QuantOm Collaboration

www.anl.gov/phy/QuantOm

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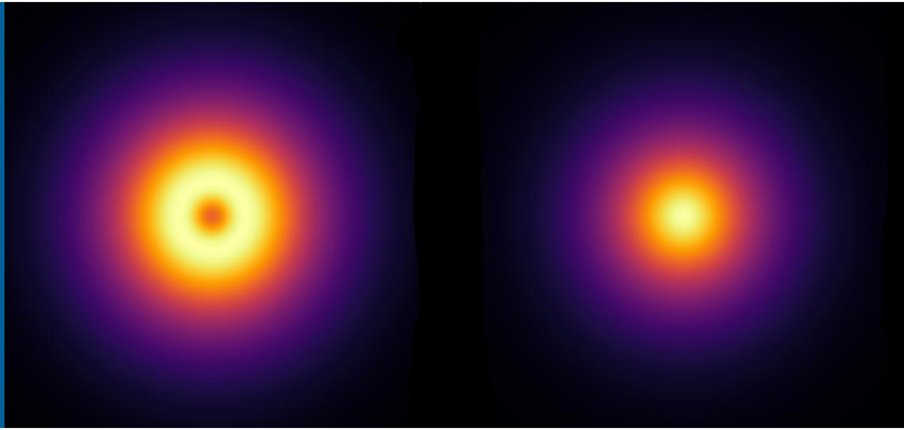
THE SCIDAC QUANTOM FRAMEWORK: A COMPOSABLE WORKFLOW



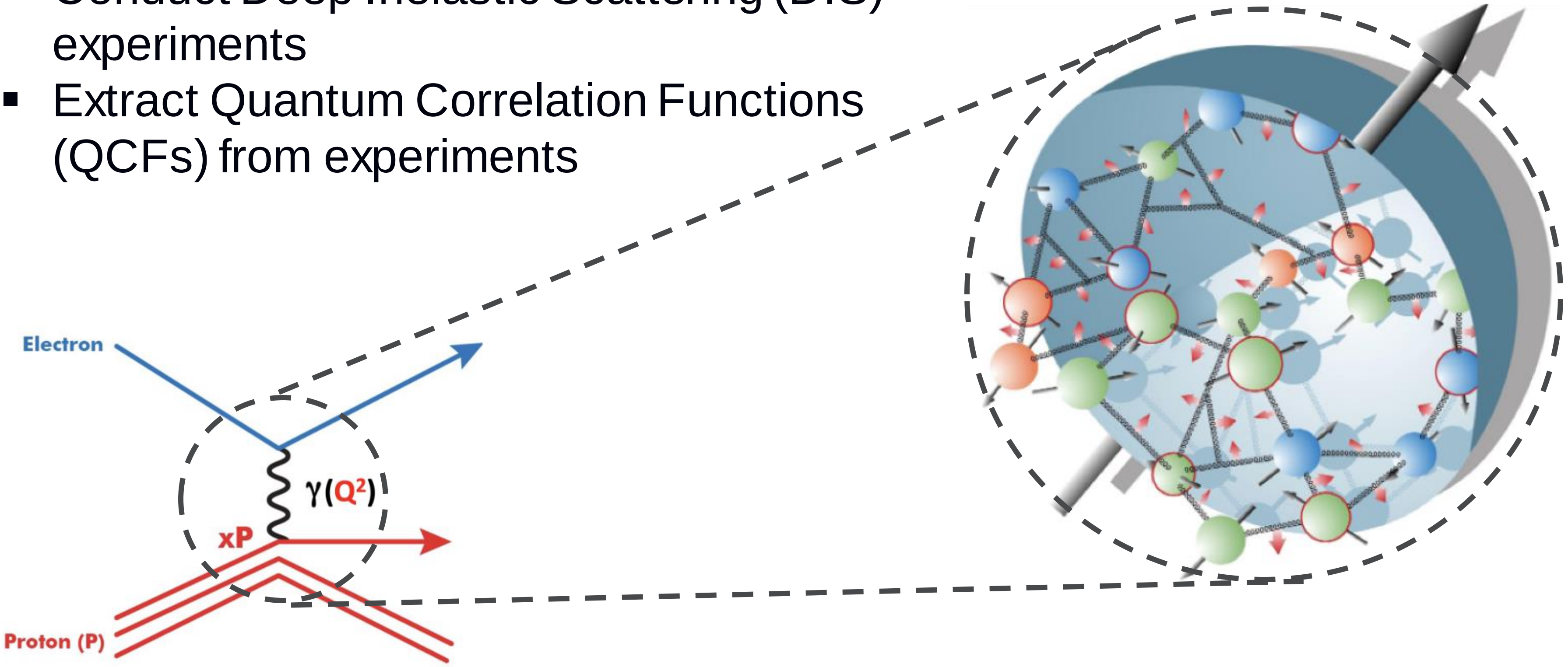
DANIEL LERSCH

for the QuantOm Collaboration

14 March 2024

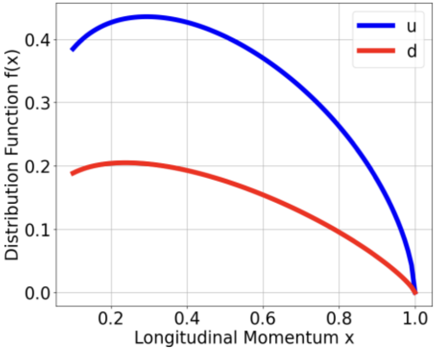
EXPLORING QUARK-GLUON STRUCTURE

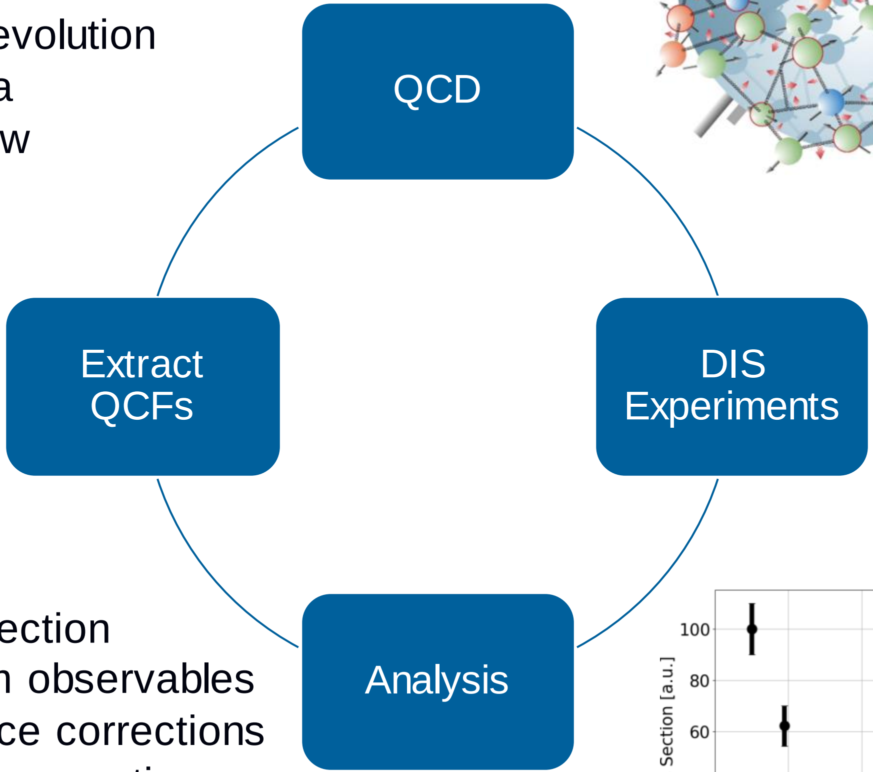
- Want to understand Quark-Gluon system
- Conduct Deep Inelastic Scattering (DIS) experiments
- Extract Quantum Correlation Functions (QCFs) from experiments

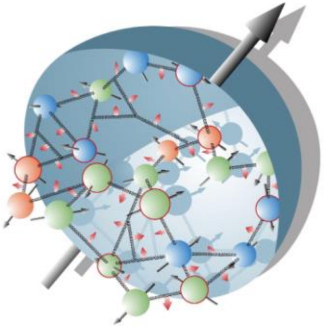


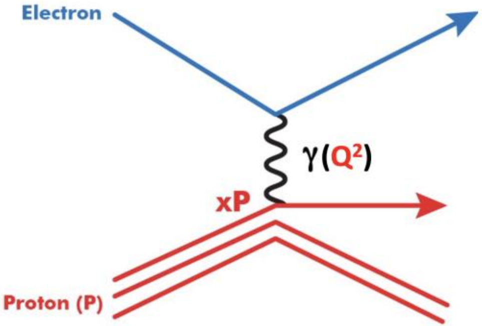
COMMONLY USED WORKFLOW

- Input from theory
- QCD factorization / evolution
- Fit experimental data
- Inspire / motivate new experiments ?

