QCD analyses for phenomenological PDF determination with comprehensive uncertainties

Bridging Theory and Experiment at the Electron-Ion Collider

BNL-INT Workshop @INT

06/02/25

Aurore Courtoy

Instituto de Física

National Autonomous University of Mexico (UNAM)

In collaboration with CTEQ-TEA collab.,
Fantômas team, and students.

Instituto de Física UNAM

Dirección General de Asuntos del Personal Académico

CTEQ

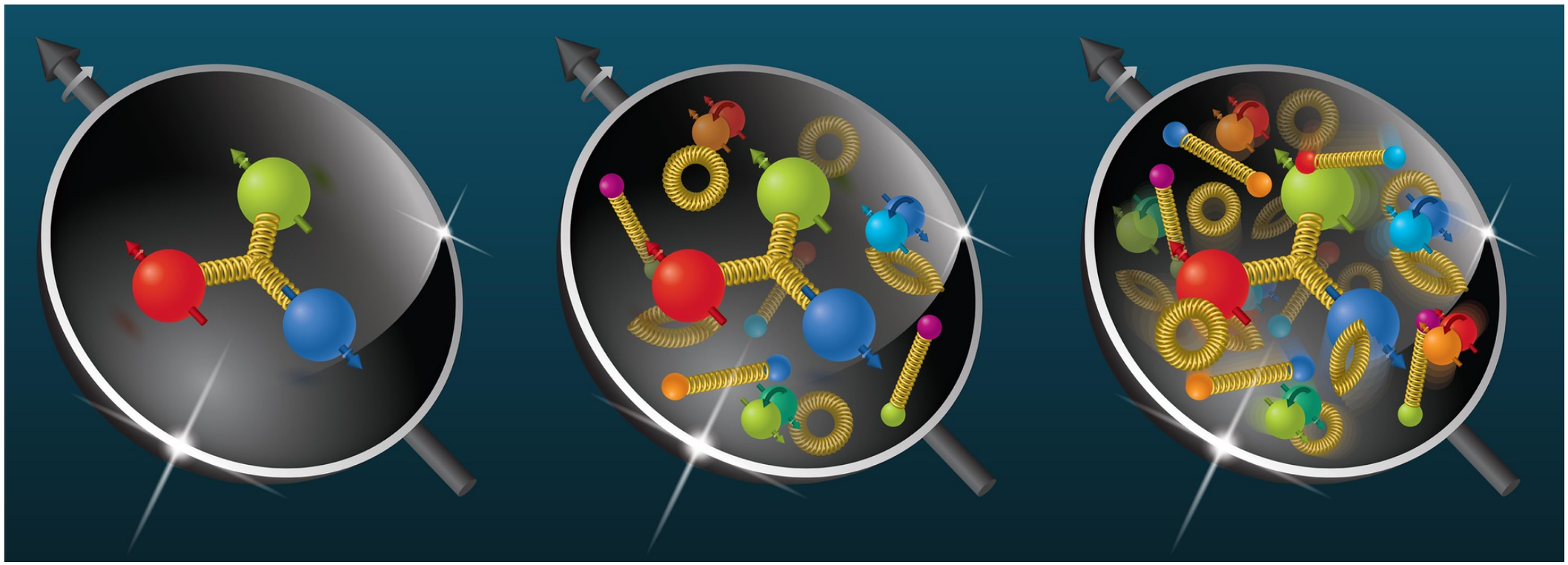
CTEQ (Wu-Ki Tung Et Al.) group

From low to high energies

PDF determination is twofold:

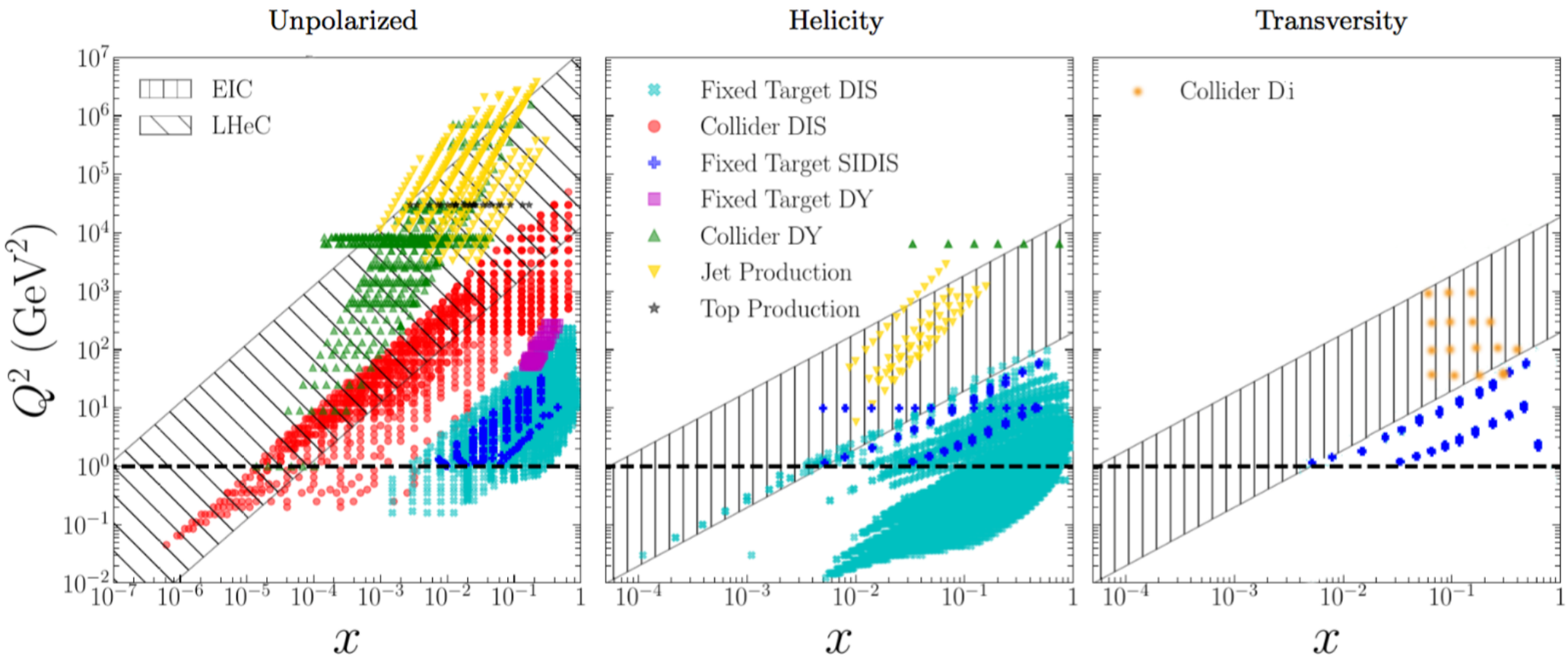
- learned from data — knowledge on low-energy dynamics and pQCD expansion
- used for precision physics at higher energies

The EIC may contribute to learning unpolarized PDFs — paradigm for this talk.



Kinematical coverage for collinear PDFs

A bit outdated…



[Prog.Part.Nucl.Phys.121]

