Inverse problems in nuclear tomography

Nobuo Sato

EIC Software AI WG (Jun 2022)

INT Program 22-1

Machine Learning for Nuclear Theory

## March 28 - April 22, 2022

Organizers:

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- Phiala Shanahan, Massachusetts Institute of Technology, pshana@mit.edu

Diversity Coordinator:

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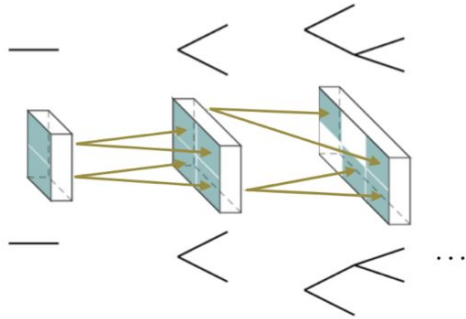
Program Coordinator:
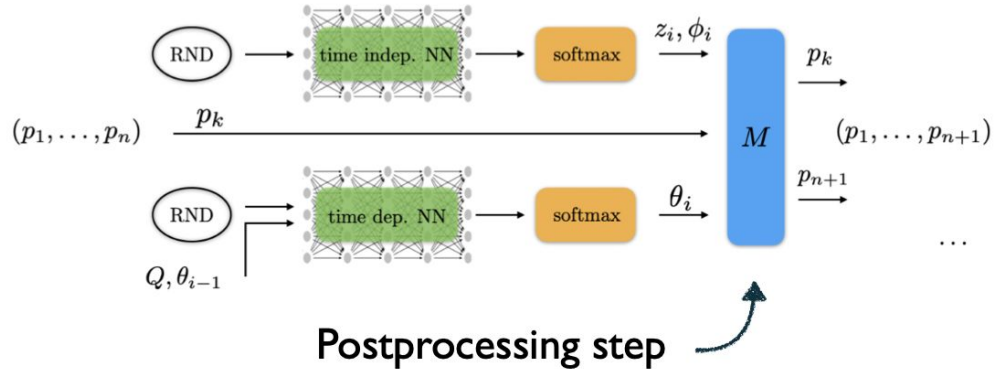
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Program Schedule
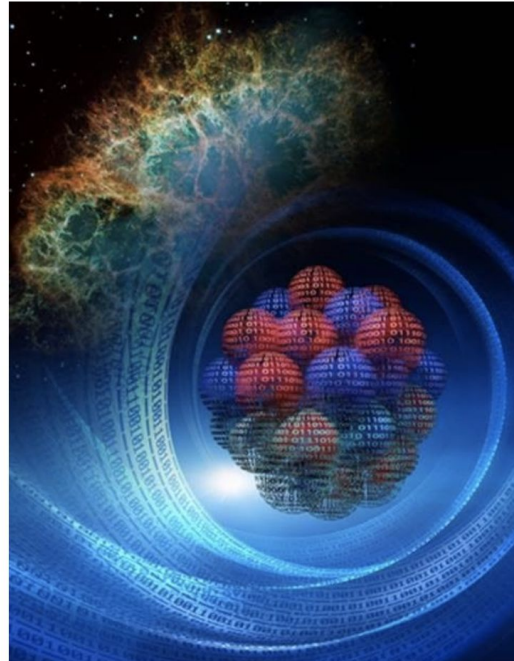
Parton showers and GANs

Lai, Ploskon, Neill, Ringer `20

- The generator sequentially generates partons $n \rightarrow n+1$

Postprocessing step

Shower history

Individual splitting

Parton showers and GANs

2. Neutron Star: EoS <=> mass-radius relation

ll, Ringer `20

TOV equations:

$$\frac{\mathrm{d}P}{\mathrm{d}r} = -\frac{(m + 4\pi r^3 P)(P + \varepsilon)}{r^2 - 2\,m\,r},$$

$$\frac{\mathrm{d}m}{\mathrm{d}r} = 4\pi r^2 \varepsilon,$$

$$\varepsilon = \varepsilon(P),$$

$\varepsilon(P)$

$M(R)$

$p_1, \ldots, p_{n+1})$

...
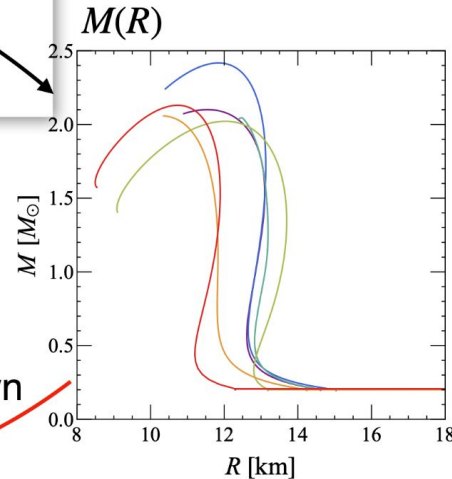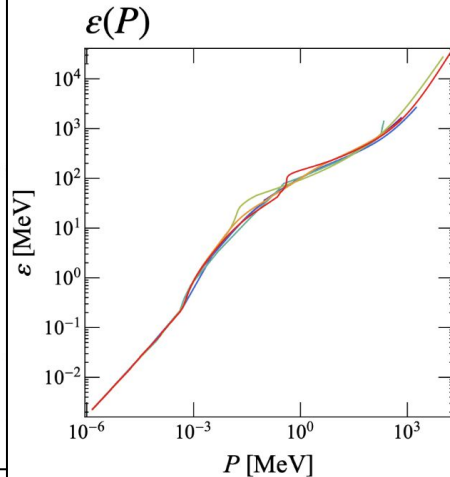
Discrete {M,R} observations?

Lindblom's algorithm
if the whole M(R) is known

Parton showers and GANs

2. Neutron Star: EoS <=> mass-radius relation

03
(repeated) *ll, Ringer `20*

Nuclear mass models based on microscopic calculations   3

**Advantage of the nuclear energy density functional**
- Include as much as possible physical ingredients
- Several parameters that can be adjusted to nuclear data
- Reasonable computational time

Mass models
- Based on skyrme : HFB1 to HFB32 -> best HFB27
- Gogny interaction : D1M -> rms = 0.788 Me
- All based on HFB (Hartree-Fock-Bogoliubov) oscillator basis

Objective
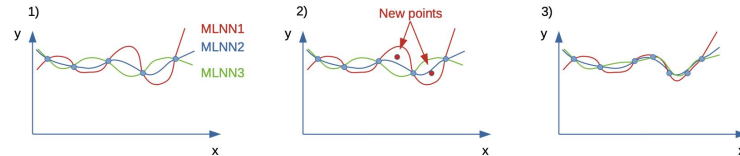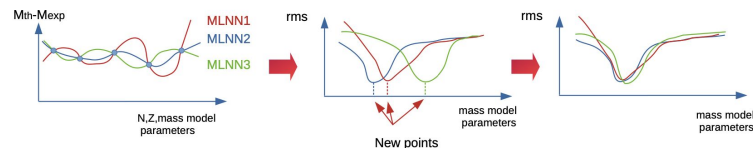We want to go further by developping a mass mod calculation.

ε [MeV]

10^4
10^3
10^2
10^1
10^0
10^{-1}
10^{-2}
10^{-6}
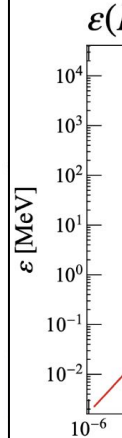
Active learning method   14

1st method,
R. Lasseri, D. Regnier, et al. Phys. Rev. Lett. 124, 162502 (2020)

Committee of Multy-layer neural network
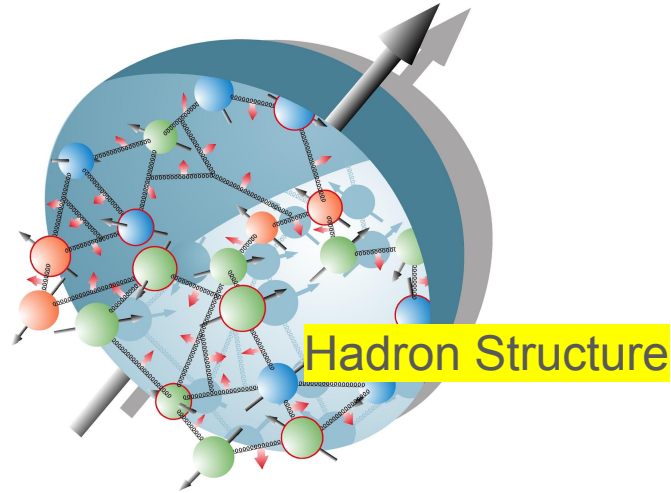
1) MLNN1 MLNN2 MLNN3   y   x
2) New points   y   x
3) y   x

Additional proposed method :

Mth-Mexp   MLNN1 MLNN2 MLNN3   N,Z,mass model parameters

rms   mass model parameters   New points

rms   mass model parameters

Quantum correlation functions (QCFs) in Nuclear femtography

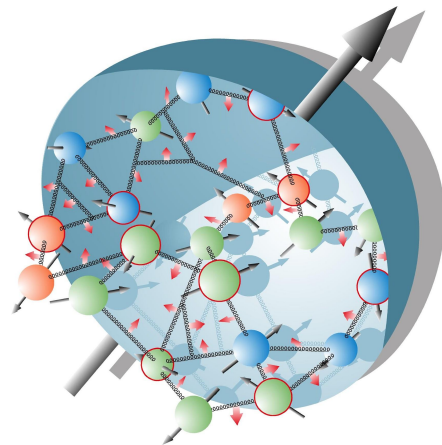Hadron Structure

Hadron formation
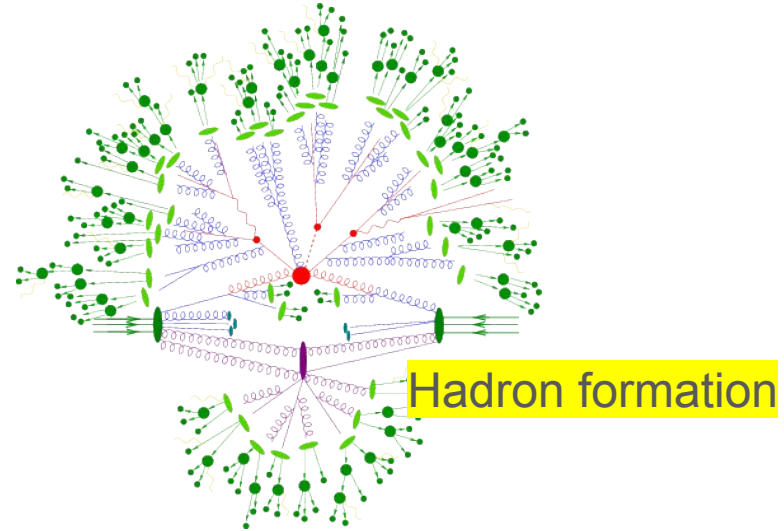
Parton distribution functions (PDFs)

Transverse momentum distributions (TMDs)

Generalized parton distributions (GPDs)

What do we mean by "hadron structure" ?

