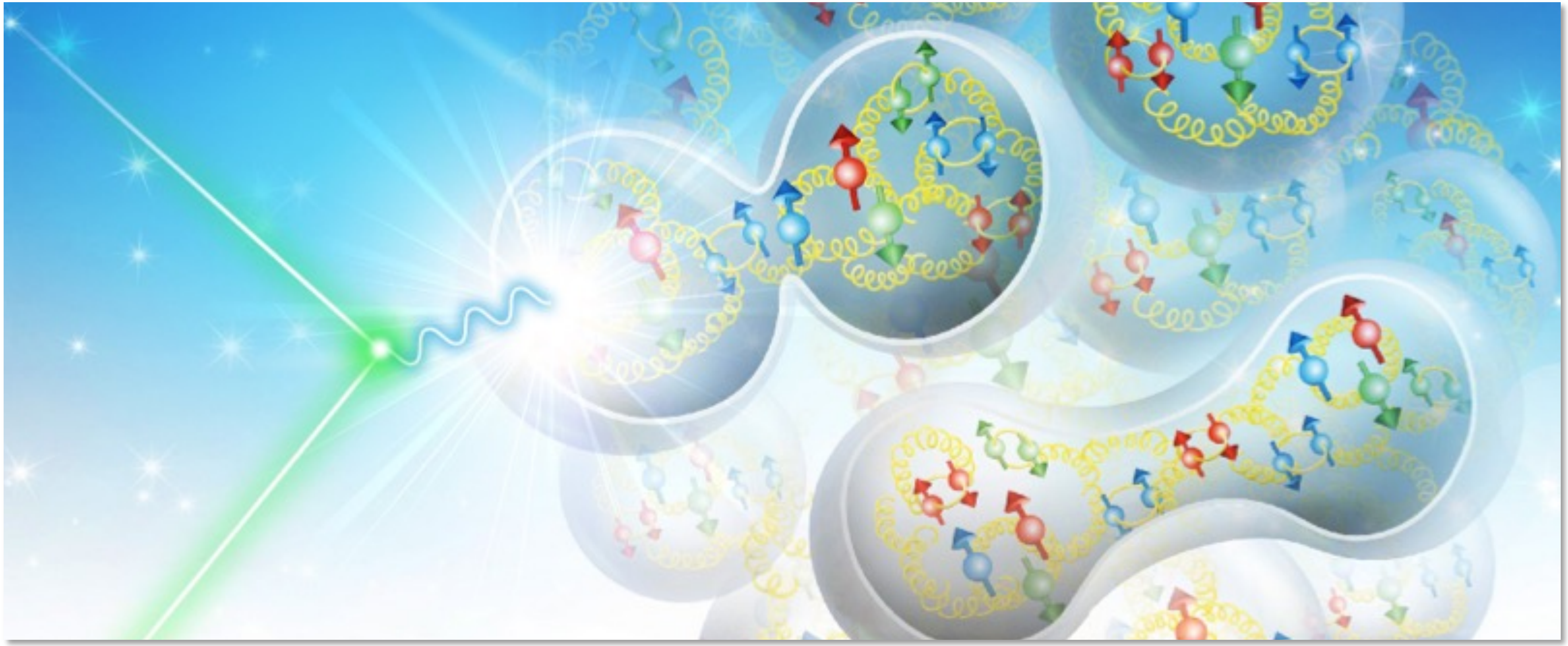
Revolutionizing the Experimental-Theoretical Workflow in Nuclear Femtography using Advanced Computing



Markus Diefenthaler

Jefferson Lab

Scientific Discovery Through Advanced Computing (SciDAC)

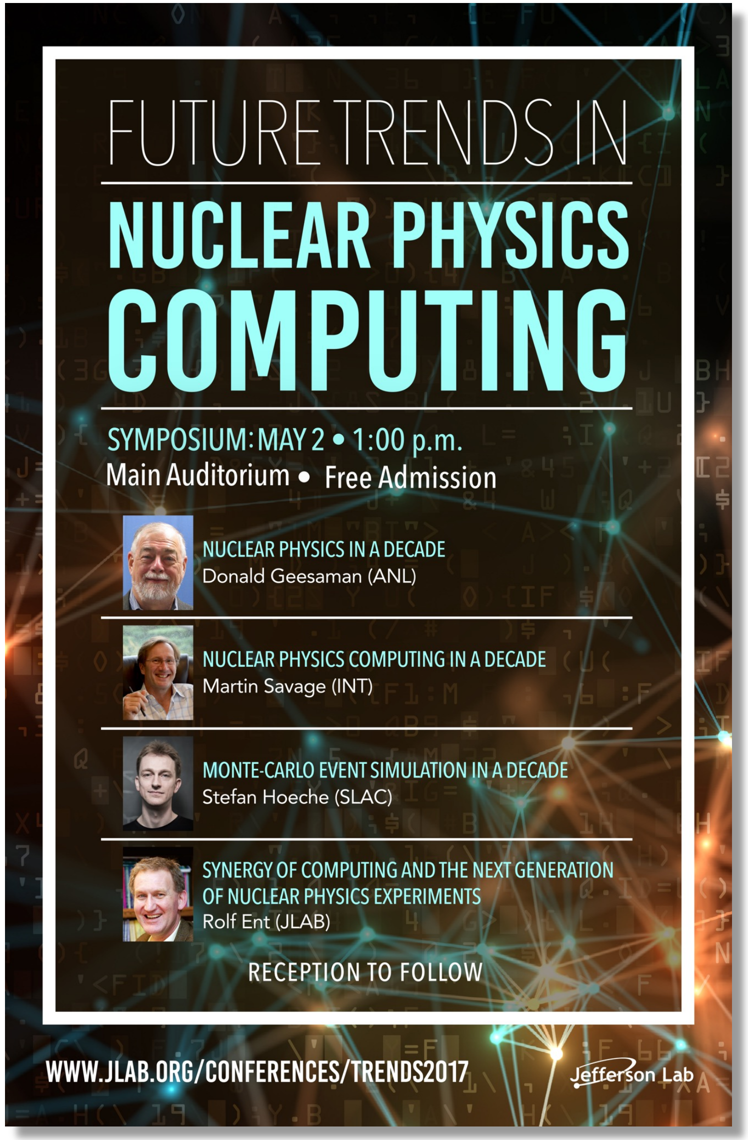
The SciDAC program was created to bring together many of the nation's top researchers to **develop new computational methods** for **tackling some of the most challenging scientific problems**.

