

High Energy Physics

Quantum Computing

Quantum Information Science in High Energy Physics at the Large Hadron Collider

PI: O.K. Baker, Yale University

Unraveling the quantum structure of QCD in parton shower Monte Carlo generators

PI: Christian Bauer, Lawrence Berkeley National Laboratory

Co-PIs: Wibe de Jong and Ben Nachman (LBNL)

The HEP.QPR Project: Quantum Pattern Recognition for Charged Particle Tracking

PI: Heather Gray, Lawrence Berkeley National Laboratory

Co-PIs: Wahid Bhimji, Paolo Calafiura, Steve Farrell, Wim Lavrijsen, Lucy Linder, Illya Shapoval (LBNL)

Neutrino-Nucleus Scattering on a Quantum Computer

PI: Rajan Gupta, Los Alamos National Laboratory

Co-PIs: Joseph Carlson (LANL); Alessandro Roggero (UW), Gabriel Purdue (FNAL)

Particle Track Pattern Recognition via Content-Addressable Memory and Adiabatic Quantum Optimization

PI: Lauren Ice, Johns Hopkins University

Co-PIs: Gregory Quiroz (Johns Hopkins); Travis Humble (Oak Ridge National Laboratory)

Towards practical quantum simulation for High Energy Physics

PI: Peter Love, Tufts University

Co-PIs: Gary Goldstein, Hugo Beauchemin (Tufts)

High Energy Physics (HEP) ML and Optimization Go Quantum

PI: Gabriel Perdue, Fermilab

Co-PIs: Jim Kowalkowski, Stephen Mrenna, Brian Nord, Aris Tsaris (Fermilab); Travis Humble, Alex McCaskey (Oak Ridge National Lab)

Quantum Machine Learning and Quantum Computation Frameworks for HEP (QMLQCF)

PI: M. Spiropulu, California Institute of Technology

Co-PIs: Panagiotis Spentzouris (Fermilab), Daniel Lidar (USC), Seth Lloyd (MIT)

Quantum Algorithms for Collider Physics

PI: Jesse Thaler, Massachusetts Institute of Technology

Co-PI: Aram Harrow, Massachusetts Institute of Technology

Quantum Machine Learning for Lattice QCD

PI: Boram Yoon, Los Alamos National Laboratory

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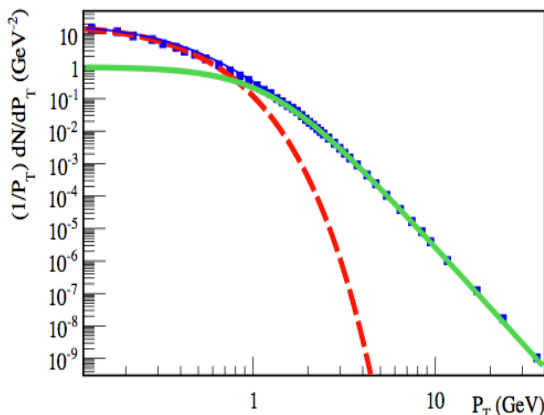
Quantum Information Science in High Energy Physics at the Large Hadron Collider

O.K. Baker, Yale University

We pursue scientific research at the interface of High Energy Physics and Quantum Information Science. This includes studies of thermal radiation and quantum entanglement in high-energy collisions at the Large Hadron Collider (LHC), with special emphasis on entanglement entropy and the Higgs boson.

Collider experiments such as proton-proton collisions at the LHC yield hadrons that exhibit an exponential behavior at low transverse momenta, P_T . Transverse momentum distributions in proton-proton scattering processes have been studied in both the ATLAS and CMS collaborations and show evidence for this exponential dependence on P_T (see Figure below for one example). This dependence can be attributed to thermal radiation that is akin to Hawking radiation or Unruh radiation that should exist at the event horizon of astrophysical black holes and neutron stars. This phenomena should not be surprising since at LHC center of mass energies, the proton-proton scattering is effectively parton-parton scattering (partons being quarks and gluons in this case). Because the scattering involves the strong nuclear force, the strongest of all of the fundamental forces in nature, the resulting deceleration gradients are so large that, in magnitude, they are comparable to the acceleration gradients that give rise to Hawking or Unruh radiation in astrophysical systems. The Principal Investigator, in collaboration with a theoretical physicist at Stony Brook University and Brookhaven National Laboratory, have shown evidence for this thermal radiation in several production and decay processes in the ATLAS and CMS data (O.K. Baker and D.E Kharzeev, Phys. Rev. D 98, 054007 (2018)). These studies and findings suggest a deep connection between quantum entanglement (entanglement entropy) and thermalization in high-energy hadron collisions that has to be investigated further as will be done during this funding period. The origin of the apparent thermalization in high-energy collisions at LHC energies will be investigated using the data of the ATLAS, CMS, and other LHC collaborations.