$$\xi = \frac{k^+}{P^+}$$

Parton momentum fraction relative to **parent hadron**

$$f_i(\xi) = \int \frac{\mathrm{d}w^-}{4\pi} e^{-i\xi p^+ w^-} \boxed{\langle N | \bar{\psi}_i(0, w^-, \mathbf{0}_{\mathrm{T}}) \gamma^+ \psi_i(0) | N \rangle}$$
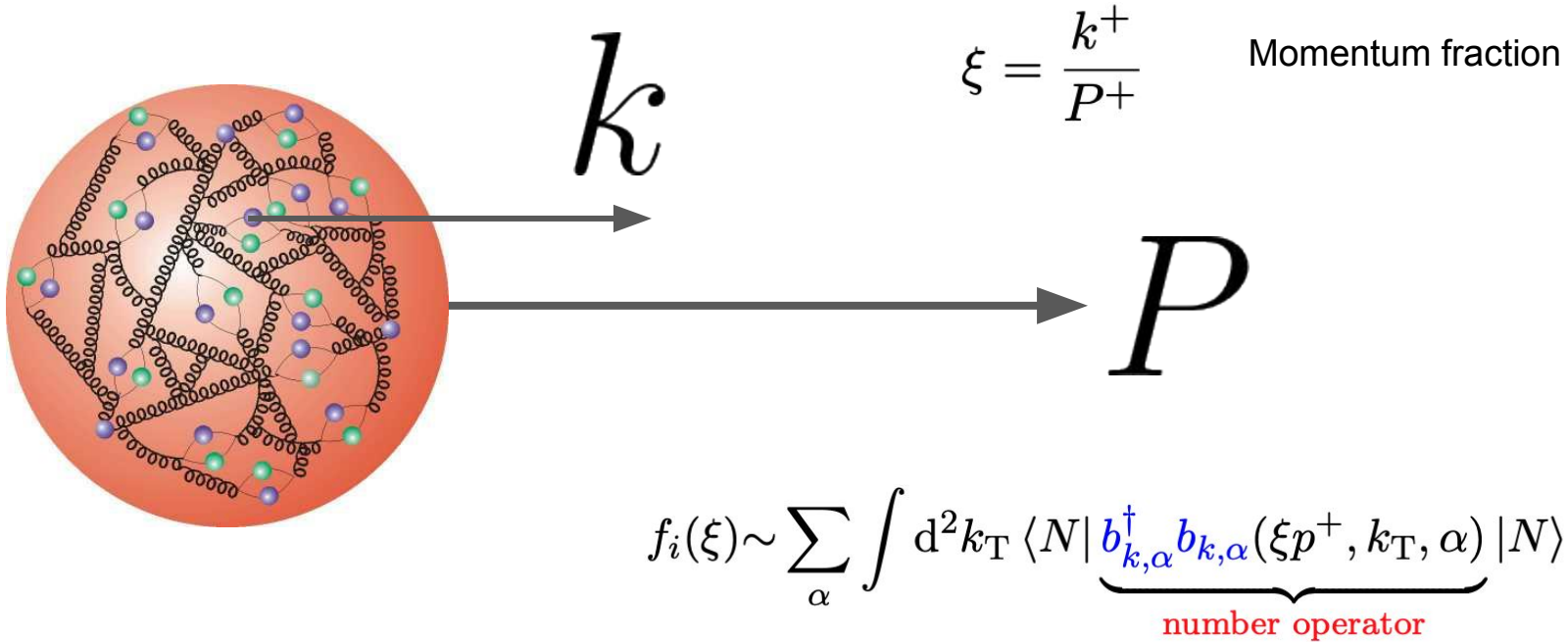
parton distribution function (PDF)
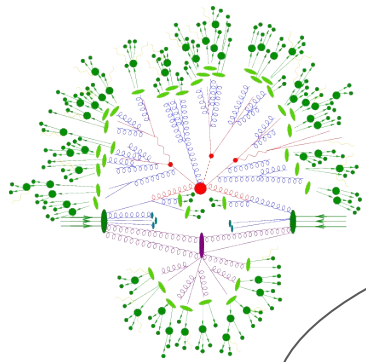
in non-interacting QCD

$$\psi_i(x) = \sum_{k,\alpha} b_{k,\alpha}(x^+) u_{k,\alpha} e^{-ik^+ x^- + ik_{\mathrm{T}} \cdot x_{\mathrm{T}}} + d^\dagger_{k,\alpha}(x^+) u_{k,-\alpha} e^{ik^+ x^- - ik_{\mathrm{T}} \cdot x_{\mathrm{T}}}$$

$$f_i(\xi) \sim \sum_\alpha \int \mathrm{d}^2 k_{\mathrm{T}} \langle N | \underbrace{b^\dagger_{k,\alpha} b_{k,\alpha}(\xi p^+, k_{\mathrm{T}}, \alpha)}_{\text{number operator}} | N \rangle$$

How quarks and gluons are distributed?

$$\xi = \frac{k^+}{P^+}$$

Momentum fraction

$$f_i(\xi) \sim \sum_\alpha \int \mathrm{d}^2 k_{\mathrm{T}} \, \langle N| \underbrace{b^\dagger_{k,\alpha} b_{k,\alpha}(\xi p^+, k_{\mathrm{T}}, \alpha)}_{\text{number operator}} |N\rangle$$

What do we mean by "hadronization" ?

$$\zeta = \frac{p_h^+}{k^+}$$
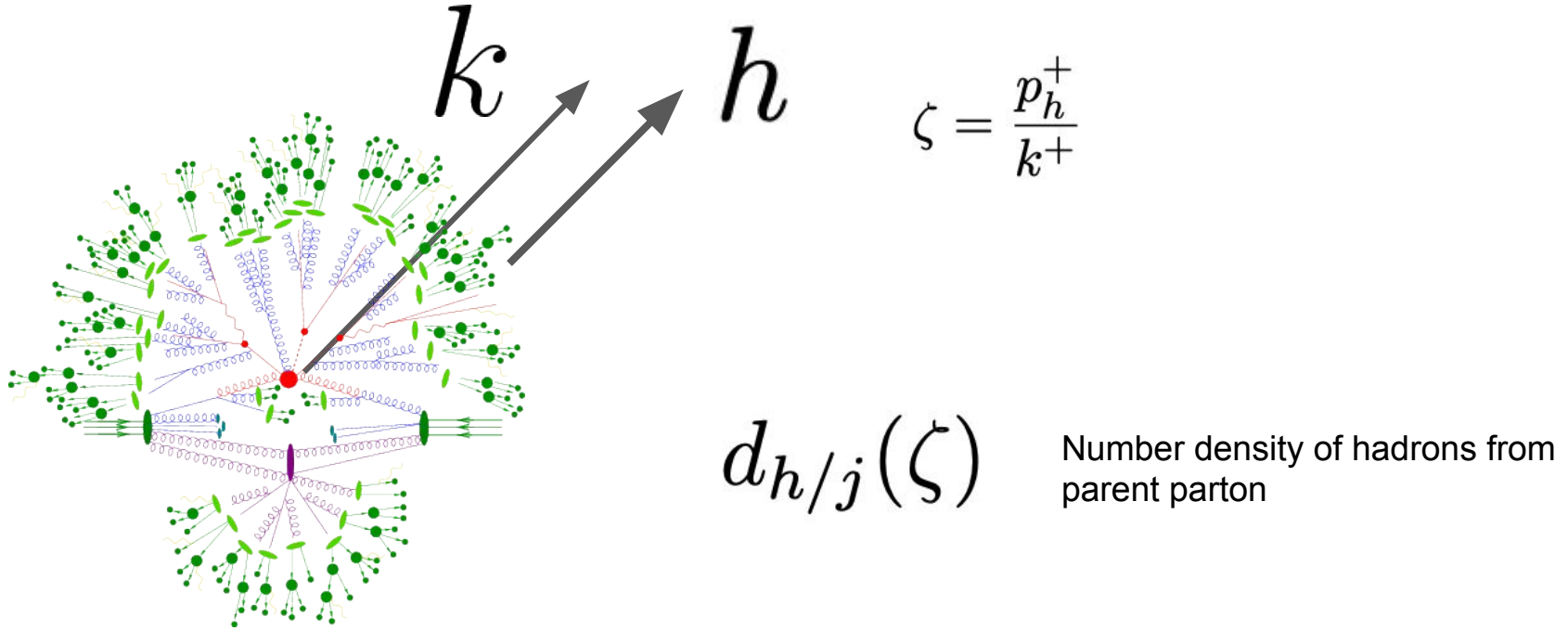
hadron momentum fraction relative to **parent parton**

$$d_{h/j}(\zeta) = \frac{\text{Tr}_{\text{color,Dirac}}}{4N_{c,j}} \sum_X \zeta \int \frac{dw^+}{2\pi} e^{i(p_h^-/\zeta)w^+}$$

$$\times \gamma^- \left\langle 0 \left| \bar{\psi}_j(0, w^+, \mathbf{0}_{\text{T}}) \right| p_h, X \right\rangle \left\langle p_h, X \right| \psi_j(0) \left| 0 \right\rangle$$

Fragmentation functions (FFs)

X = all states except detected hadron **h**

How hadrons emerges from quarks and gluons

$$k \qquad h$$

$$\zeta = \frac{p_h^+}{k^+}$$

$$d_{h/j}(\zeta)$$

Number density of hadrons from parent parton

Hadron structure in interacting theory

Definition of PDFs in field theory requires renormalization

PDFs will depend on renormalization scale and its RGEs are the famous DGLAP equations

UV singularity when the field separation is zero

$$f_i(\xi) \overset{!}{=} \int \frac{\mathrm{d}w^-}{4\pi} e^{-i\xi p^+ w^-} \langle N|\bar{\psi}_i(0, w^-, \mathbf{0}_\mathrm{T})\gamma^+ \psi_i(0)|N\rangle$$

Renormalization

Dokshitzer–**G**ribov–**L**ipatov–**A**ltarelli–**P**arisi

$$f = Z_F \otimes f_\mathrm{bare}$$

$$f(\xi) \rightarrow f(\xi, \mu)$$

$$\frac{\mathrm{d}f_i(\xi, \mu^2)}{\mathrm{d}\ln\mu^2} = \sum_j \int_\xi^1 \frac{\mathrm{d}y}{y} P_{ij}(\xi, \mu^2) f_j\left(\frac{y}{\xi}, \mu^2\right)$$
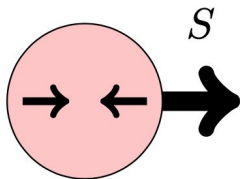
aka   **DGLAP**

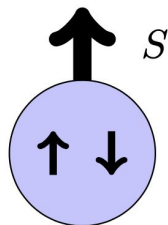# Spin structures
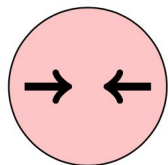
$$f = f_\rightarrow + f_\leftarrow$$

Unpol pdfs

$$\langle N|\bar{\psi}_i(0, w^-, \mathbf{0}_{\mathrm{T}})\gamma^+\psi_i(0)|N\rangle$$

$$\Delta f = f_\rightarrow - f_\leftarrow$$

Helicity distribution

$$\langle N|\bar{\psi}_i(0, w^-, \mathbf{0}_{\mathrm{T}})\gamma^+\gamma_5\psi_i(0)|N\rangle$$

$$\delta_{\mathrm{T}} f = f_\uparrow - f_\downarrow$$

Transversity

$$\langle N|\bar{\psi}_i(0, w^-, \mathbf{0}_{\mathrm{T}})\gamma^+\gamma_\perp\gamma_5\psi_i(0)|N\rangle$$
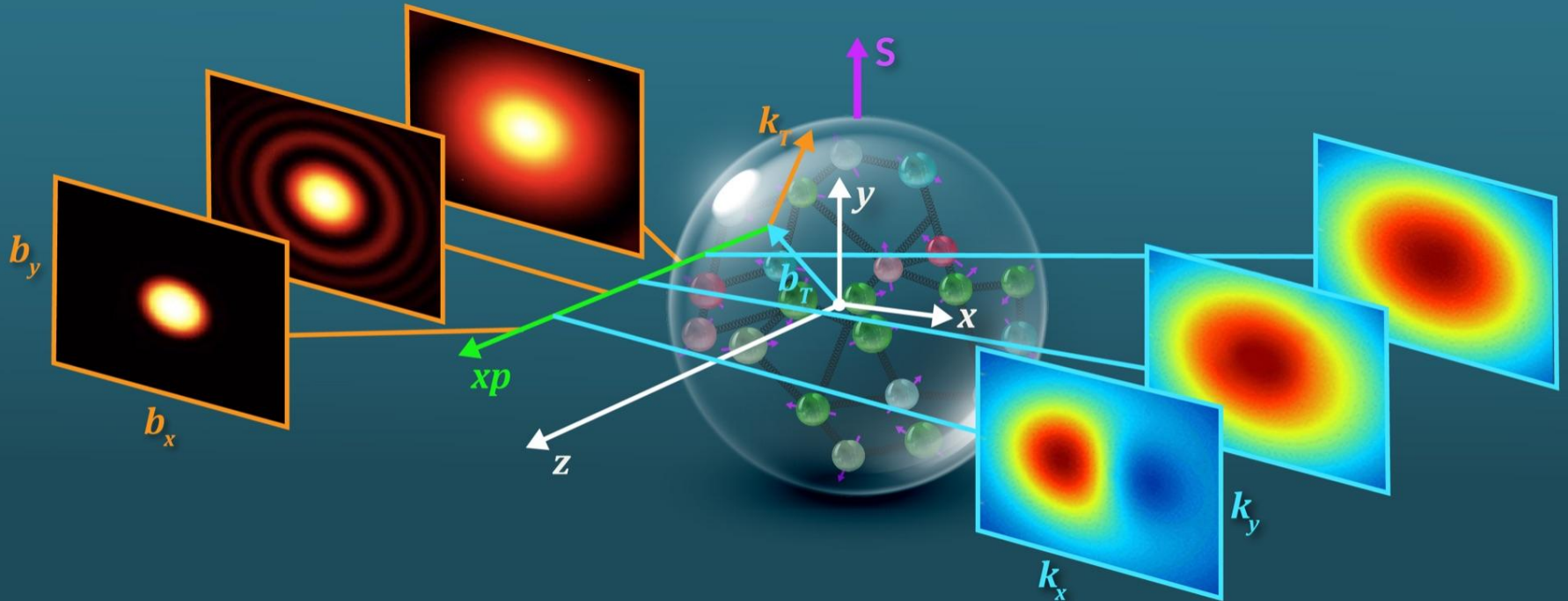
Extensions to 3D