Department of Energy Announces $35 Million for Scientific Discovery through Advanced Computing (SciDAC) Partnership in Nuclear Physics

Annoucement Number: *DE-FOA-0002589* *List Posted:* *9/6/2022*

Principal Investigator	Title	Institution	City	State	9-digit zip code
Cloet, Ian	Femtoscale Imaging of Nuclei using Exascale Platforms	Argonne National Laboratory	Lemont	IL	60439-4803
Qiu, Jianwei	Femtoscale Imaging of Nuclei using Exascale Platforms	Thomas Jefferson National Accelerator Facility	Newport News	VA	23606-4468
Feng, Wu-chun	Femtoscale Imaging of Nuclei using Exascale Platforms	Virginia Polytechnic Institute and State University	Blacksburg	VA	24061-0001

The Role of Advanced Computing in Nuclear Physics



Future Trends in Nuclear Physics Computing

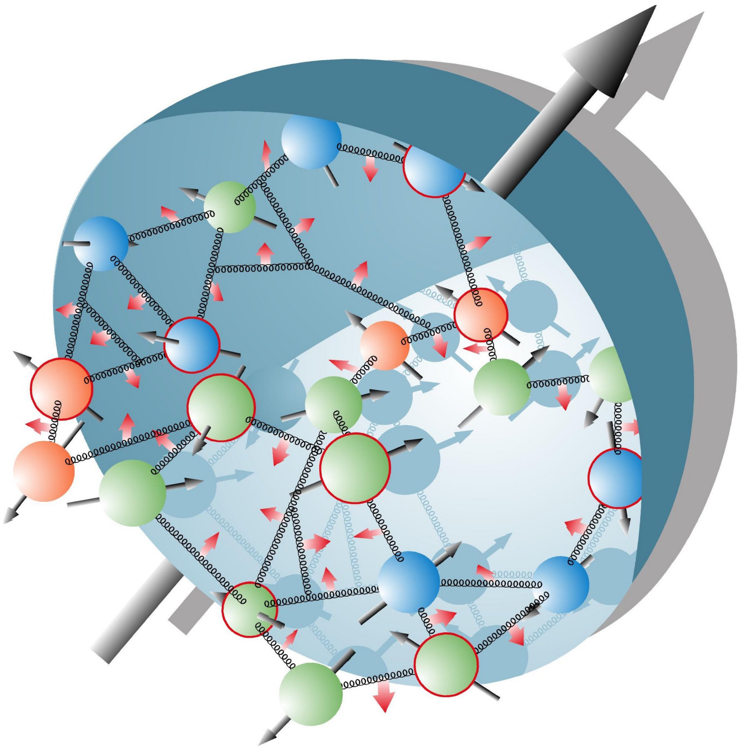
- **Recent years** Discussion about the next generation of data processing and analysis workflows that will maximize the science output.
- **One context for this discussion**
  - Workshop series on Future Trends in Nuclear Physiscs Computing

Donald Geesaman (ANL, former NSAC Chair) *"It will be **joint progress of theory and experiment** that moves us forward, not in one side alone"*

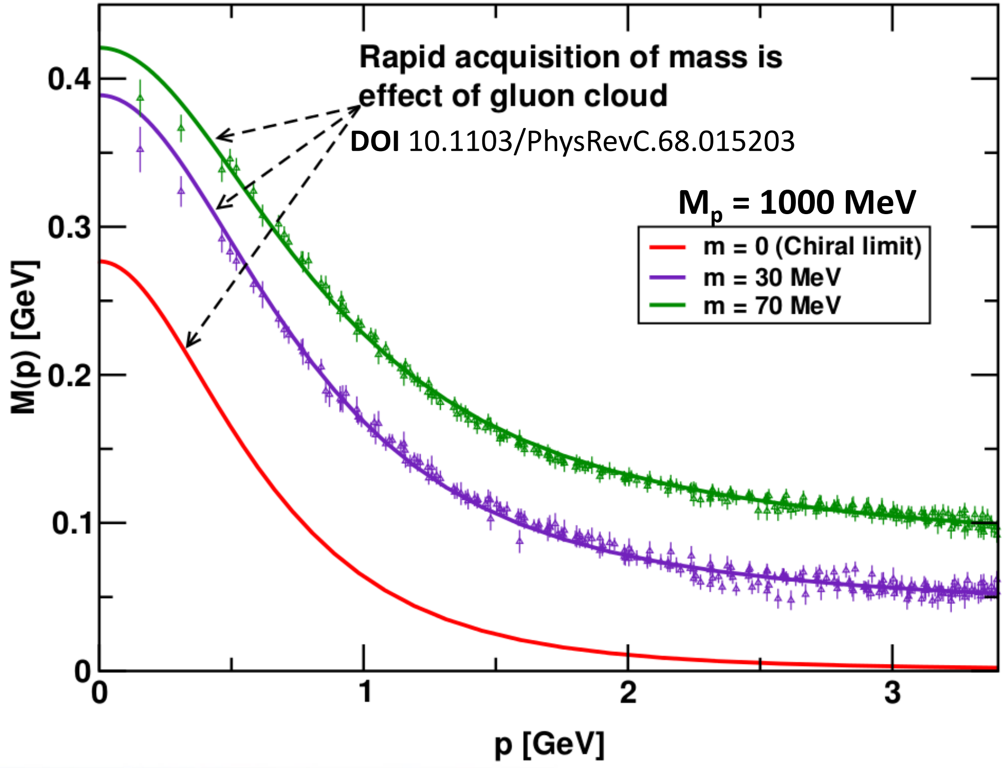
Martin Savage (INT) *"The next decade will be looked back upon as a **truly astonishing period in Nuclear Physics** and in our understanding of fundamental aspects of nature. This will be **made possible by advances in scientific computing** and in how the Nuclear Physics community organizes and collaborates, and how DOE and NSF supports this, to take full advantage of these advances."*

