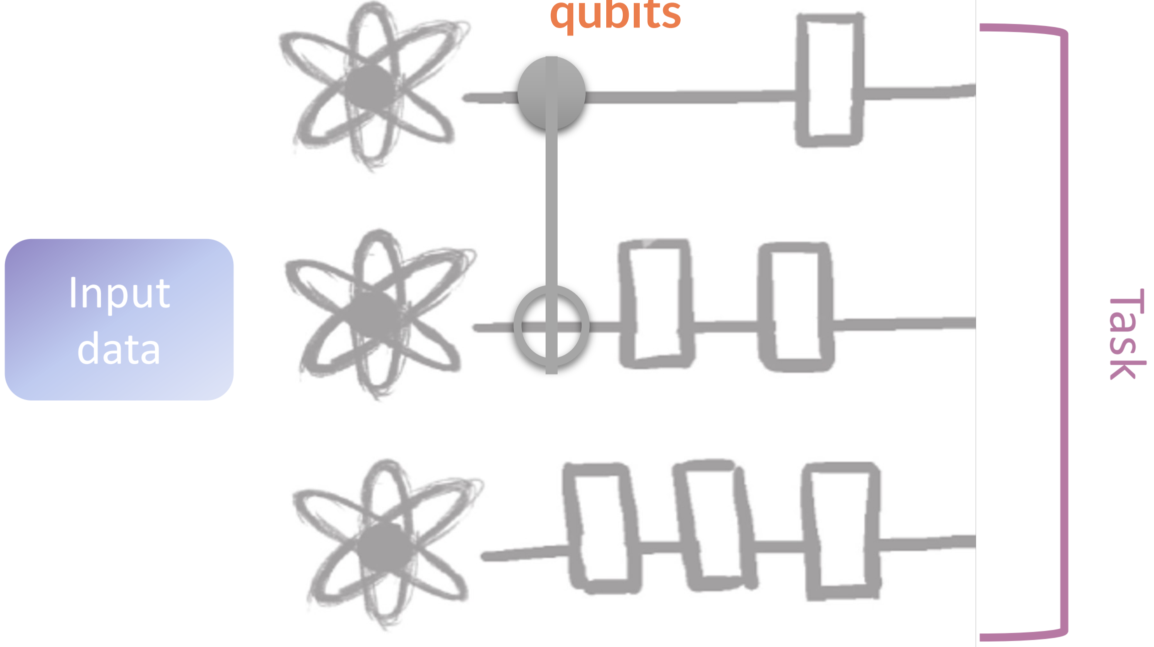
Machine Learning

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

Can we speed up some tasks, better generalization, faster training?

How do QML models compare to ML models?

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

Quantum Machine Learning in the NISQ Era

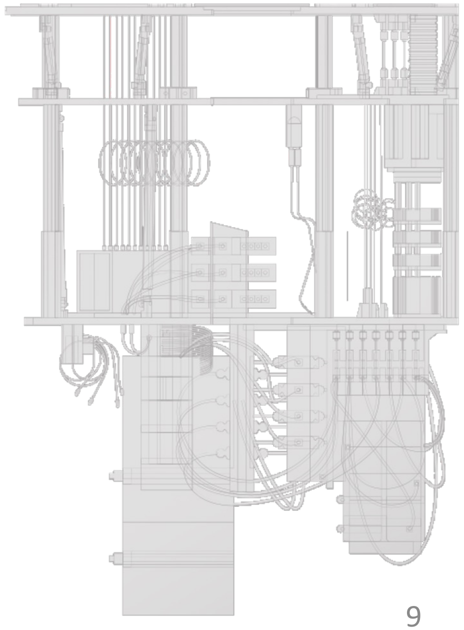
★ Motivated by access to **cloud-based** NISQ processors and commercial applications.

★ Developed for deployment on **Noisy Intermediate-Scale Quantum (NISQ)** devices.
  - Few qubits,
  - Noisy,
  - Low gate fidelity – limits the number of operations that can be executed.

★ Applications in **Quantum Machine Learning (QML)** spurred by the release of Xanadu's PennyLane / Google's Tensorflow.