$$f(\xi, b_{\mathrm{T}})$$

Impact parameter
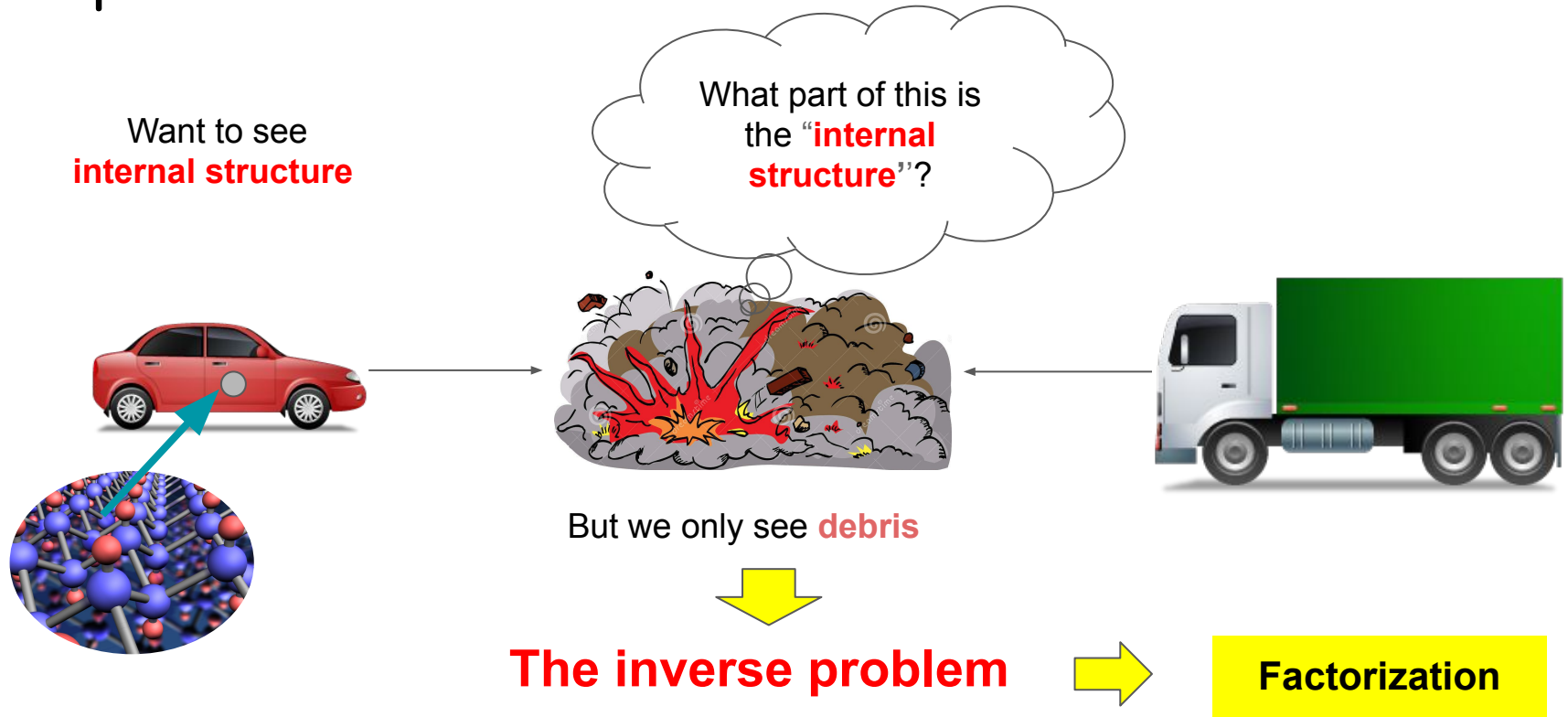distribution -> **GPDs**
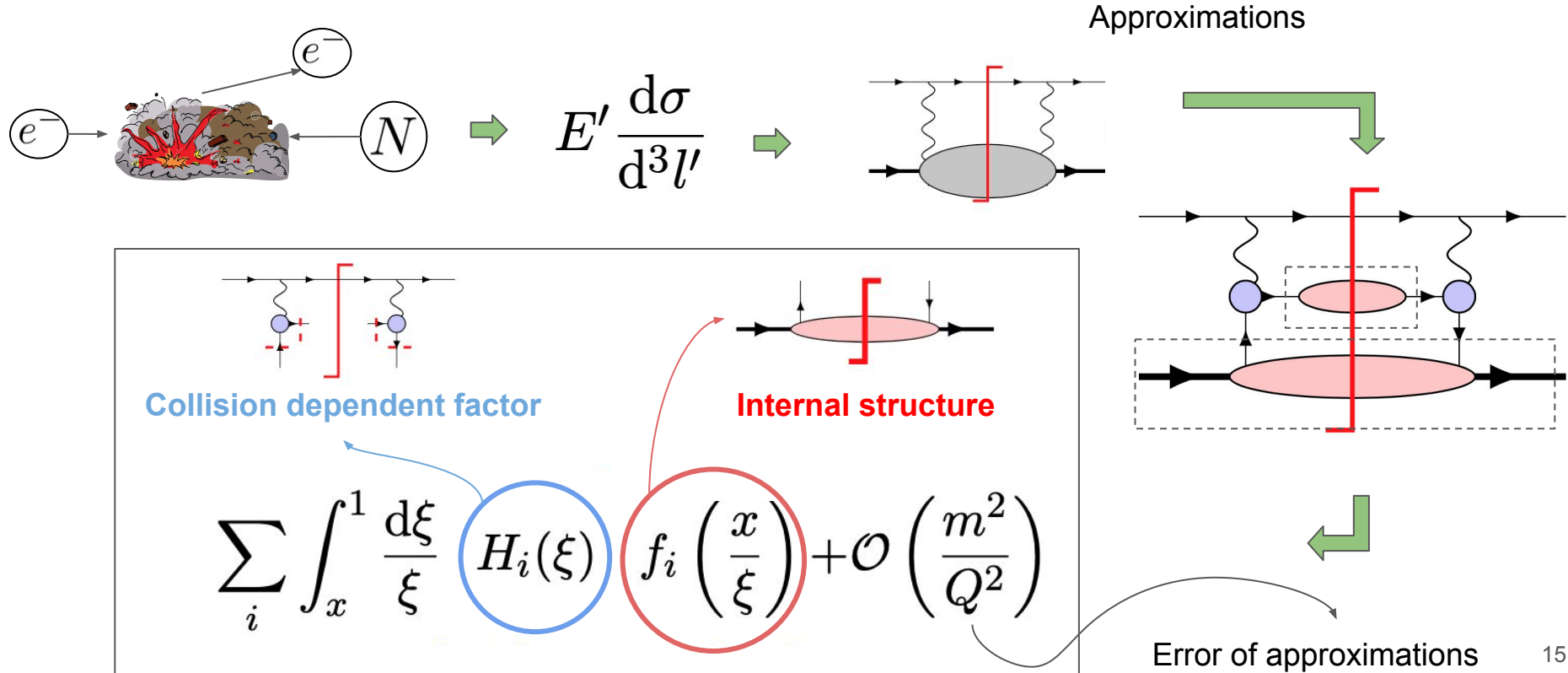
$$f(\xi)$$

PDFs

$$f(\xi, k_{\mathrm{T}})$$

Transverse momentum
distribution -> **TMDs**

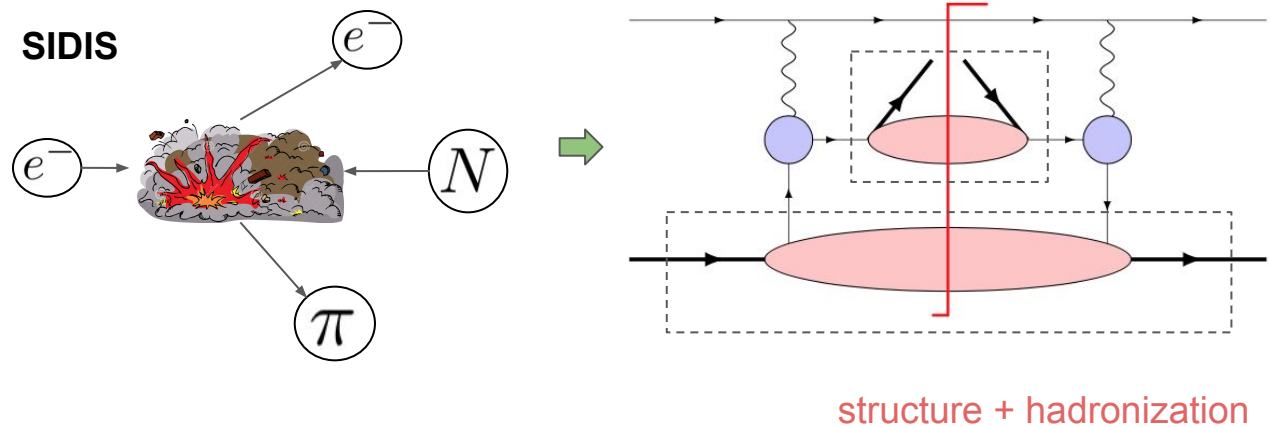# So how do we get hadron structure from experimental data?

Want to see
internal structure

What part of this is the "**internal structure**"?

But we only see **debris**

The inverse problem   **Factorization**

Factorization in deep-inelastic scattering

Approximations

Collision dependent factor

Internal structure

$$\sum_i \int_x^1 \frac{\mathrm{d}\xi}{\xi} H_i(\xi) f_i\left(\frac{x}{\xi}\right) + \mathcal{O}\left(\frac{m^2}{Q^2}\right)$$

Error of approximations

15

Factorization in other reactions

SIA

hadronization

$$\mathrm{d}\sigma = \sum_i H_i^{\mathrm{SIA}} \otimes d_i$$

SIDIS

$$\mathrm{d}\sigma = \sum_{ij} H_{ij}^{\mathrm{SIDIS}} \otimes f_i \otimes d_j$$

structure + hadronization
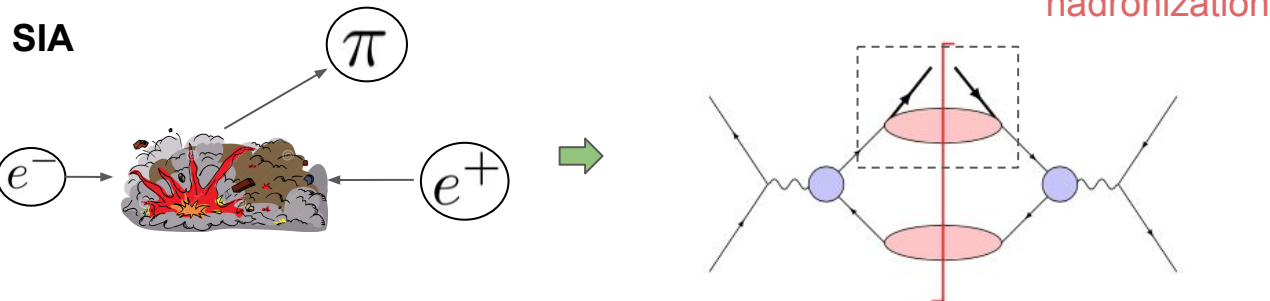
..and many more