The Scientific Challenge of Understanding Nuclear Matter

Nuclear Matter Interactions and structures are inextricably mixed up



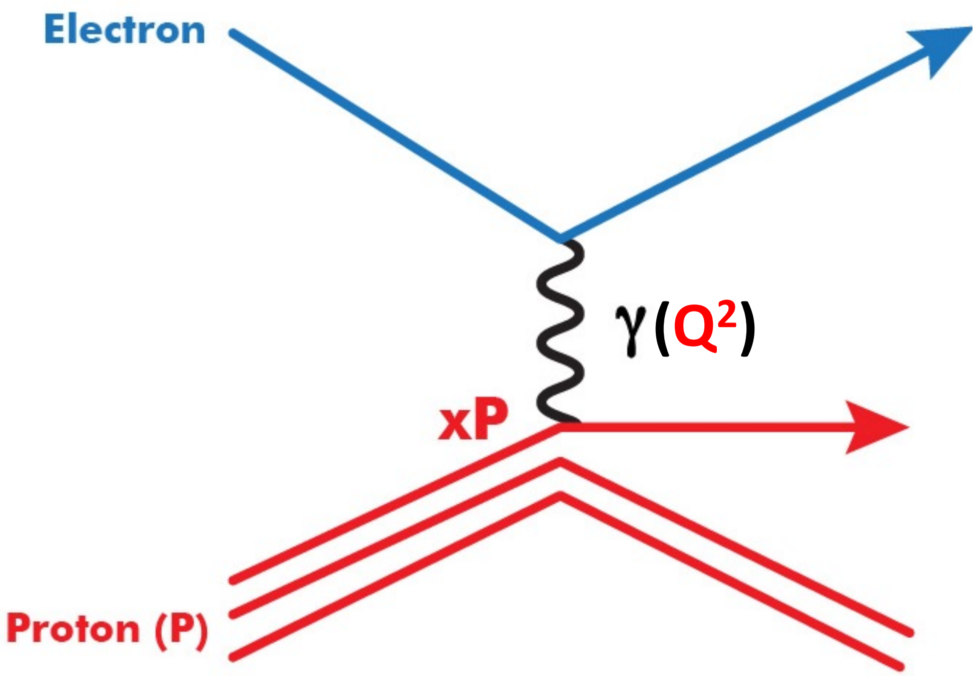
Observed properties such as mass and spin emerge out of the complex system



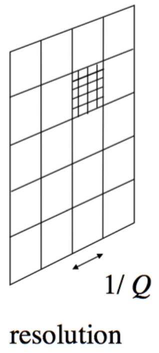
Ultimate goal Understand how matter at its most fundamental level is made

To reach goal precisely image quarks and gluons and their interactions (Nuclear Femtography)

Deep-Inelastic Scattering (DIS) of Electrons off Protons

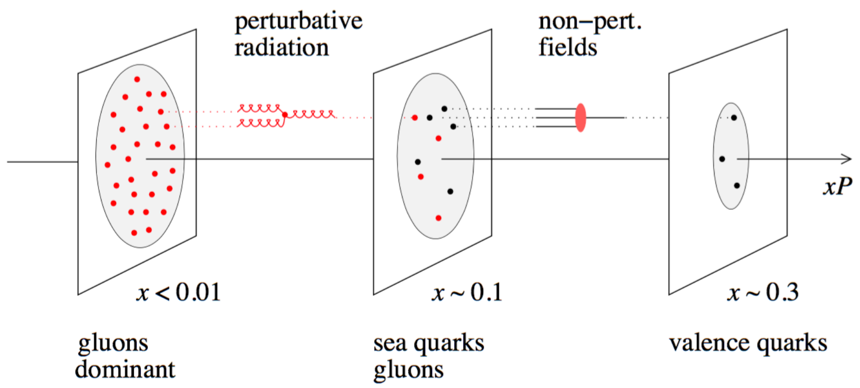


Ability to change Q^2 changes the resolution scale



$Q^2 = 400\ GeV^2$
$\Rightarrow 1/Q = 0.01$ fm

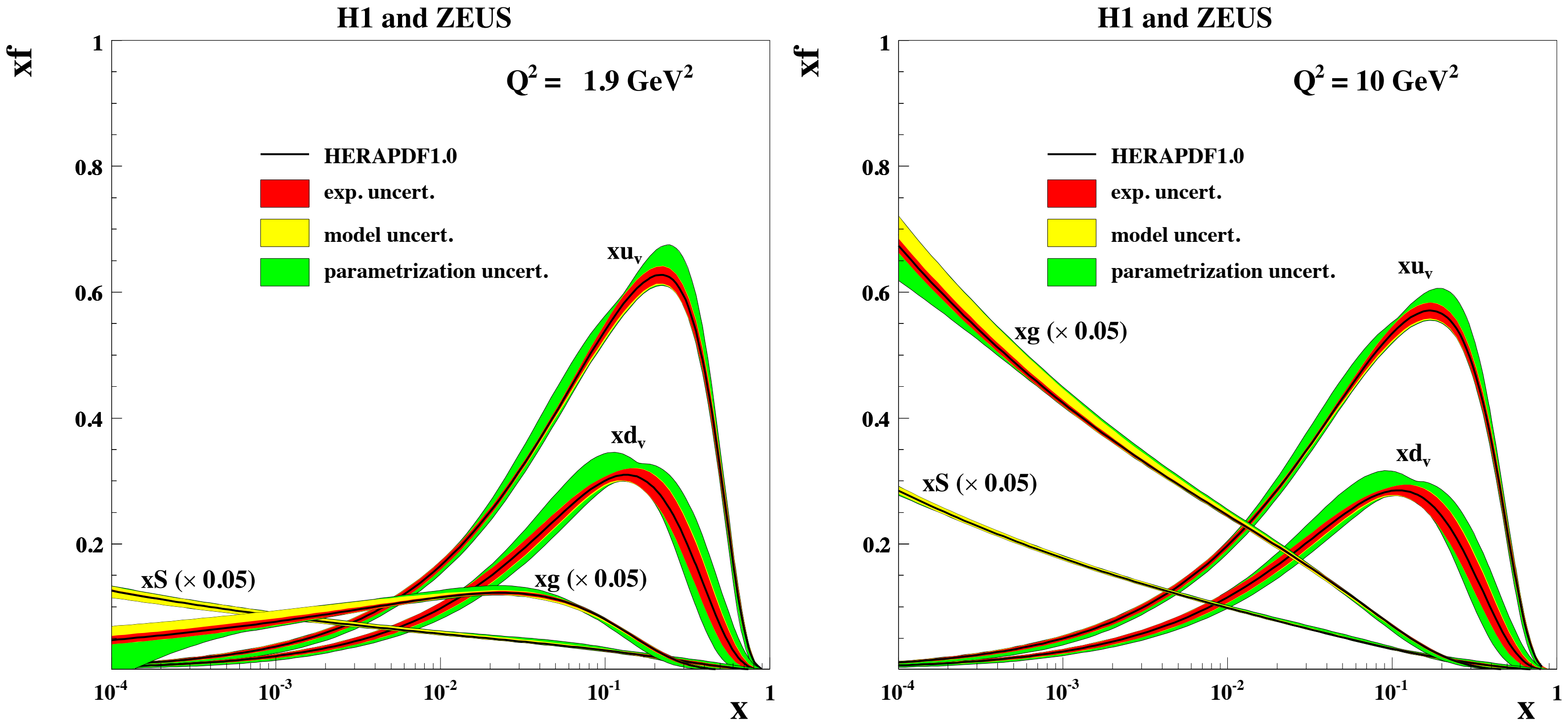
Ability to change x projects out different configurations where different dynamics dominate



