Quantum simulation and theory for high-energy physics at CERN

Dorota M. Grabowska

QUANTUM TECHNOLOGY INITIATIVE

10.03.2022

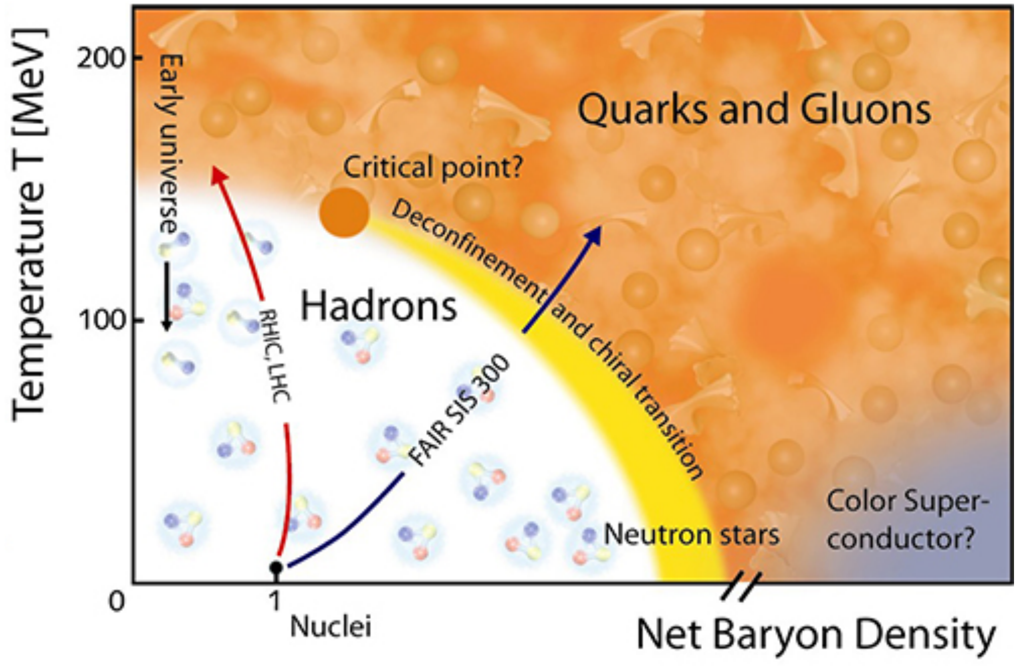
Non-perturbative Phenomena in Particle Physics

Rich phenomena of non-perturbative quantum field theories is a profitable place to look for new answers to the big questions

Studying the properties of strongly coupled theories from first principles is necessary to fully understand the Standard Model

Quantum Chromodynamics (QCD)

- Provides precise and quantitative description of the strong nuclear force over an broad range of energies
- *Ab-initio* calculations crucial for comparing theoretical predictions of the Standard Model to experimental results
- Gives rise to complex array of emergent phenomena that cannot be identified from underlying degrees of freedom



Proposed QCD Phase Diagram

Quantum Simulations of the Standard Model

Quantum computers have a fundamentally different computational strategy and will provide novel probes of fundamental questions in nuclear and particle physics

- The last decade has seen the rapid evolution of real-world quantum computers, with increasing size and decreasing noise
- It is imperative to begin exploratory studies of the applicability of this emerging technology

Quantum Simulations of the Standard Model

Quantum computers have a fundamentally different computational strategy and will provide novel probes of fundamental questions in nuclear and particle physics

- The last decade has seen the rapid evolution of real-world quantum computers, with increasing size and decreasing noise
- It is imperative to begin exploratory studies of the applicability of this emerging technology

Two Complementary Directions

Probe theories that are inaccessible through classical computing techniques

Real-Time Dynamics

Finite-Density Nuclear Matter

Decrease cost for computationally expensive but feasible calculations

Augmentation of Monte Carlo Event Generation via Quantum Machine Learning

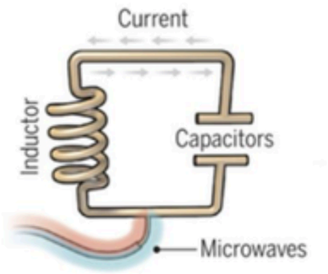
Different approaches with different timescales

Digital Quantum Computing

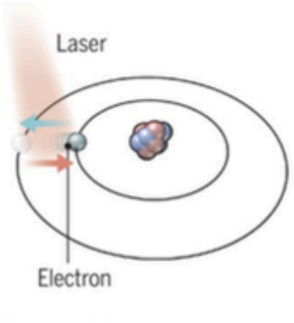
General Idea: Utilize collective properties of quantum states (superposition, interference, entanglement) to perform calculations

Computational Strategy: Quantum circuit is created by acting on collection of two-state systems (qubits) with unitary operations (gates)

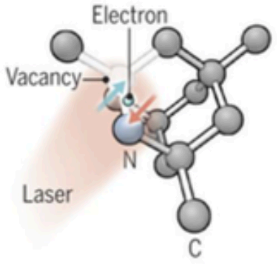
- Superconducting loops



- Trapped ions



- Diamond vacancies



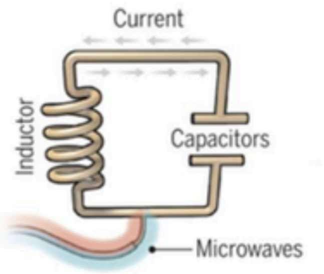
Graphics by C. Bickle, Science
Data by Gabriel Popkin

Digital Quantum Computing

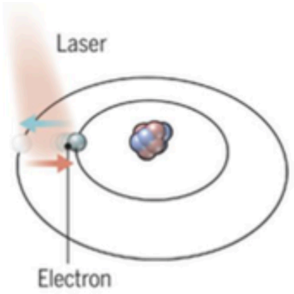
General Idea: Utilize collective properties of quantum states (superposition, interference, entanglement) to perform calculations

Computational Strategy: Quantum circuit is created by acting on collection of two-state systems (qubits) with unitary operations (gates)