Universality
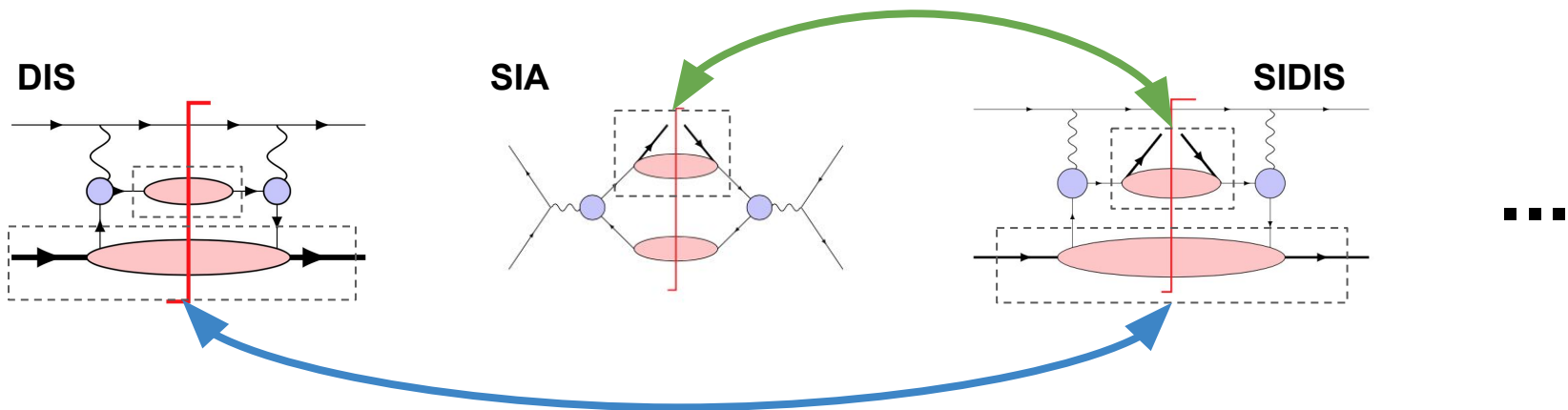
cross sections described by **universal non-perturbative** functions, e.g. PDFs, FFs

The Bayesian inference

Experiments = theory + errors

$$d\sigma_{\mathrm{DIS}} = \sum_i H_i^{\mathrm{DIS}} \otimes f_i$$

$$d\sigma_{\mathrm{DY}} = \sum_{ij} H_{ij}^{\mathrm{DY}} \otimes f_i \otimes f_j$$

$$d\sigma_{\mathrm{SIA}} = \sum_i H_i^{\mathrm{SIA}} \otimes d_i$$

$$d\sigma_{\mathrm{SIDIS}} = \sum_{ij} H_{ij}^{\mathrm{SIDIS}} \otimes f_i \otimes d_j$$

RGE boundary conditions (QCF modeling)

$$f_i(\xi, \mu_0^2) = N_i \xi^{a_i} (1 - \xi)^{b_i} (1 + ...)$$

$$d_i(\zeta, \mu_0^2) = N_i \zeta^{a_i} (1 - \zeta)^{b_i} (1 + ...)$$

$$\mathbf{a} = (N_i, a_i, b_i, ...)$$

$$\rho(\mathbf{a}|\mathrm{data}) \sim \mathcal{L}(\mathbf{a}, \mathrm{data})\pi(\mathbf{a})$$

$$\mathcal{L}(\boldsymbol{a}, \mathrm{data}) = \exp\left[-\frac{1}{2}\chi^2(\boldsymbol{a}, \mathrm{data}) \right]$$

$$\chi^2(\boldsymbol{a}) = \sum_{i,e} \left(\frac{d_{i,e} - \sum_k r_e^k \beta_{i,e}^k - T_{i,e}(\boldsymbol{a})/N_e}{\alpha_{i,e}} \right)^2$$

$$\mathrm{E}[f_i(\xi, \mu^2)] = \int d^n\mathbf{a} \, \rho(\mathbf{a}|\mathrm{data}) f_i(\xi, \mu^2; \mathbf{a})$$

$$\mathrm{V}[f_i(\xi, \mu^2)] = \int d^n\mathbf{a} \, \rho(\mathbf{a}|\mathrm{data}) \left[f_i(\xi, \mu^2; \mathbf{a}) - \mathrm{E}[f_i(\xi, \mu^2)] \right]^2$$

How do we deal with the posterior?

$$E[f_i(\xi, \mu^2)] = \int d^n\mathbf{a} \; \rho(\mathbf{a}|\text{data}) f_i(\xi, \mu^2; \mathbf{a})$$

$$V[f_i(\xi, \mu^2)] = \int d^n\mathbf{a} \; \rho(\mathbf{a}|\text{data}) \left[f_i(\xi, \mu^2; \mathbf{a}) - E[f_i(\xi, \mu^2)] \right]^2$$

Maximum likelihood
+ Hessian
+ Lagrange

MC methods
+ Data resampling
+ Markovian
 approaches

Maximum likelihood (+Hessian)

Hunt-Smith, Accardi, Melnitchouk, NS, Thomas, White (in prep)

$$E\{\mathcal{O}(\boldsymbol{a})\} = \int \mathrm{d}^n t \; p(\boldsymbol{t}|\boldsymbol{m}) \, \mathcal{O}(\boldsymbol{a}(\boldsymbol{t})) \approx \mathcal{O}(\boldsymbol{a}_0) \, .$$

$$V\{\mathcal{O}(\boldsymbol{a})\} = \int \mathrm{d}^n t \; p(\boldsymbol{t}|\boldsymbol{m}) \big[\mathcal{O}(\boldsymbol{a}(\boldsymbol{t})) - E\{\mathcal{O}(\boldsymbol{a})\}\big]^2$$

$$\approx \prod_k \int \mathrm{d}t_k \; p\Big(t_k \frac{\boldsymbol{e}_k}{\sqrt{w_k}}\Big|\boldsymbol{m}\Big) \Big(\sum_l \frac{\partial \mathcal{O}(\boldsymbol{a}(\boldsymbol{t}))}{\partial t_l}\Big|_{\boldsymbol{a}_0} t_l\Big)^2$$

$$= \sum_k T_k^2 \left(\frac{\partial \mathcal{O}(\boldsymbol{a}(\boldsymbol{t}))}{\partial t_k}\Big|_{\boldsymbol{a}_0}\right)^2, \qquad \Longrightarrow \qquad T_k^2 = \int \mathrm{d}t_k \; p_k(t_k|\boldsymbol{m}) \, t_k^2.$$

$$V\{\mathcal{O}(\boldsymbol{a})\} \approx \sum_k \frac{1}{4}\Big[\mathcal{O}\Big(\boldsymbol{a}_0 + T_k\frac{\boldsymbol{e}_k}{\sqrt{w_k}}\Big) - \mathcal{O}\Big(\boldsymbol{a}_0 - T_k\frac{\boldsymbol{e}_k}{\sqrt{w_k}}\Big)\Big]^2$$
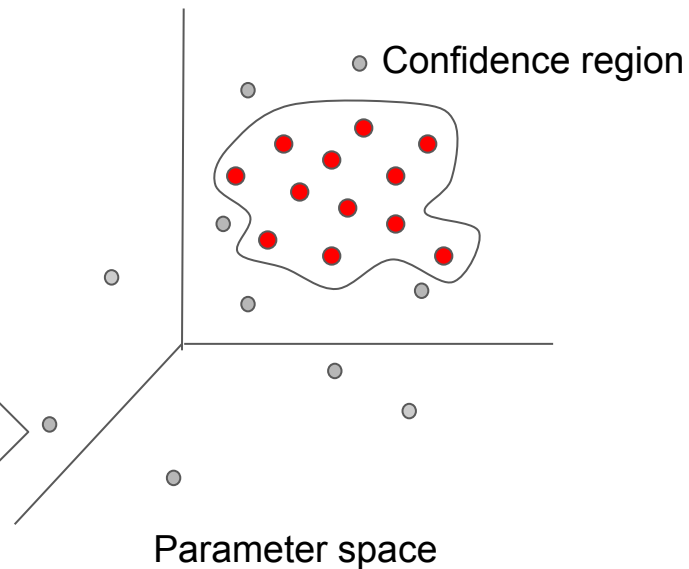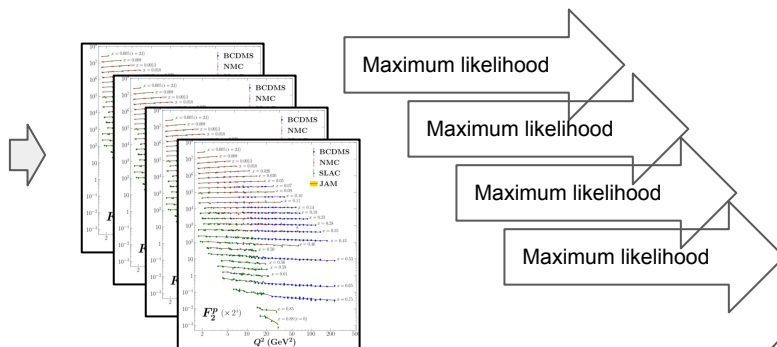
Data resampling

$$E_{\text{freq}}\{\mathcal{O}(\boldsymbol{a})\} = \frac{1}{n_{\text{rep}}} \sum^{n_{\text{rep}}} \mathcal{O}(\boldsymbol{a}_{\text{rep}}),$$

$$V_{\text{freq}}\{\mathcal{O}(\boldsymbol{a})\} = \frac{1}{n_{\text{rep}}} \sum^{n_{\text{rep}}} \left[\mathcal{O}(\boldsymbol{a}_{\text{rep}}) - E_{\text{freq}}\{\mathcal{O}(\boldsymbol{a})\}\right]^2.$$

$$d_{k,i}^{(\text{pseudo})} = d_i^{(\text{original})} + \alpha_i \, R_{k,i}$$

Confidence region

Original data

Replica data

Maximum likelihood

Maximum likelihood

Maximum likelihood

Maximum likelihood

Parameter space
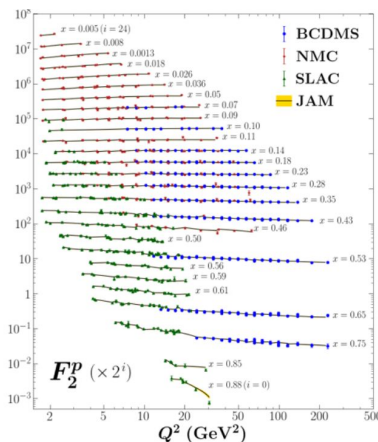
Jefferson Lab Angular Momentum Collaboration
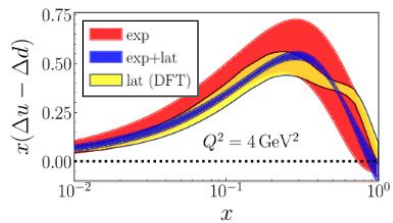
First global analysis with lattice off-the-light cone matrix elements for polarized and unpolarized PDFs. Polarized lattice data compatible with experimental data *PRD* 103 (2021)

