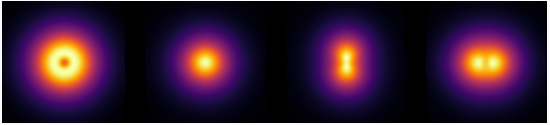
Femtoscale Imaging of Nuclei using Exascale Platforms



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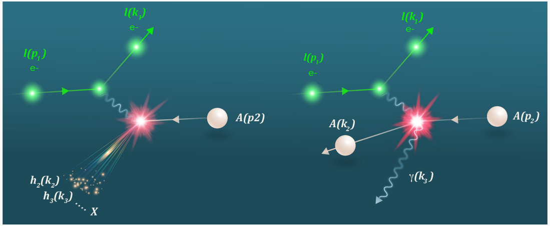
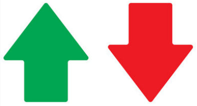
Workshop on Software Infrastructure
for Advanced Nuclear Physics Computing (SANPC 2024)
20—22 June 2024

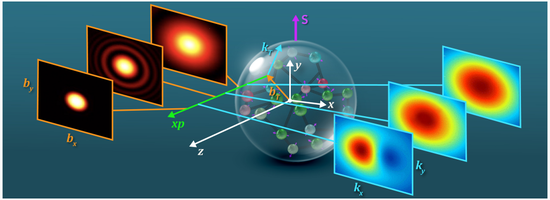
QuantOm Collaboration

Motivation for this SciDAC

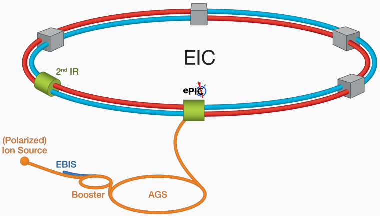
- **Goal:** To develop a new paradigm for the interface between theory and experiment for the analysis of data to infer femtoscale *images* of proton's and nuclei to reveal their 3D quark and gluon structure
- **Science Motivation:** To make optimal use of the petabytes of data from JLab, EIC, etc. to shed light on some of the key questions in nuclear physics:
  - What is the 3D confined motion and spatial distribution of quarks and gluons in nucleons and nuclei?
  - How do quark-gluon dynamics produce proton mass and thereby vast bulk of mass in the visible universe?
- To deliver these goals need a diverse team: domain experts in QCD theory and experiment, in collab with applied math, AI/ML, data science, and high-performance computing expertise

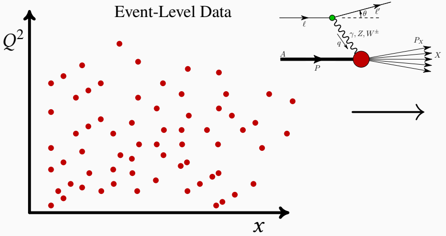


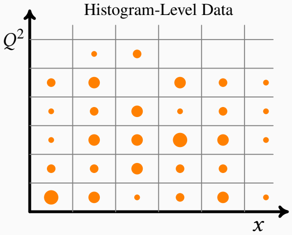




Current Paradigm



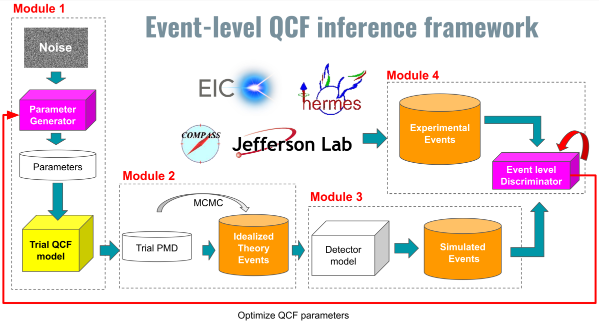


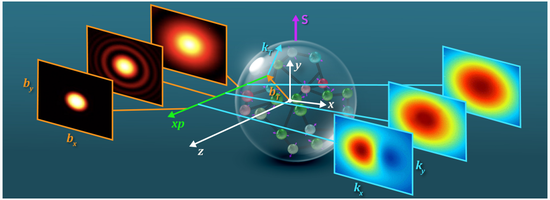


- Events are the basic *quantum of information* for our SciDAC – EIC will produce PBs of event data
- Current approach takes measured events and puts them in "bins" to obtain an average result over the phase space of the bin (histogram) – several shortcomings to this process, including:
  - Information is lost in this process
  - Limited resolution on events can cause bin migration effects
  - Detector effects need to be unfolded which is much more difficult the folding in the detector effects
- Histograming events works well enough in low dimensions with a sufficient amount of data, however, taking 3D pictures of the proton requires events in 5 or more dimensions
  - Loss of correlations/information in the data which could greatly impact the experimental program

