QuantOm Collaboration

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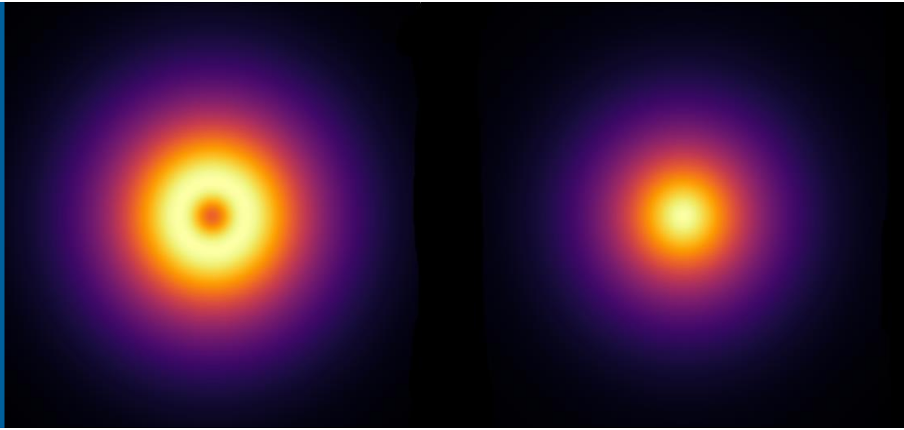
https://quantom-collab.github.io

SAGIPS: A SCALABLE FRAMEWORK FOR SCIDAC QUANTOM

SCIDAC-5: FEMTOSCALE IMAGING OF NUCLEI USING EXASCALE PLATFORMS



DANIEL LERSCH
For the QuantOm collaboration

AI4EIC 2025, MIT, Boston

October 29, 2025

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Argonne NATIONAL LABORATORY

Jefferson Lab

VIRGINIA TECH

FASTMATH

NREL NATIONAL RENEWABLE ENERGY LABORATORY

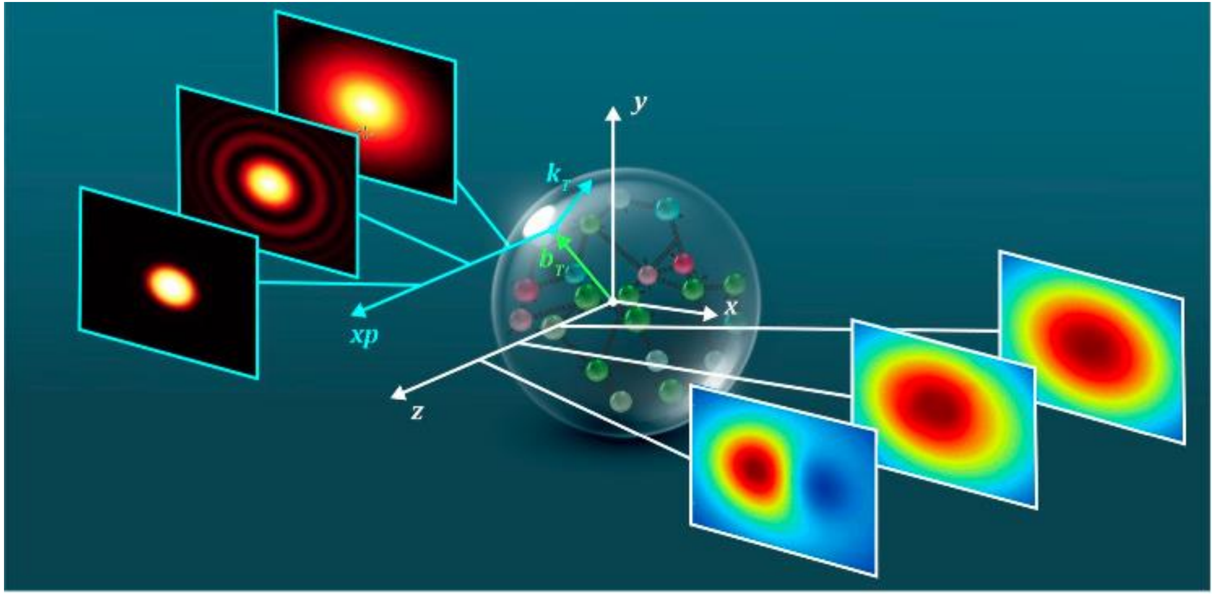
OLD DOMINION UNIVERSITY

THE OHIO STATE UNIVERSITY

RAPIDS

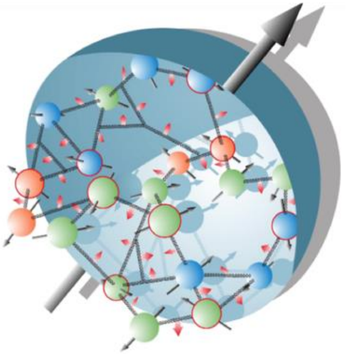
Exploring the Quark-Gluon Structure

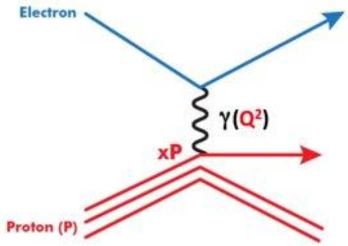
- QUAntum Nuclear TOMography (QUANTOM)
- Extract Quantum Correlation Functions (QCFs) from Deep Inelastic Scattering (DIS) experiments
- Joint theoretical-experimental analysis
- 3D imaging of nuclei



Towards a joint Theoretical-Experimental Analysis of QCF

QCD → Experiments → Observables → Analysis





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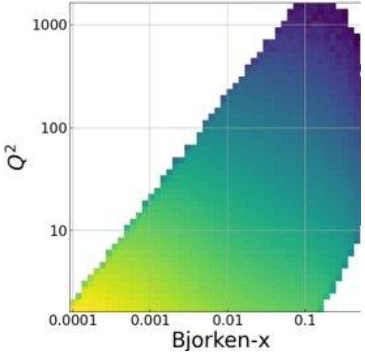