New combined analysis of pdfs and ffs including unidentified charged hadron SIDIS and SIA data. The update analysis from JAM19 indicates again the strong nucleon suppression PRD 104 (2021)
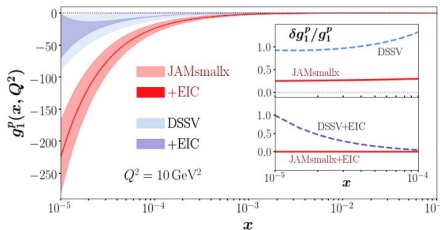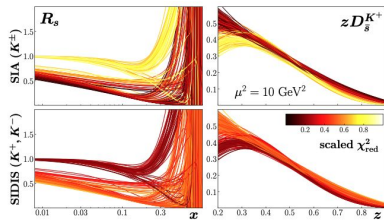
First global QCD analysis of polarized PDFs using small x evolution. The constrained small x indicates a strong preference for negative g1p at small x. Provides important guidance for EIC simulations PRD 104 (2021)
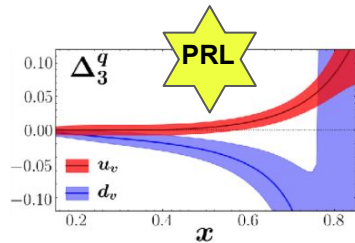
PDF analysis with the inclusion of collider W/Z data and the MARATHON d/p, Helium , Triton DIS data. Evidence for iso-vector effects illuminating nuclear effects in light nuclei arXiv:2104.06946 - accepted in PRL
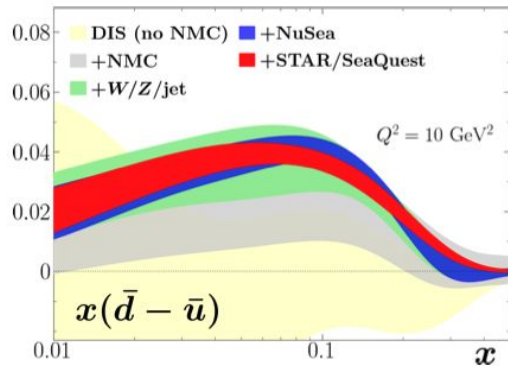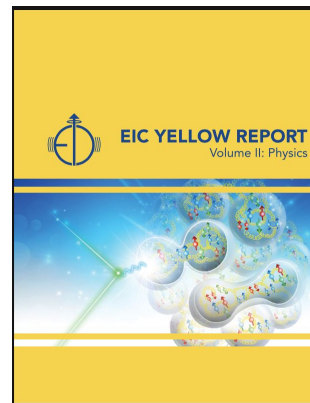
Including of RHIC W+/- data and Seaquest DY data. New constraints on antimatter asymmetry in the nucleon PRD 104 (2021)
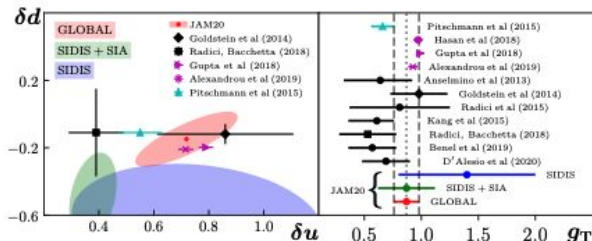
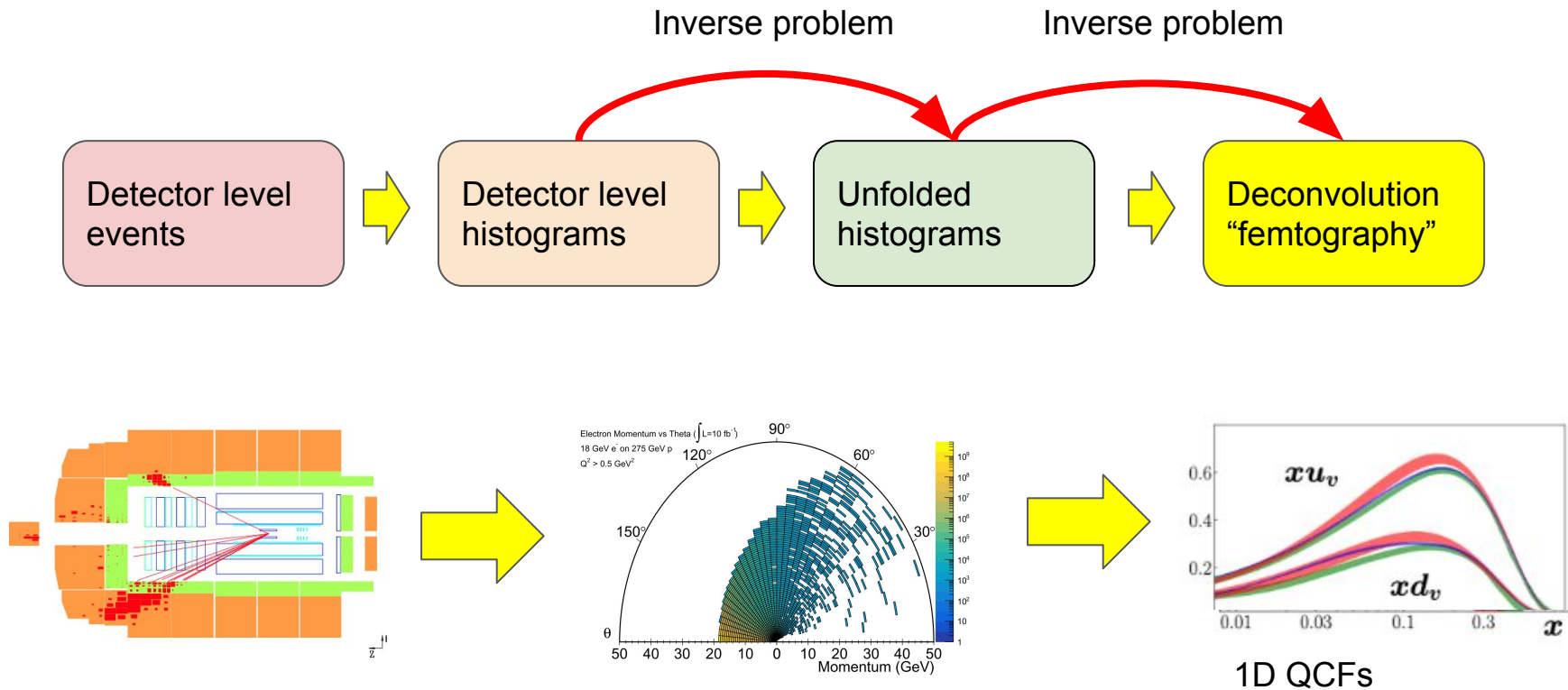First global analysis of all SSA in TMD+CT3 framework. New constraints on nucleon tensor charges PRD 102 (2020)
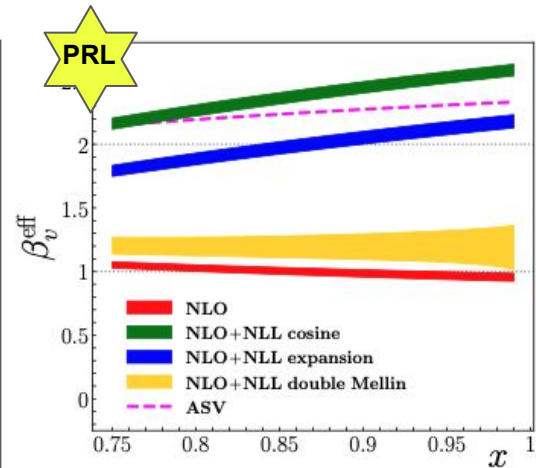
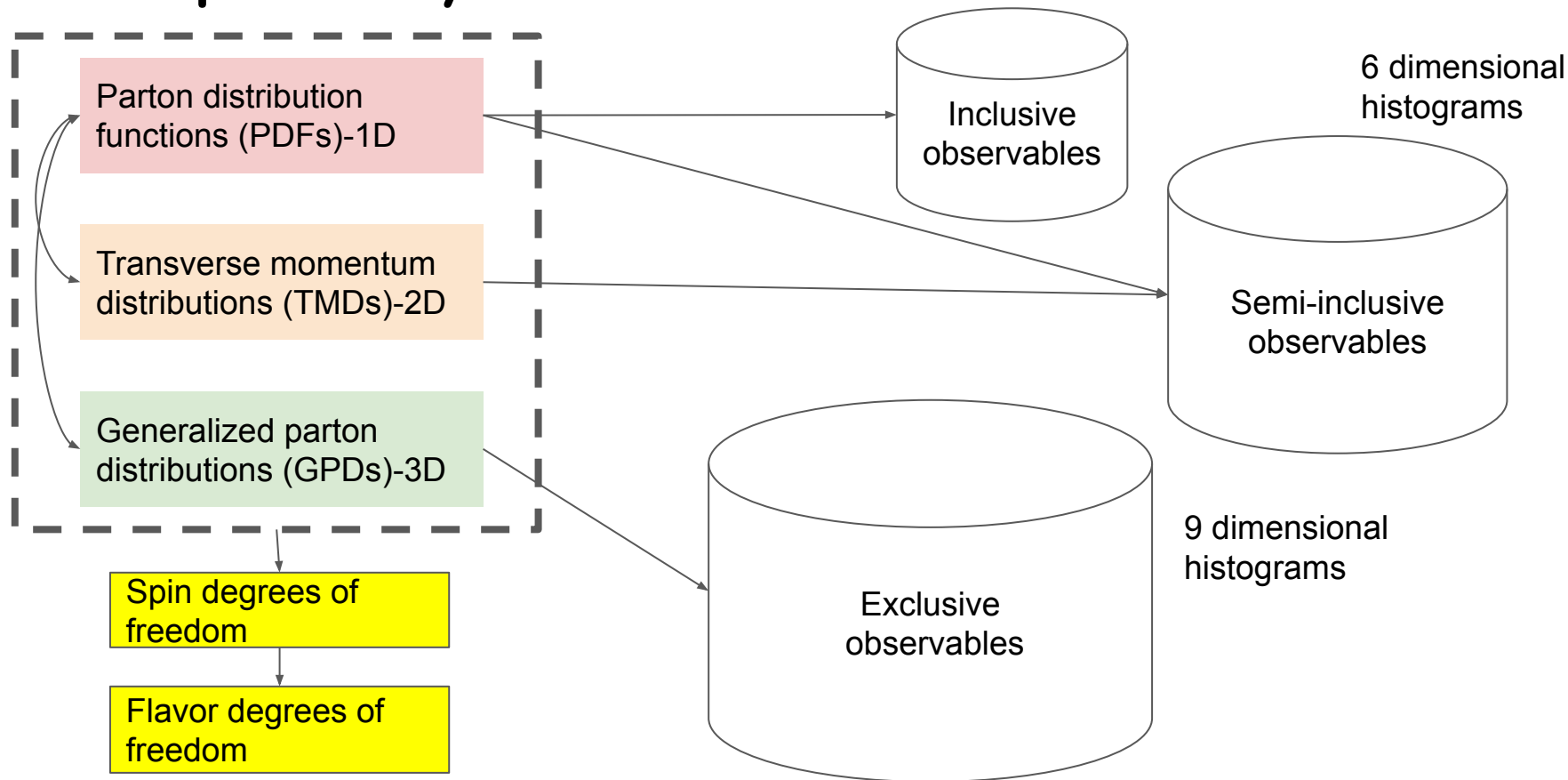New results on pion pdfs providing the effective large x asymptotic and its theory uncertainties PRL 127 2021

Support for EIC yellow report including unpolarized and polarized nucleon pdfs, electroweak parameters, meson structure and TMD arXiv:2103.05419
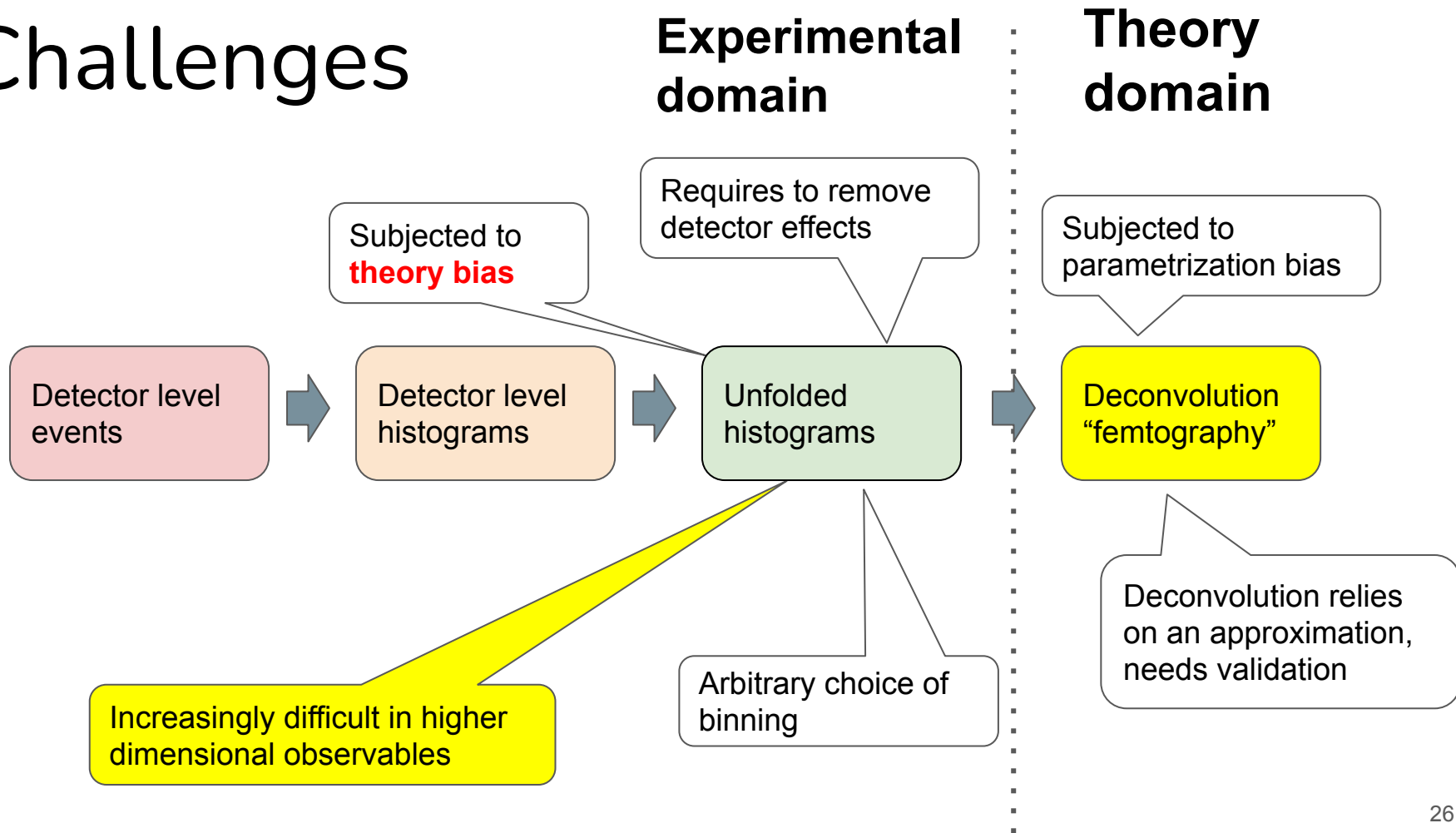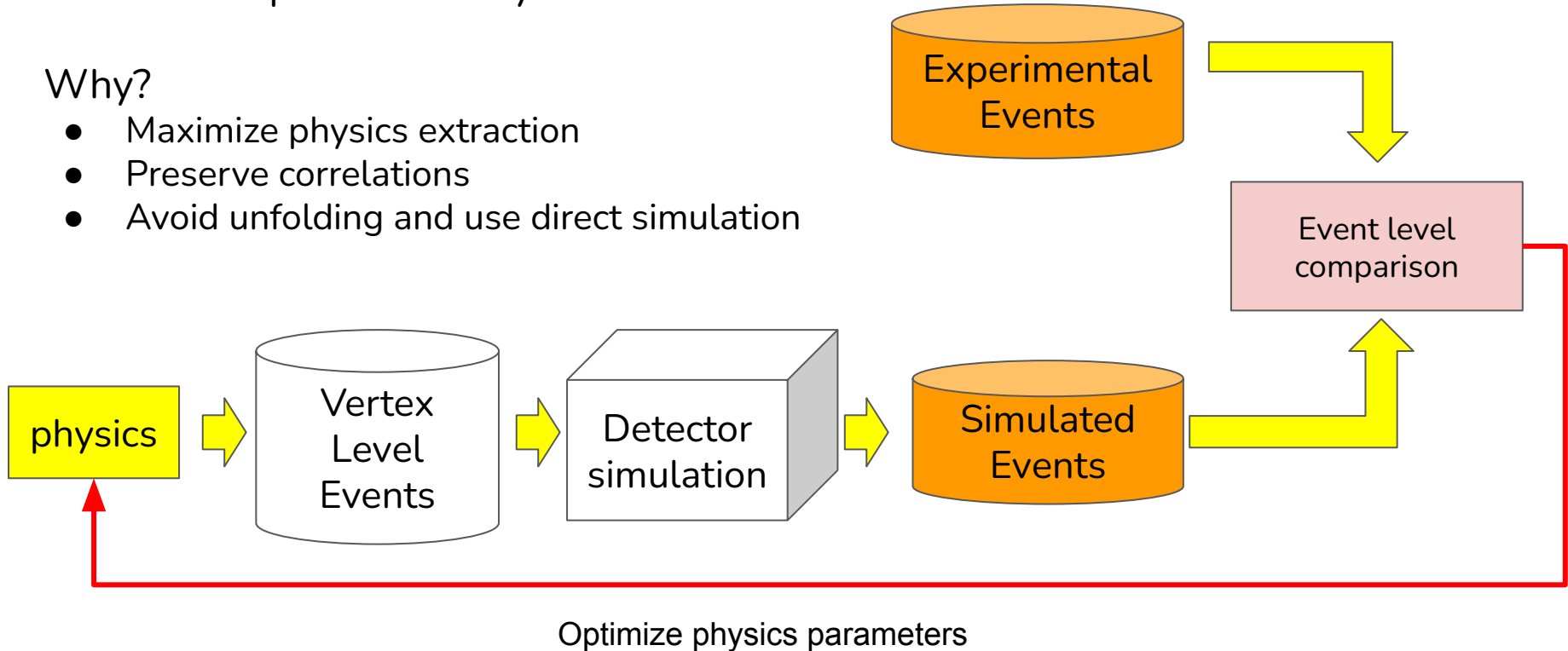
EIC YELLOW REPORT
Volume II: Physics