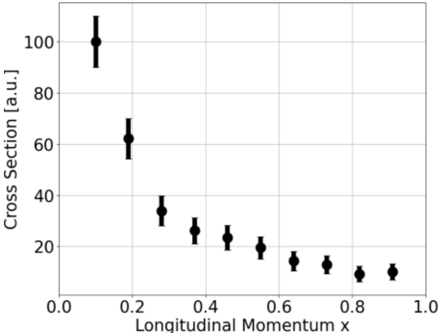








- Event selection
- Histogram observables
- Acceptance corrections
- Radiative corrections
- ...



EIC²

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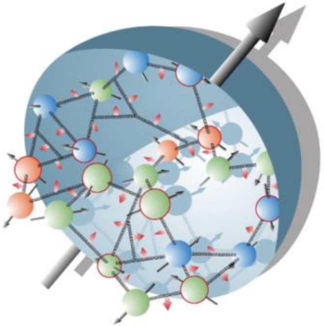

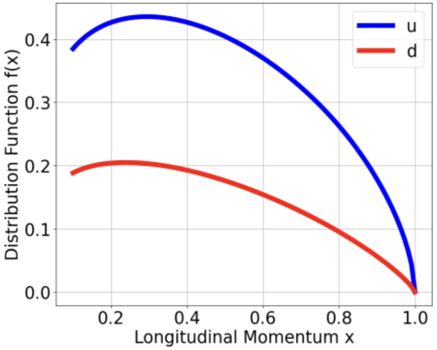

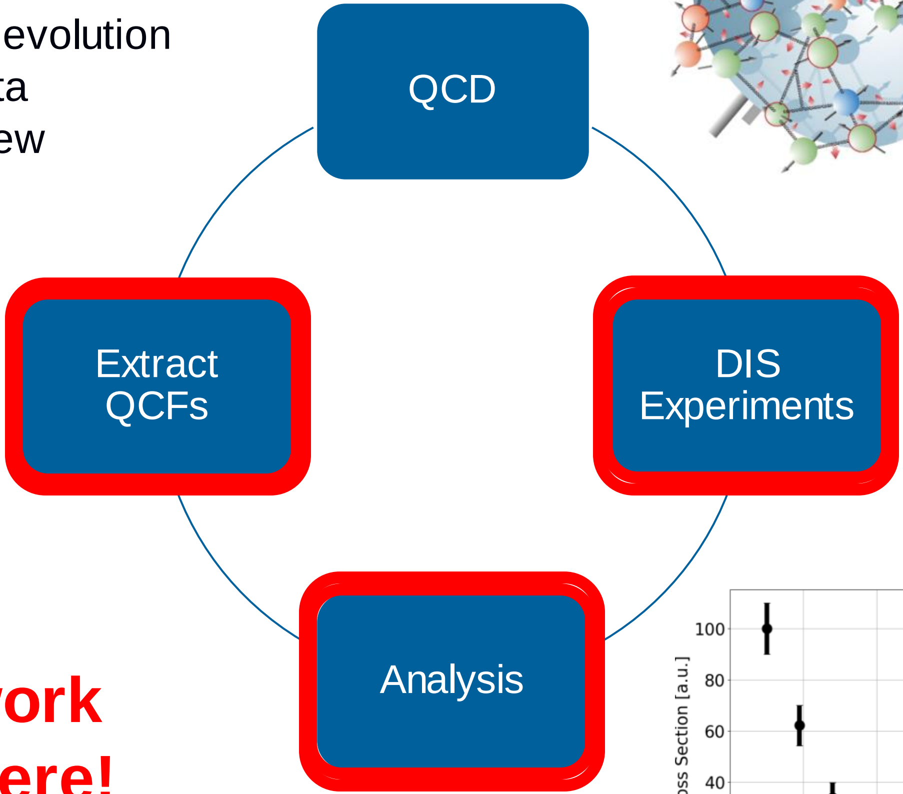

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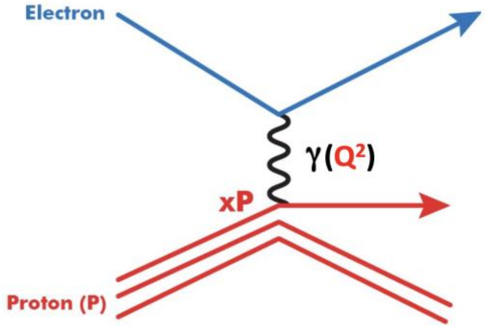

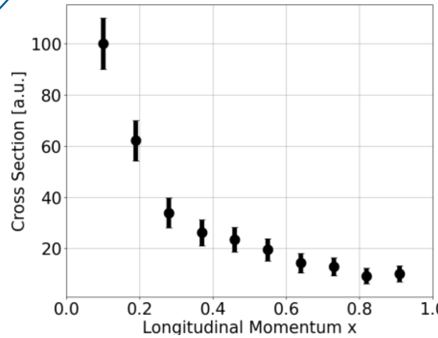

A lot of work goes in here!

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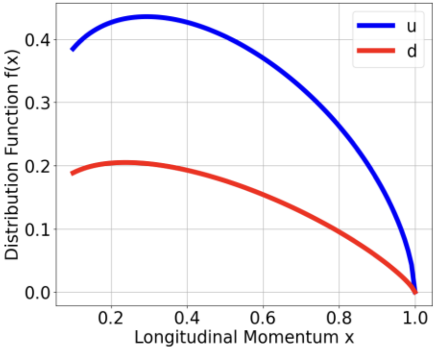
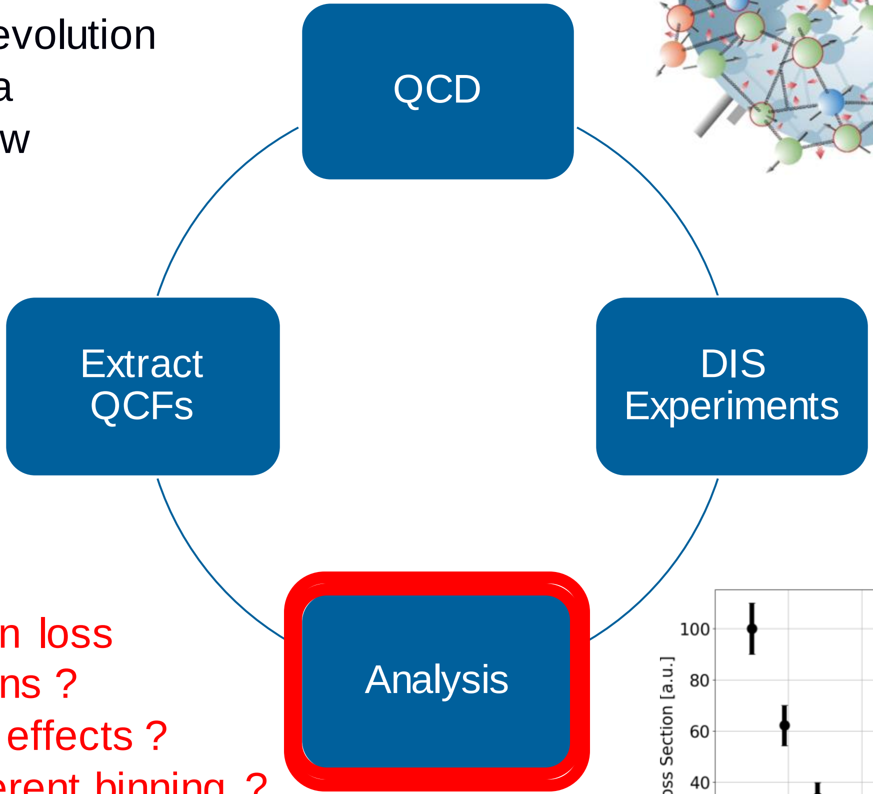
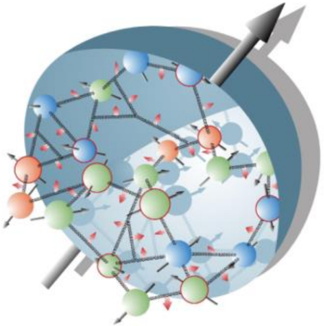
COMMONLY USED WORKFLOW

- Input from theory
- QCD factorization / evolution
- Fit experimental data
- Inspire / motivate new experiments ?