Parton Distribution Functions (PDF)

Observable cross section → structure functions → **QCD analysis** PDFs

process-dependent | **universal**



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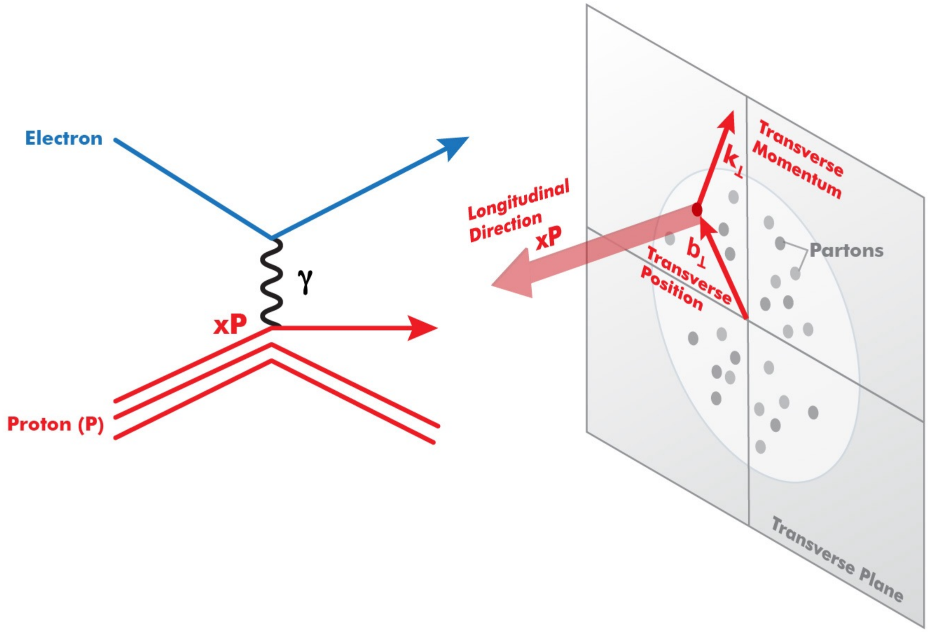
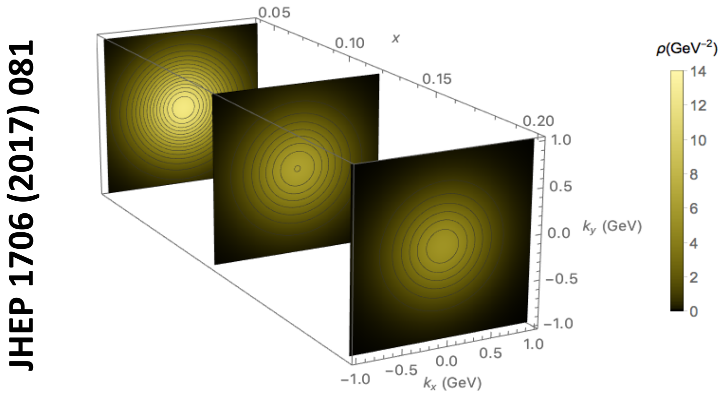
From PDFs to 3D Imaging (Nuclear Femtography)

3D Imaging in Space and Momentum

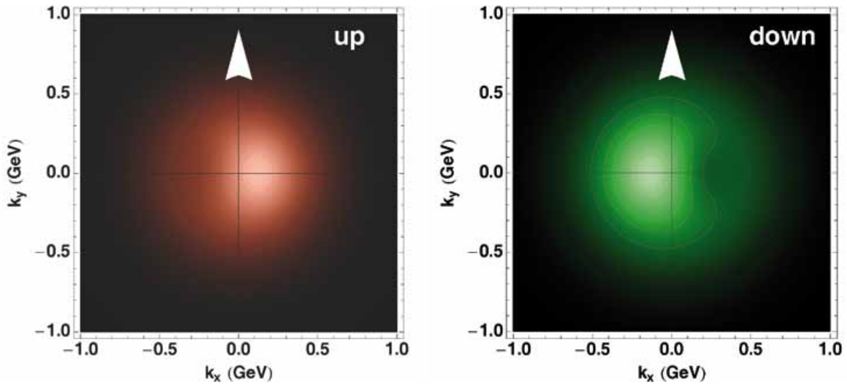


longitudinal structure (PDF)
+ transverse position information (GPDs)
+ transverse momentum information (TMDs)