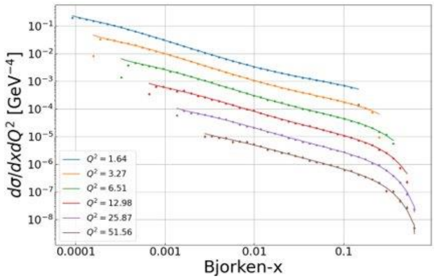

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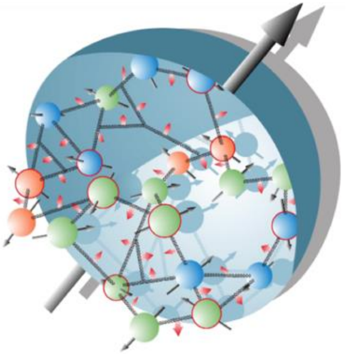
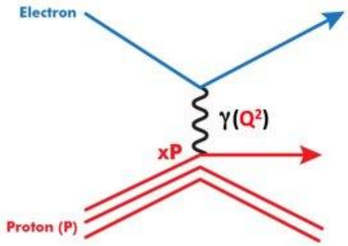
Towards a joint Theoretical-Experimental Analysis of QCF

conventional

- Binned analysis
- Acceptance corrections
- Fit experimental data
- Extract QCFs

QCD → Experiments → Observables → Analysis





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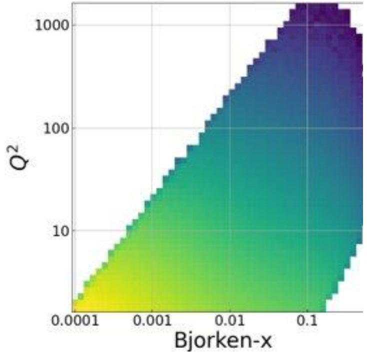

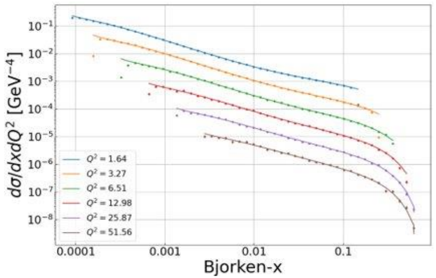

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Towards a joint Theoretical-Experimental Analysis of QCF

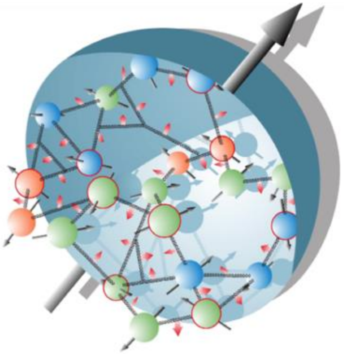
Event-Level Fit

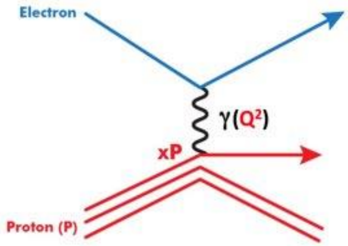
- Unbinned analysis
- Extract QCFs directly from experimental data
- Access to higher dimensional correlated data

conventional

- Binned analysis
- Acceptance corrections
- Fit experimental data
- Extract QCFs

QCD → Experiments → Observables → Analysis





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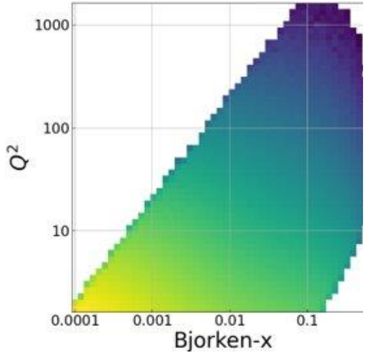

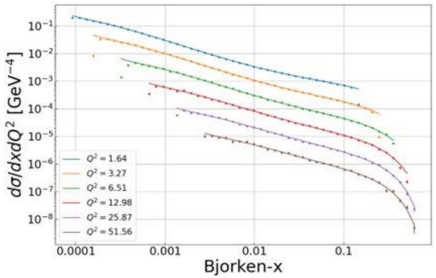

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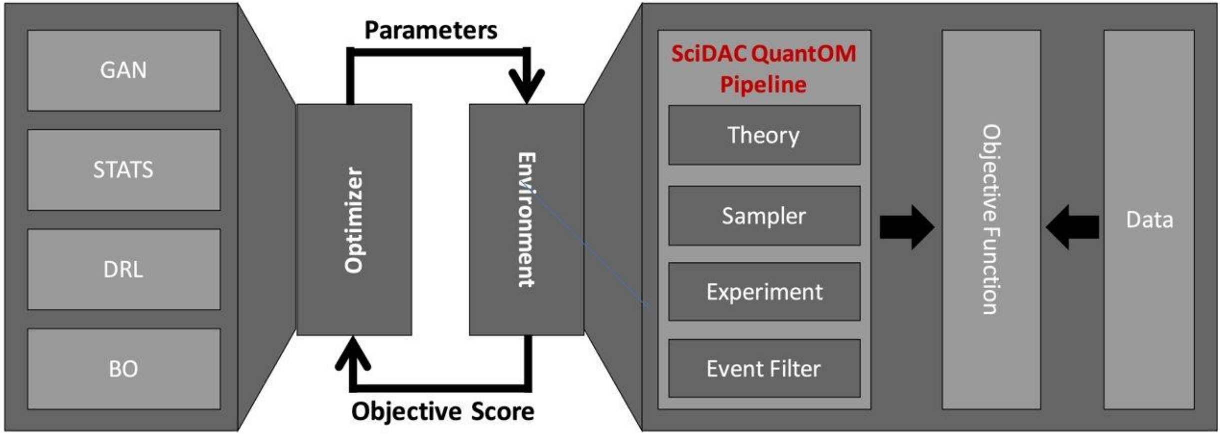
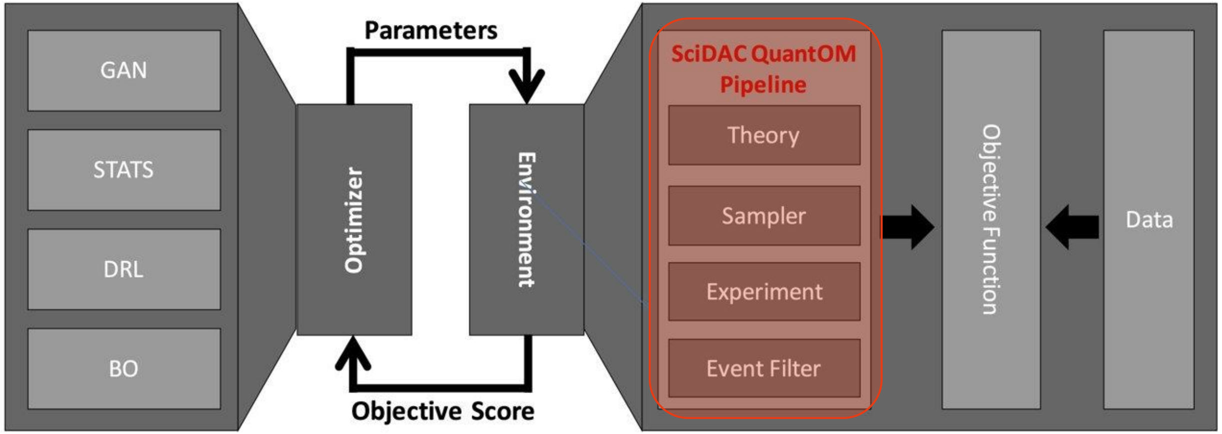
SAGIPS: Scalable Asynchronous Generative Inverse Problem Solver