An Event-Level Approach and Framework

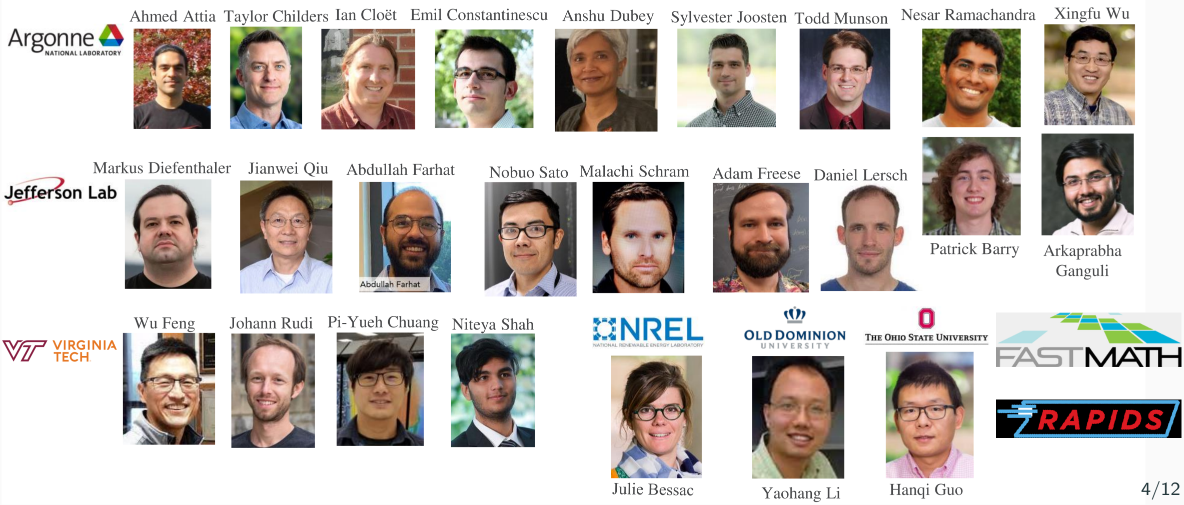
- In general, our approach is to represent the pictures of the proton in some manner e.g., as images, using piecewise polynomials, etc. that are governed by a large number of parameters (up to millions)
- Use these pictures, together with QCD theory, sampling, detector models, etc., to create set of simulated events
- We then use some approach to adjust the parameters until the simulated events and experimental events can be attributed to the same theory
- Workflow requires numerous methods from applied math, AI/ML, HPC, etc.
  - Statistical methods, Generative Adversarial Networks, event-level loss functions, distributed learning, . . .



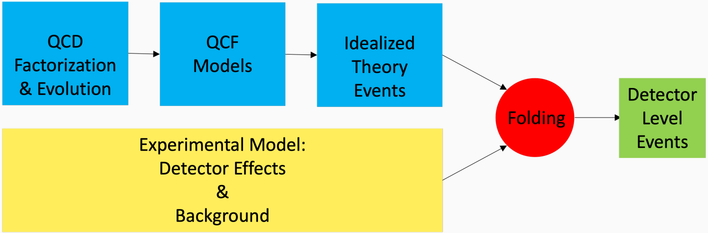


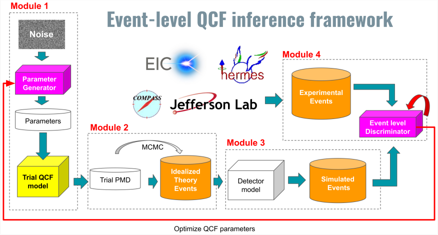
QuantOm Collaboration

QuantOm (QUAntum chromodynamics Nuclear TOMography) **Collaboration** is the team that will deliver the *"Femtoscale Imaging of Nuclei using Exascale Platforms"* SciDAC Project