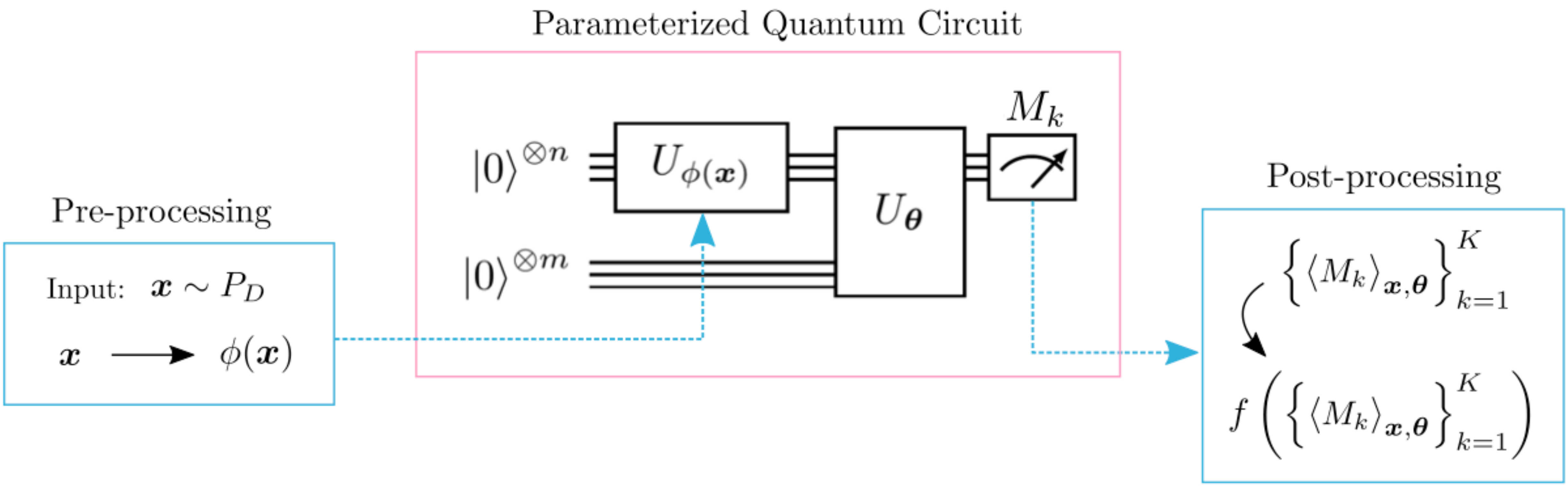
★ **Co-design**:
  - *Algorithmic development/research is adapting to match the pace of hardware development.*

★ Hybrid frameworks to leverage benefits of both classical and quantum computing - ***variational quantum circuits***.