- Modular framework
- Adjustable pipeline translates predictions to physics events
- Leverage input from theory and experiment
- Currently 2 optimization approaches available

1. Statistical workflow
2. GAN workflow (today's focus)

SAGIPS: Scalable Asynchronous Generative Inverse Problem Solver



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Domain Science

1. Statistical workflow
2. GAN workflow (today's focus)

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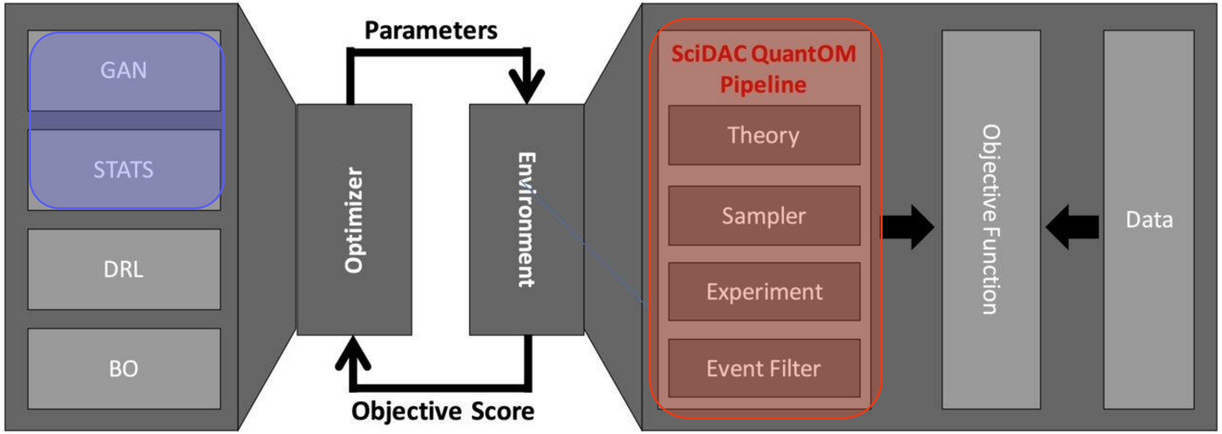

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- Currently 2 optimization approaches available