Unifying Theory and Experiment via Folding

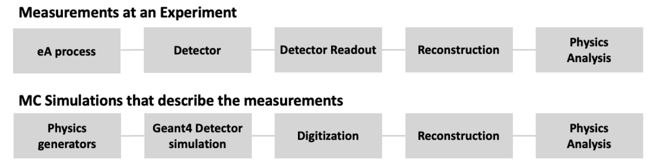




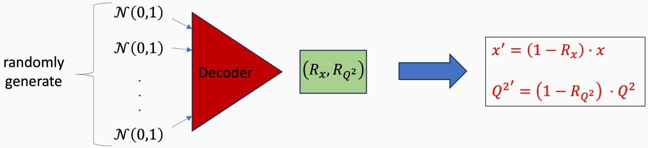
- Theory and Experiment usually meet at the differential cross-section level
  - Requires the *unfolding* of detector effects, backgrounds, etc.
- Folding in detector effects, backgrounds, etc. much more robust
  - Folding is not an invertible transformation, so reduces systematic uncertainties associated with unfolding
- Folding enables theory and experiment to be treated in an equal and unified manner, and variations in the theory can be much more rigorously studied

Experimental Modeling

- To develop an AI/ML enabled QuantOm workflow for event-level analysis need a differentiable detector module
  - Need to develop surrogate models for detectors



- Developed an event-level approach to model experimental effects from detailed simulations of the experiment, including background, e.g., Variational Autoencoder (VAE)



- Found that VAE demonstrates better performance over Deep Neural Networks for the cases studied

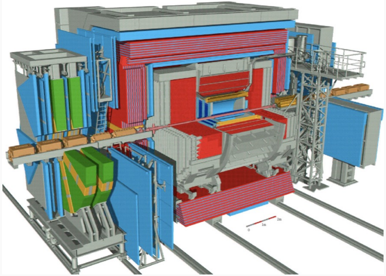
ZEUS Example

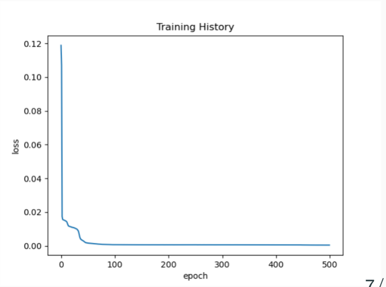
- Selected inclusive DIS events from detailed simulations of the ZEUS experiment at HERA.

- Used electron method for (x, Q^2) reconstruction

- AE detector surrogate specifications:
  - Encoder hidden layers and units: [50,50,50,100,100]
  - Decoder Hidden layers and units: [100,100,50,50,50]
  - Latent Dimension 128, RELU activation function

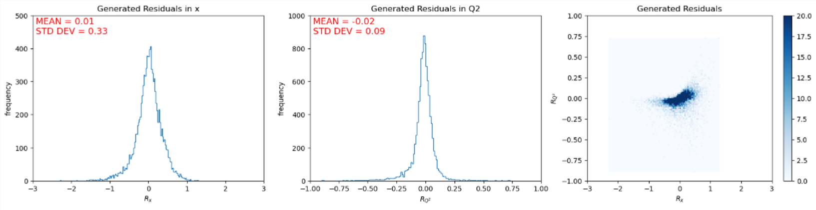
- Training: 20k events, 80/20 train/test split, outliers removed



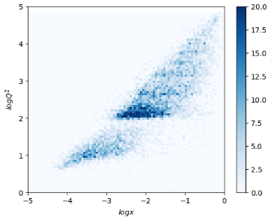


ZEUS Example: Residual and (x, Q^2) Distributions

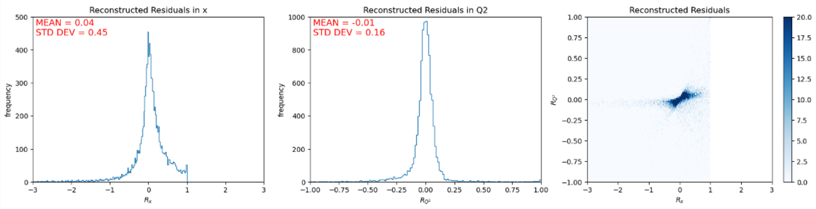
VAE Detector Surrogate



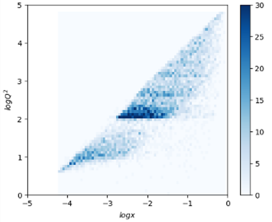
VAE Detector Surrogate



ZEUS Simulation (electron method only)