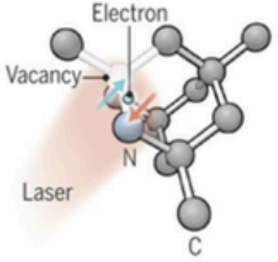
- Superconducting loops



- Trapped ions



- Diamond vacancies



Graphics by C. Bickle, Science
Data by Gabriel Popkin

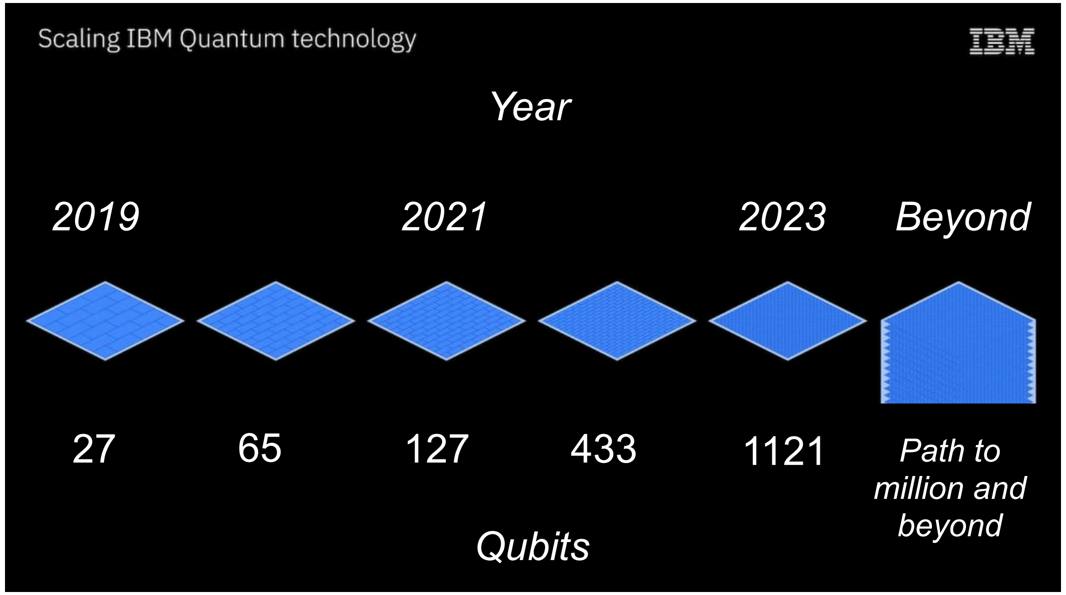
Currently in ***Noisy Intermediate-Scale Quantum*** (NISQ)-era

- Machines contain $\mathcal{O}(100)$ noisy qubits without error corrections
- Sensitive to various sources of noise, including decoherence and dephasing

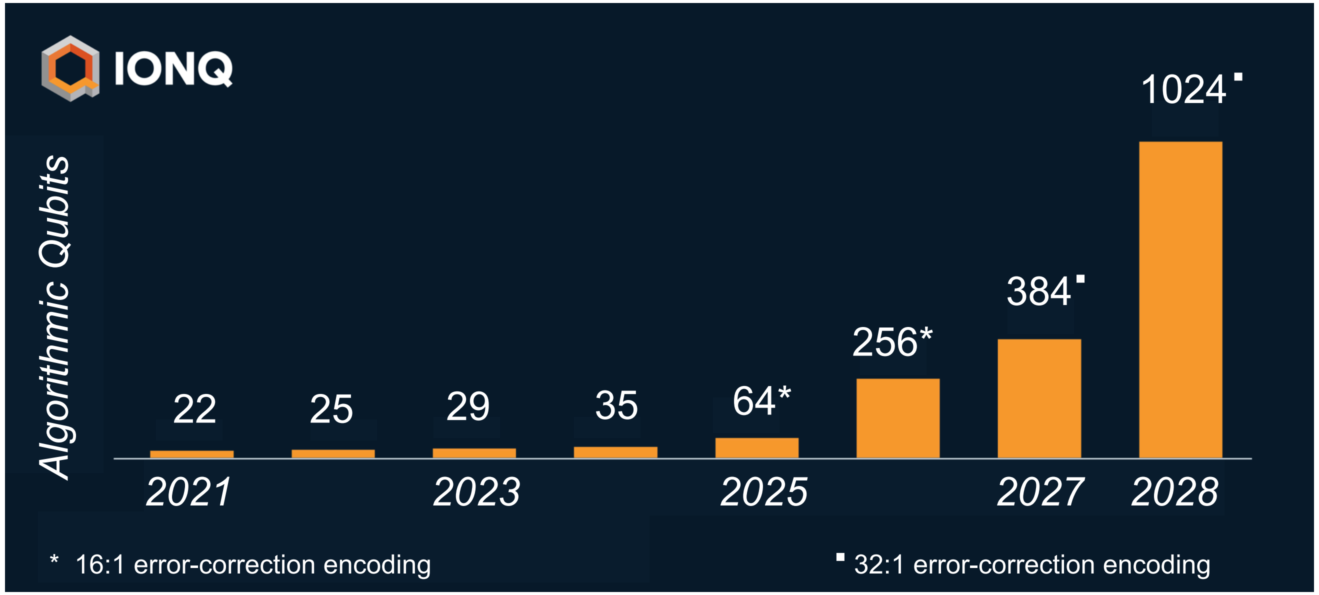
Hope to see exponential improvement in run-time scaling for physically-relevant calculations

Projection for Near-Future Digital Quantum Computers

Increasing Qubit Count: Many companies projecting 1k+ qubit quantum machines on this timescale



IBM Quantum Roadmap, 2020
Superconducting Qubits



IonQ Roadmap, 2020
Trapped Ion

Gate Noise: Expect decreasing noise which will allow for longer circuits

Quantum Technology Initiative (QTI)

Hub for Collaborative Developments in Quantum Information Science and Technology

Main Branches and Coordinators

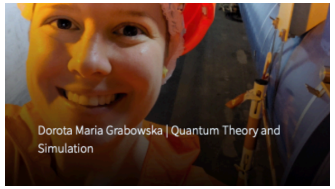
Michael Doser

Sensing, Metrology and Materials
EP Department

talked yesterday

Dorota Grabowska

Theory and Simulation
TH Department

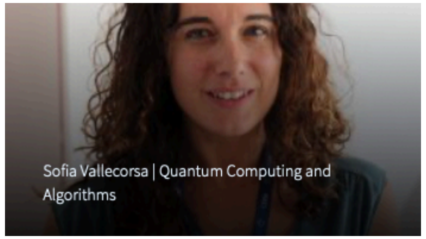


Alberto Di Meglio

HEAD COORDINATOR
CERN OpenLab Head
IT Department

Sofia Vallecorsa

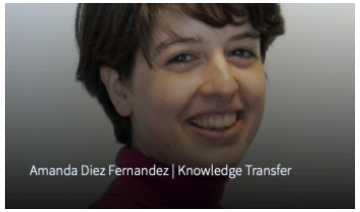
Computing and Algorithms
IT Department

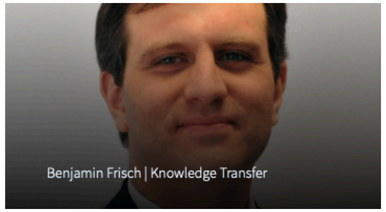


talking today

Amanda Diez Fernandez
Benjamin Frisch

Knowledge Transfer
IPT Department





High Level Goals of QTI

Guiding CERN's involvement in many rapidly advancing fields of quantum technology

QTI has developed a roadmap document to define and guide the activities of the initiative during the first three years and lay the foundations for a continuing program

This Strategy is based on four top-level objectives

1. Scientific and Technical Development and Capacity Building
2. Co-Development
3. Community Building
4. Integration with National and International Initiatives and Programs

Roadmap Document has now been approved and released to the public!
https://doi.org/10.5281/zenodo.5553774

Theory + Simulation Branch

Four Top-Level Objects in the Roadmap Document

Identify possible applications of quantum simulations and support worldwide experimental efforts to probe and measure both Standard Model and beyond the Standard Model physics.