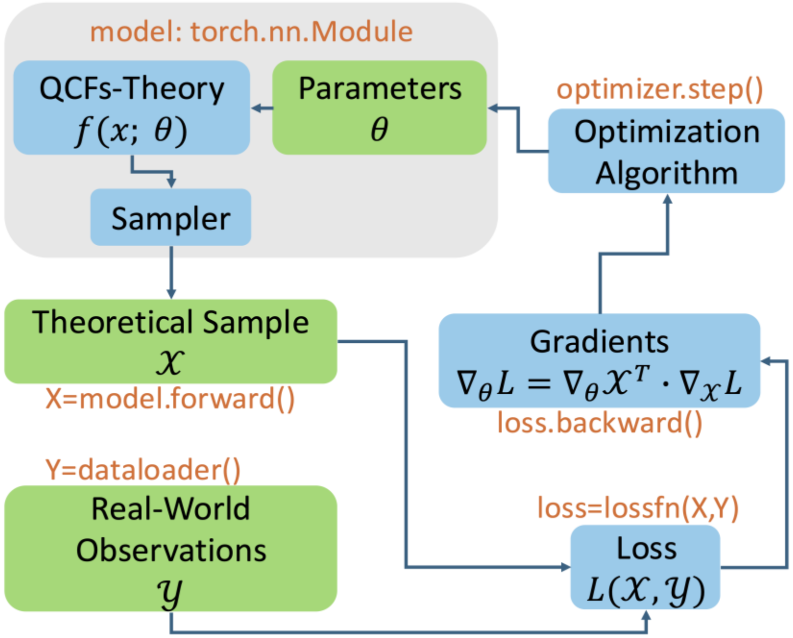
Domain Science

1. Statistical workflow
2. GAN workflow (today's focus)

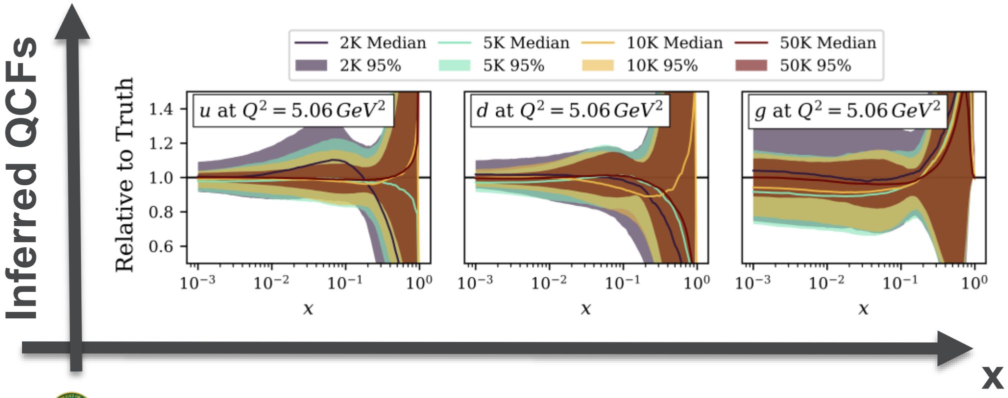
Data Science

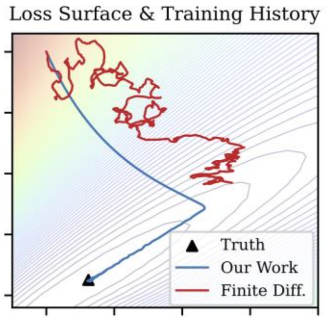
Statistical Workflow

- Pi-Yueh Chuang (Argonne) et al.
- Determine gradients for non-differentiable components: **DistroSA** (Distribution Sensi tivity Analysis)
- Support any event sampling routine
- First tests on proxy problem
- GPU accelerated loss function

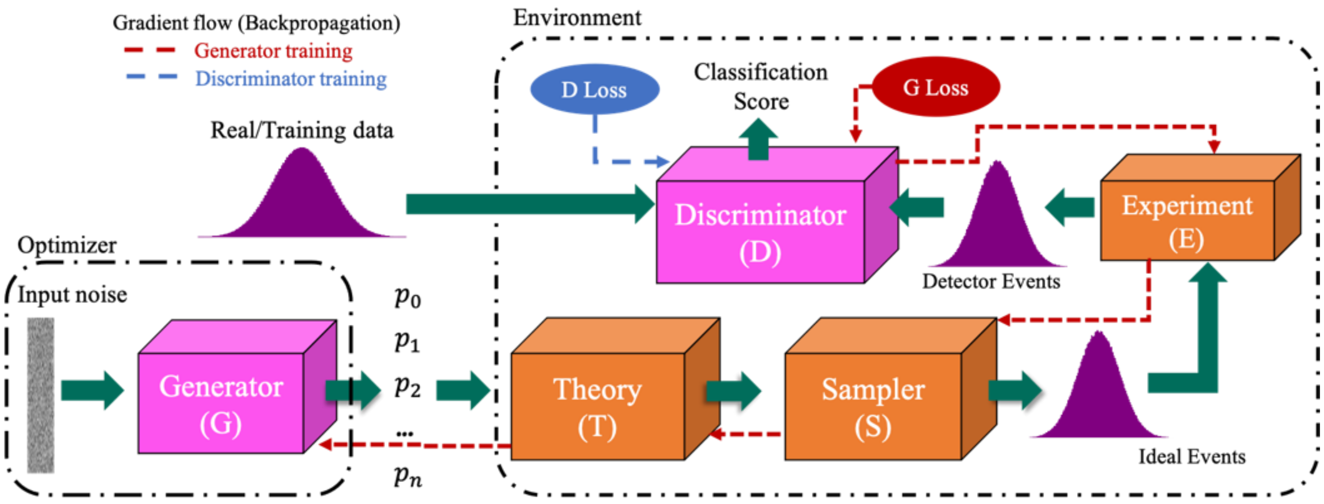


Orange texts are corresponding PyTorch code.





GAN Workflow



- All components need to be differentiable
- Use proxy problems to evaluate workflow
- 3 evaluation phases

Phase	Proxy Problem Dimensionality	Complexity
1	1D	low
2	2D	mid
3	5D	high

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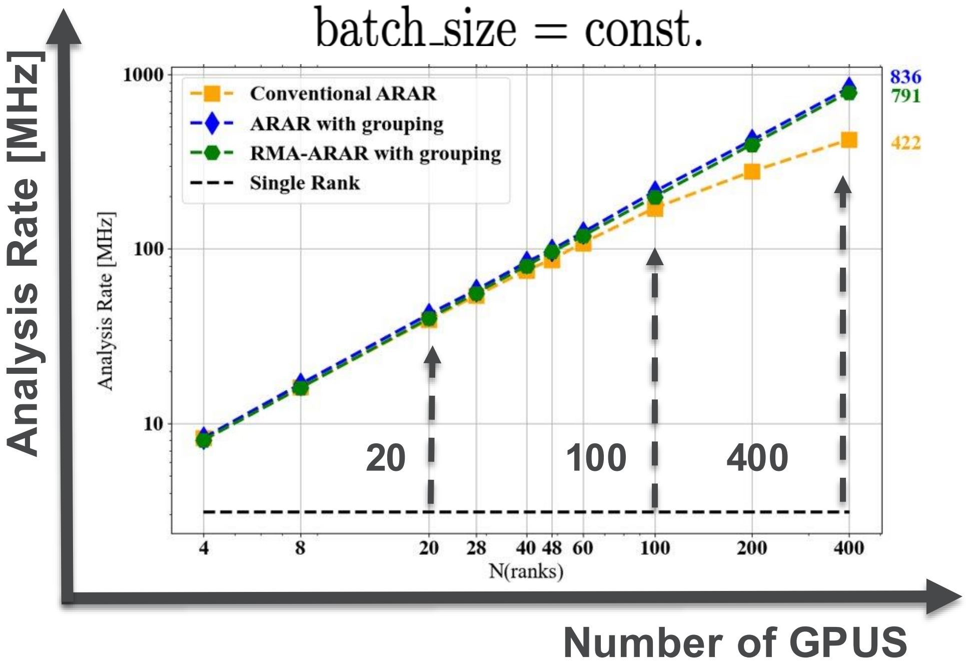
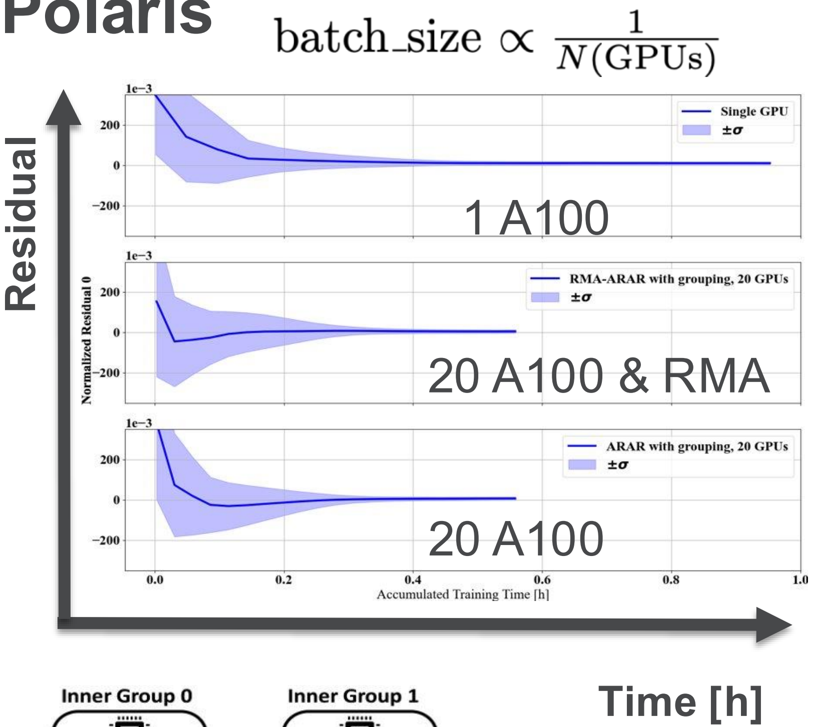
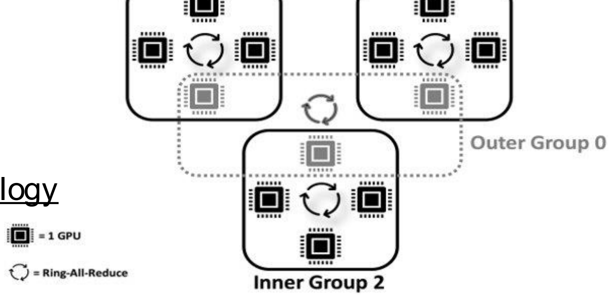
Phase 1: Distributed Analysis on Polaris