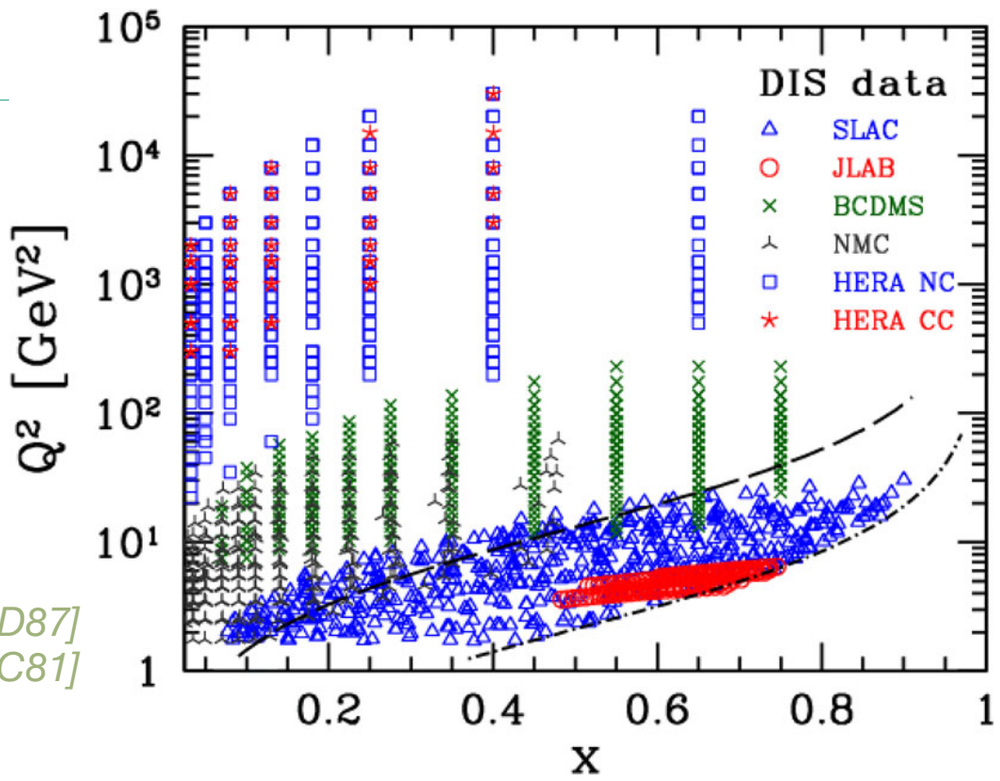
Extrapolation regions for unpolarized PDFs

- very small x — $x < 10^{-6}$.
- large x: $x \gtrsim 0.2$, includes the valence region.

Both regions involve physics *at the end-points* —non-perturbative and more effects.