TMDs of unpolarized nucleon



TMDs of transversely polarized nucleon



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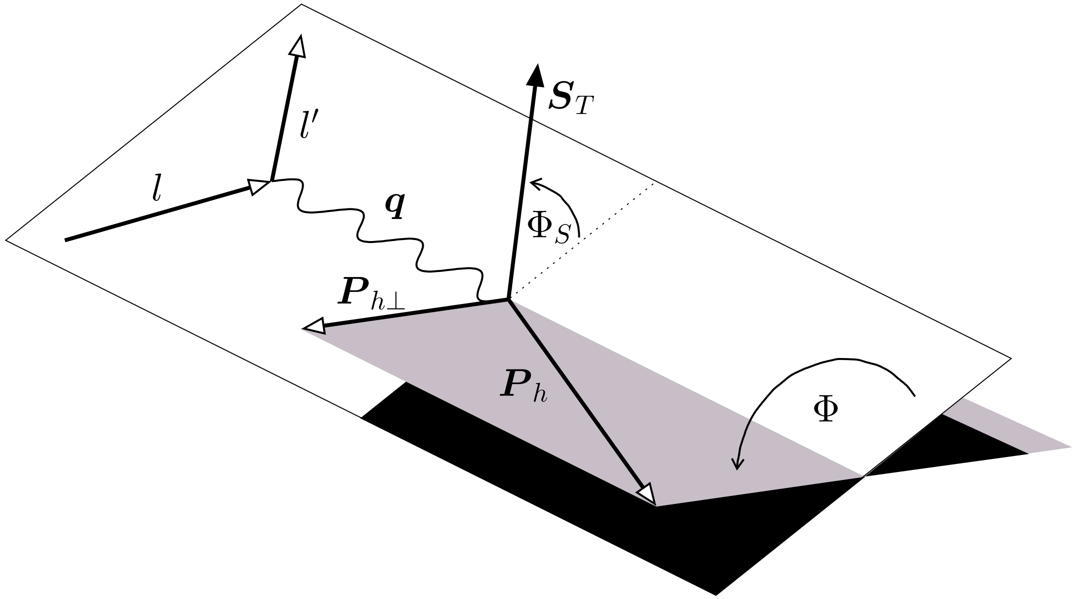
Advances in Nuclear Physics (NP)

Advances in Experimental NP: Measurements of Semi-Inclusive Deep-Inelastic Scattering (SIDIS)

- **Hadron h** is detected
- in **coincidence** with the scattered lepton l’



Observable

SIDIS cross section

Observable for TMD PDFs and TMD FFs

Advances in Theoretical NP: Factorization Theorem for SIDIS

Distribution functions (PDF, TMD PDF) empirical description of non-perturbative structure (confinement)

Perturbative part Cross section for elementary photon-quark interaction **Calculable** (asymptotic freedom)

Fragmentation functions (FF, TMD FF) empirical description of non-perturbative structure (hadronization)

Signals for TMD PDFs and TMD FFs

Differential cross section

Cross section decomposition in terms of structure functions

$$\frac{d\sigma^h}{dx\,dy\,d\phi_S\,dz\,d\phi\,d\mathbf{P}_{h\perp}^2} = \frac{\alpha^2}{xyQ^2}\frac{y^2}{2(1-\varepsilon)}\left(1+\frac{\gamma^2}{2x}\right)$$

$$\Big\{ \Big[F_{\mathrm{UU,T}} + \varepsilon F_{\mathrm{UU,L}} + \sqrt{2\varepsilon(1+\varepsilon)}\cos(\phi) F_{\mathrm{UU}}^{\cos(\phi)} + \varepsilon\cos(2\phi) F_{\mathrm{UU}}^{\cos(2\phi)}\Big]$$

Sivers effect

$$+ \; S_T \Big[\sin(\phi-\phi_S)\left(F_{\mathrm{UT,T}}^{\sin(\phi-\phi_S)} + \varepsilon F_{\mathrm{UT,L}}^{\sin(\phi-\phi_S)}\right)$$

Collins effect

$$+\varepsilon\sin(\phi+\phi_S) F_{\mathrm{UT}}^{\sin(\phi+\phi_S)} + \varepsilon\sin(3\phi-\phi_S) F_{\mathrm{UT}}^{\sin(3\phi-\phi_S)}$$
$$+\sqrt{2\varepsilon(1+\varepsilon)}\sin(\phi_S) F_{\mathrm{UT}}^{\sin(\phi_S)}$$
$$+\sqrt{2\varepsilon(1+\varepsilon)}\sin(2\phi-\phi_S) F_{\mathrm{UT}}^{\sin(2\phi-\phi_S)}\Big]$$

Factorized results in terms of TMD PDFs and TMD FFs

at tree-level and twist-2 and twist-3 accuracy

Assuming one-photon exchange, current fragmentation only, TMD factorization hold, small transverse momenta, Gaussian Ansatz valid

Sivers TMD and spin-independent FF

$$F_{\mathrm{UT,T}}^{\sin(\phi-\phi_S)} = \mathscr{C}\left[-\frac{\hat{\mathbf{h}}\cdot\mathbf{p}_T}{M} f_{1T}^{\perp} D_1\right]$$

Transversity PDF and Collins FF

$$F_{\mathrm{UT}}^{\sin(\phi+\phi_S)} = \mathscr{C}\left[-\frac{\hat{\mathbf{h}}\cdot\mathbf{k}_T}{M_h} h_1 H_1^{\perp}\right]$$

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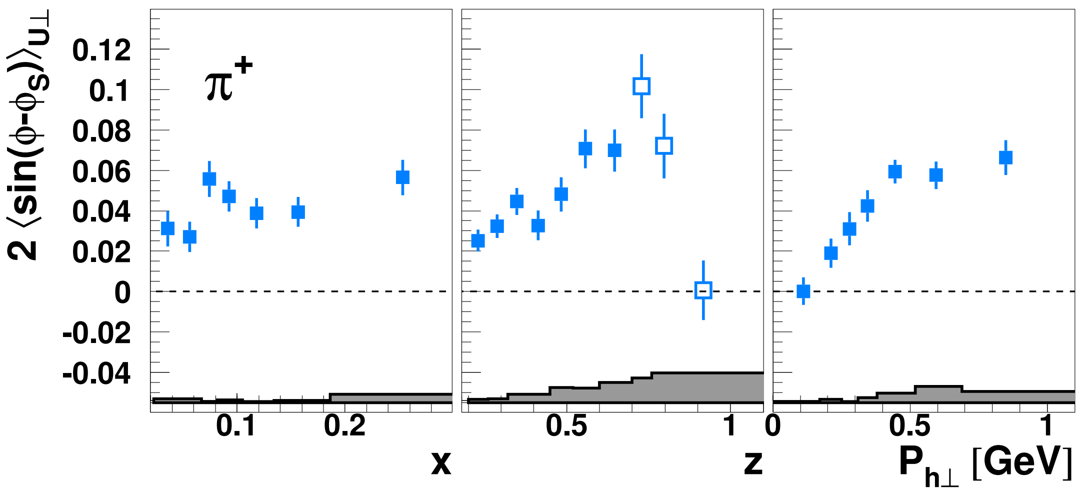
Tackling Some of the Most Challenging Scientific Problems

What are the challenges in extracting TMDs…

… and how will we address them in our SciDAC project?