Applications of Quantum Technology To Particle and Nuclear Physics

Assist the computing and sensing activities in identifying theoretically promising regions of parameter space in which quantum technology could provide an advantage over classical methods.

Benchmark the current and potential performance of quantum simulations against state-of-the-art classical computations.

Host workshops, summer institutes and visitors, establishing global collaborations with other institutes, national labs and companies.

Simulation of Lattice Gauge Theories

Sign Problems in Lattice Gauge Theories

Lattice Simulations: Numerically estimation of lattice-regulated quantum path integral via Monte Carlo importance sampling requires the existence of a positive probability measure

$$\mathcal{Z} = \int [DU] \det D_F(U)\, e^{-S[U]}$$

Must be real and positive

Sign Problems in Lattice Gauge Theories

Lattice Simulations: Numerically estimation of lattice-regulated quantum path integral via Monte Carlo importance sampling requires the existence of a positive probability measure

$$\mathcal{Z} = \int [DU] \, \text{det}\, D_F(U)\, e^{-S[U]}$$

Must be real and positive

"Sign Problem" prohibits first-principles study of phenomenologically-relevant theories

<u>Real-Time Dynamics</u>

Early Universe Phase Transitions

Requires Minkowski space simulations

<u>Chiral Gauge Theories</u>

Fully defined Standard Model

Complex fermion determinant

<u>Finite-Density Nuclear Matter</u>

Neutron stars and QCD phase diagram

Complex fermion determinant

Can quantum computing help?

Hamiltonian Formulations of Lattice Gauge Theories

Lattice Hamiltonian: Requires basis of states, set of operators and commutation relations

Two Key Considerations

Gauge Invariance and Redundancies

- ***Problem:*** Gauss' Law is not automatically satisfied in Hamiltonian formulations
  - Allows for charge-violating transitions
- ***Problem:*** Naive basis of states is over-complete
  - Requires more quantum resources than strictly necessary

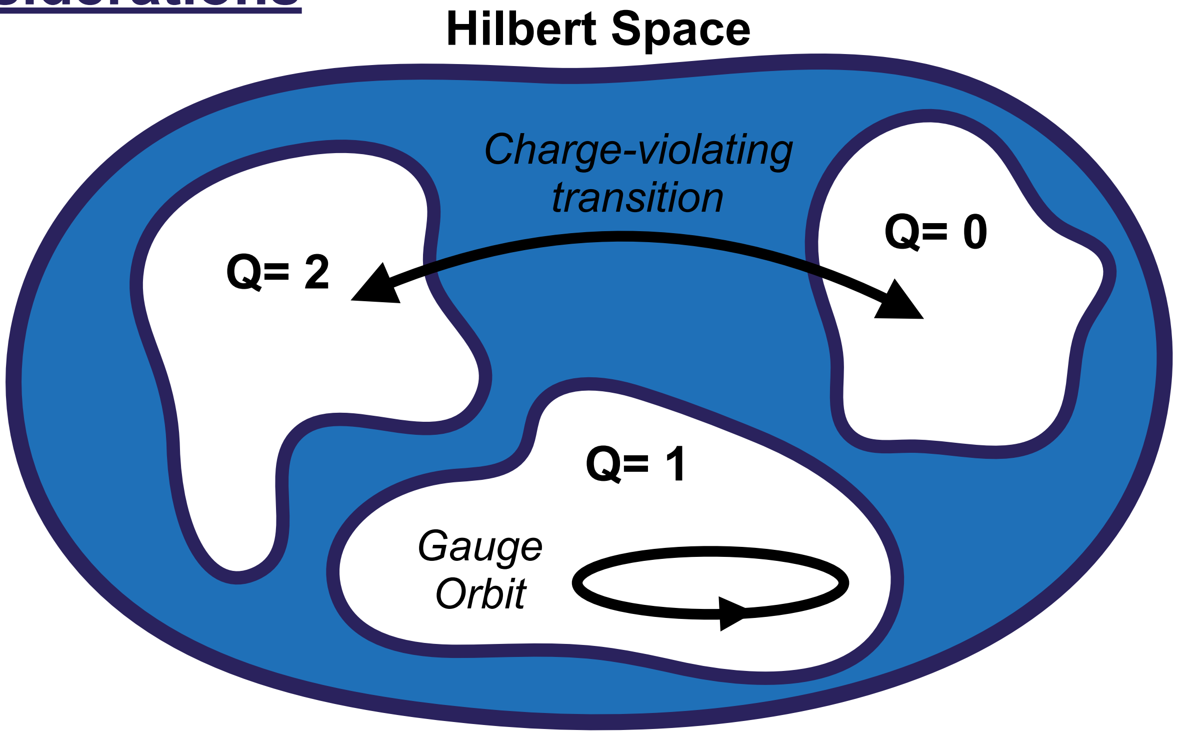
Hamiltonian Formulations of Lattice Gauge Theories

Lattice Hamiltonian: Requires basis of states, set of operators and commutation relations

Two Key Considerations

Gauge Invariance and Redundancies

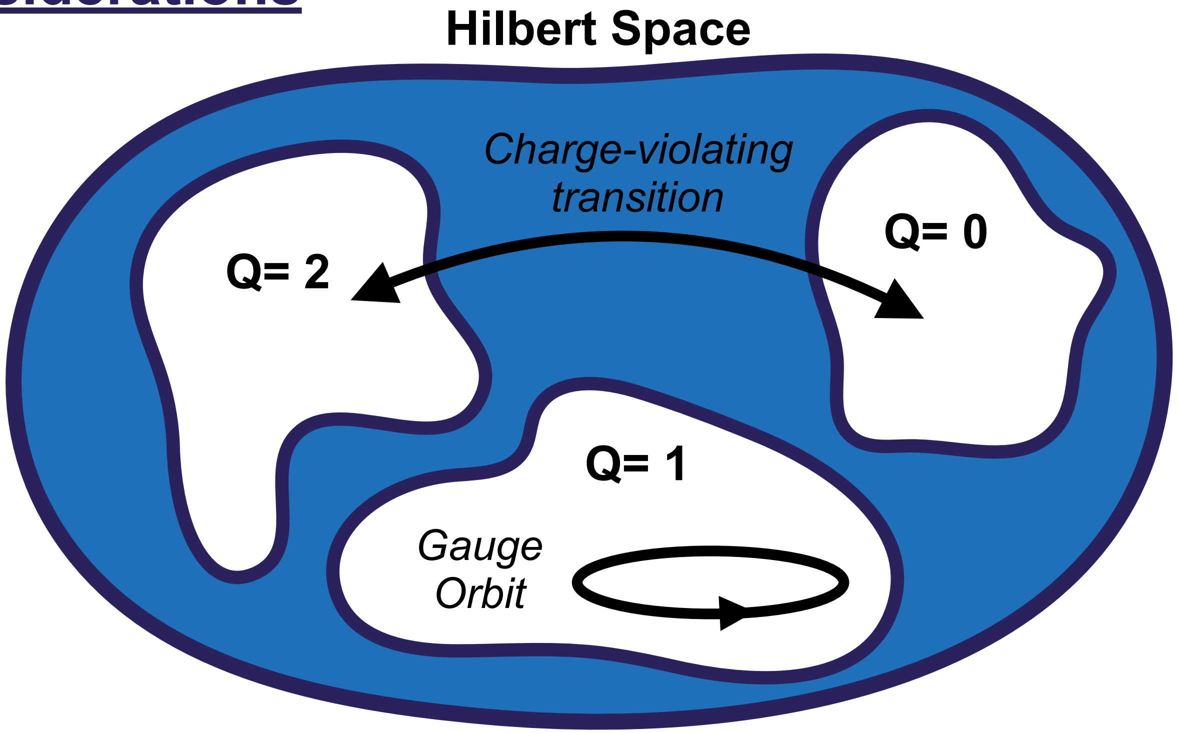
- ***Problem:*** Gauss' Law is not automatically satisfied in Hamiltonian formulations
    - Allows for charge-violating transitions
- ***Problem:*** Naive basis of states is over-complete
    - Requires more quantum resources than strictly necessary