- Analyzed 1D proxy problem: $x \sim \rho(x, p_0, \ldots, p_5)$
- Share generator gradients across GPUs
- Asynchronous ring communication w/ grouping mechanism
- Optional: Remote Memory Access
- Published in: IOPScience: Machine Learning: Science and Technology



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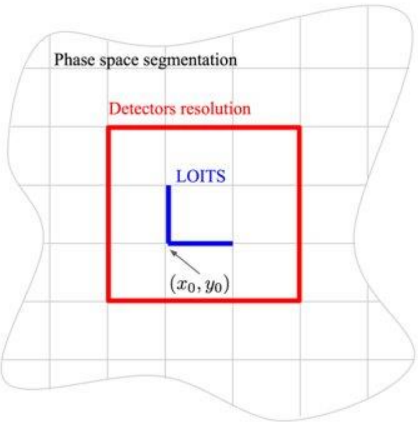
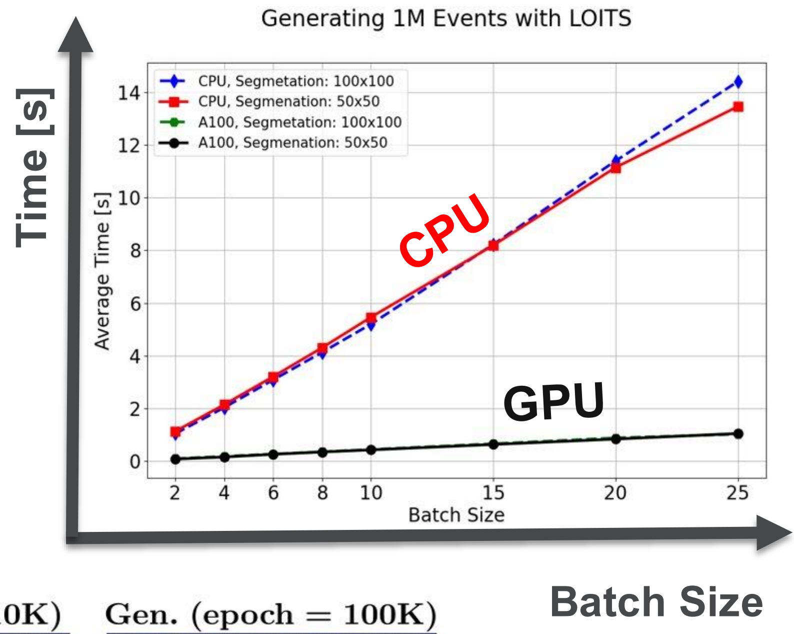
Differential Sampling in 2D

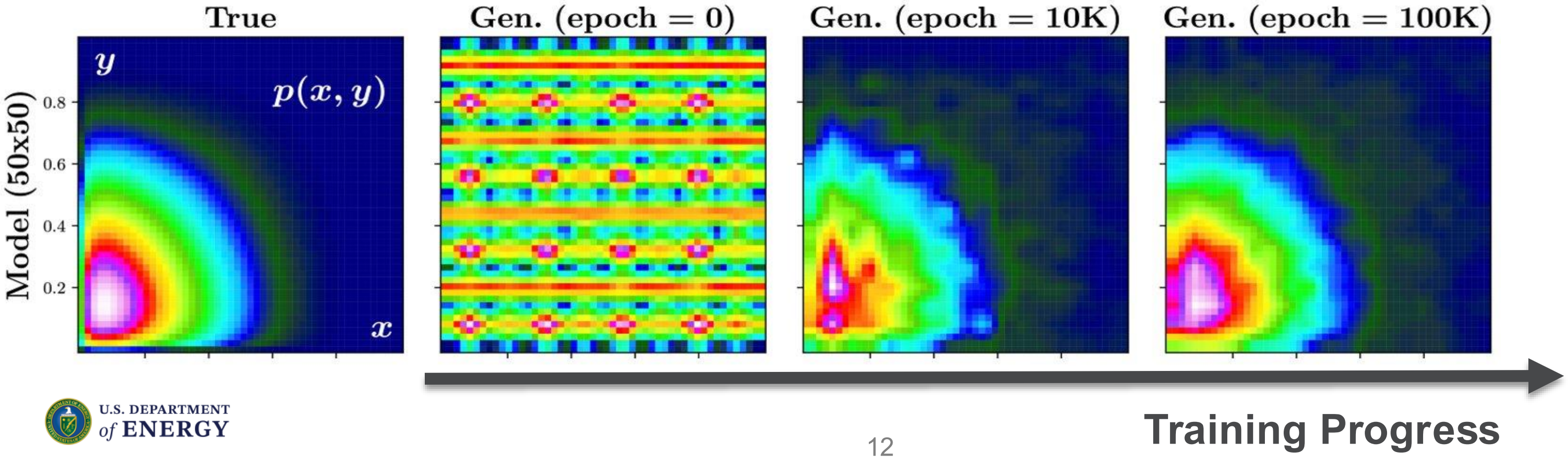
- **L**ocal **O**rthogonal **I**nverse **T**ransform **S**ampler – **LOITS**
- Provide gradients for backpropagation
- Optimal performance on GPU
- Tested on 2D proxy problem:

$$(x, y) \sim \rho(x, y)$$

- Submitted to Physics Letter B







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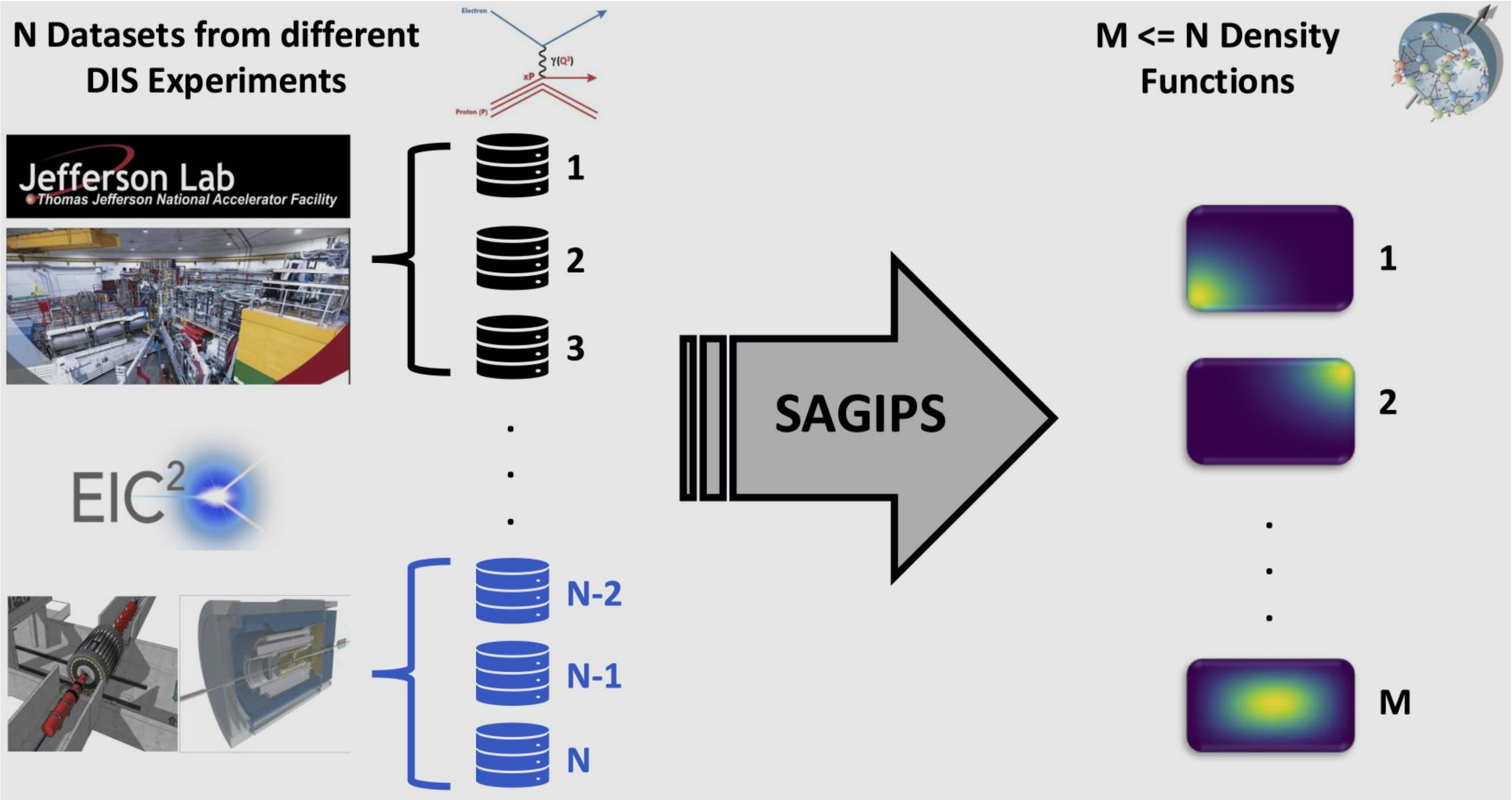
Multi-Dataset Analysis