Experimentalists measure signals for TMDs



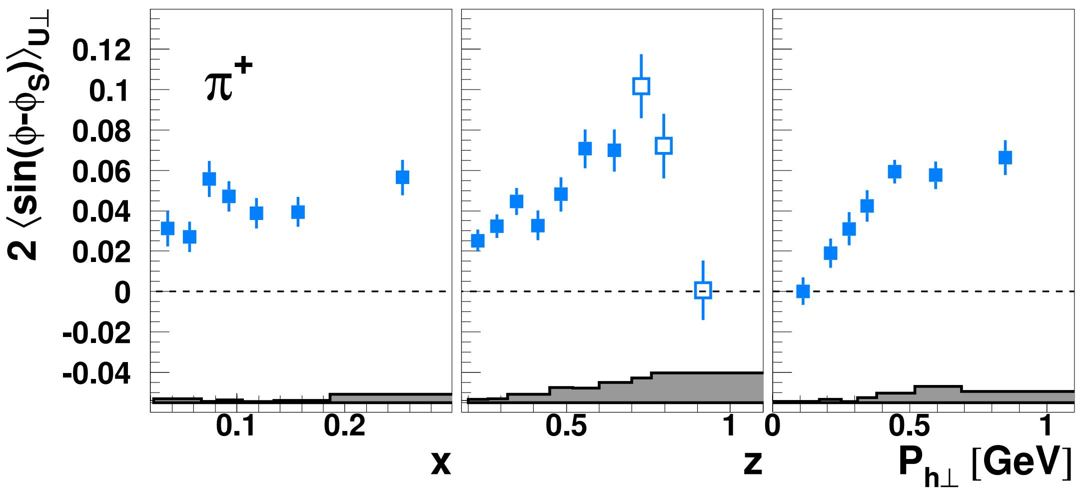
Experimentalists measure signals for TMDs
One Example: Pioneering TMD studies by HERMES

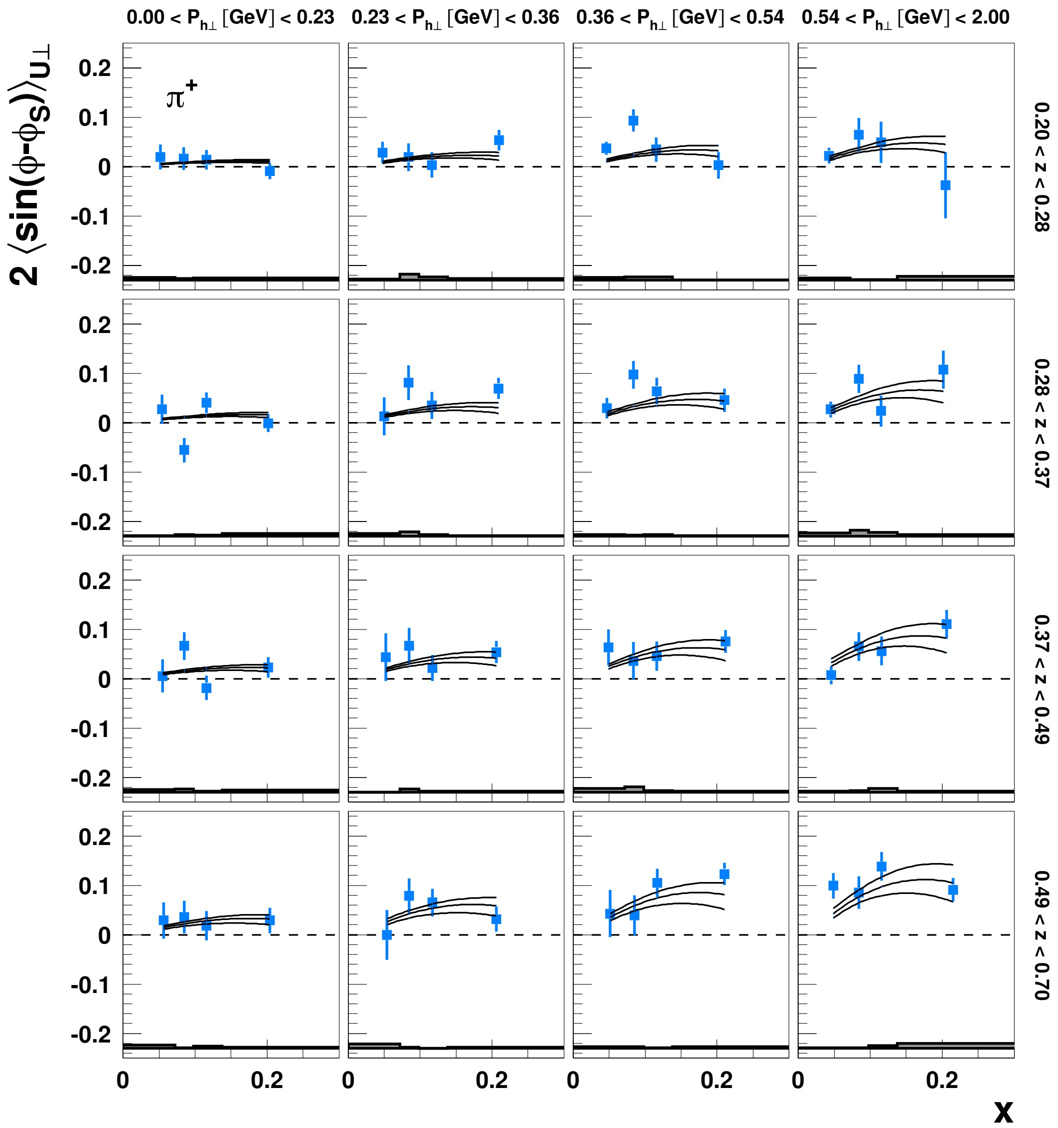
- SIDIS measurement of π^+
- Plot shows structure function related to Sivers effect
  - Allows extraction of Sivers TMD
- Information about 755k π^+ compressed in 24 data points