We will confirm or refute the proposed relation between the effective temperature



and the hard scattering scale observed at lower energies, and show that it extends even to the Higgs boson production process. This research tests the hypothesis about the link between quantum entanglement and thermalization in high-energy collisions.

Figure: Charged hadron transverse momentum distribution; thermal (exponential) behavior in red, hard scattering (power law) behavior in green, data in blue squares.

Unraveling the quantum structure of QCD in parton shower Monte Carlo generators

Christian Bauer (PI) (LBNL), Wibe de Jong (LBNL), Ben Nachman (LBNL)

The goal of high-energy physics is to test our understanding of nature at the most fundamental level. Our current understanding is captured by the standard model of particle physics, which is currently being tested at the Large Hadron Collider (LHC) in Geneva, Switzerland. To compare events produced at the LHC against our expectations from the standard model, one uses so-called event generators, which simulate events very similar to those observed at the LHC, but purely from theoretical calculations in the standard model. A clear deviation between data and simulation would indicate physics not described by our current understanding of nature.

A key challenge is that such simulations need to represent a complex quantum process, but are currently limited to using inherently classical algorithms. As a result, the standard event generators are limited in their precision for describing crucial entanglement phenomena observed in the data. We propose to investigate modeling the quantum nature of a event generators with an inherently quantum algorithm, exploiting the recent exciting progress in quantum computation.

The goal of the project is to develop quantum algorithms that allow for event simulation in theories resembling the standard model. This will allow to ultimately test the standard model at currently unattainable precision, deepening our fundamental understanding of nature at the smallest scales. We will build collaborations between High Energy Physics and Quantum Information Science experts developing quantum hardware, software and algorithmic approaches to deliver innovative solutions required to enable such algorithms to run effectively on near-term quantum computers.

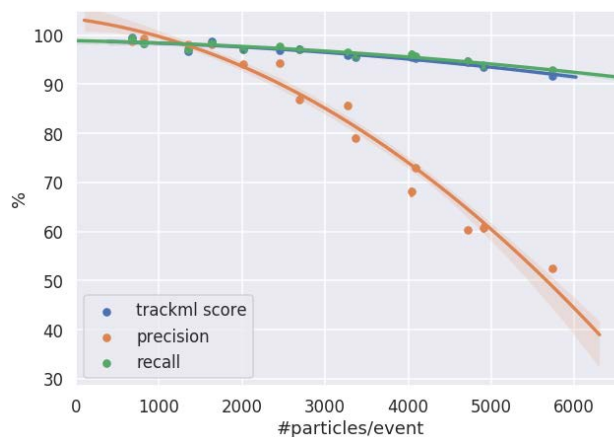
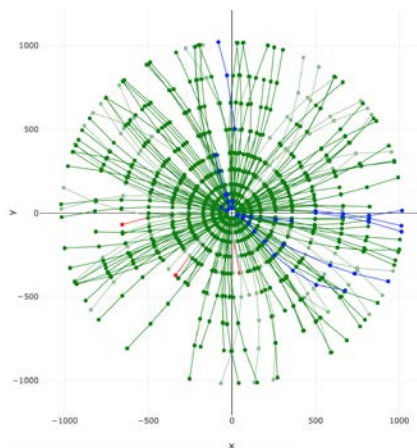
The HEP.QPR Project: Quantum Pattern Recognition for Charged Particle Tracking

Authors: Wahid Bhimji, Paolo Calafiura, Steve Farrell, Heather Gray, Wim Lavrijsen, Lucy Linder, Illya Shapoval (LBNL)

The era of Universal Quantum Computing may still be a few years away, but we have already entered into the Noisy Intermediate-Scale Quantum era. This ranges from D-Wave commercial Quantum Annealers to a wide selection of gate-based quantum processor prototypes. This hardware provides us with the opportunity to evaluate the potential of the Quantum Computing paradigm for HEP applications. We will present early results from the DOE HEP.QPR project on the impact of Quantum Computing on charged particle tracking.