Current paradigm

Inverse problem   Inverse problem

Detector level events	⇨	Detector level histograms	⇨	Unfolded histograms	⇨	Deconvolution "femtography"

Electron Momentum vs Theta (∫L=10 fb⁻¹)
18 GeV e⁻ on 275 GeV p
Q² > 0.5 GeV²

1D QCFs

Complexity

Parton distribution functions (PDFs)-1D

Transverse momentum distributions (TMDs)-2D

Generalized parton distributions (GPDs)-3D

Spin degrees of freedom

Flavor degrees of freedom

3 dimensional histograms

Inclusive observables

6 dimensional histograms

Semi-inclusive observables

9 dimensional histograms

Exclusive observables

Challenges

Experimental domain

Theory domain

Subjected to **theory bias**

Requires to remove detector effects

Subjected to parametrization bias

Detector level events

Detector level histograms

Unfolded histograms

Deconvolution "femtography"

Increasingly difficult in higher dimensional observables

Arbitrary choice of binning

Deconvolution relies on an approximation, needs validation

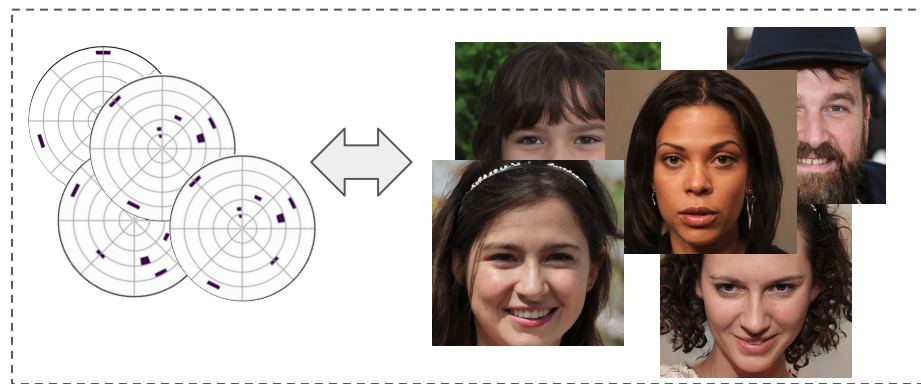# Event-based analysis?

Can we compare real vs synthetic events?

Why?
- Maximize physics extraction
- Preserve correlations
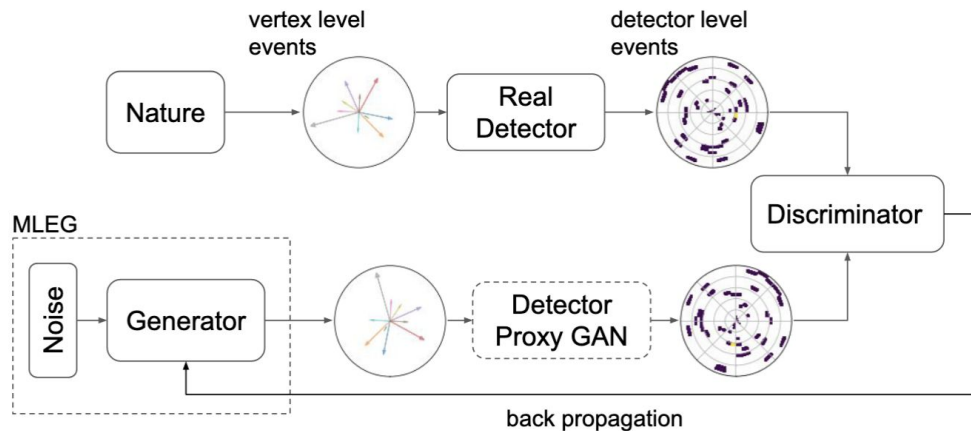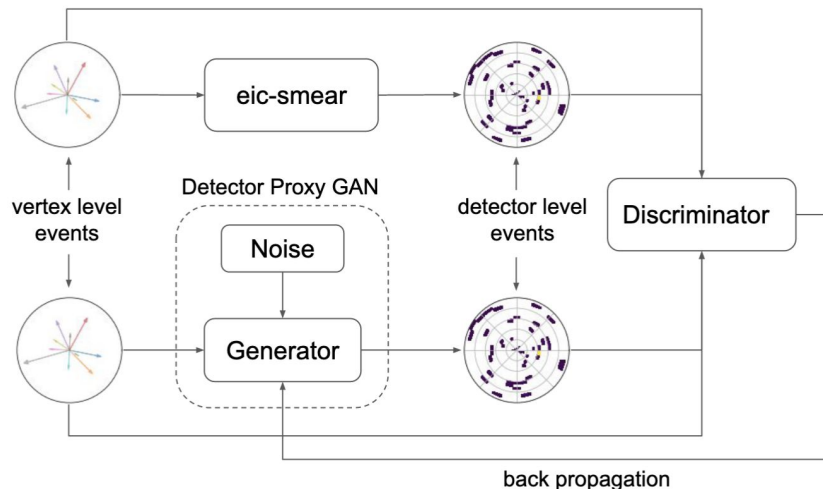- Avoid unfolding and use direct simulation

Experimental Events

Event level comparison

physics → Vertex Level Events → Detector simulation → Simulated Events

Optimize physics parameters

GANs

Random noise → Generator
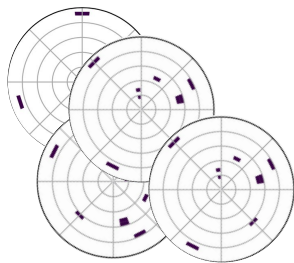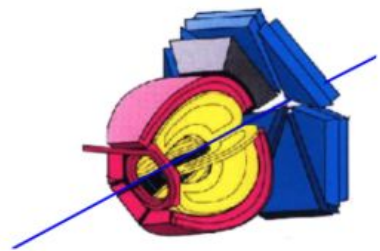
Discriminator → Real / Fake
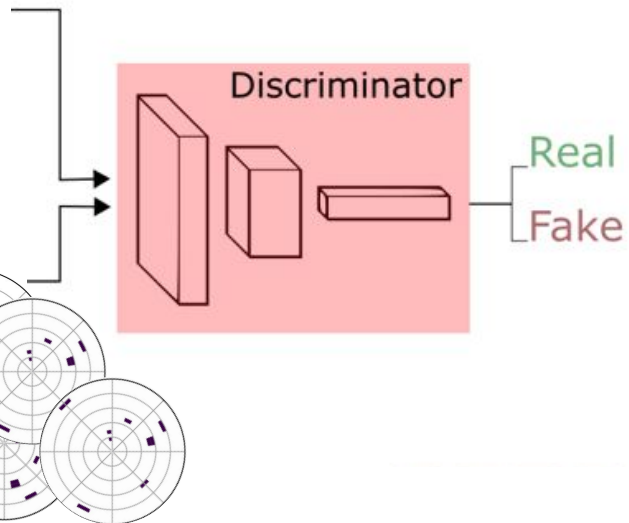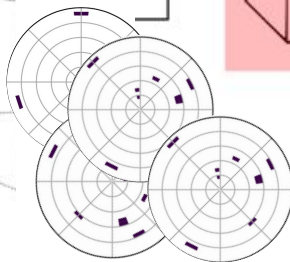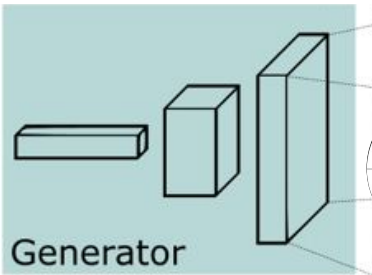
Application to inclusive DIS
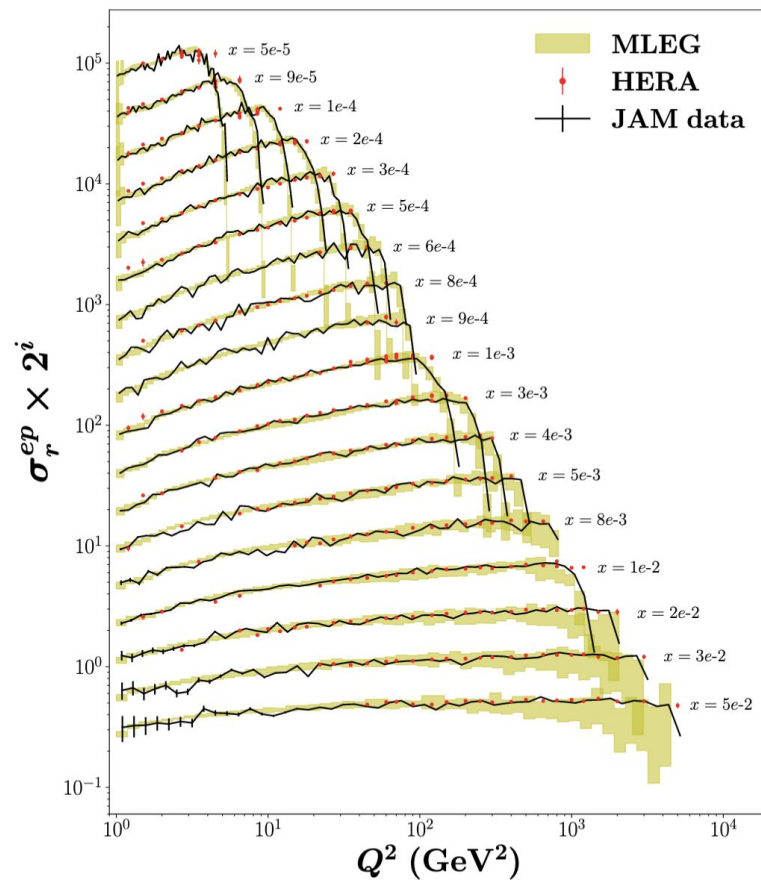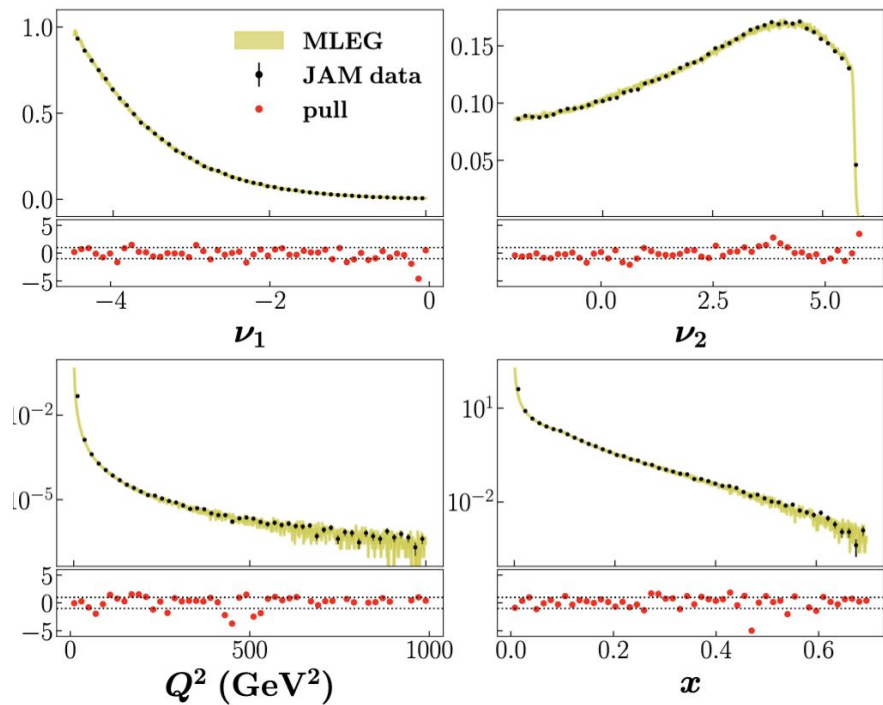
$$k + p \rightarrow k' + X$$