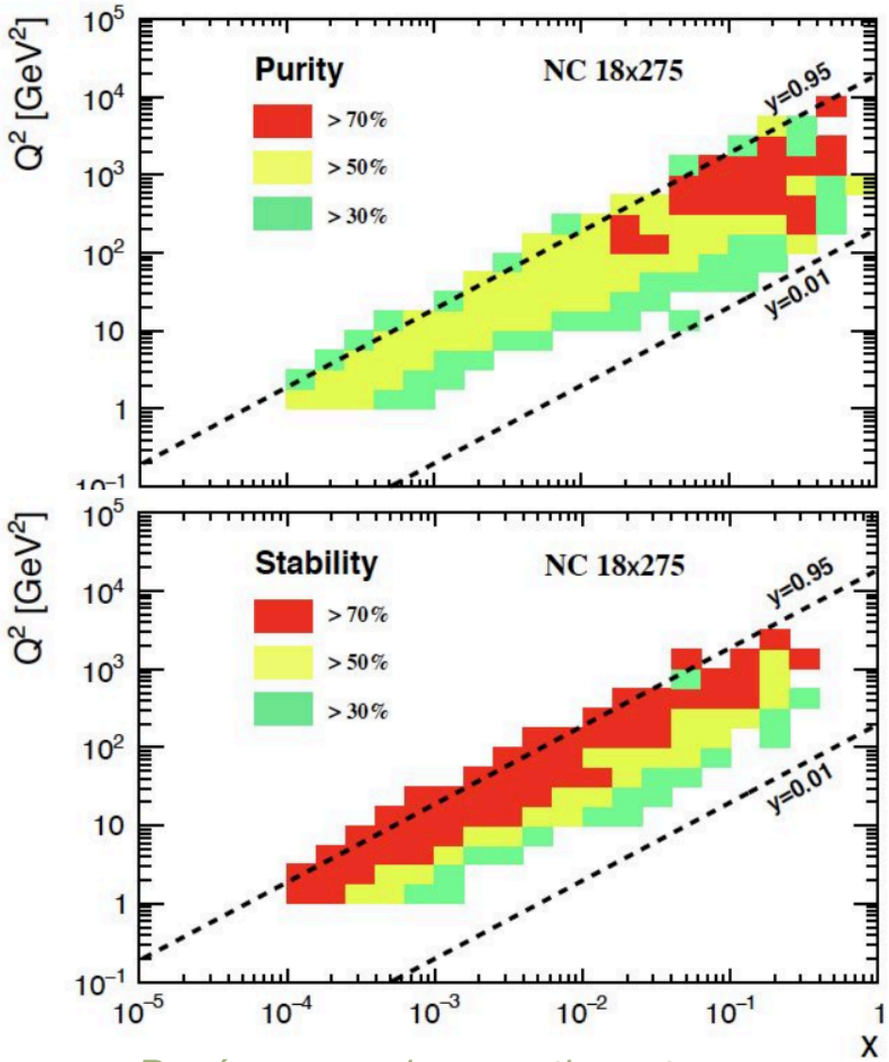
Kinematics for future experiments

Old kinematic coverage showing the impact of the W^2 cuts on data selection.

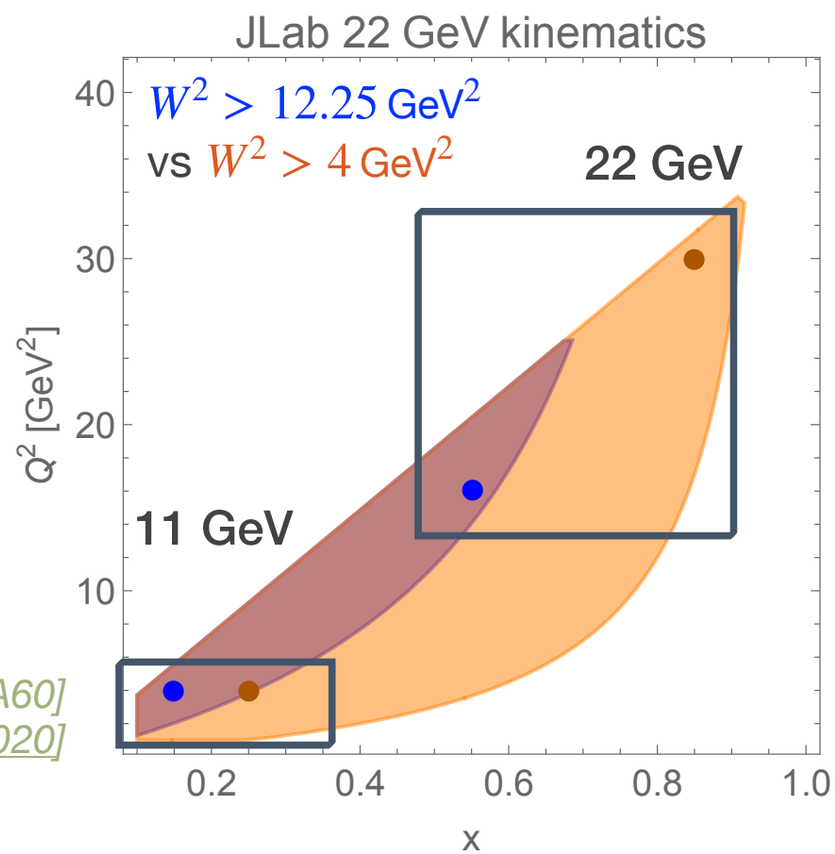


[Owens et al, PRD87]
[Accardi et al, EPJC81]

EIC



Renée, somewhere on the net
See Salvatore's talk this morning, too!