Parameterized Quantum Circuits as ML Models

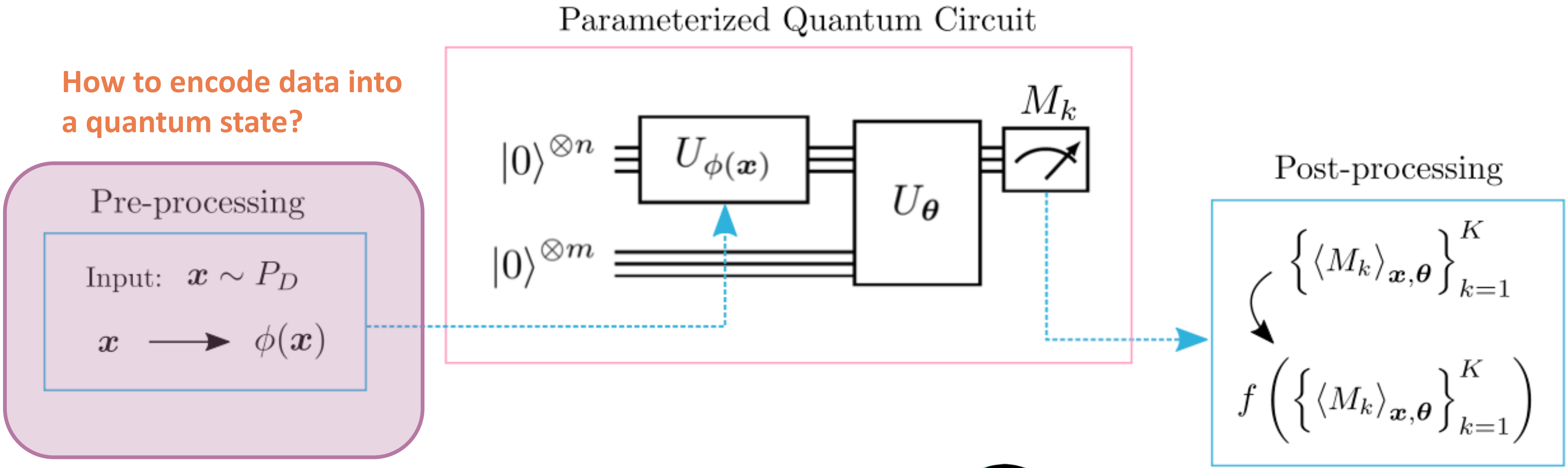
Benedetti, arXiv:1906.07682



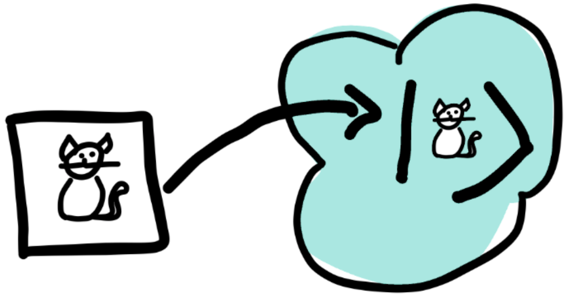
Parameterized Quantum Circuits as ML Models

Benedetti, arXiv:1906.07682

How to encode data into a quantum state?



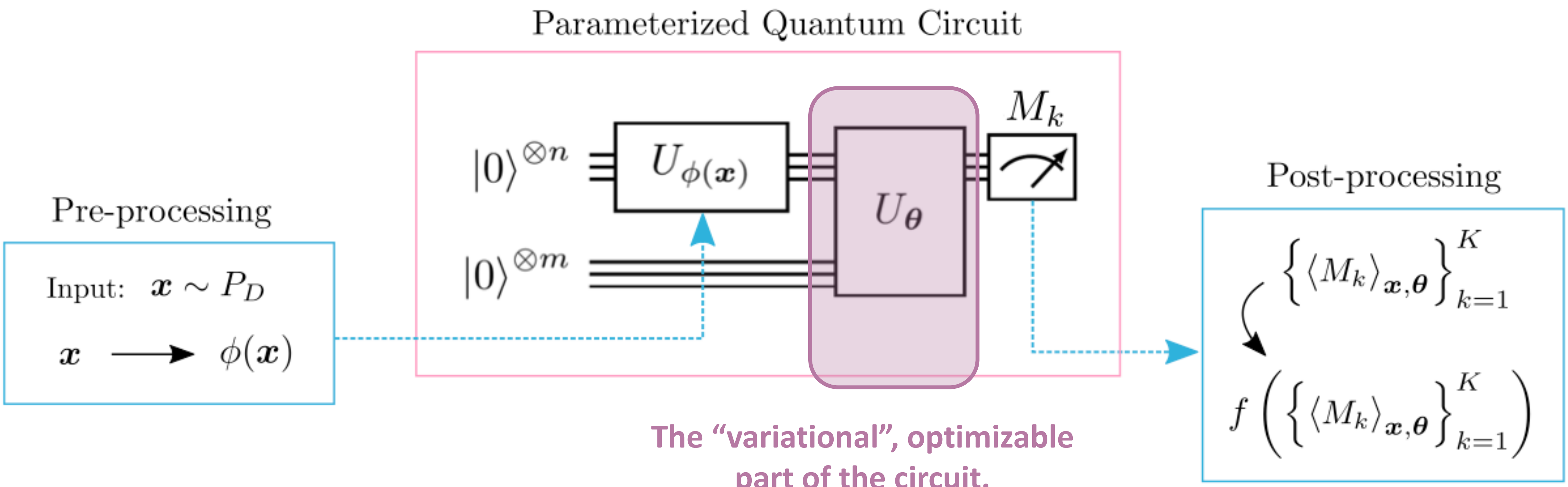
1. Start from a feature vector ***x***.
2. Optional: dimensionality reduction, PCA, etc.
3. Quantum embedding through a quantum feature map: *Basis embedding, amplitude embedding.*