Hamiltonian Formulations of Lattice Gauge Theories

Lattice Hamiltonian: Requires basis of states, set of operators and commutation relations

Two Key Considerations



Gauge Invariance and Redundancies

- ***Problem:*** Gauss' Law is not automatically satisfied in Hamiltonian formulations
  - Allows for charge-violating transitions
- ***Problem:*** Naive basis of states is over-complete
  - Requires more quantum resources than strictly necessary

Truncation and Digitization

- ***Problem:*** Must choose maximum field value and how many field values included
  - Incorrectly chosen values lead to poor representation of desired theory

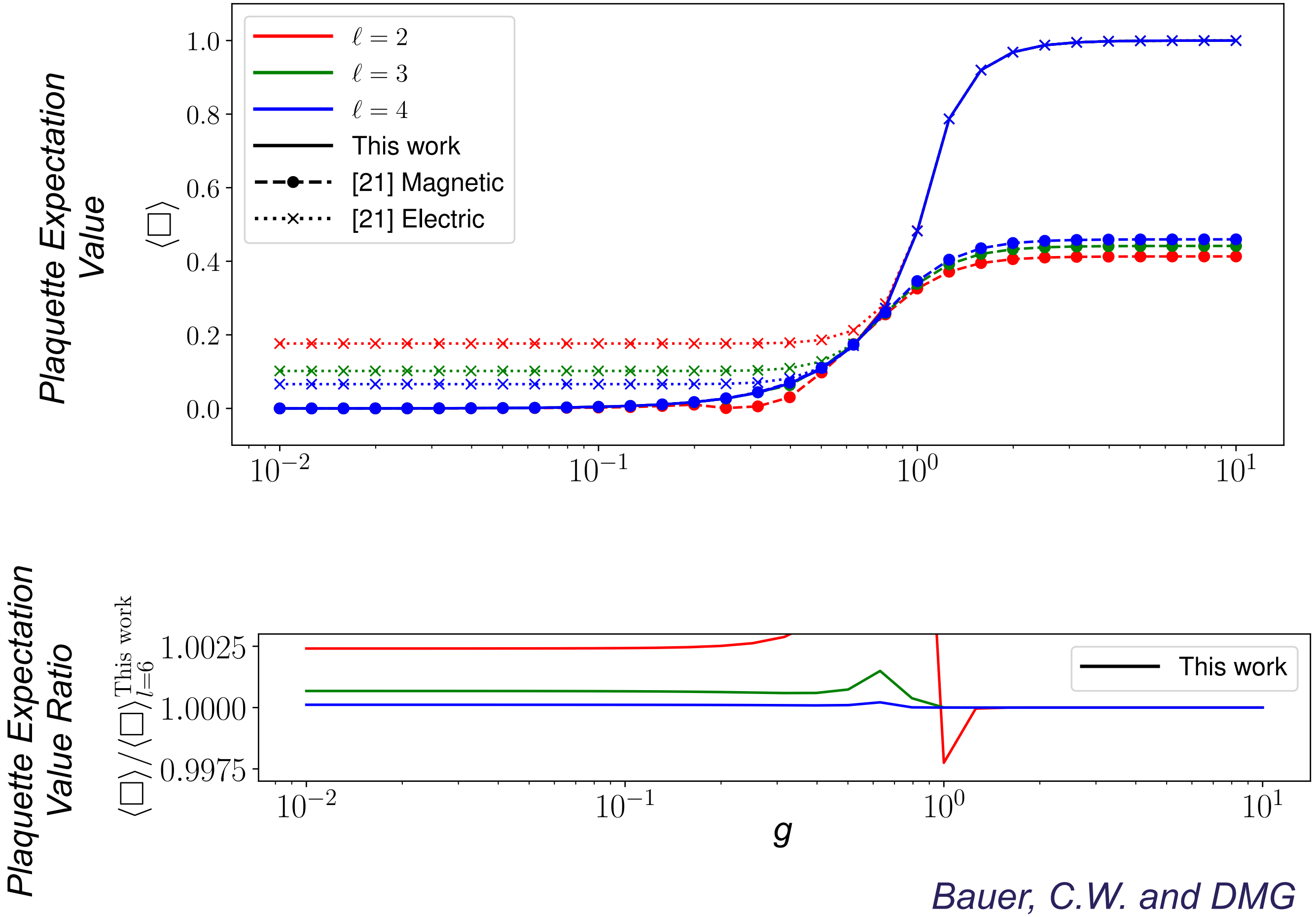
U(1) Gauge Theories in 2+1 Dimensions

General Idea: Combine "gauge-redundancy free" dual representation with digitization method that strives to minimize violation of commutation relations

- Hamiltonian defined in terms of plaquette variables: rotors and magnetic loops

$$[B_p, R_{p'}] = i\delta_{pp'}$$

- Gauss' law automatically satisfied
- No redundant degrees of freedom
- Formulations works well for all values of the gauge coupling