[Accardi et al, EPJA60]
[Ablat et al., 2408.04020]

Parton Distribution Functions as an inverse problem

Parton Distribution Functions: are determined from data through an inverse problem.

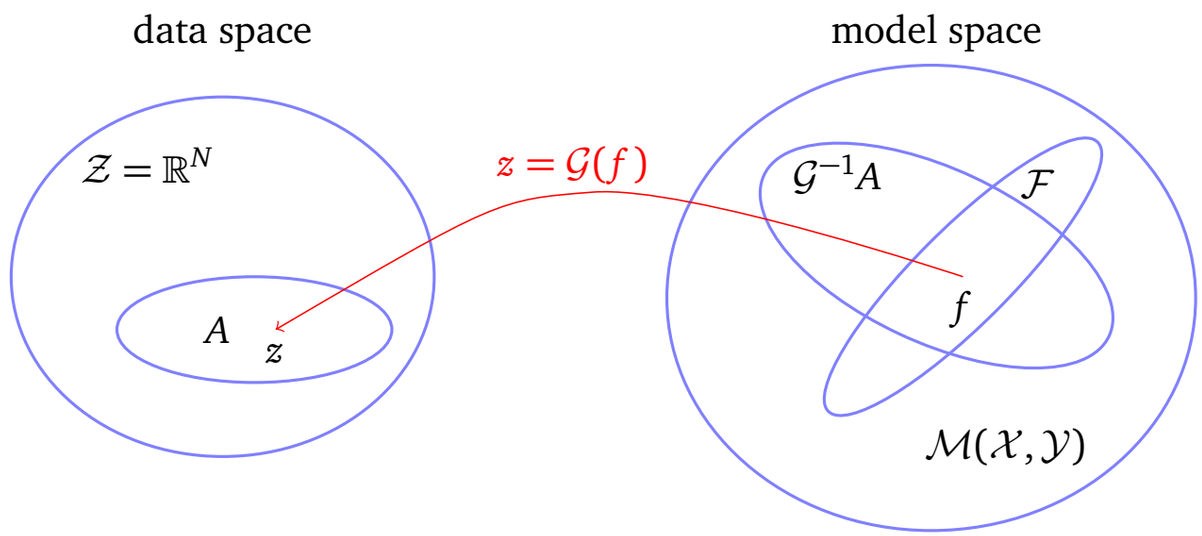


Image from: del Debbio, SciPost Phys. Proc. 15, 028 (2024)

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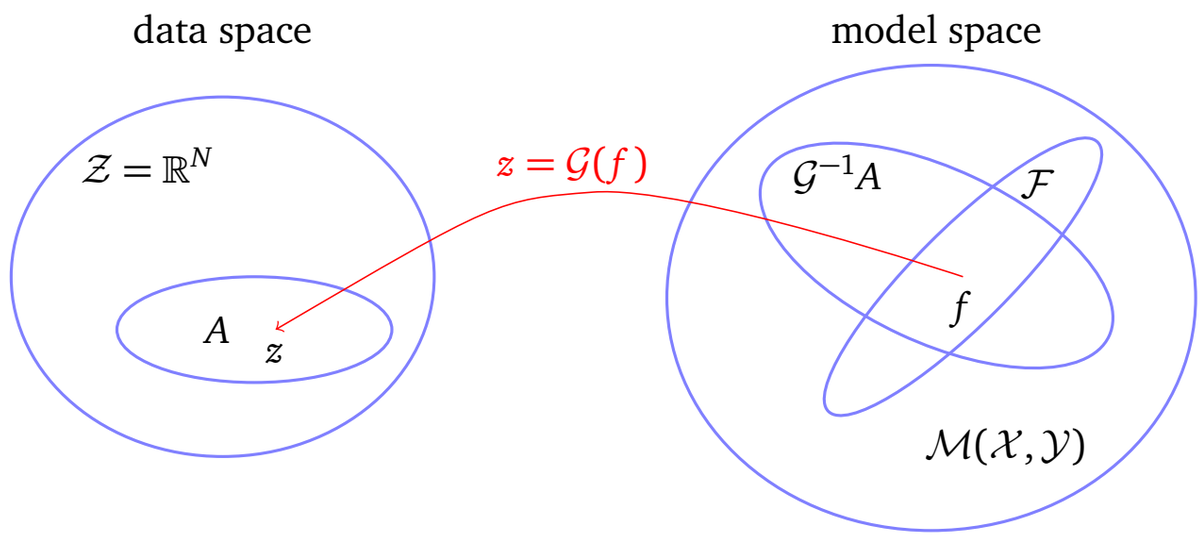