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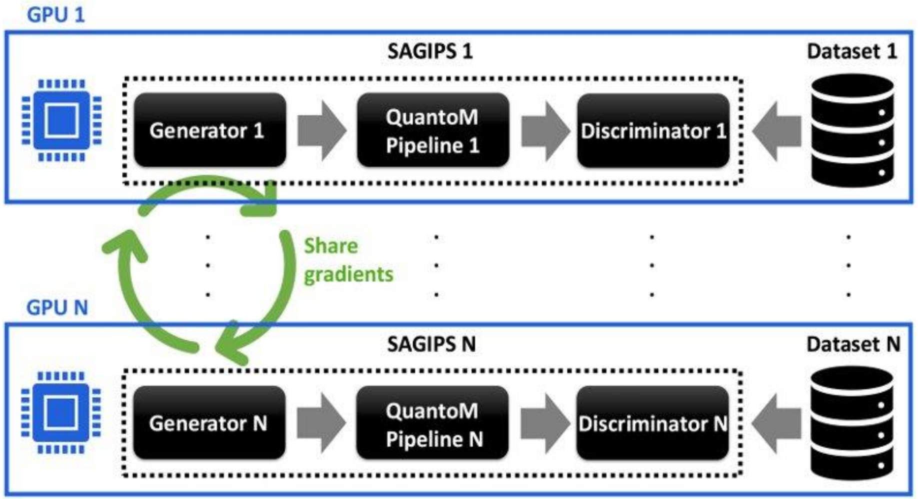
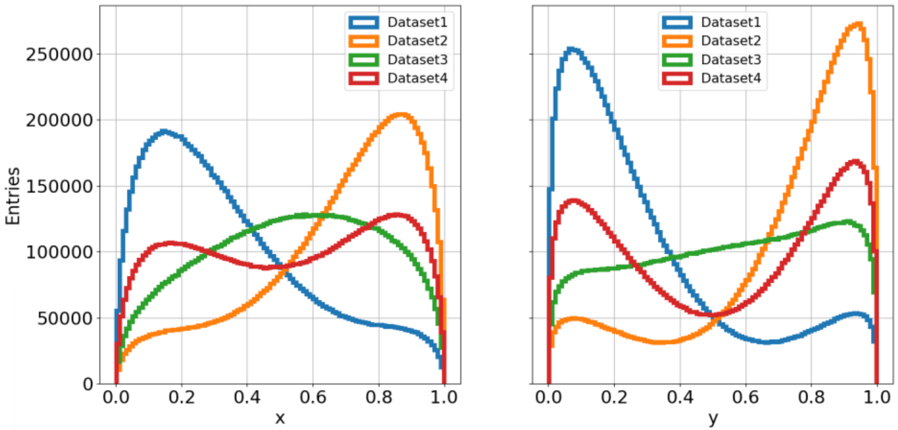
Phase 2: Multi-Dataset Analysis on 2D Proxy Problem

- Simultaneously fit 4 datasets and extracted 3 densities

$$(x_i, y_i) \sim \sum_{j=1}^{3} \left[m_{ij} \cdot \rho_j(x, y) \right], \; i = 1, ..., 4$$

- Apply distributed data parallel technique





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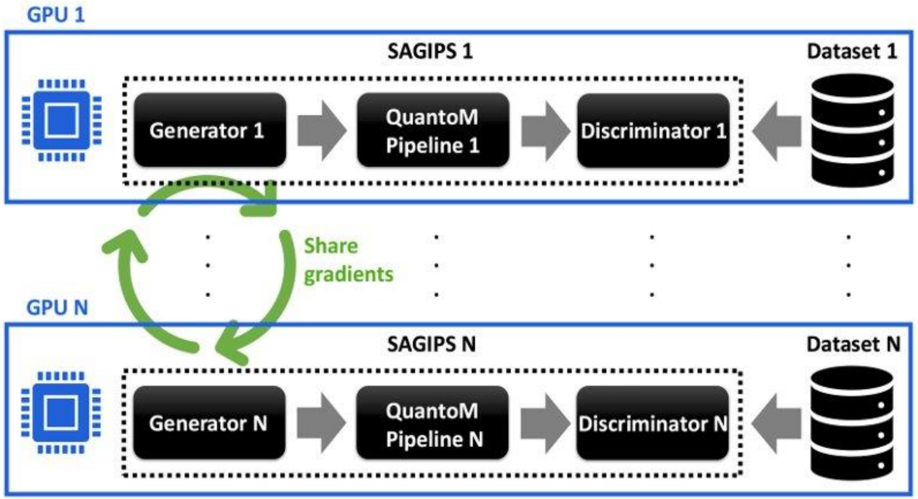
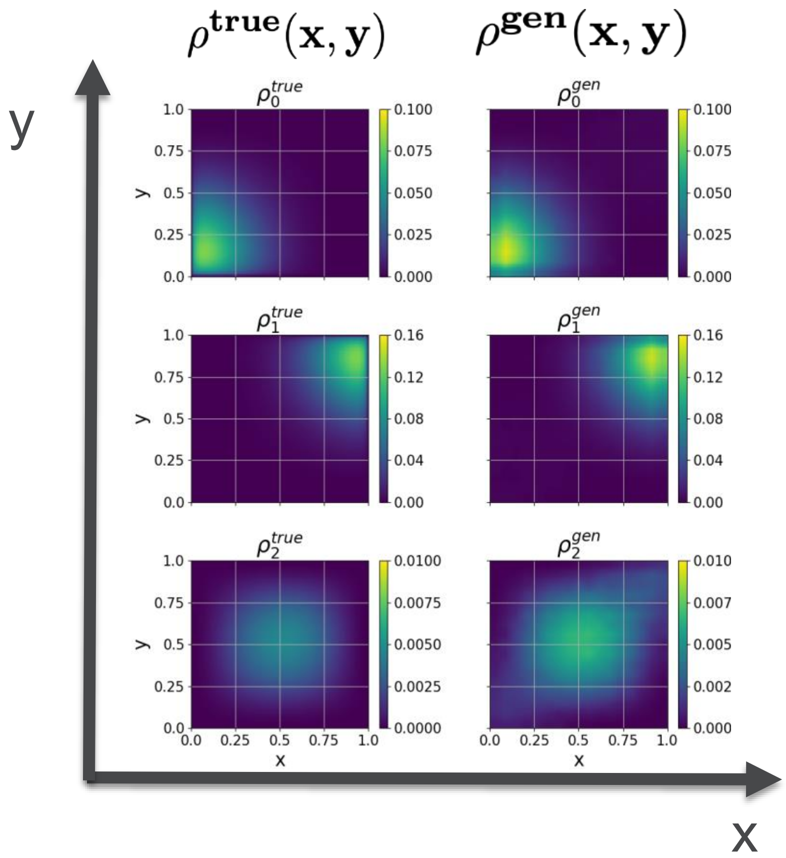
- Apply distributed data parallel technique
- Utilized 160 Polaris GPUs
- Detailed evaluation ongoing