- ★ Havlicek, et al, arXiv:1804.11326
- ★ Schuld, Killoran, arXiv:1803.07128
- ★ Lloyd, Schuld, et al, arXiv:2001.03622

Parameterized Quantum Circuits as ML Models

Benedetti, arXiv:1906.07682

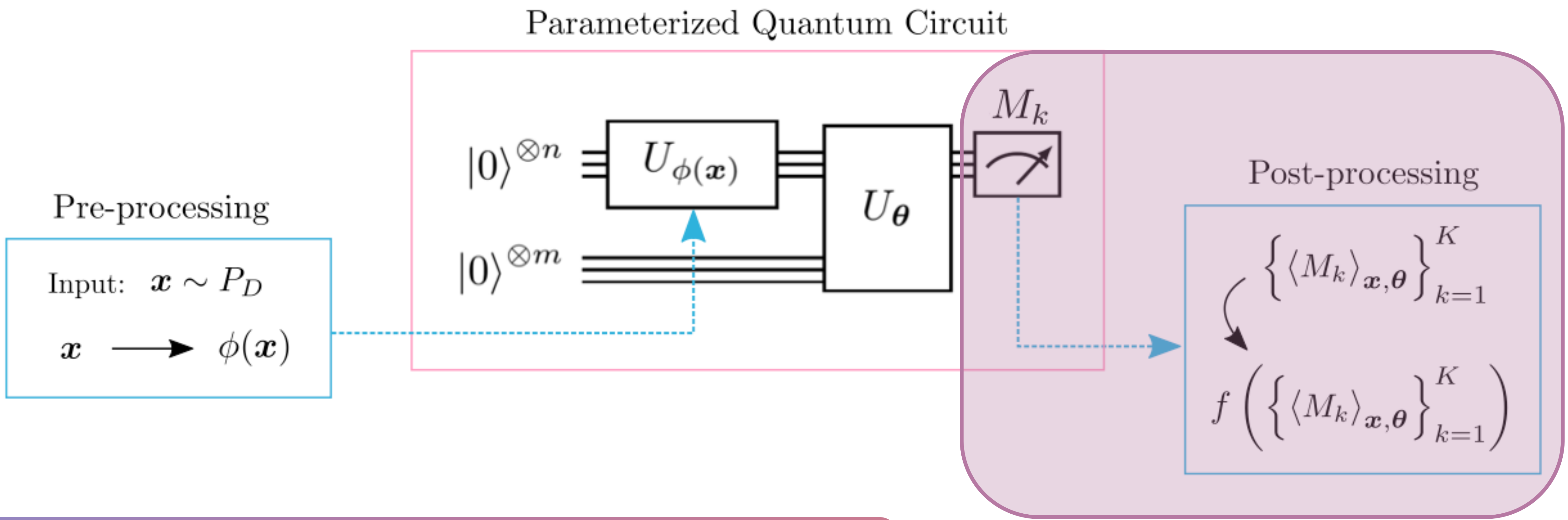


The "variational", optimizable part of the circuit.

The "guess" or trial function is the unitary U parameterized by a set of free parameters θ that will be updated during training.