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Reasons for complexity of inverse problems

- direct products
- convolutional problems ← most common for PDF analyses
- Hausdorff moment problem

Ill-posed problem that accepts no unique solution:
determining PDFs will involve defining a set of solutions.

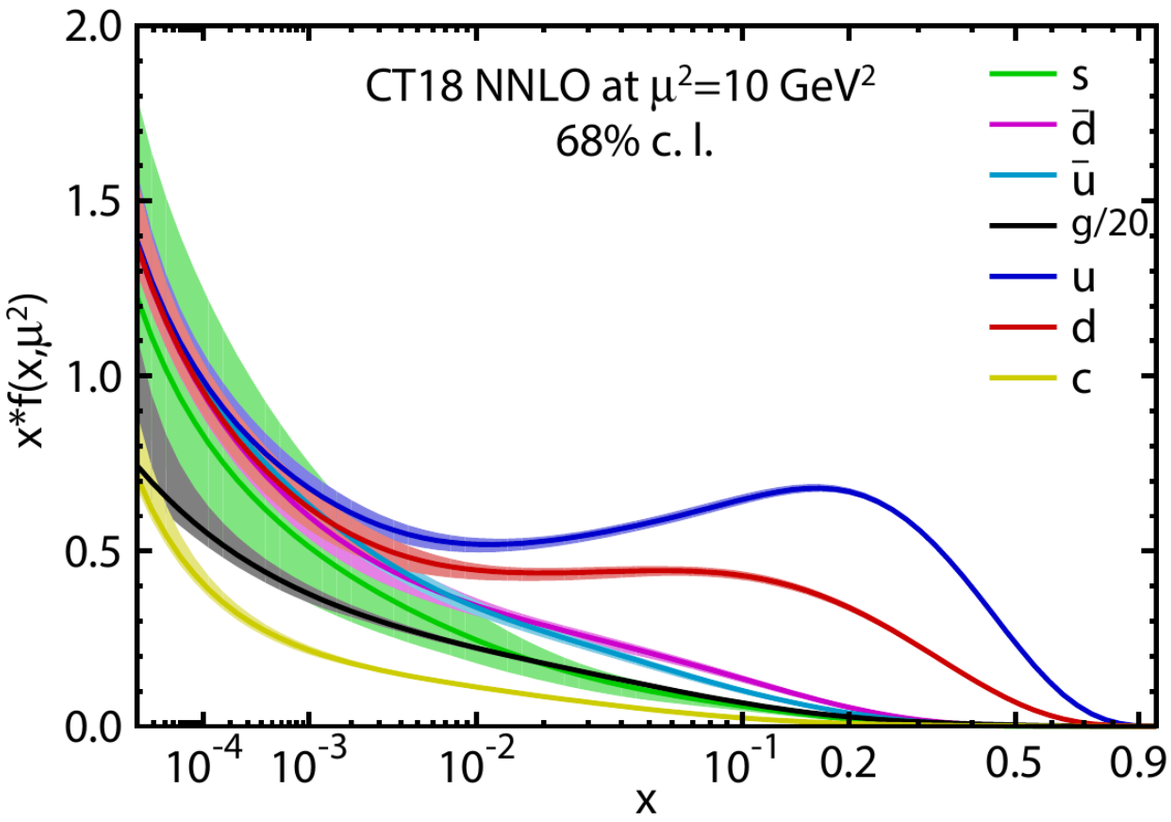
CT18 unpolarized PDFs

CTEQ (Wu-Ki Tung Et Al.) group

CT18NNLO is the general-purpose PDF set published in 2019.