GAN detector

- A GANs to train a detector emulator
- Train particle generator using GAN detector
- change of variables to improve discriminator
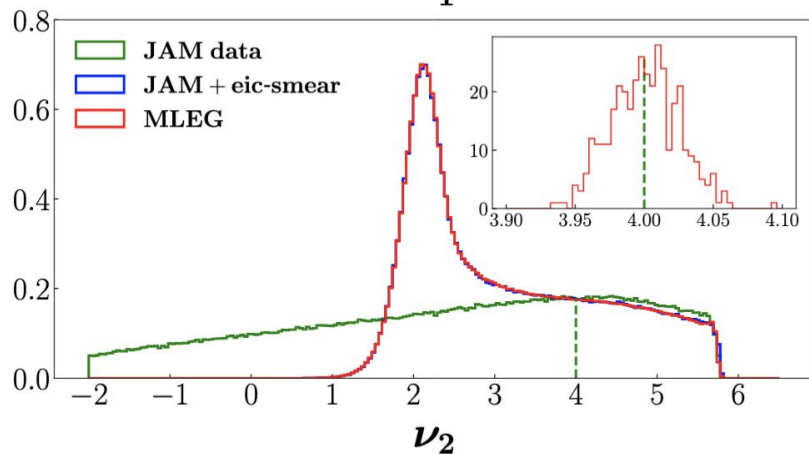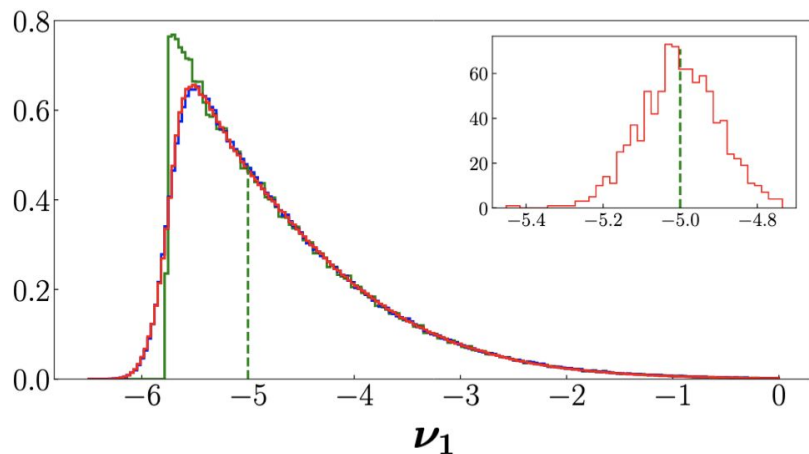
$$\nu_1 = \ln\left((k'_0 - k'_z)/1\,\text{GeV}\right),$$
$$\nu_2 = \ln\left((2E_e - k'_0 - k'_z)/1\,\text{GeV}\right),$$

Y. Alanazi,[1] P. Ambrozewicz,[2] M. Battaglieri,[3] A. N. Hiller Blin,[4] M. P. Kuchera,[5] Y. Li,[1] T. Liu,[6] R. E. McClellan,[2] W. Melnitchouk,[2] E. Pritchard,[5] M. Robertson,[7] N. Sato,[2] R. Strauss,[7] and L. Velasco[8]
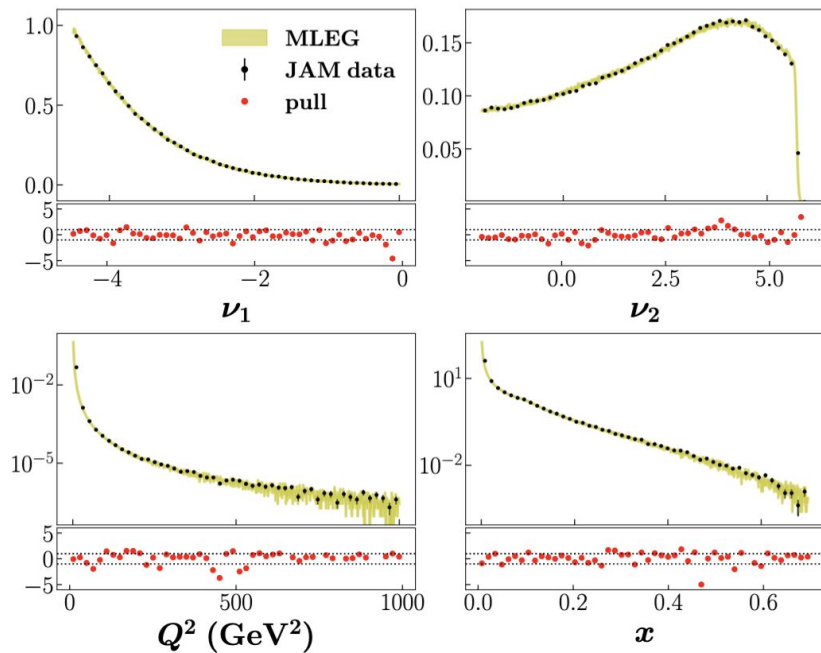
Case 1: no detector effects
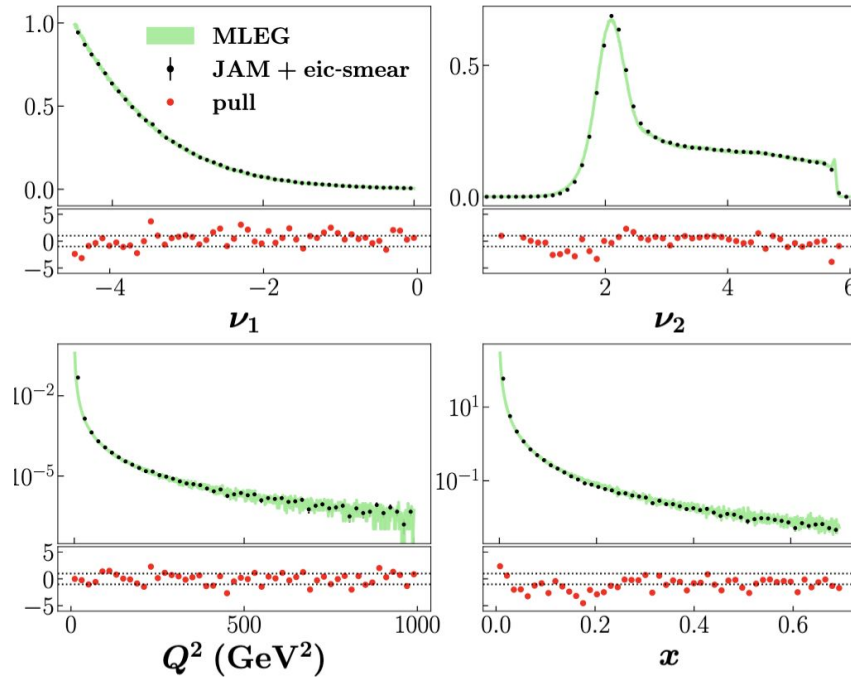
Detector GAN proxy

- Use simple detector parametrization (EICSmear)
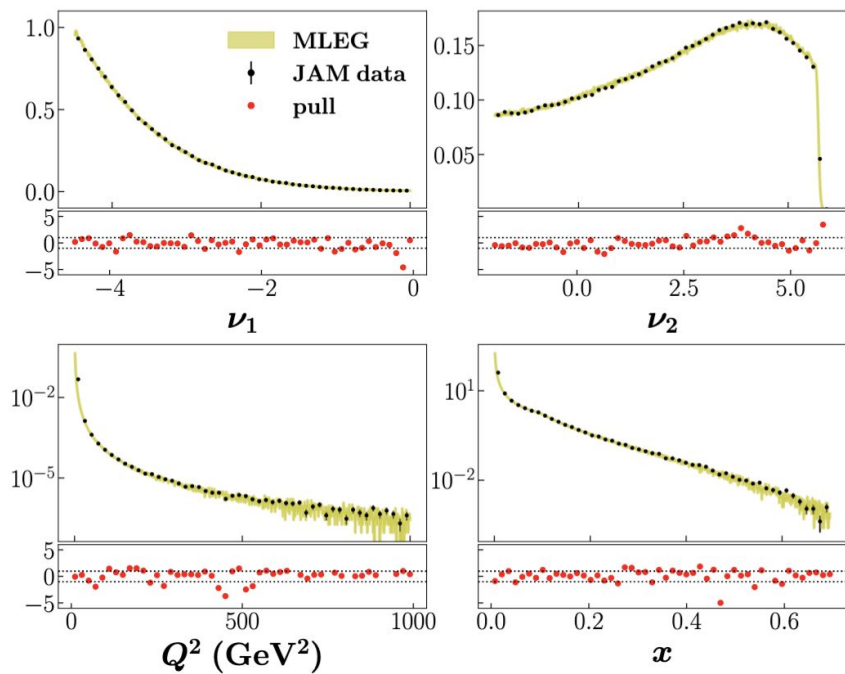
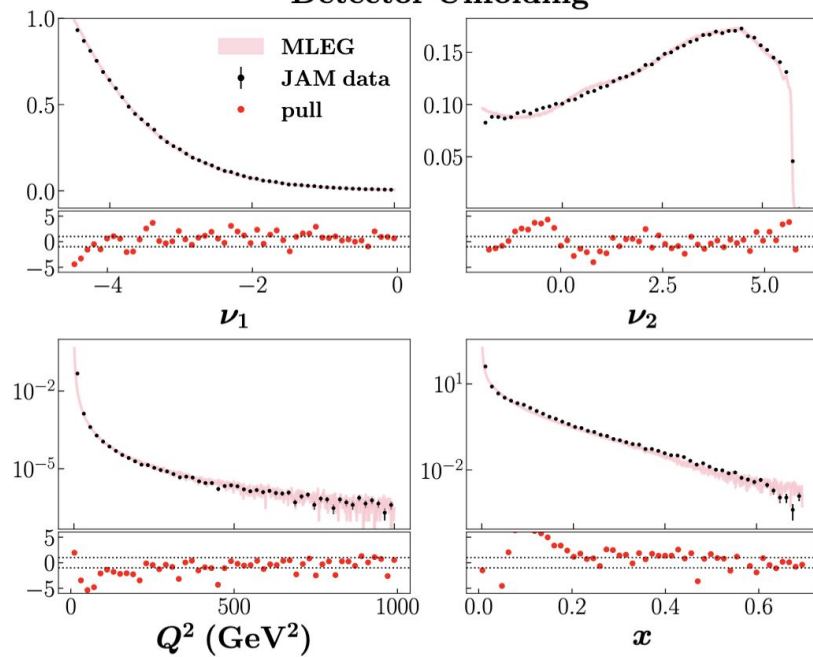- Train detector GAN proxi using EICSmear