Due to increasing data rates and event complexities, tracking has become one of the most pressing computational problems facing the HEP community. In HEP.QPR, we are studying the potential of the Quantum Associative Memory (QuAM) and Quantum Annealing (QA) algorithms. QuAM provides in principle an exponential increase in storage capacity compared to classical Associative Memory used in the context of LHC data triggering. We examine the practical limits of storage capacity, as well as store and recall errorless efficiency, from the viewpoints of the state-of-the-art IBM quantum processors and LHC real-time charged track pattern recognition requirements. We present a software prototype implementation of the QuAM protocols and analyze the topological limitations for porting the simplest QuAM instances to the public IBM 5Q and 14Q cloud-based superconducting chips.

We will also present some promising results we achieved expressing the LHC track finding problem as a Quadratic Unconstrained Binary Optimization (QUBO), that can be solved using a D-Wave Quantum Annealer. We generated QUBOs that encode the pattern recognition problem at the LHC using the TrackML dataset and solved them using D-Wave qbsolv and its Leap Cloud Service. Those early experiments achieved a performance exceeding 99% purity, efficiency, and TrackML score at low track densities. We plan to extend the performance of such algorithms at higher track densities by improving seeding algorithms, geographic partitioning, and our QUBO models. We plan to evaluate if the combined classical/quantum annealing approach used by qbsolv provides performance improvements compared to classical QUBO solvers.



Neutrino-Nucleus Scattering on a Quantum Computer

Rajan Gupta, Joseph Carlson (LANL), Alessandro Roggero (UW), Gabriel Purdue (FNAL)

Neutrinos are fascinating elusive particles that interact very weakly with normal matter. Determining the mass hierarchy of the three flavors of neutrinos and studying CP violation in their interactions is a very important part of the DOE HEP program. Neutrino properties are and will be inferred by detecting how neutrinos interact with complex nuclei like Argon in the short-baseline and DUNE experimental neutrino programs at Fermilab. An accurate understanding of the quantum dynamics of a struck Argon nucleus with 18 protons and 22 neutrons is very challenging but crucial to extract detailed information on the subtle nature of the neutrino and its interactions. Quantum computers can, in principle, provide an exponential increase in our capabilities of simulating neutrino-nucleus dynamics and more generally linear response in quantum systems[1].

We are developing algorithms for quantum computers to study linear response in quantum systems. In particular we have developed simplified lattice models to implement on present-day quantum computers, models that can later be extended to more realistic treatments as their capabilities increase. Studying high energy and momentum neutrino scattering on present day quantum computers is interesting because the high energy and momentum scales correspond to short-time (requiring smaller circuits) and small spatial lattices.

In a simple model we have designed circuits to (1) accurately reproduce the ground state, (2) simulate the coupling of neutrinos to the nucleons, and (3) propagate the nucleons for short times to gain information about the energy dependence of the cross section. These are the three key ingredients in simulating neutrinos interacting with nuclei. We are running these algorithms on classical computers and quantum simulators, with the goal of running on actual quantum devices in the near future. We will present our results for the ground state, for the time correlation function and how it can be used to reconstruct the energy dependence of the cross section.

We are also simulating larger systems on classical computers to understand how we can best simulate neutrino-nucleus dynamics using a combination of quantum computer algorithms and the traditional classical event generators. Even in the short-term we should be able to gain fascinating information about this transition from quantum to classical dynamics.