Bauer, C.W. and DMG
arXiv: 2111.08015

U(1) Gauge Theories in 2+1 Dimensions

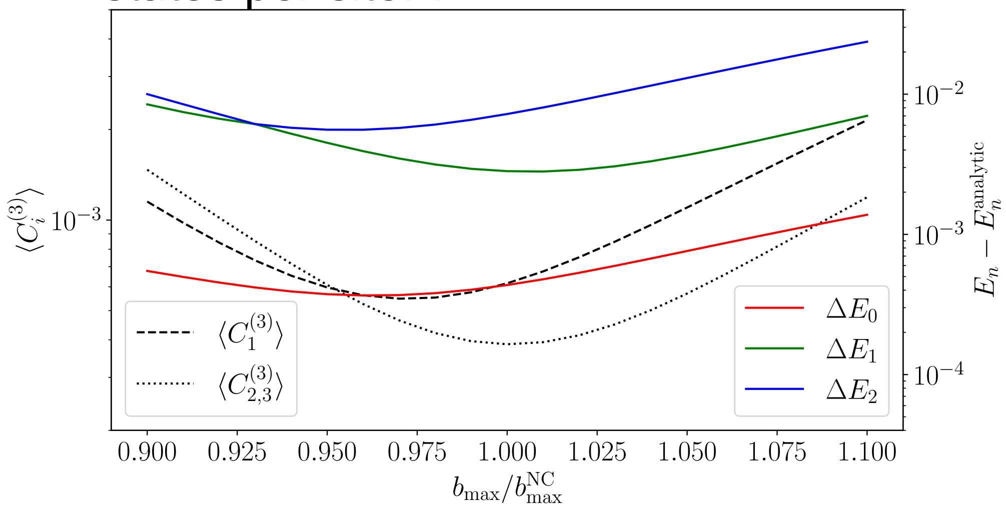
General Idea: Combine “gauge-redundancy free” dual representation with digitization method that strives to minimize violation of commutation relations

- Gauss’ law is automatically satisfied and there are no redundant degrees of freedom
- Truncation scale and digitization scale are not independent and there is an optimal choice
- Canonical commutation relations are minimally violated for that optimal choice

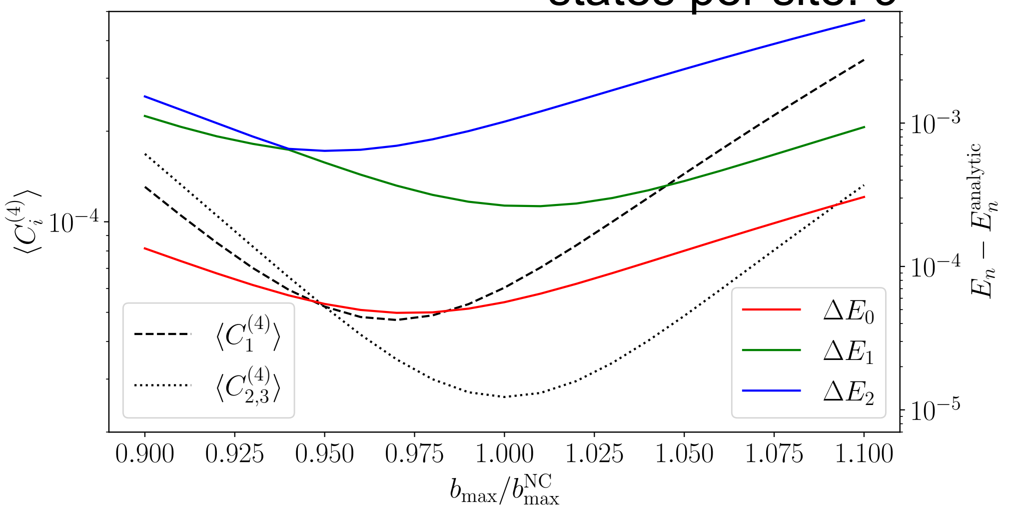
Comparison to exact solution

Violation of Commutation Relations

states per site: 7



states per site: 9



Precision in Low-Lying Energy Eigenvalue

Scanning through truncation scale, compared to optimal truncation scale

Bauer, C.W. and DMG
arXiv: 2111.08015

Circuit Implementation and Gate Cost

Complication: Imposing magnetic Gauss' law without any gauge redundancy seems to be exponentially expensive in circuit length

Cause: Total magnetic flux conservation results in non-local term

$$H_B \propto \sum_{p=1}^{N_P} \cos\left(B_p\right) + \cos\left(\sum_{p=1}^{N_P} B_p\right)$$

$N_P \sim (\text{Lattice Sites})^2$

Naive Cost: $\sim \left(2^{N_P}\right) N_P$

Work in Progress

Circuit Implementation and Gate Cost

Complication: Imposing magnetic Gauss' law without any gauge redundancy seems to be exponentially expensive in circuit length

Cause: Total magnetic flux conservation results in non-local term

$$H_B \propto \sum_{p=1}^{N_P} \cos\left(B_p\right) + \cos\left(\sum_{p=1}^{N_P} B_p\right)$$

$N_P \sim (\text{Lattice Sites})^2$

Naive Cost: $\sim \left(2^{N_P}\right) N_P$

Approach One: Rotate to different operator basis to minimize cost

Rotated Cost : $\dfrac{N_P^2}{4\log_2 N_P}\left(\log_2\left(\dfrac{N_P}{\log_2 N_P}\right) + \dfrac{2\log_2^2 N_P}{N_P} + 1\right)$

Quadratic vs Exponential!

Approach Two: Allow gauge redundancy in time evolution and correct for later

Work in Progress

Generalizations and Applications

Next Steps: Generalize formulation to more physically-relevant theories

Standard Model

3+1 dimensional gauge theory

$$SU(3) \times SU(2)_L \times U(1)_Y$$

Higher Dimensions

Imposing Gauss' law in 3+1 dimensions is more complicated

Fermions

Introduce fermions with good chiral symmetry

Non-Abelian Groups

Self-interaction of gauge fields introduces additional complications

Works in Progress

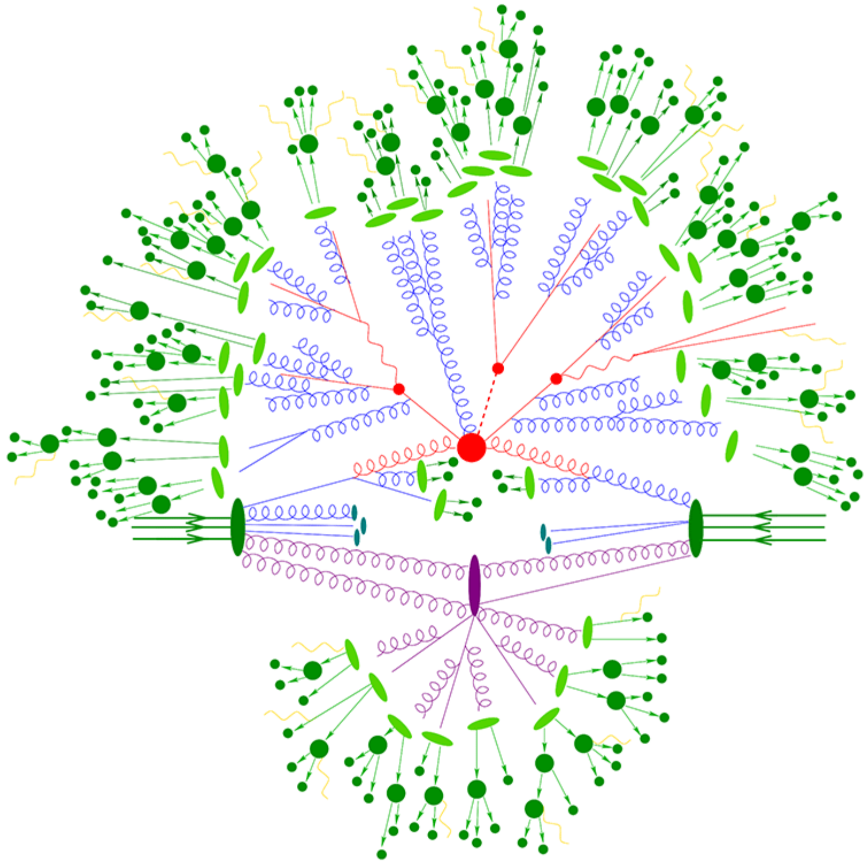
Quantum Machine Learning* For Monte Carlo Event Generation