Theoreticians extract TMDs from these data points

- And many other data points in a global analysis
- They wait years for the data points to become available.
- HERMES example:
  - Data taking in 2002–2005
  - Publications in 2005
    - *Phys.Rev.Lett.* 94 (2005) 012002, 755 citations, only 2002 data
    - *Phys.Rev.Lett.* 103 (2009) 152002, 378 citations
    - *Phys.Lett.B* 693 (2010) 11-16, 240 citations
    - *JHEP* 12 (2020) 010, 24 citations

Multi-Dimensional Data Challenge





Fully differential approach with small bin-sizes

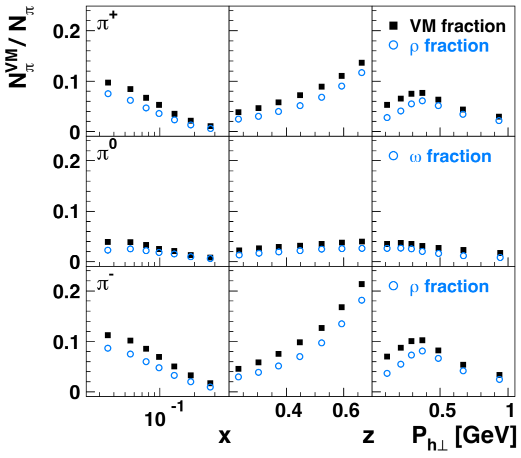
- minimizes the dominant contributions to the systematic uncertainty, and therefore maximizes the attainable experimental precision
- maximize information for QCD analysis

To advance this even further

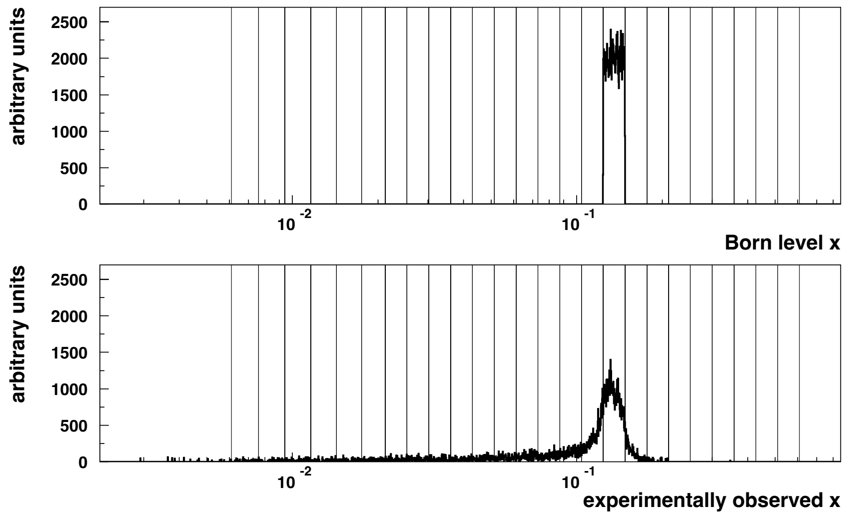
- Analysis on **event level**

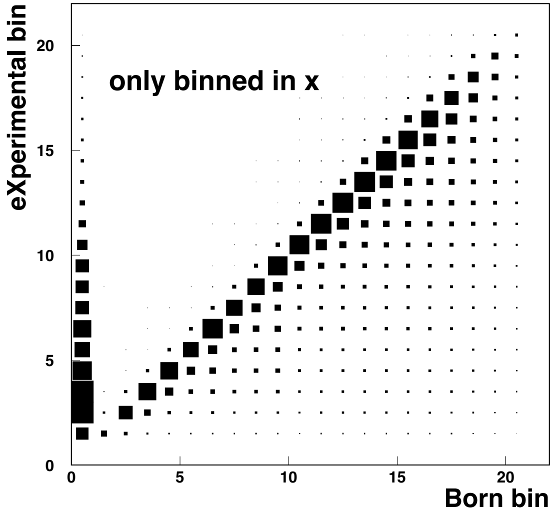
Joint Experimental-Theoretical Analysis

- Avoid mismatches between experimental-theoretical analysis
  - E.g.:
    - Some experimental analyses remove final-state hadrons originating from decay of diffractively produced vector-mesons.
    - However, these final-state hadrons are not removed in factorization proofs. Removing them in the experimental analysis would result in a mismatch between the experimental-theoretical analyses.



- Treat theoretical calculations and assumptions consistently
  - E.g.:
    - Treatment of QED radiative effects and detector smearing



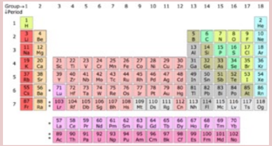
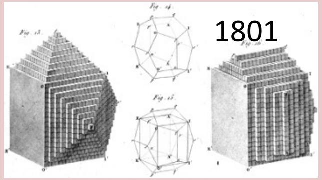
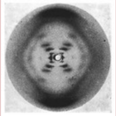
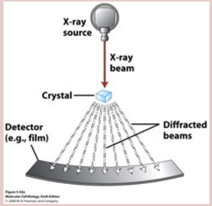
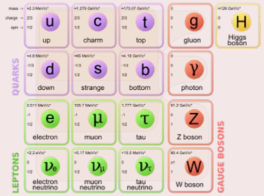
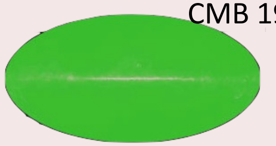
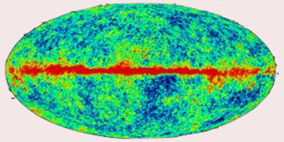
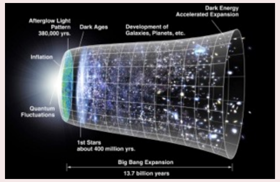
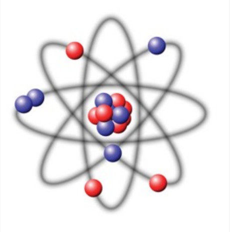
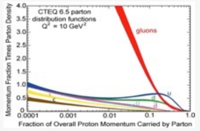
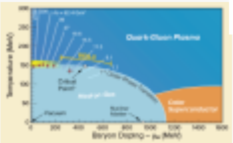
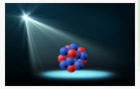
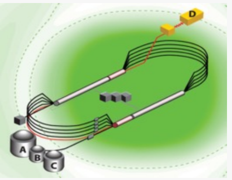
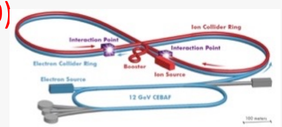