[1] A. Roggero and J. Carlson, 'Linear Response on a Quantum Computer', arXiv:1804.01505

Particle Track Pattern Recognition via Content-Addressable Memory and Adiabatic Quantum Optimization

Lauren Ice¹, Gregory Quiroz¹, and Travis Humble²

This project will evaluate employing content-addressable memory (CAM) recall in combination with adiabatic quantum optimization (AQO) to improve the pattern matching algorithm for particle track pattern recognition in high energy physics (HEP) detection systems. Track recognition and reconstruction is a challenging and necessary part of most high energy physics (HEP) experiments. To simplify track reconstruction, pattern matching algorithms are commonly employed to prune data of random noise and to help discriminate signals that potentially correspond to particle tracks of interest from background events. Pattern matching quickly identifies potential track candidates by comparing the pattern of detector signals to a library of patterns known to be from events of interest. The time to search the library is decreased by organizing the library patterns into a tree structure however, the speed and effectiveness of the tree search algorithm is sensitive to the amount of random detector noise, background processes, and the spatial resolution of the detector. For this project, the quantum CAM (QCAM) approach will be compared to the tree search method by examining the quality of track reconstruction and computational speed.

CAM represents an associative memory structure in which key-value data is recalled based on its value as opposed to its key. Incorporating AQO, an approach designed to exploit quantum phenomena to find the global minimum of an objective function, CAM recall is cast as a problem of finding the energetic minimum of an Ising model constructed from a database of known key-value pairs. The track recognition problem will be cast as a CAM recall problem and study the performance of AQO via the D-Wave Systems, Inc. 2000Q quantum processing unit (QPU), the newest generation 2048 quantum bit QPU.

The effort will focus on data collected from the OLYMPUS experiment, an experiment designed to measure the two-photon exchange contribution to lepton-proton elastic scattering. This effort will be the first of its kind, in which QCAM is applied to a practical application. The objectives of this study will be to characterize and optimize QCAM performance for a practical application and to compare QCAM to classical methods (here, the tree search method used for the OLYMPUS dataset) commonly used in HEP experiments with respect to the quality of track reconstruction, rejection of noise, and computational speed.

Ultimately, observed improvements provided by QCAM will give insight into the potential advantages of future track reconstruction algorithms that incorporate quantum hardware. The team will begin by applying QCAM to pattern matching in a simulated toy dataset and then will apply the methods to Monte Carlo and experimental data from the OLYMPUS experiment. QCAM performance will be evaluated and optimized with respect to recall accuracy, while exploring bounds on recall capacity. Ultimately, QCAM will be compared to the tree search method by examining the quality of track reconstruction and computational speed.

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Towards practical quantum simulation for High Energy Physics.

Peter Love, Gary Goldstein, Hugo Beauchemin, Tufts University

Over the last decade quantum algorithms for quantum simulation of electronic structure have become accepted as the most promising early application of quantum computing. They form a major focus of both Google and IBMs commercial efforts to construct a medium-scale quantum computer. The refinement of these algorithms has involved the development of numerous new quantum algorithmic techniques and small-scale experimental demonstrations in various quantum computing hardware platforms.

Quantum algorithms for HEP problems, including algorithms for the simulation of quantum field theory, remain in a more nascent state. Several important results have recently been established but the algorithms proposed to date require many more qubits than are likely to be available in the next five to ten years. We will therefore use the results and techniques developed for quantum chemistry over the course of the last decade to improve the practicality of simulation algorithms for quantum field theories with application to specific HEP questions.

The LHC has entered into a precision era where many of the LHC flagship measurements have systematic uncertainties dominated by theoretical sources, among which the uncertainty in the proton parton distribution functions (PDF) is often the largest. We choose the computation of the proton PDF as a high-impact long-range target for quantum computation applied to HEP.

For example, the W mass measurement (<https://arxiv.org/abs/1701.07240>) has reached a precision of $\sim 0.02\%$. As can be seen in the table below (Table 13 from <https://arxiv.org/abs/1701.07240>), the largest uncertainty is clearly from the pdf. This is a particularly notable example as the difference in W^+ and W^- mass is obtained as 29.2 ± 28 MeV, with the pdf uncertainty accounting for 23.9 MeV, or 85% of this uncertainty.