*QML

High-Energy Collisions at the Large Hadron Collider

LHC Collisions: Extremely complex events that span many different energy scales, further complicated by detector construction and experimental configuration

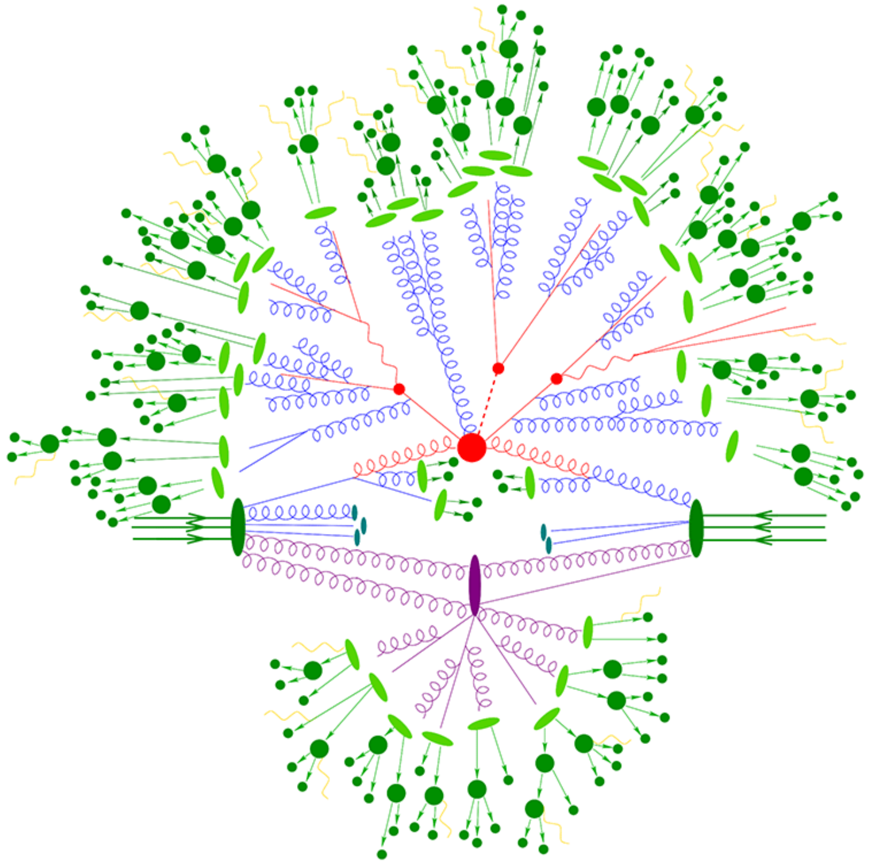
- No simple one-to-one mapping between Standard Model parameters and experimental measurements
- Monte Carlo event generation is necessary to compare theoretical expectation to experimental reality



High-Energy Collisions at the Large Hadron Collider

LHC Collisions: Extremely complex events that span many different energy scales, further complicated by detector construction and experimental configuration

- No simple one-to-one mapping between Standard Model parameters and experimental measurements
- Monte Carlo event generation is necessary to compare theoretical expectation to experimental reality



Monte Carlo Event Generation: Pipeline that transforms Standard Model parameters into event distributions

- Feasible on classical machines, but computationally expensive

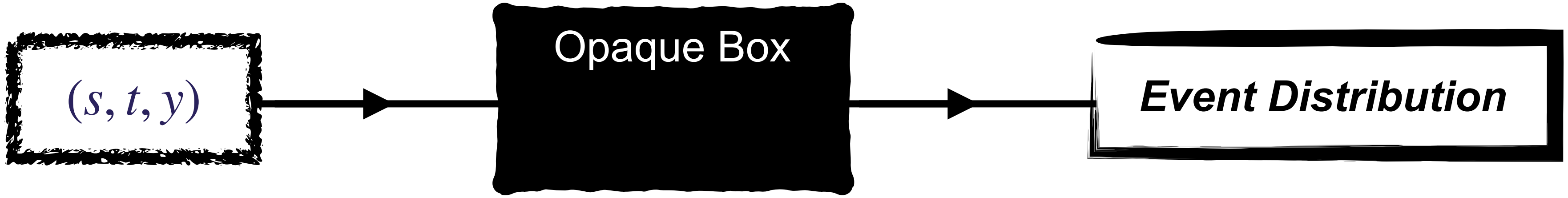
Can quantum machine learning help?

(Quantum) Machine Learning

Machine Learning: Computer algorithm that improves automatically through experience and use of data

Intuitive Definition: Algorithm creates improvable opaque box that transforms input variables to output distributions

Ex: Transform set of Mandelstam variables plus rapidity into underlying event distribution of these variables

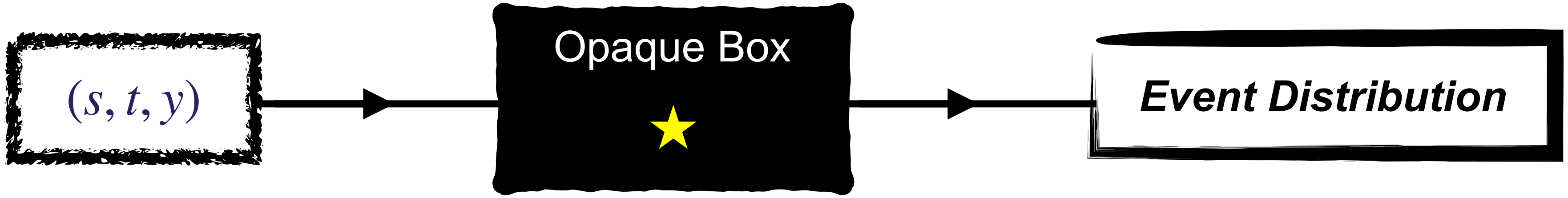


(Quantum) Machine Learning

Machine Learning: Computer algorithm that improves automatically through experience and use of data