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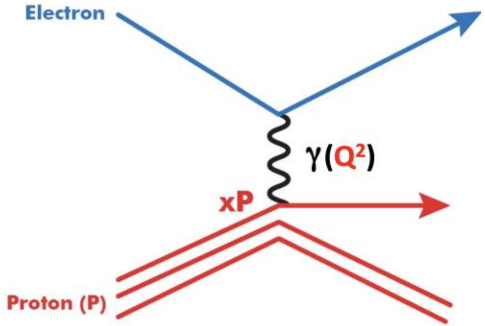
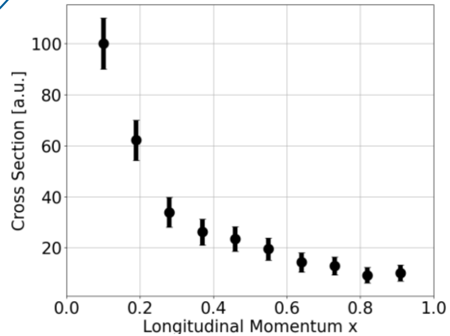


- Possible information loss
- Handling correlations ?
- Binning / smearing effects ?
- Re-iterate with different binning ?
- ...



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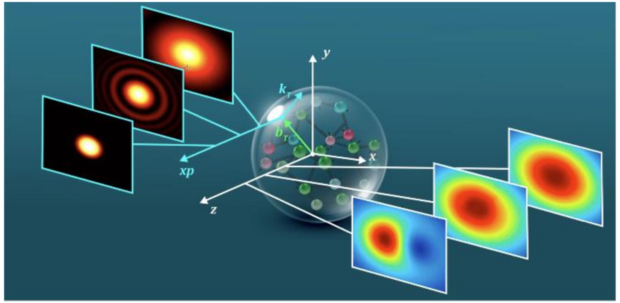
TOWARDS AN EVENT-LEVEL ANALYSIS

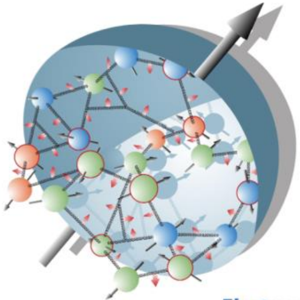


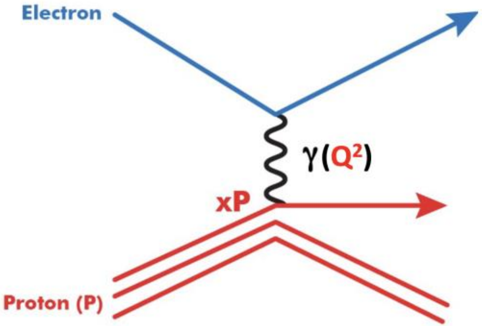
QCD

3D Imaging of QCFs

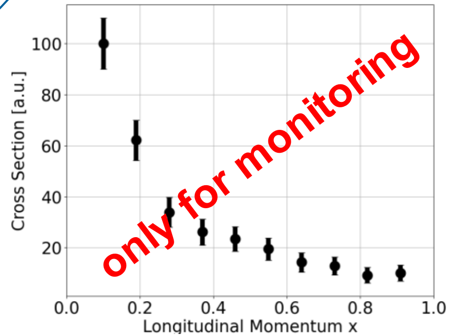
DIS Experiments

Event-Level Analysis





- Utilize all available information (i.e. theory, experiment,..)
- Explore entire feature space in experimental data
- Analyze experimental data "on the fly"



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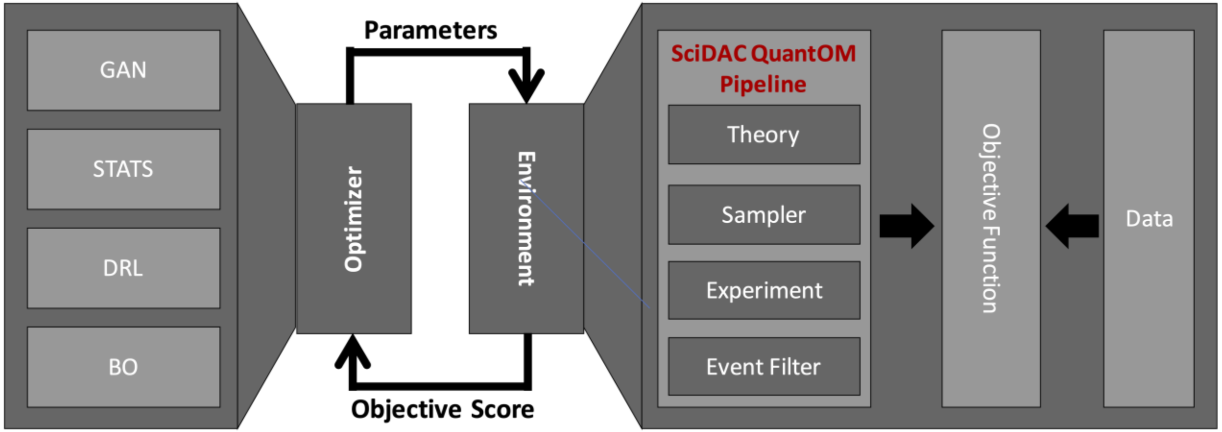
THE QUANTUM NUCLEAR TOMOGRAPHY (QUANTOM) COLLABORATION

- Part of **Sci**entific **D**iscovery through **A**dvanced **C**omputing (**SciDAC**)
- Interdisciplinary research
  - Applied mathematics
  - Computer and data science
  - Theoretical and experimental nuclear physics
  - High performance computing
- Collaboration between multiple national research institutions
  - Jefferson Lab
  - Argonne National Laboratory
  - Old Dominion University
  - Virginia Tech

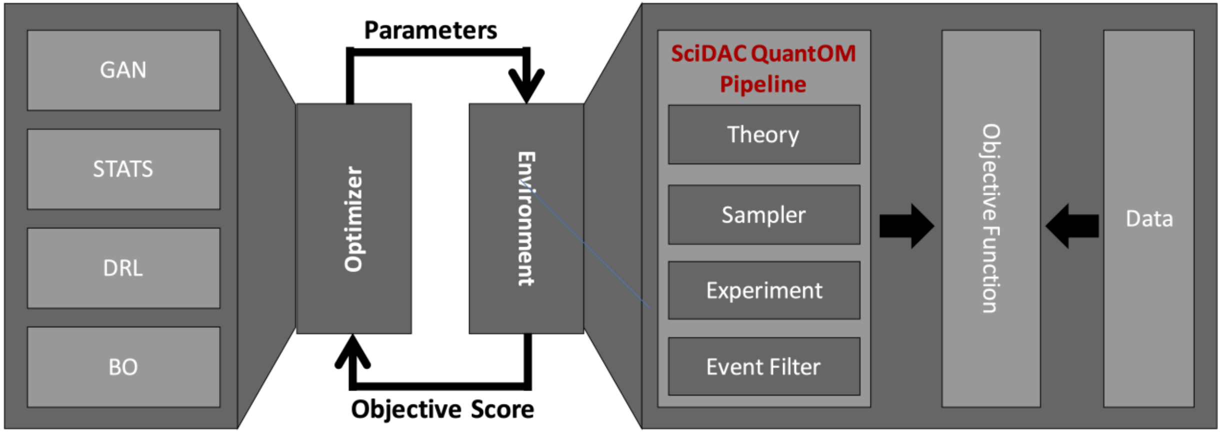
INVERSE PROBLEMS

- Measure observable y
- Interested in underlying mechanisms, encoded in x
- x is experimentally not accessible
- Known: $y = f(x)$
- $f(\cdot)$ can not be trivially inverted
- Theory provides a model: $x \approx \hat{x}(p)$
- Find $\tilde{p}$ that minimizes: $F[y, f(\hat{x}(p))]$
- Use $\hat{x}(\tilde{p})$ as an approximation for unknown x