Parameterized Quantum Circuits as ML Models

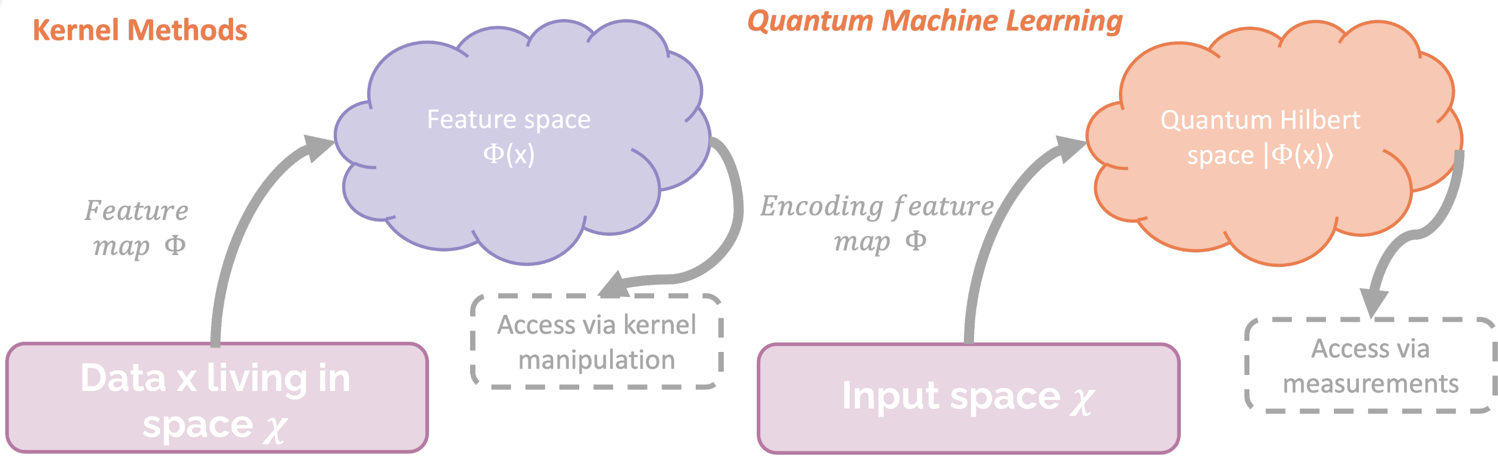
Benedetti, arXiv:1906.07682



Quantum information is turned back into classical information by evaluating the expectation value of an observable, or measurement.

The measurement output is then used to construct a decision function, a probability distribution, a boundary, etc.

Supervised Learning



How is this useful for HEP?

- Parameterized quantum circuits *are kernel methods*.
- **Potentially** more expressive models in QML, requiring less data to train.

Why quantum?

- When feature space become large, kernel functions become computationally expensive to estimate.

Extensively studied in HEP applications

- In the form of parameterized quantum circuits trained for classification, clustering and anomaly detection tasks.
- Applications in event reconstruction and classification, tracking, jet reconstruction and tagging ...
- Check out the arXiv pre-prints: [1908.04480], [2002.09935], [2010.07335], [2012.11560], [2012.12177], [2103.12257], [2103.03897], [2104.07692], [2003.08126], [2007.06868], [2012.01379], [2109.12636], and more.

Unsupervised Learning

How is this useful for HEP?