Intuitive Definition: Algorithm creates improvable opaque box that transforms input variables to output distributions

Ex: Transform set of Mandelstam variables plus rapidity into underlying event distribution of these variables



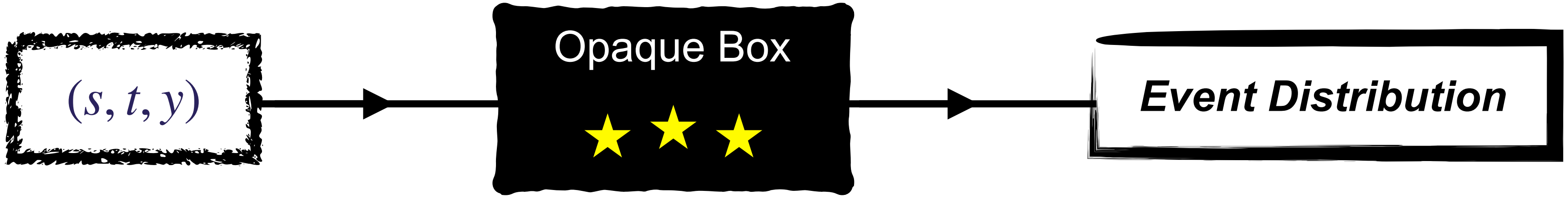
Training improves how well the opaque box replicates the underlying distribution

(Quantum) Machine Learning

Machine Learning: Computer algorithm that improves automatically through experience and use of data

Intuitive Definition: Algorithm creates improvable opaque box that transforms input variables to output distributions

Ex: Transform set of Mandelstam variables plus rapidity into underlying event distribution of these variables



Training improves how well the opaque box replicates the underlying distribution

Opaque box is reproducible and can generate same distributions in the future

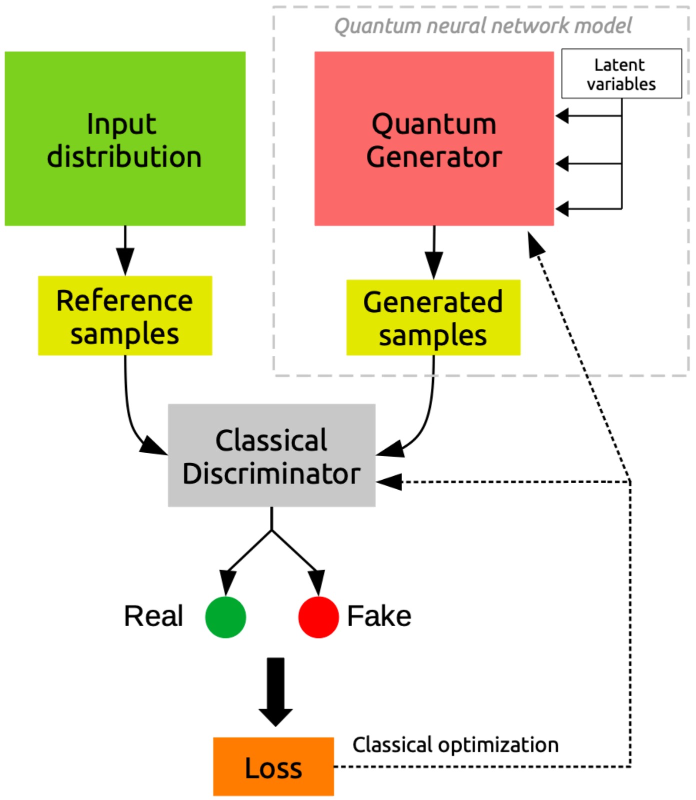
Quantum Machine Learning Strategy

General Idea: Use a trained neural network to augment data produced by classical Monte Carlo event generation

- Data augmentation decreases classical computational cost due to "filling in" the distribution without having to rerun entire pipeline
- Quantum approach may be beneficial due to small number of highly correlated input variables

Generative Adversarial Network (GAN): Two networks compete against one another and through this competition, one network learns the underlying distribution

- Hybrid approach as no viable quantum training algorithm



Bravo-Prieto, C., Baglio, J., Cè, M., Francis, A., DMG and Carrazza, S.; arXiv: 2110.06933

Real Quantum Machine, Real Monte Carlo Data

Key Result: Create new qGAN architecture that learns underlying distribution for LHC scattering process

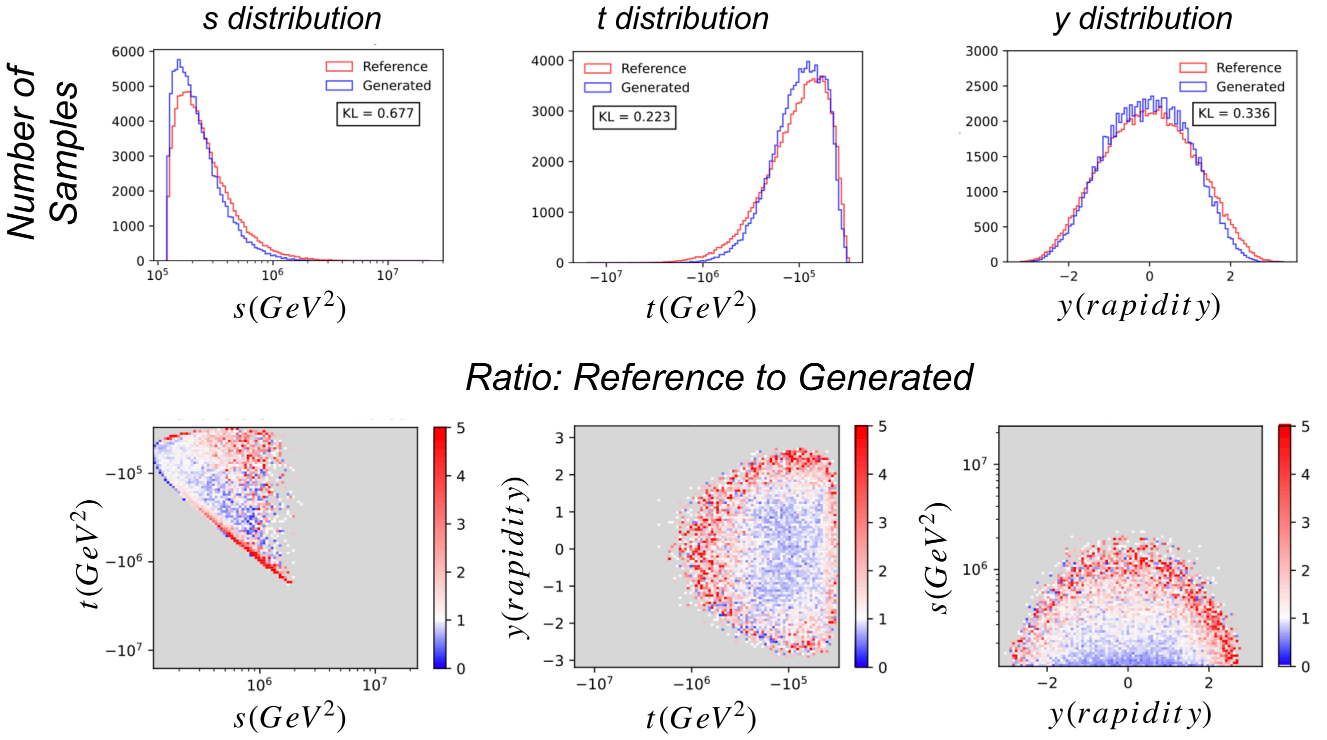
Key Result: See successful data augmentation on noisy machine