THE GENERATIVE INVERSE PROBLEM SOLVER: GIPS



THE GENERATIVE INVERSE PROBLEM SOLVER: GIPS

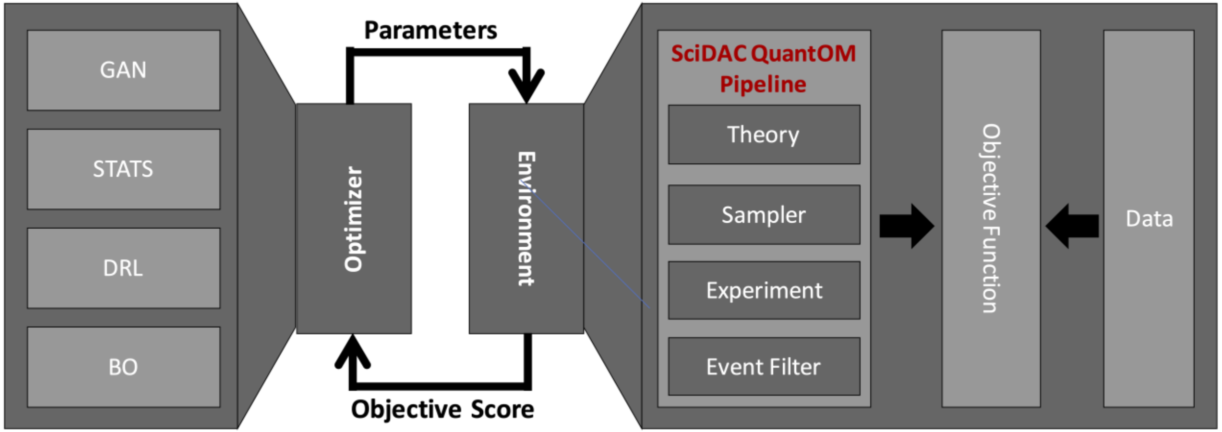


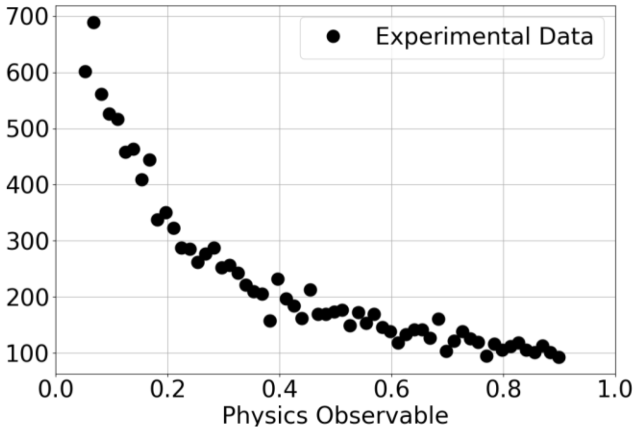
$$F[y, f(\hat{x}(p))]$$

p

$f(\hat{x}(p))$ $F[\cdot,\cdot]$ y

THE GENERATIVE INVERSE PROBLEM SOLVER: GIPS





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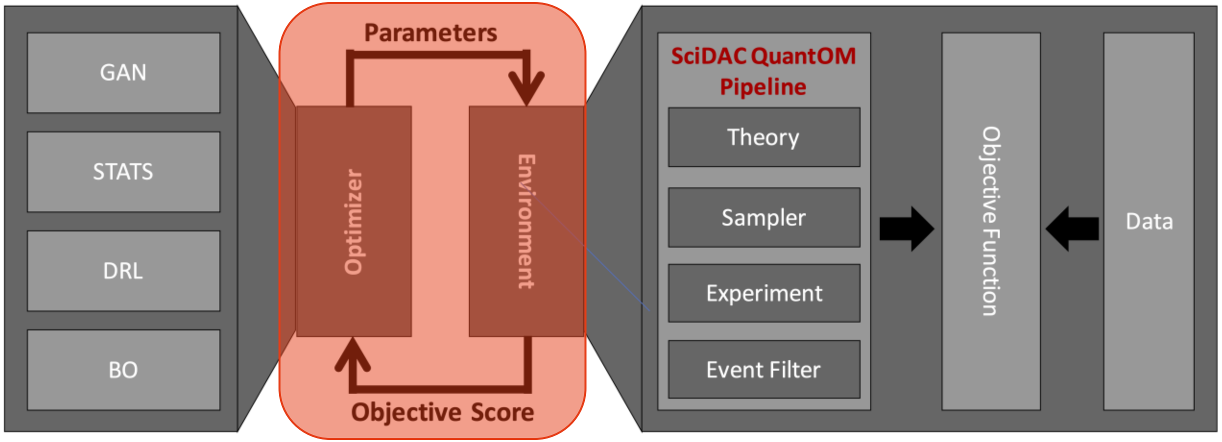

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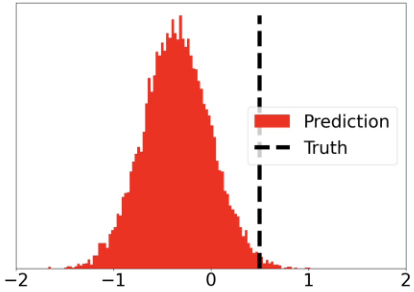
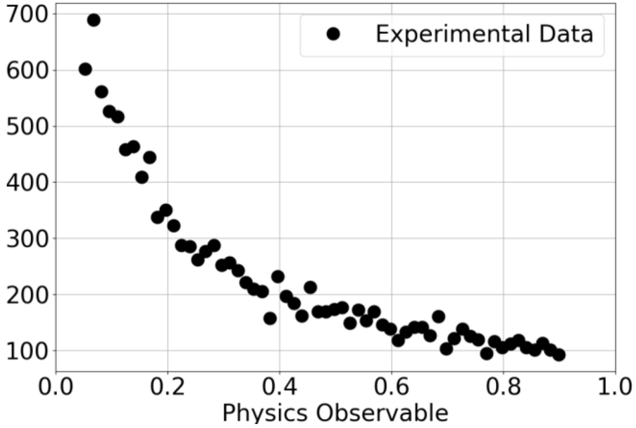
Iteration 0



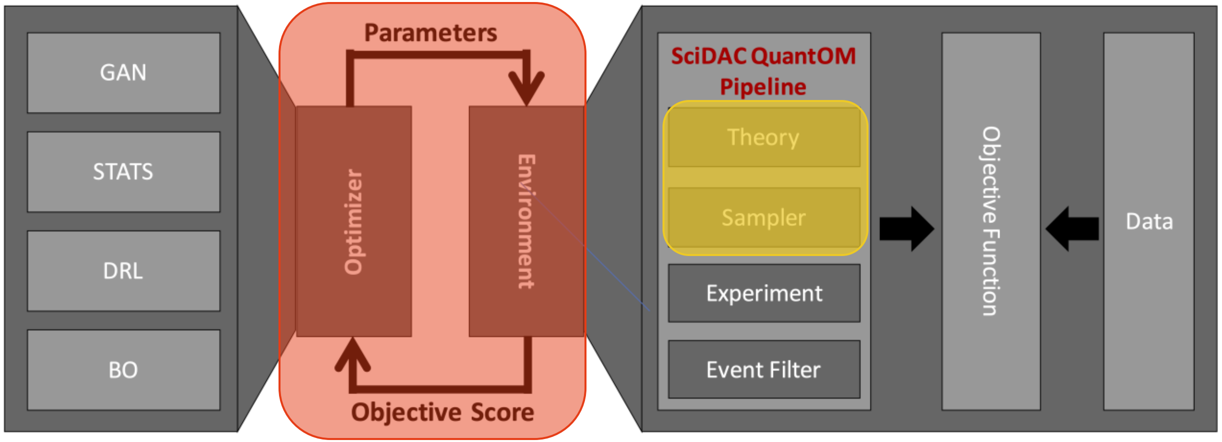
Parameters p

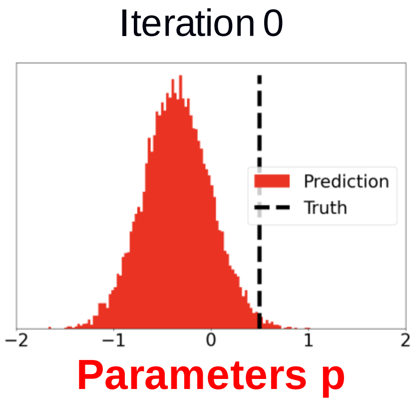
≠

Can not directly compare

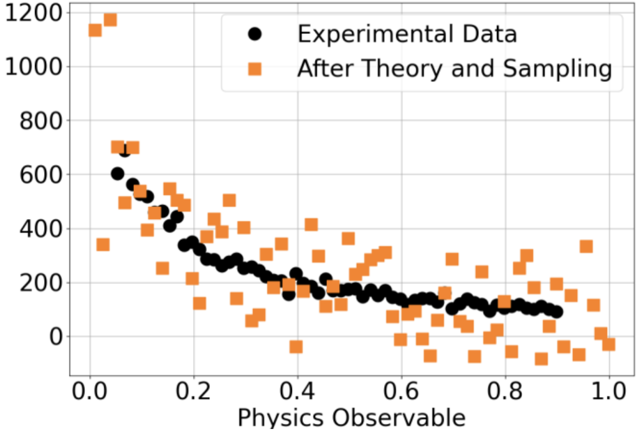


THE GENERATIVE INVERSE PROBLEM SOLVER: GIPS

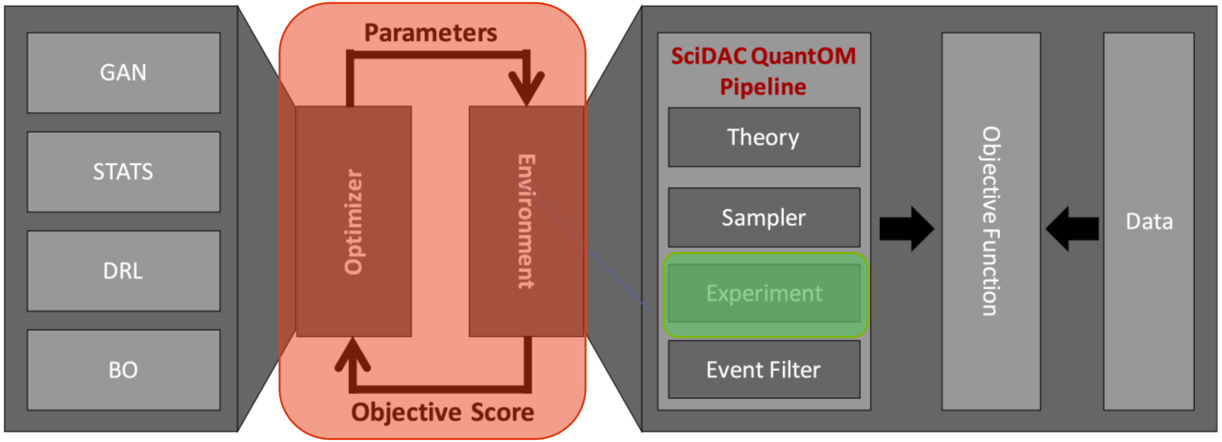




- Convert parameters to parton density functions (PDFs)
- Include higher order and radiate corrections
- Sample events from PDFs (e.g. via MCMC)