No Detector Effects

With Detector Effects

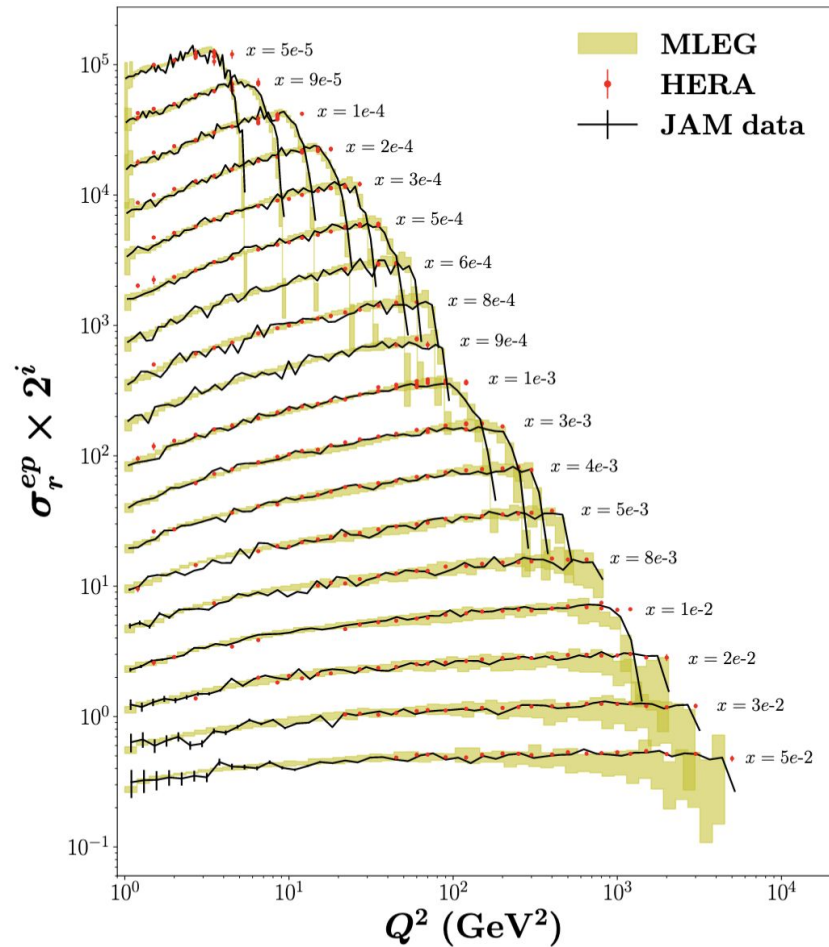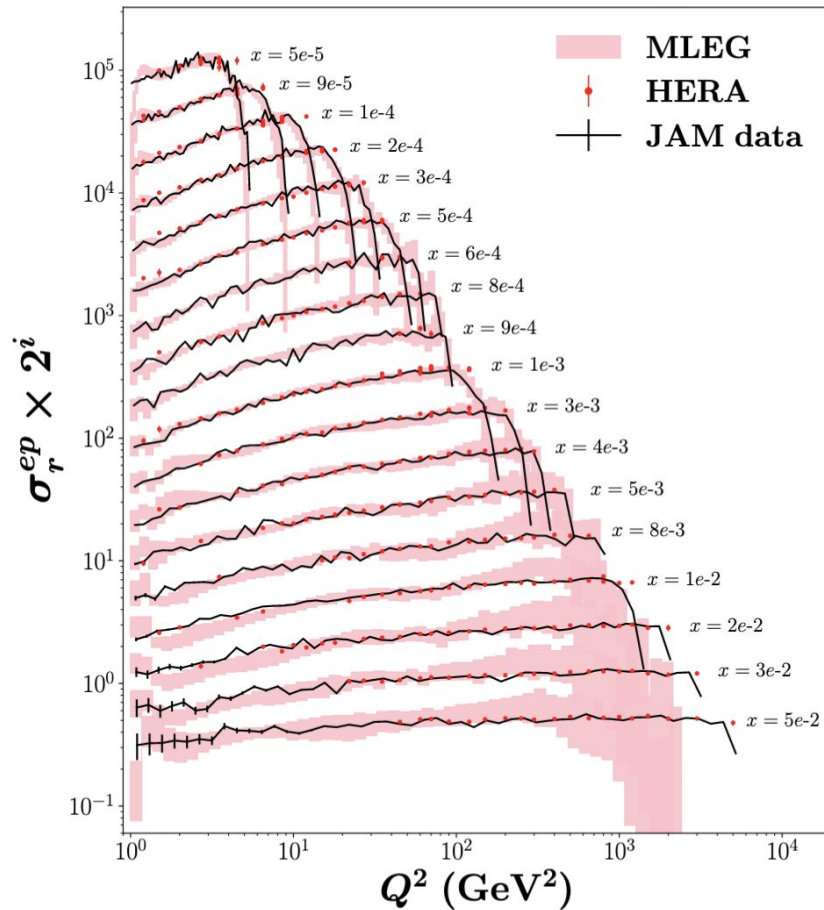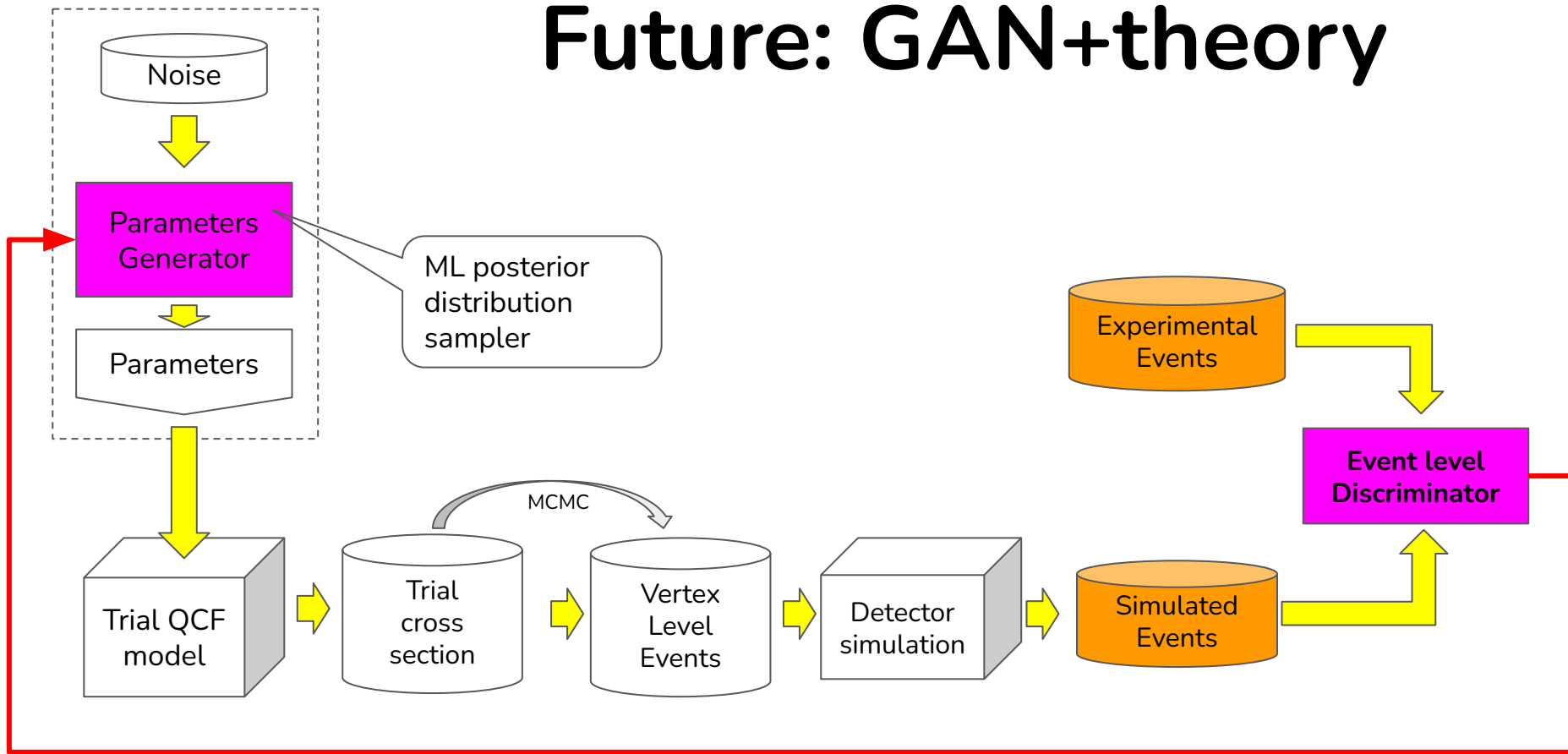## No Detector Effects

Detector Unfolding

No Detector Effects

Detector Unfolding

Plots of $\sigma_r^{ep} \times 2^i$ versus Q^2 (GeV^2) for MLEG, HERA, and JAM data at various values of x: $x = 5e\text{-}5$, $x = 9e\text{-}5$, $x = 1e\text{-}4$, $x = 2e\text{-}4$, $x = 3e\text{-}4$, $x = 5e\text{-}4$, $x = 6e\text{-}4$, $x = 8e\text{-}4$, $x = 9e\text{-}4$, $x = 1e\text{-}3$, $x = 3e\text{-}3$, $x = 4e\text{-}3$, $x = 5e\text{-}3$, $x = 8e\text{-}3$, $x = 1e\text{-}2$, $x = 2e\text{-}2$, $x = 3e\text{-}2$, $x = 5e\text{-}2$.
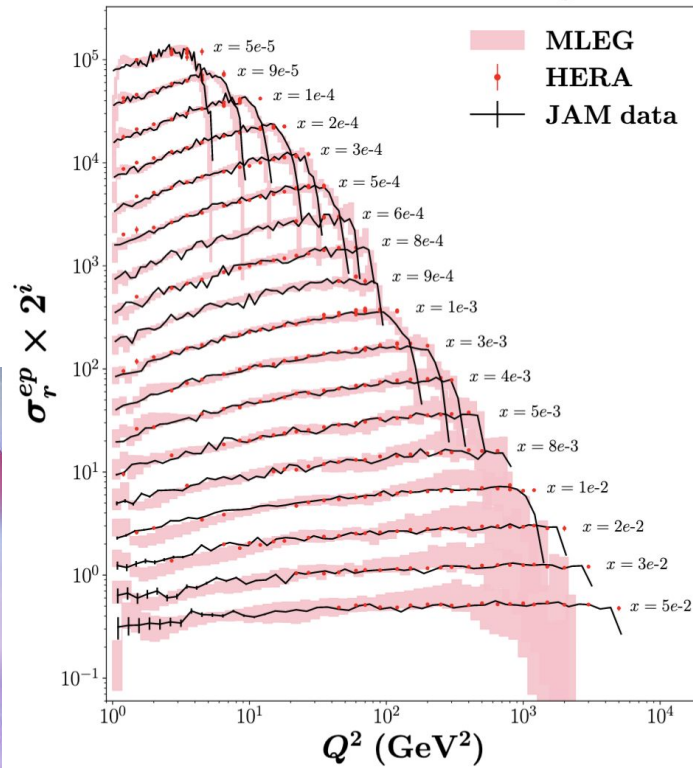
Future: GAN+theory

Optimize physics parameters

Summary/Outlook

- Even-level interpolators can be constructed using generative models

- Discriminators have the unique feature to compare data at the event-level

- ML unifies theory and experiment by solving inverse problems in hadronic physics at the event-level

Detector Unfolding

$$\mathcal{L}_{\mathrm{QCD}} = \sum_q \overline{\psi}_q (i\gamma_\mu D^\mu - m_q)\psi_q - \frac{1}{2}\mathrm{Tr}[G_{\mu\nu}G^{\mu\nu}]$$