- Non-trivial proof-of-principles test as data is non-gaussian and highly correlated
- Significantly simpler algorithm than corresponding classical neural network
- See similar results on different classes of quantum hardware

$pp \to t\bar{t}$

Distributions: 10^5 *samples*

ibmq_santiago



Bravo-Prieto, C., Baglio, J., Cè, M., Francis, A., DMG and Carrazza, S.; arXiv: 2110.06933

Different Quantum Architectures

Comparison between (superconducting) transmon and trapped ion machines

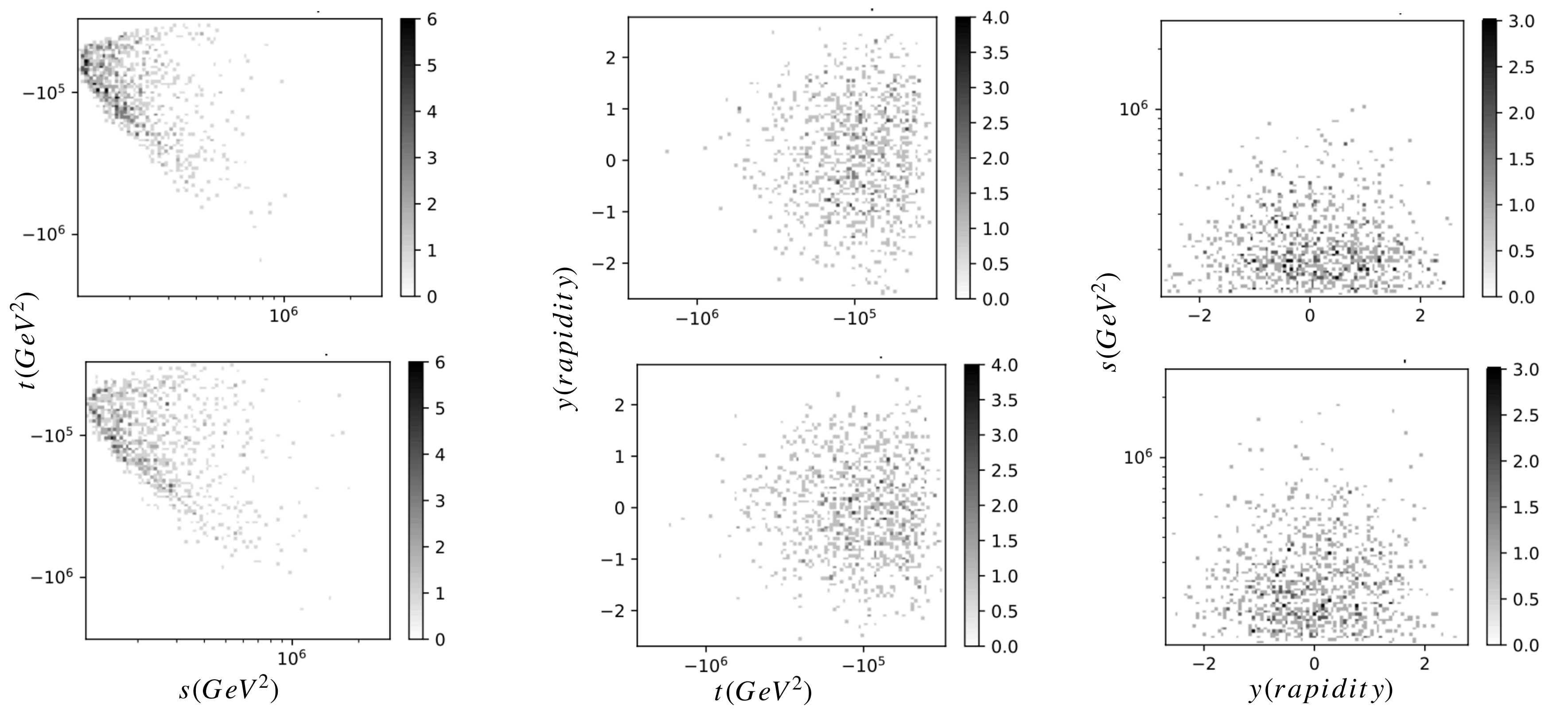
Ratio: Reference to Generated

Transmon

ibmq_santiago

Trapped Ion

IonQ



10^3 *Samples*

Bravo-Prieto, C., Baglio, J., Cè, M., Francis, A., DMG and Carrazza, S.; arXiv: 2110.06933

Benchmarking, Transfer Learning and Future Directions

Recall: For calculations that are feasible but expensive on classical hardware, performing comparison studies is imperative

Does QML data augmentation improve total run-time?

Are there other processes that could be similarly augmented via QML?

How does QML compare to ML, especially in number of hidden parameters?

Benchmarking, Transfer Learning and Future Directions

Recall: For calculations that are feasible but expensive on classical hardware, performing comparison studies is imperative

Does QML data augmentation improve total run-time?

Are there other processes that could be similarly augmented via QML?

How does QML compare to ML, especially in number of hidden parameters?

Transfer Learning

Can we recycle neural net trained on one scattering process and use it for other processes

$pp \to t\bar{t}$ — *partial re-training* → $pp \to WW$

Work in Progress

Benchmarking, Transfer Learning and Future Directions

Recall: For calculations that are feasible but expensive on classical hardware, performing comparison studies is imperative

Does QML data augmentation improve total run-time?

Are there other processes that could be similarly augmented via QML?

How does QML compare to ML, especially in number of hidden parameters?

Transfer Learning

Can we recycle neural net trained on one scattering process and use it for other processes

$pp \to t\bar{t}$ — *partial re-training* → $pp \to WW$

Work in Progress

Fully Quantum Approach

Can we create a fully quantum approach to machine learning that benefits from quantum speed-up?

MAJOR ROADBLOCK

No good quantum training algorithms

Concluding Remarks

Conclusions

Quantum computers have a fundamentally different computational strategy and will provide novel probes of fundamental questions in nuclear and particle physics

Important to think carefully about what particle and nuclear physics problems would be most amenable to this novel computational strategy

Two Complementary Directions

Probe gauge theories that are inaccessible through classical computing techniques

Real-Time Dynamics

Finite-Density Nuclear Matter

Decrease cost for computationally expensive but feasible calculations

Augmentation of Monte Carlo Event Generation via Quantum Machine Learning

Different approaches with different timescales