CT methodology is based on minimizing a χ^2 expressed in terms of *parametrizations* for the PDFs, finding the global minimum, and providing Hessian error PDFs to estimate the uncertainty.

CT25 in the making — stay tuned!



[Hou et al, Phys.Rev.D 103 (2021)]

Uncertainty Quantification in CT involves a two-tier analysis

Fixed tolerance criterion T^2 — beyond the $\Delta\chi^2 = 1$ prescription
Experiment-based penalty

} encompasses both the propagation of experimental and methodological uncertainties

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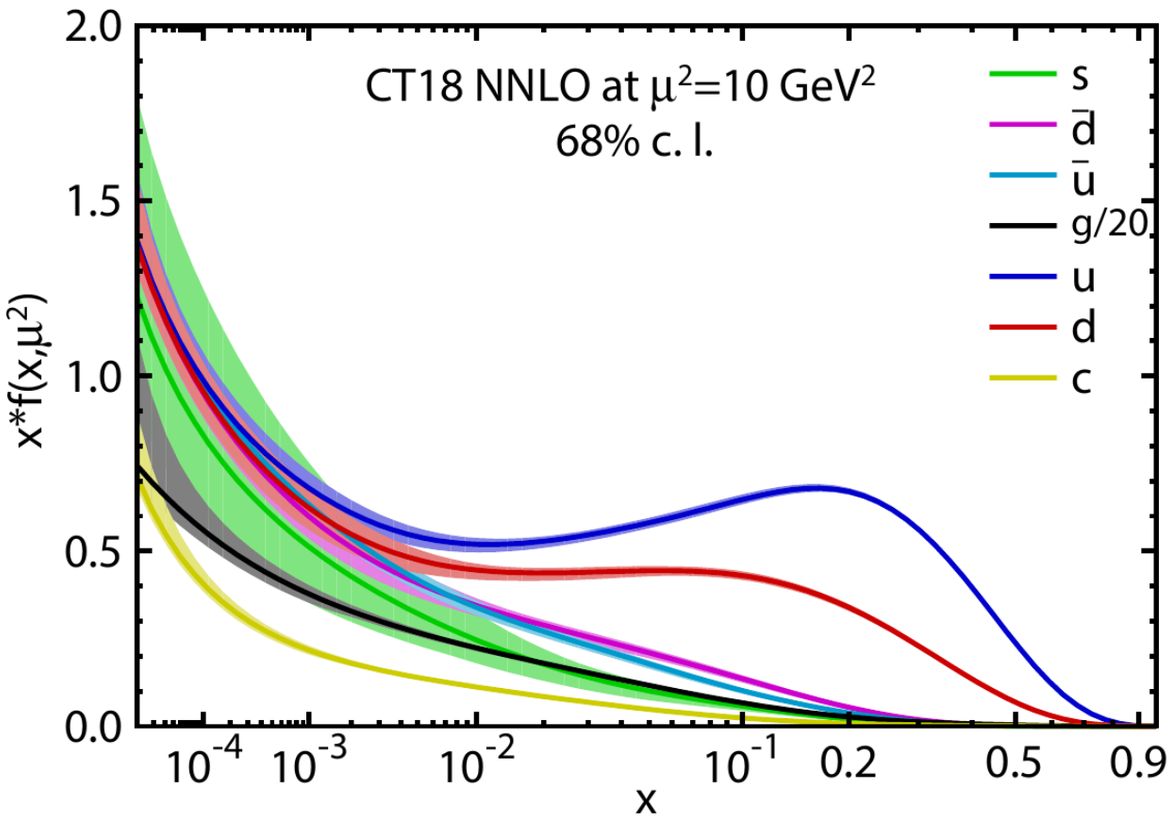