Channel	$m_{W^+} - m_{W^-}$ [MeV]	Stat. Unc.	Muon Unc.	Elec. Unc.	Recoil Unc.	Bckg. Unc.	QCD Unc.	EW Unc.	PDF Unc.	Total Unc.
$W \rightarrow e\nu$	-29.7	17.5	0.0	4.9	0.9	5.4	0.5	0.0	24.1	30.7
$W \rightarrow \mu\nu$	-28.6	16.3	11.7	0.0	1.1	5.0	0.4	0.0	26.0	33.2
Combined	-29.2	12.8	3.3	4.1	1.0	4.5	0.4	0.0	23.9	28.0

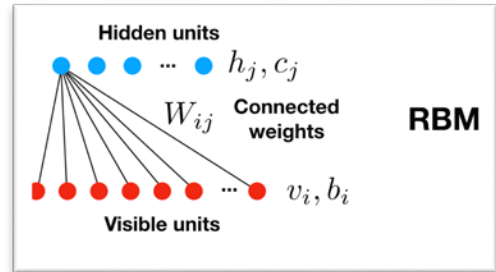
Table 13 from (<https://arxiv.org/abs/1701.07240>). The uncertainty in the W mass is dominated by the theoretical uncertainty in the proton pdf.

These theoretical errors arise due to limitations of current classical approaches for which the errors are on the order of 5%. Determining the quantum computational requirements to compute the proton PDF's to better accuracy than this, and ultimately to reduce the theoretical error below the experimental error, would significantly improve the sensitivity of many LHC measurements to new physics searches. We therefore focus on the proton pdf and the proton-proton multiply differential cross section as targets for quantum computation, with examples of those target impacts on HEP that set energy ranges and precision requirements for the computation.

High Energy Physics (HEP) ML and Optimization Go Quantum

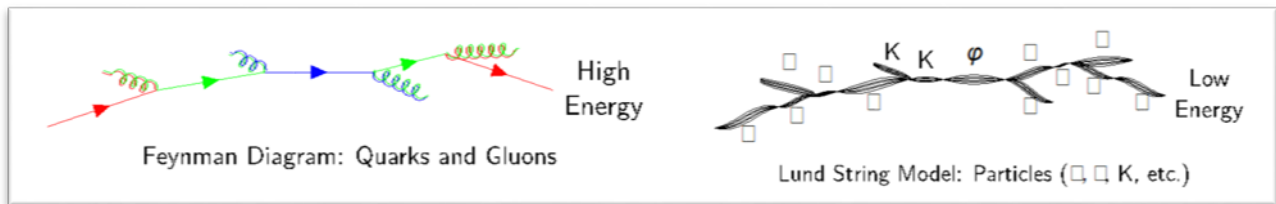
Gabriel Perdue (PI), Jim Kowalkowski, Stephen Mrenna, Brian Nord, Aris Tsaris – Fermilab
 Travis Humble (Co-PI), Alex McCaskey – Oak Ridge National Lab

We will explore machine learning (ML) and optimization problems from HEP that can be formulated using Restricted Boltzmann Machines (RBMs) or as Binary Constraint Satisfaction Problems (CSPs). Solutions to these types of problems are feasible with existing quantum annealers, simulators, and gate-based hardware. This project forms a collaboration between HEP and QIS domain scientists from FNAL and ORNL, bringing together the resources necessary to construct and run successful HEP ML and optimization quantum workflows using existing QC systems.



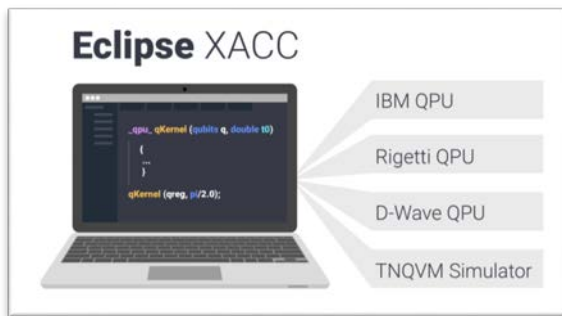
We will study two classification problems from the Energy and Cosmic Frontiers using ML and optimization techniques within the ORNL quantum development and execution environment. For ML, studies include: (1) multi-object detection used in classifying supernova and separating galaxies from stars, (2) compressing and generating simulations to accelerate analyses, and (3) unsupervised learning to detect anomalous objects. The goal is to demonstrate solving an ML problem with scientific data using a quantum annealer.