- Correction via unfolding approach requires theoretical model for QED radiative.
- Irreversable. Limits re-use and re-interpretability of experimental analysis.
- **Solution**: Consistent treatment of QED effects in joint experimental-theoretical analysis.

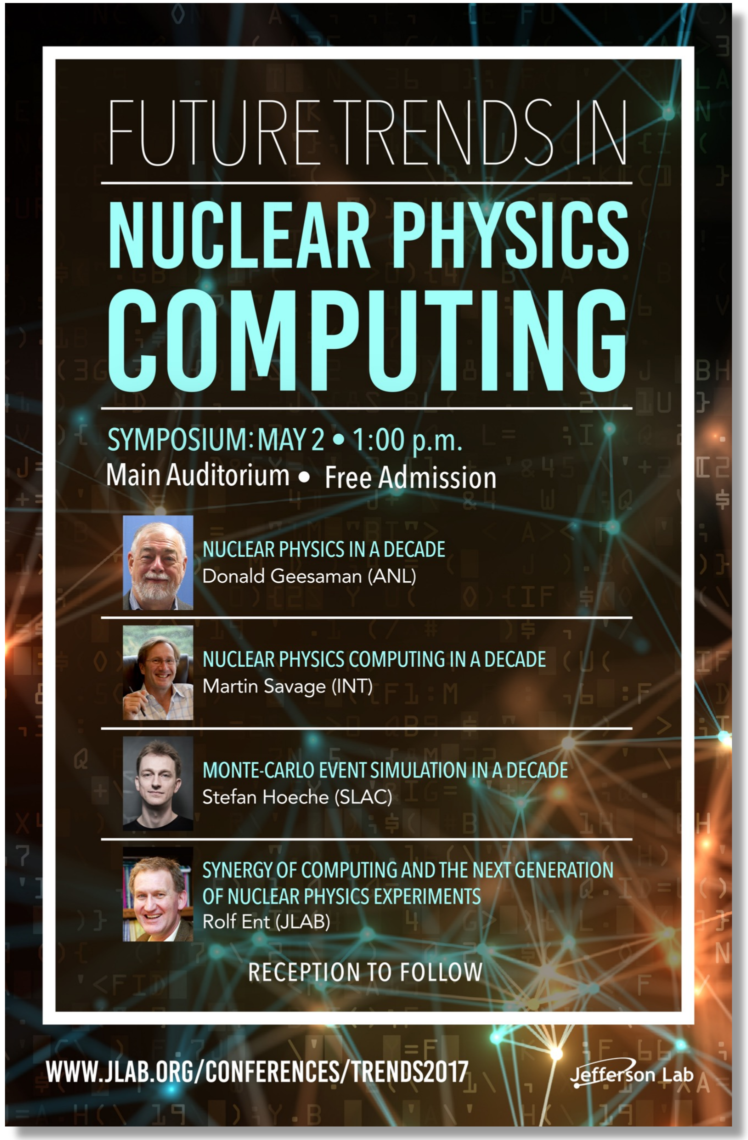
How We Advance the Experimental-Theoretical Workflow

- **Developing a workflow on the event level**:
  - The extraction of PDFs, TMDs, and GPDs is a multidimensional data challenge. We analyze high statistics data sets with strong correlations in five or more kinematics and with various final-state particles. Access to the data on event level allows theoreticians to studying these correlations directly.
- **Developing a joint experimental-theoretical workflow**:
  - Extracting PDFs, TMDs, or GPDs directly from the experiment allows experimentalists and theoreticians to work closely together. This not only removes the delay in providing the experimental measurement but truly enables joint experimental-theoretical wok.
- **Developing a HPC workflow**:
  - The extremely parallelized architecture allows to study the strong correlations in the data in an unprecedented manner, while maximizing the experimental precision at the same time.
  - The accelerated hardware of the new HPC systems is ideal for AI/ML, allowing us to do the parallelized workflow at the event level in near real-time.
    - Future experiments will produce analysis-ready data in near real-time using streaming readout and AI/ML.

What Does This Mean for Science?

Dynamical System	Fundamental Knowns	Unknowns	Breakthrough Structure Probes (Date)	New Sciences, New Frontiers
Solids 	Electromagnetism Atoms 	Structure  1801	X-ray Diffraction (~1920)  	Solid state physics Molecular biology  DNA
Universe 	General Relativity Standard Model 	Quantum Gravity, Dark matter, Dark energy. Structure CMB 1965 	Large Scale Surveys CMB Probes (~2000)  	Precision Observational Cosmology 
Nuclei and Nucleons 	Perturbative QCD Quarks and Gluons $\mathcal{L}_{QCD} = \overline{\psi}(i\partial\!\!\!/ - gA\!\!\!/)\psi - \frac{1}{2}\mathrm{tr}\, F_{\mu\nu}F^{\mu\nu}$	Non-perturbative QCD Structure 2017   	CEBAF12 (2018)   Electron-Ion Collider (~2030) 	Structure & Dynamics in QCD 

The Role of Advanced Computing in Nuclear Physics



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Our developments

- Comparing experiment and theory at the event level
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- HPC for multi-dimensional data challenge
- AI/ML on HPC to accelerate workflow