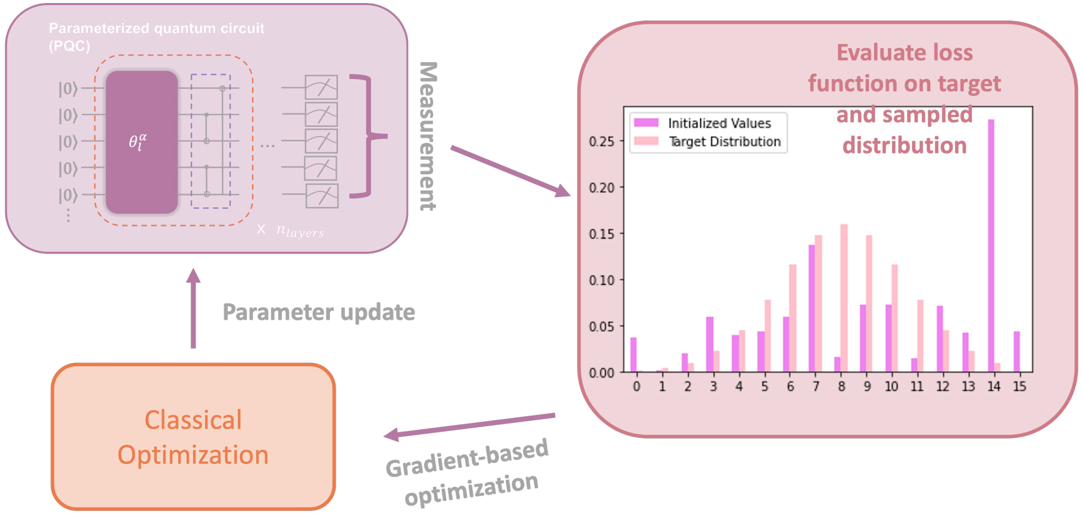
- Generative models *can act as surrogate* to generate data similar to previous observations.
- Valuable tool when the underlying process which generated a given set of data is unknown or poorly characterized, or when generating data has high overhead.

Why quantum?

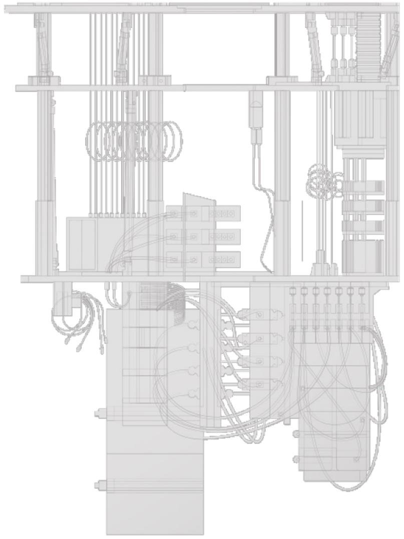
- Projection onto a fixed basis maps the state prepared by a circuit onto a set of classical bitstrings and yields a probability distribution -> ***Easy to obtain new samples***

Extensively studied in HEP applications

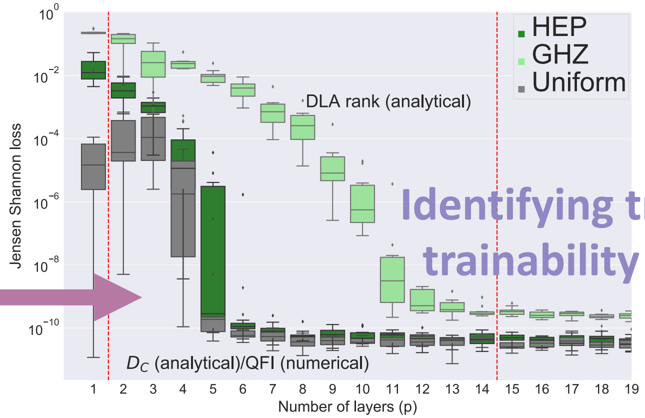
- In the form of Quantum Generative Adversarial Networks (QGANs) and Quantum Circuit Born Machines (QCBMs) for anomaly detection, generative modeling, etc.
- Applications in data augmentation, detector simulation,
- Check out the arXiv pre-prints: [2112.04958], [2101.11132], [2110.06933], [2201.01547], [2203.03578], [2011.13934].



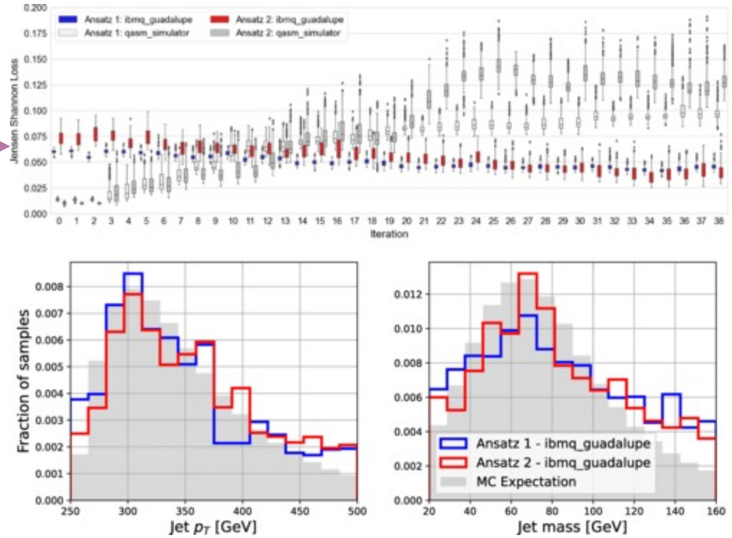
Quantum Computing for Data Analysis in HEP