For optimization, we will study the color reconnections (CR) phenomenon at particle colliders, which involves



a minimization of the lengths of QCD strings. This involves: (1) formulation of the string minimization problem as a binary CSP, (2) solution of this problem for realistic partonic configurations, and (3) determination of the phenomenological impact of global solutions and identification of deficiencies in the underlying models. The goal is to reduce the uncertainty on the top quark mass as extracted from HEP data.

The ML and the optimization components will be implemented as classical/quantum hybrid applications. A



challenge is to determine the number of states required to solve physics problems given the available QC space. Simplifications necessary to fit within current constraints will be studied. The structure of these problems is well suited to ORNL's XACC (<https://ornl-qci.github.io/xacc/>) quantum programming framework. The structure also provides a setting for Fermilab HEPCloud (<http://hepccloud.fnal.gov>) integration. We will develop realizations of the above-described applications using mixed-language programs, targeting D-Wave and Google's quantum hardware, with C++ and

Python to classical processing, while offloading of optimization to quantum hardware.

**Quantum Machine Learning and Quantum Computation Frameworks for HEP
(QMLQCF)
PUBLIC ABSTRACT**

Several technologies for building quantum computing systems and devices have made considerable progress over the past few of years. Photonic gates can be imprinted in devices to form quantum circuits, microwave cavities are becoming more performant, ion traps are getting more reliable, and the number of qubits in quantum annealing systems has grown to the thousands. It is thus becoming practical to realize quantum algorithms on hardware testbeds, rather than simulators, to perform algorithmic validation and benchmarking experiments. We propose a multi-prong program of research for the investigation of applications of quantum algorithms, technologies, and simulations on challenging areas in High Energy Physics and an associated program of benchmarking and validation. Specifically within this project we target to explore quantum-assisted tracking, vertexing, and particle-based reconstruction algorithms and methods, real-time decision making and inference algorithms with various time and flow constraints, data anomaly detection, rapid data access & indexing schemes and hybrid computation architectures. We also target to investigate possible deep connections between deep learning networks and renormalization group flow. These studies could lead to new physical insights about both. The project proposed is designed to impact High Energy Physics while developing quantum methodologies that can be used in other computation and data intensive sciences.

Lead PI: M. Spiropulu (California Institute of Technology)
(Co-Investigator) Panagiotis Spentzouris, Fermilab
(Co-Investigator) Daniel Lidar, USC
(Co-Investigator) Seth Lloyd, MIT

Quantum Algorithms for Collider Physics

*Prof. Jesse Thaler and Prof. Aram Harrow
Massachusetts Institute of Technology*

The goal of our research is to unite powerful analysis techniques in high energy physics with cutting-edge advances in quantum computation. Broadly speaking, Thaler's research is aimed at discovering new physics at the Large Hadron Collider (LHC) and Harrow's research is aimed at unlocking the capabilities of quantum computers. Through this innovative work at the interface of high energy physics and quantum information science, we aim to maximize the discovery potential of the LHC and future colliders by demonstrating how quantum algorithms can expose important features in collision events that would otherwise be intractable with classical methods.

To search for new physics at colliders like the LHC, one relies on a series of algorithms to enhance signals of interest and mitigate backgrounds. Many of these algorithms are related to identifying and classifying jets—collimated sprays of particles that are copiously produced in high-energy collision events. Almost every LHC collision involves jets in some way, but the algorithms that are currently used to identify and classify jets are constrained by the limits of classical computation. Quantum algorithms could fundamentally change the way that collider data is analyzed, either by speeding up existing classical algorithms or by enabling quantum representations of the collision debris.