THE GENERATIVE INVERSE PROBLEM SOLVER: GIPS



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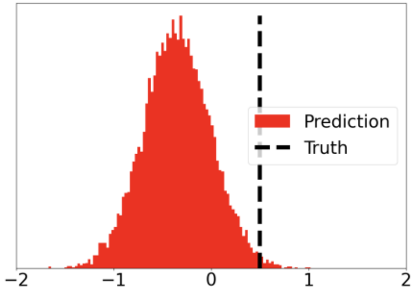
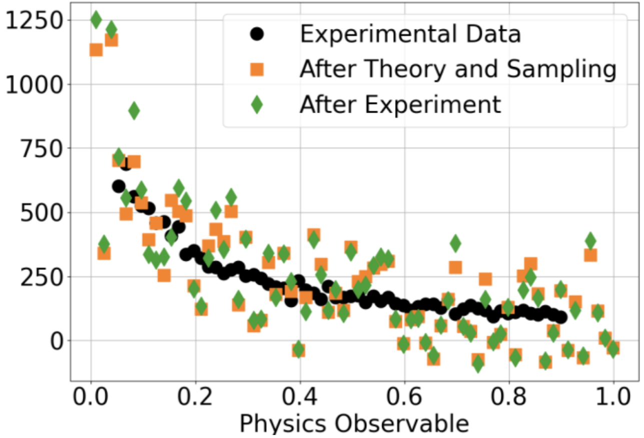


Parameters p

- Apply experimental effects (e.g. resolution, acceptance)
- Handle background contributions
- Use surrogate for detector



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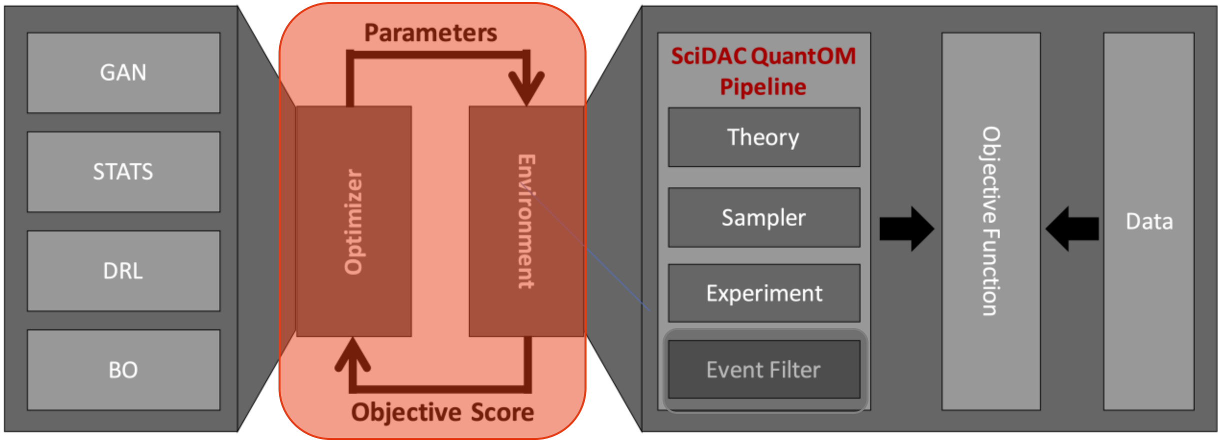
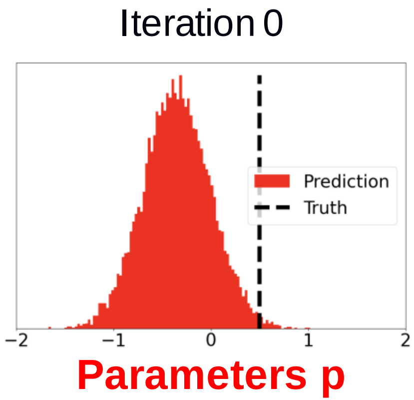
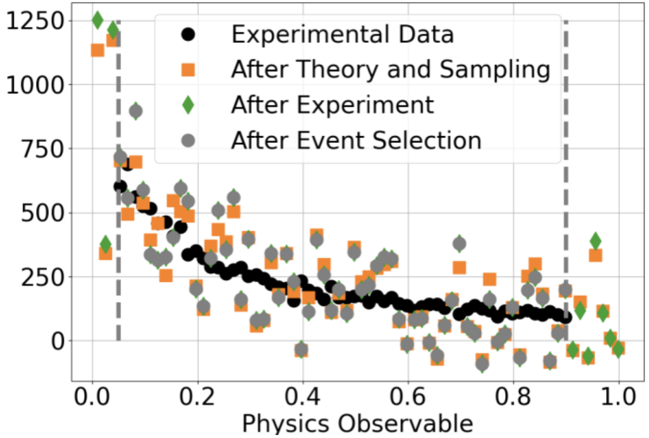
THE GENERATIVE INVERSE PROBLEM SOLVER: GIPS





- Exclude un-physical data points
- Match experimental and synthetic data



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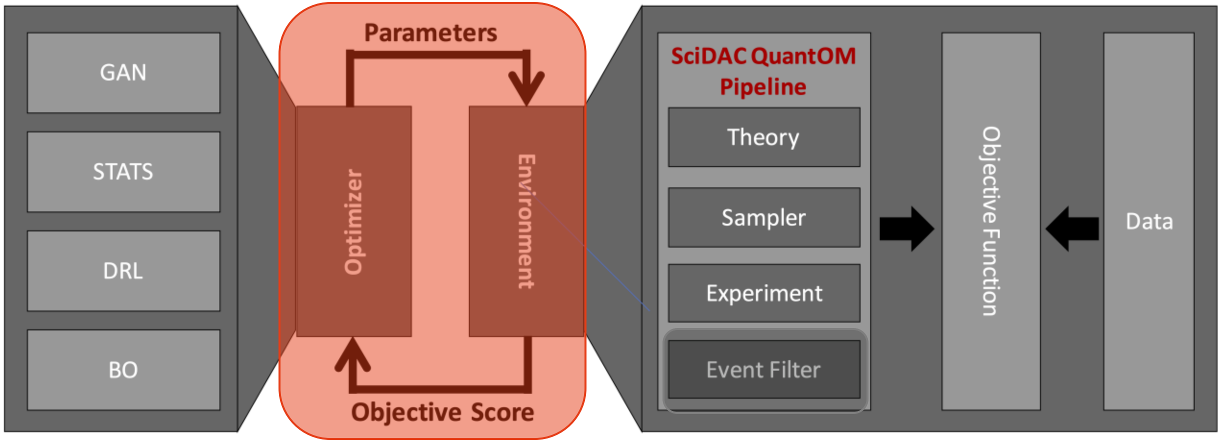
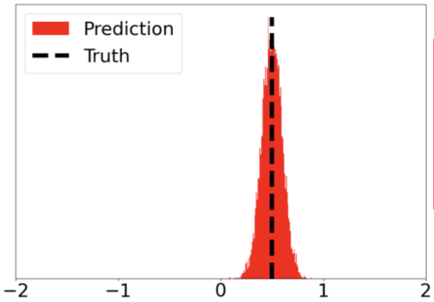
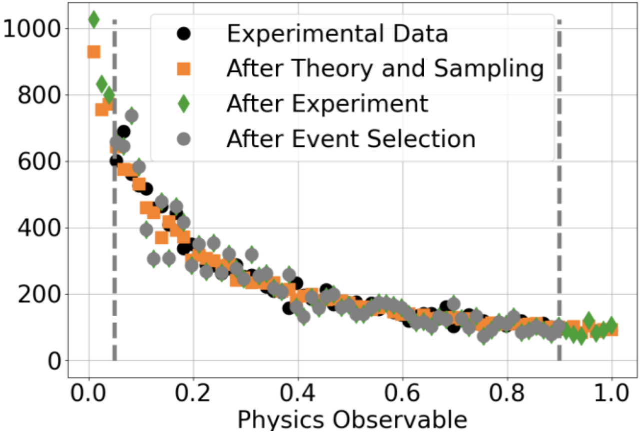