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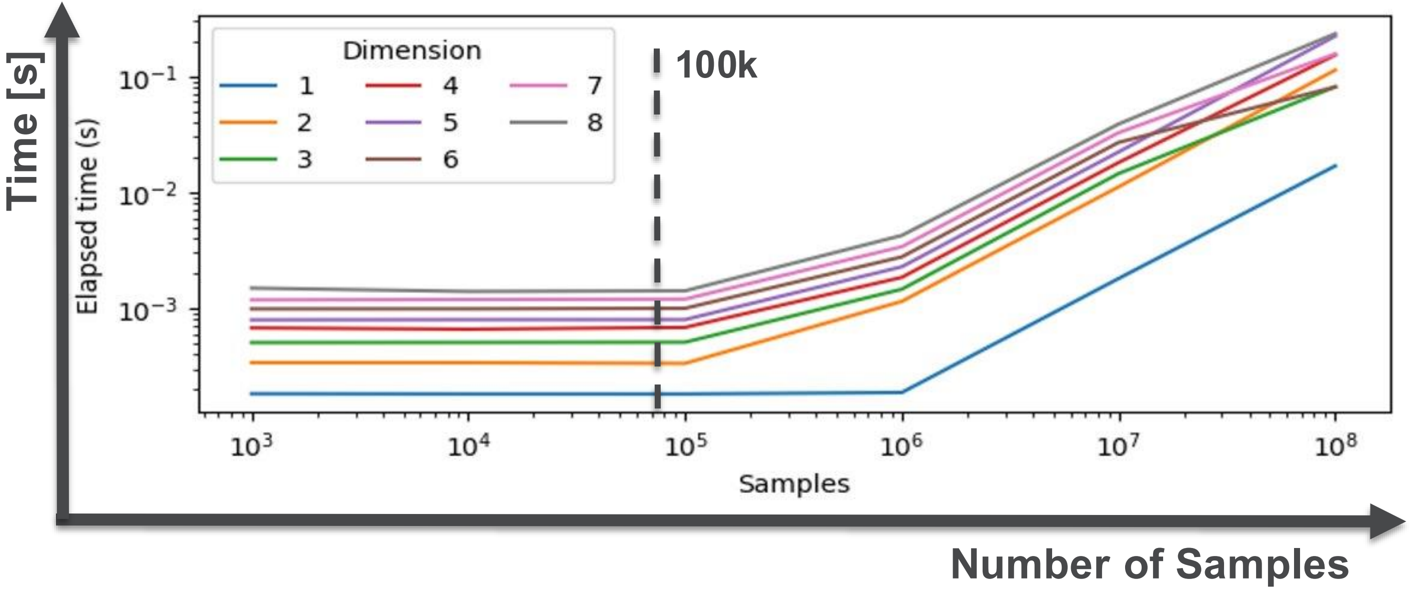
Towards Phase 3 with N-D Sampling



- Extension of LOITS to run in 5D
- Dimensional scaling tests on A800
- Observe nearly linear scaling
- Integrate N-D sampler into workflow and run performance tests

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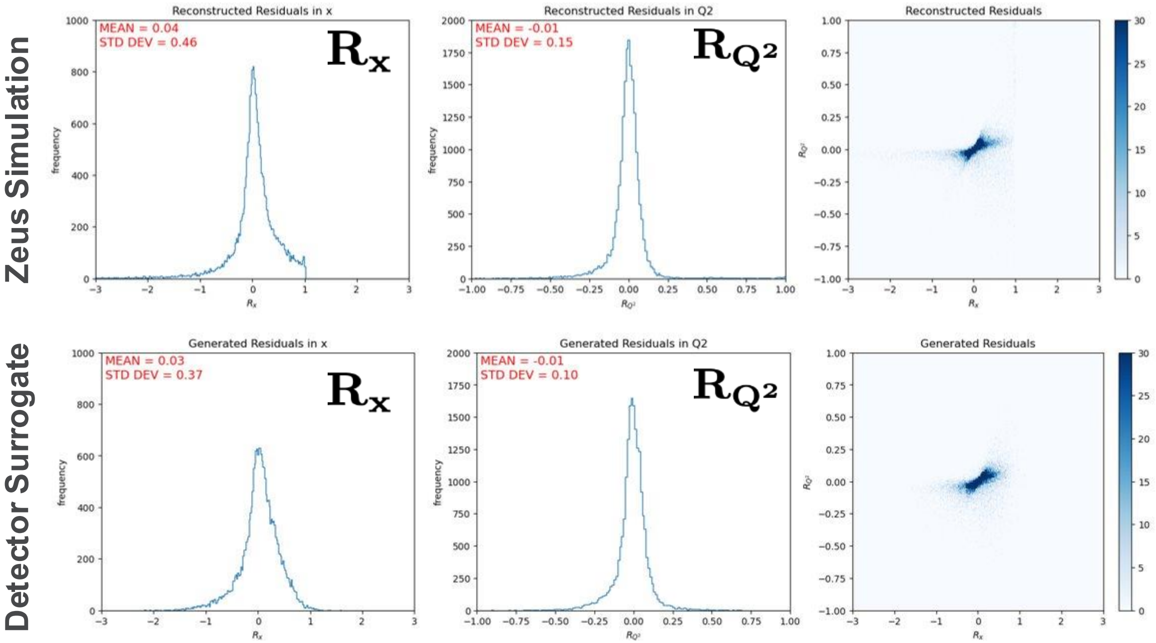
Experimental Effects

- Events generated by SAGIPS need to match experimental data
- Include experimental effects
  - Accelerator and physics backgrounds
  - Detector misalignment and inefficiencies
  - Acceptance and resolution effects
  - Particle misidentification
- Full simulation chain not applicable --> Use surrogate instead
- Detector modeling mostly finished
- Work on background handling ongoing



- Surrogate generates residuals: $R_x = \frac{x_0 - x'}{x_0}$, x_0: ideal, x' : after detector
- Apply resolution effects (folding): $x \mapsto x \cdot (1 - R_x)$
- First test: Trained VAE detector surrogate on Zeus simulations

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Summary & Outlook

- 3D Imaging of nuclei through simulation based inference
- Joint theoretical-experimental analysis of QCFs
- Generative AI for inverse problem solving
    - Modular workflow
    - Asynchronous ring communication
    - Deployed on Polaris HPC system
    - Differentiable sampling
    - Simultaneous fit of multiple data sources
- Integrate uncertainty quantification
- Work on detector surrogate and background modeling ongoing
- Run analysis on real experimental data

BACKUP SLIDES

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