We are currently exploring two directions where quantum computation could have a direct impact on collider physics. The first direction is to use quantum machine learning algorithms to classify jets. The detailed pattern of particles within a jet (i.e. its substructure) contains valuable information about its origin, and classical machine learning algorithms have already seen numerous applications in jet classification. This research will address situations where efficiently finding the optimal classifier requires quantum manipulations, either through quantum annealing or through quantum superposition. The second direction is to use quantum clustering algorithms to identify jets. Jet clustering can be viewed as a kind of optimization problem, though most classical algorithms in use at the LHC only find approximate solutions. This research will develop quantum jet clustering algorithms that can efficiently find optimal jet configurations, as relevant for new physics searches involving multiple overlapping jets.

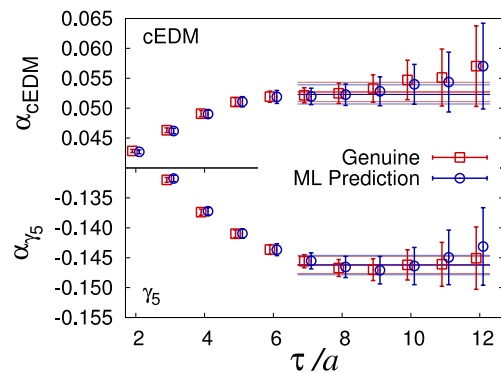
By exploiting the capabilities of quantum computation, this research confronts the challenge of data analysis in collider physics. Moreover, the work described above may pave the way for future applications of quantum machine learning beyond high energy physics, in particular clustering problems in other application domains.

Quantum Machine Learning for Lattice QCD

Boram Yoon (PI), Nga T. T. Nguyen, Garrett Kenyon, Tanmoy Bhattacharya and Rajan Gupta
Los Alamos National Laboratory

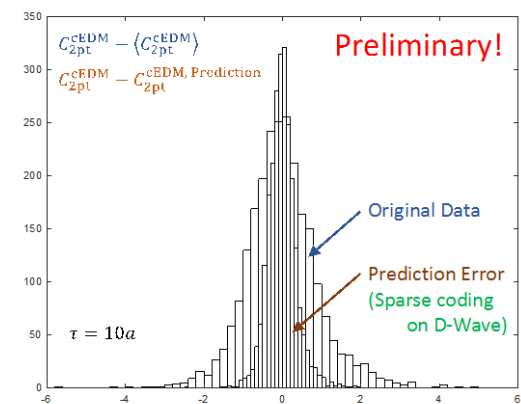
Lattice QCD is a non-perturbative formulation of QCD, the theory of strongly interacting quarks and gluons. It is solved using Monte Carlo simulations by first discretizing the theory on a hypercubic Euclidean space-time grid. In the lattice QCD Monte Carlo simulations, multiple observables are simultaneously measured on a series of Monte-Carlo samples of gluon fields as calculate expectation value, and the fluctuations of these observables over the Monte-Carlo samples are correlated. By exploiting these correlations between observables, one can build a machine learning (ML) algorithm that predicts values of a set of observables using the information on other observables. Such algorithm allows us to measure only partial of the observables, and to reduce the computational cost for the measurement. The right-hand side plot shows the ML prediction on the lattice QCD calculation of the CP Violating (CPV) phase. After trained on 30% of total simulation data, a boosted decision tree classical ML regression algorithm was able to predict the CPV phase for the remaining 70% of data only using the two-point correlation functions calculated without any CPV interactions.

Prediction of CPV Phase using Classical ML



Recently, sparse coding algorithm has been implemented on the DWave quantum annealing system by our team members. Sparse coding is a representation learning algorithm, which builds a dictionary inferred from the input data and finds a sparse representation, the linear coefficients of the dictionary elements reconstructing the input data. The representation is sparse as the algorithm enforces it to use minimal set of dictionary elements for the reconstruction of a given input data. Because the representation is sparse, the reconstruction picks up only the key features of the data, wiping out unseen fluctuations, and reconstructs

Distribution of CPV correlators and ML predictions



input data in a way that can be explained by the dictionary elements. Therefore, by taking array of observables as an input data and setting the target observable to an arbitrary value, the reconstruction fills up the target observable with its prediction value based on the dictionary obtained from a training data set, so it can be used as a regression algorithm. The left-hand side plot shows a preliminary study of the sparse coding regression performed using DWave quantum annealer. Narrower spread of the prediction error than the distribution of original data indicates that the prediction algorithm is working as expected.