Iteration 100



Parameters p

- Run workflow iteratively
- Use objective score to update optimizer

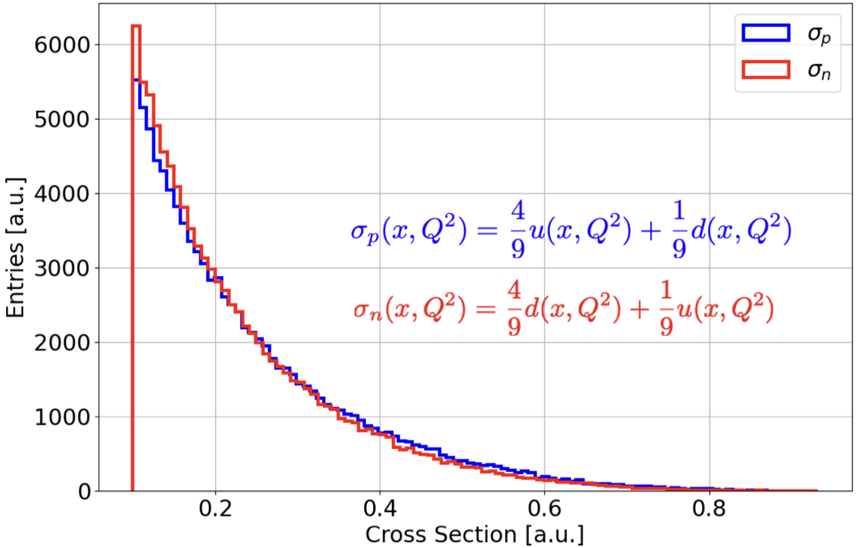


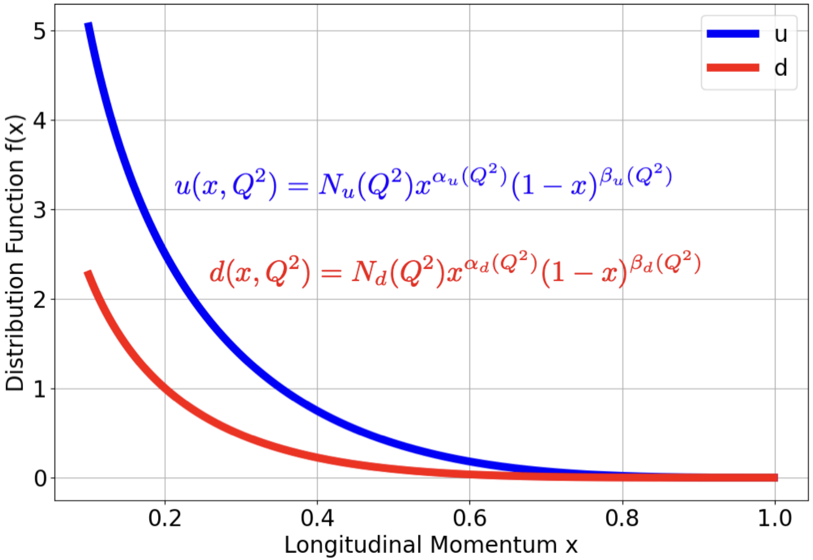
WORKFLOW SPECS

- Written in python
- Supports Tensorflow, Keras, PyTorch,…
- Runs on CPU / GPU
- Modular
  - Change / update / add individual modules
  - Customize entire pipeline
- Each module has its dedicated working group (e.g. theory, experiment,…)
- Fit multiple experiments simultaneously <--> Each experiment has its dedicated module

THE 1D PROXY APP

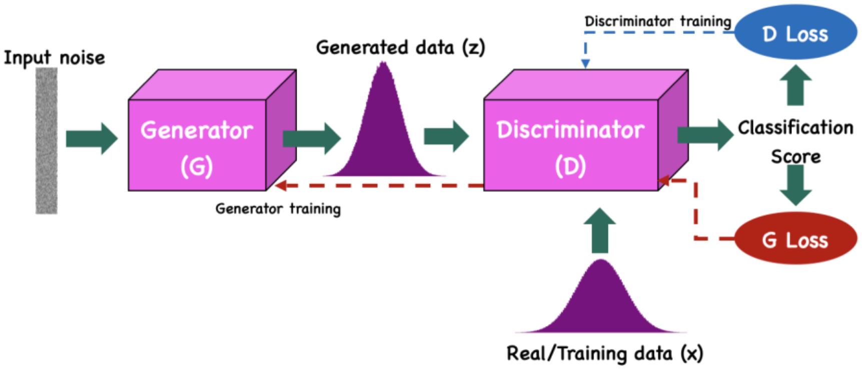
- **Test, debug and benchmark workflow**
- **Given:** Toy data set consisting of cross section "measurements"
- **Goal:** Extract the underlying PDFs that determine the cross sections

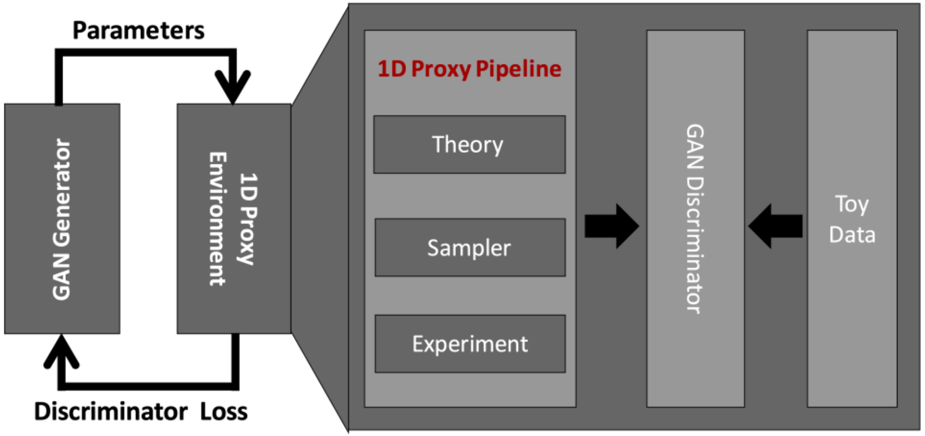




- **Approach:** Use workflow to find PDFs
- Truth, i.e. inputs, is known here
- Perform loop closure tests

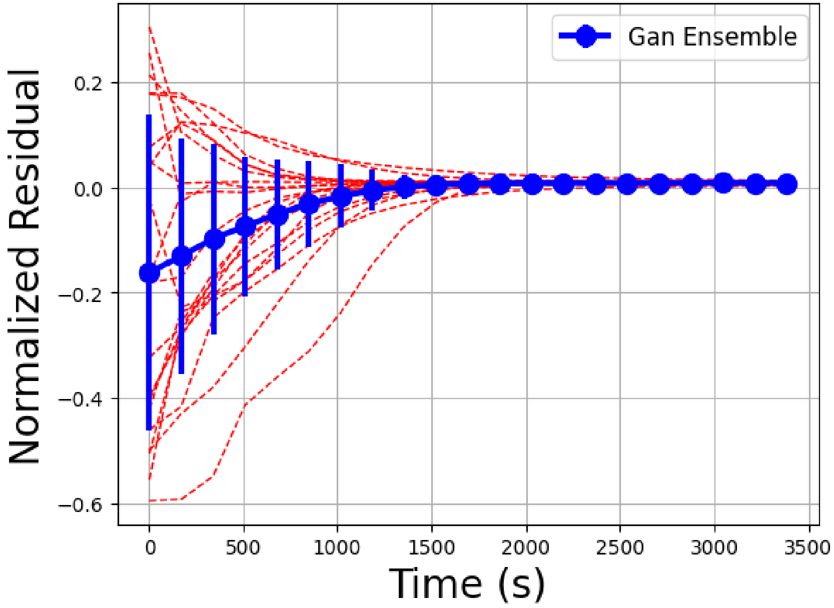
THE 1D PROXY APP WITH GIPS



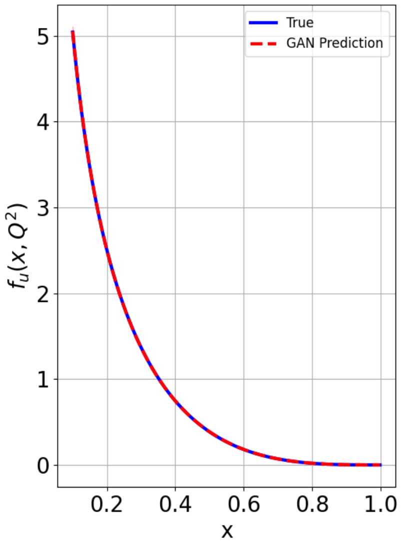


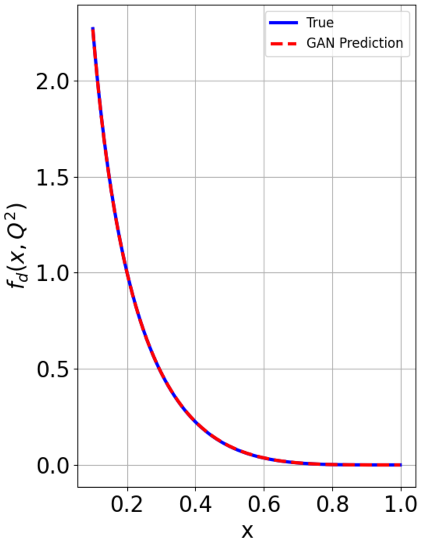
1. Generator predicts 6 parameters
2. Parameters are translated to synthetic events by environment
3. Discriminator (part of environment) is trained on synthetic and toy data
4. Use discriminator loss on synthetic data to update generator
5. Repeat steps 1 – 4 until convergence