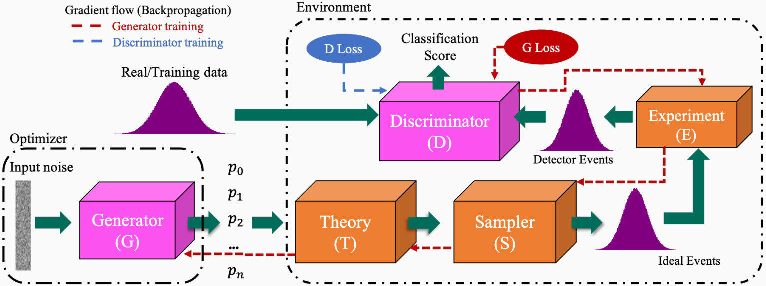
Ground Truth



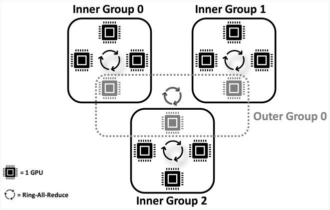
Developed a detector surrogate and training procedure to model various eA experiments

Scaling QuantOm Workflow using GANs

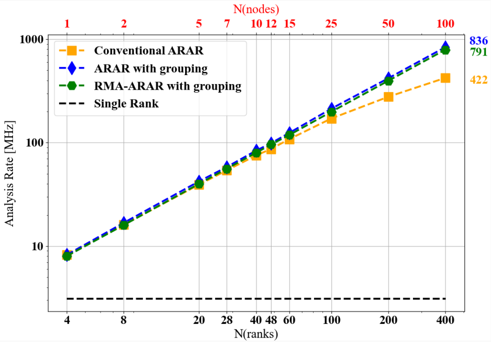
- **Goal:** Want to run workflow across multiple GPUs
  - Handle data size
  - Distribute computational load, e.g. sampler module

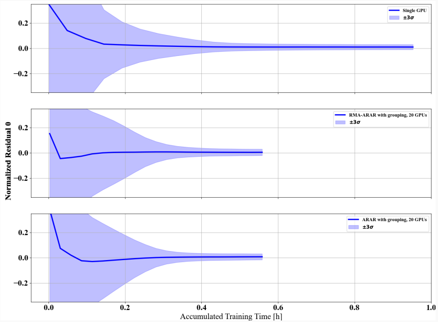


- **Approach:** Asynchronous Ring All-Reduce (ARAR)
  - Data is shared across GPUs
  - Each GPU trains discriminator locally
  - Generator gradients are transferred between GPUs
  - GPUs are bundled into groups
  - Enabled usage of Remote Memory access (RMA-ARAR)



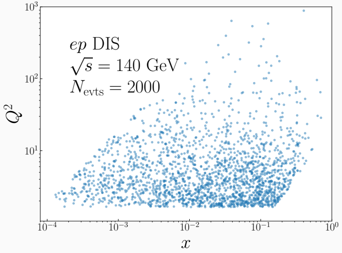
Results on Distributed Learning Approaches using Polaris

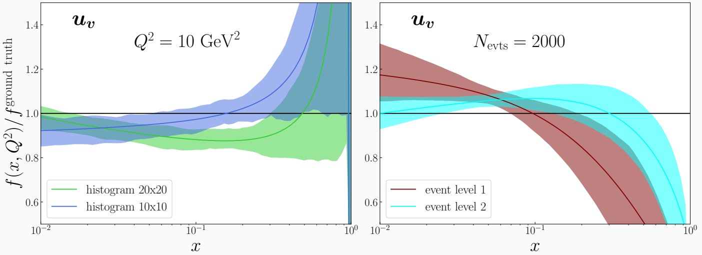




- Test distributed learning approaches on for event-level PDF analysis using Polaris
  - Used ensemble technique to determine convergence quality
  - ARAR/RMA-ARAR with grouping allow for earlier convergence
  - Observe weak nearly linear scaling
- Method will be further tested and developed on Aurora at Argonne
- Demonstration that we can develop an event-level analysis framework at scale

First Event-Level Analysis for DIS





- Generated 2000 simulated DIS events, which were sampled from a differential cross-section generated from ground-truth PDFs
- Analyzed these events using the traditional histogram approach and two event-level approaches
  - The histogram approach and event-level 2 perform about the same
  - However, a different binning produces different results
- Event-level approach removes a key systematic uncertainty: *How does different binning schemes impact the extraction of quantum correlation functions?*

Conclusion and Outlook

- Performing an analysis of scattering data at the event level requires significantly more upfront computing resources
  - Real-world deployment will require exascale resources, however, this will compress the time scales from measurement to discovery, which is often years to up to more than a decade
  - Real-time data analysis becomes a possibility, and when combined with autonomous optimization, could lead to autonomous discovery at facilities like the EIC
- The success of this SciDAC project should represent paradigm shift in the way science is conducted at high-energy accelerator facilities
  - Will remove the artificial wall between theory and experiment and seamlessly connect them into a single analysis framework