- ★ Lots of applications and use cases developed over the last couple of years.
  - ★ *"Quantum computing for data analysis in HEP"*, Delgado, A., Hamilton, K.E., arXiv:2203.08805
- ★ Challenges to overcome:
  - ★ Noisy devices, limiting performance.
  - ★ Encoding of classical data into quantum states.
  - ★ Circuit depth limited by coherence times.
- ★ Borrowing tools form classical ML to characterize quantum models
  - ★ Over/under parameterization.
  - ★ Trainability – hardware noise.
  - ★ Generalization.
- ★ What else?



Identifying transitions in trainability landscape.



Flat landscapes when training in hardware.

But also… can we re-evaluate our current HEP experiments?

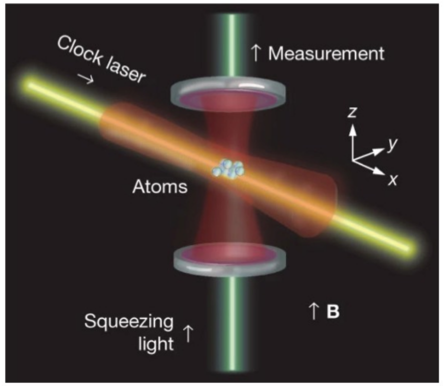
Recent developments in **quantum sensing** has inspired novel ideas for dark matter detection through quantum-enhanced techniques.

- Quantum sensors are able to detect very small changes in motion, electric and magnetic fields.

★ Open questions:

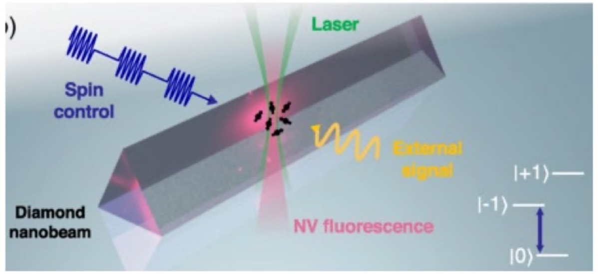
- Could they complement BSM searches at large-scale facilities such as the LHC?
- Can we couple QML algorithms to these devices?
- Opportunities for co-design.

entanglement-enhanced atomic sensors



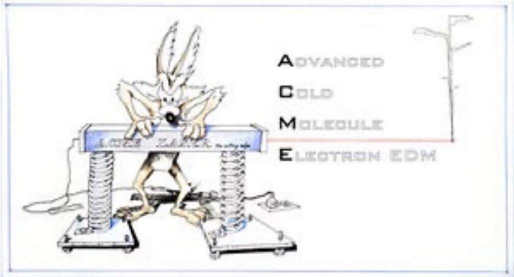
[Nature **588**, 414 (2020)]
[arXiv:2106.03754 (2021)]

NV centers in diamond



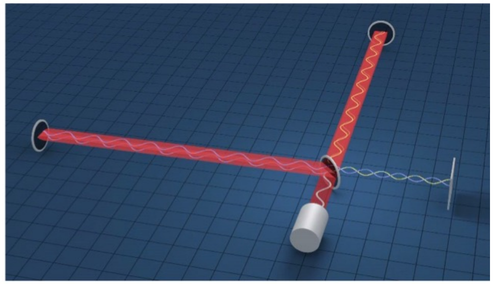
[PRX **10**, 031003 (2020)]

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)]

Thank you!

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