ENSEMBLE ANALYSIS ON 1D PROXY APP



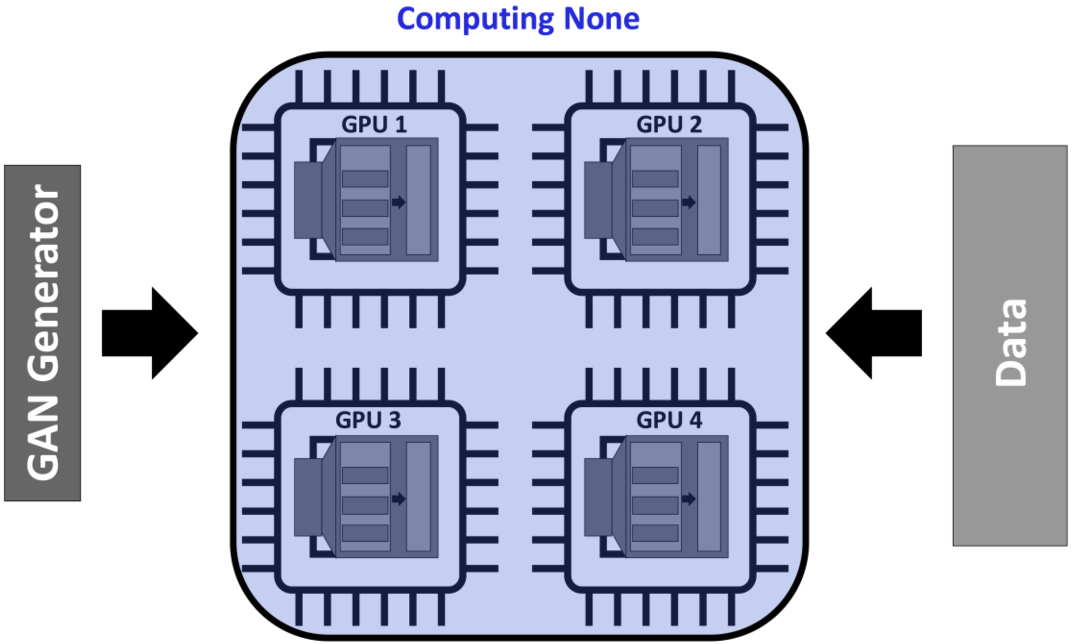
- Used ensemble with 20 GANs
- Benefit from individual parameter initialization
- Ensemble converges earlier to expected solution than individual GAN





- Ran loop closure tests with / without resolution effects
- Reproduced input PDFs
- Need to include uncertainty quantification

SCALING GIPS WITH THE 1D PROXY APP

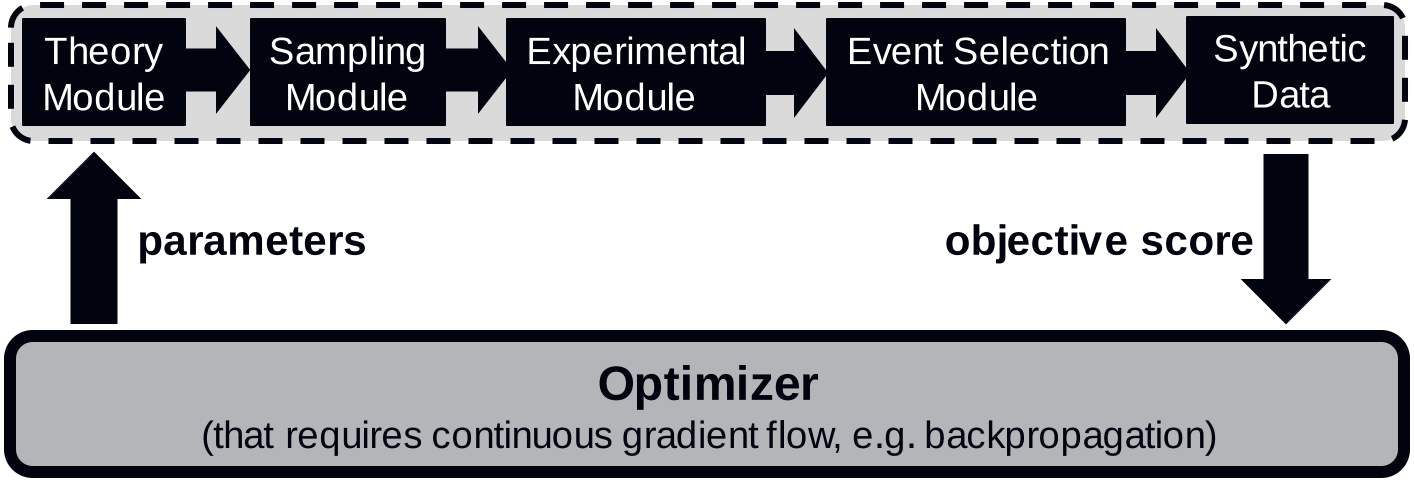


- Handle data volume --> run GIPS across multiple nodes
- Tricky due to stochastic nature of sampling process
- Each GPU has its own environment
- Use asynchronous data parallel training to update GAN generator
- **Ran tests on Polaris --> See poster: "Scaling the SciDAC QuantOm Workflow"**

MANAGING THE GRADIENT FLOW

Forward pass

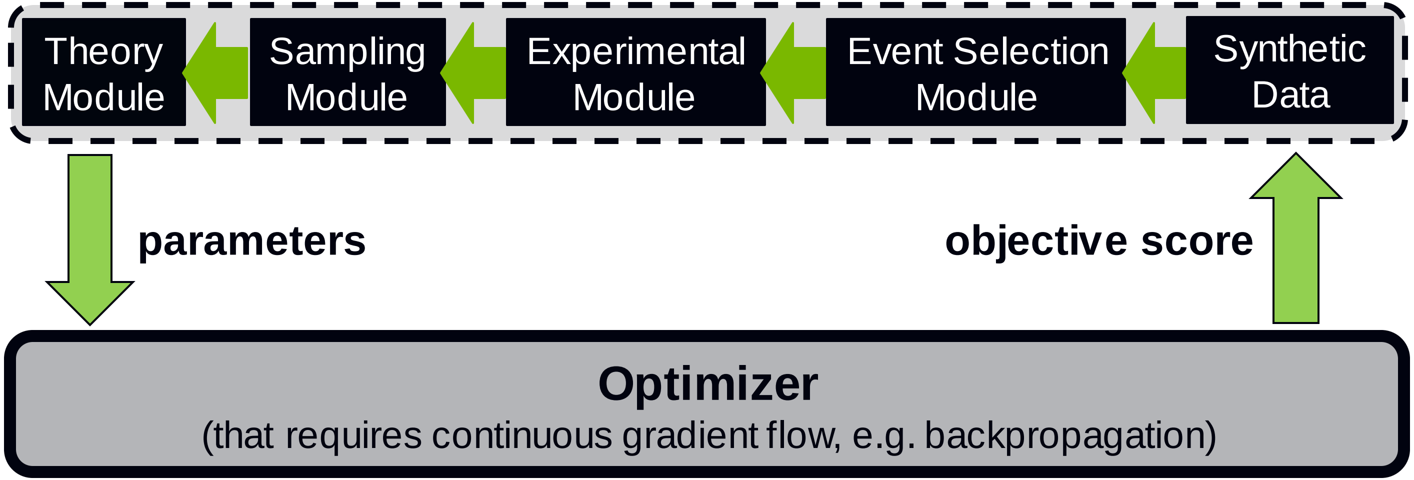
- Optimizer predicts parameters
- Parameters are translated to synthetic data
- Synthetic data defines, together with experimental data, an objective score



MANAGING THE GRADIENT FLOW

Backward pass

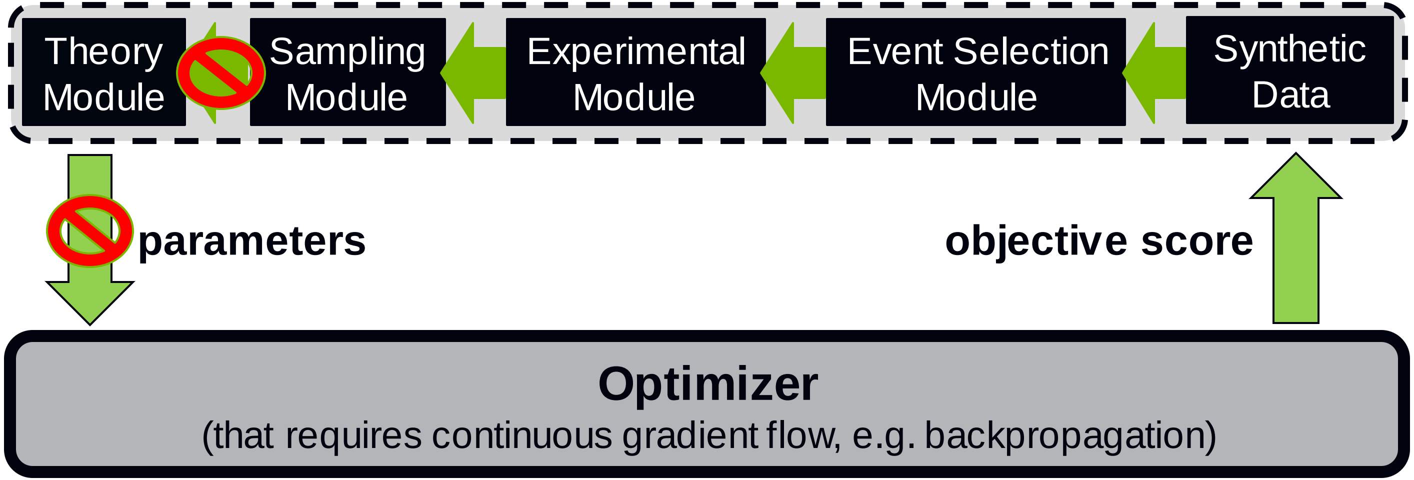
- Rely on chain rule to update optimizer state
- Propagate gradients back through entire pipeline
- **Every module needs to be differentiable**



MANAGING THE GRADIENT FLOW

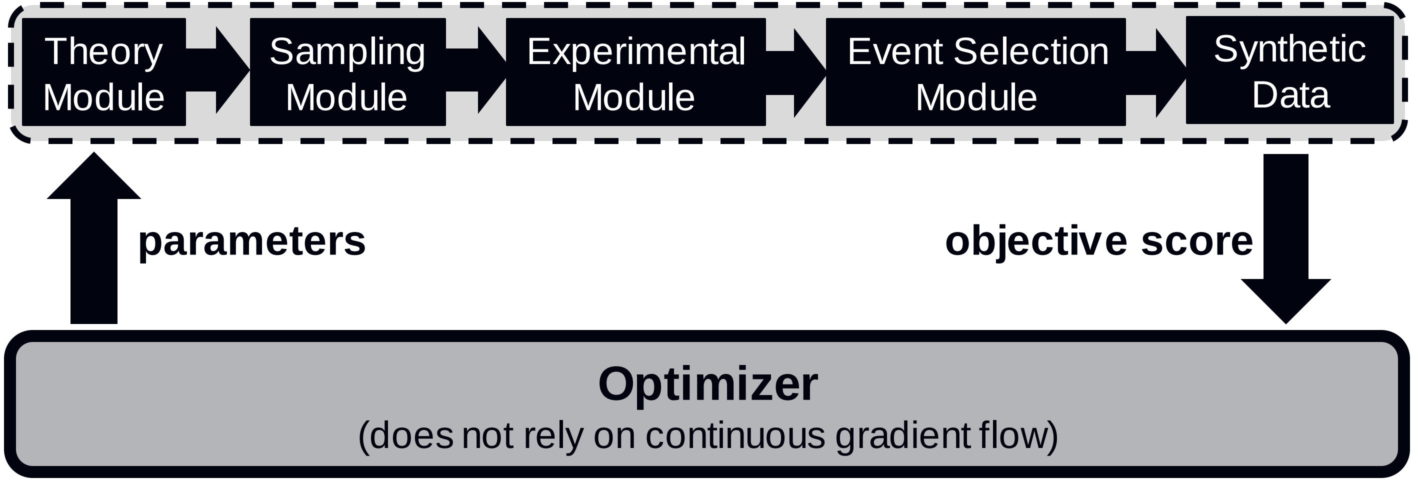
Trouble

- Rely on chain rule to update optimizer state
- Gradient flow is disturbed
- **At least one module is not differentiable (e.g. sampler)**

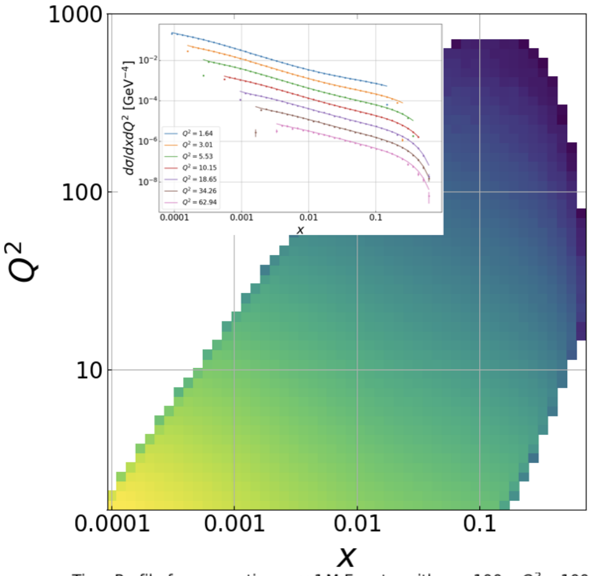


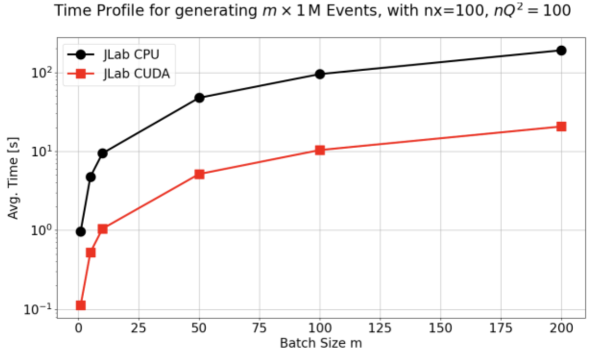
ALTERNATIVE: AVOID GRADIENT FLOW

- Do not care about differentiability
- Minimize / Maximize objective score w.r.t predicted parameters
- Currently exploring: Reinforcement Learning, Genetic Algorithms, Simulated Annealing,...

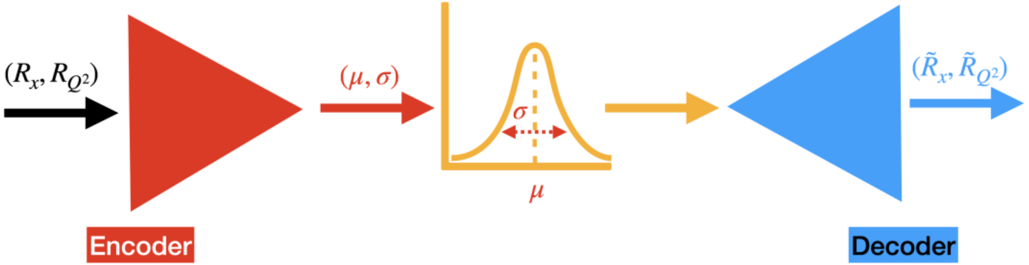


TOWARDS A 2D PROXY APP AND DIS ANALYSIS





- DIS Theory following Duke & Owens
- Generate DIS events in x and Q
- Differentiable sampler with GPU capability
- Use VAE as a detector surrogate ==> Model residuals in x and Q
- Enable analysis of real measured DIS data
- Workflow already set up for 2D proxy analysis
- Currently in testing and debugging phase



Loss $\sim \|(R_x, R_{Q^2}) - (\tilde{R}_x, \tilde{R}_{Q^2})\|$ + **KL-Divergence**

$$R_i \equiv \frac{i - i'}{i}, i = x, Q^2$$

SUMMARY AND OUTLOOK

- Generative Inverse Problem Solver - GIPS
  - Composable workflow
  - Successful loop-closure tests on 1D proxy app
  - Enable faster convergence with ensemble analysis
  - Need to formulate proper uncertainty quantification (UQ)
  - Define proper convergence metric (truth is unknown in "real" measurement)

- Currently summarizing scaling efforts in paper
- Explore non-gradient based optimizers
- 2D proxy analysis in the pipeline
- Extend experimental module ==> Include effects other than detector resolution / acceptance (e.g. background)
- Deploy workflow to HPC machines, e.g. Aurora, Sunspot,...

THE END