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UQ glossary

- **aleatoric**/statistical uncertainties — fixed once for all
- **epistemic**/systematic uncertainties — *e.g.* from methodology, can be reduced

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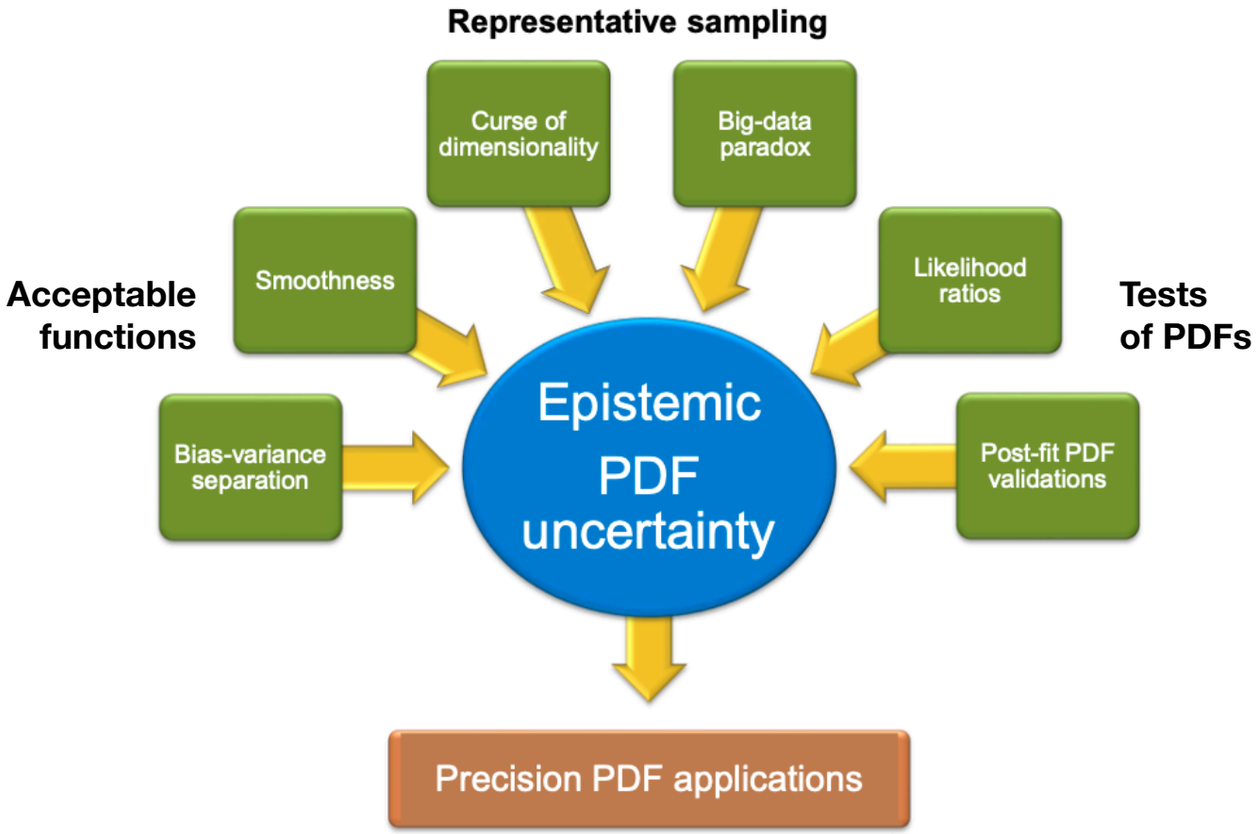
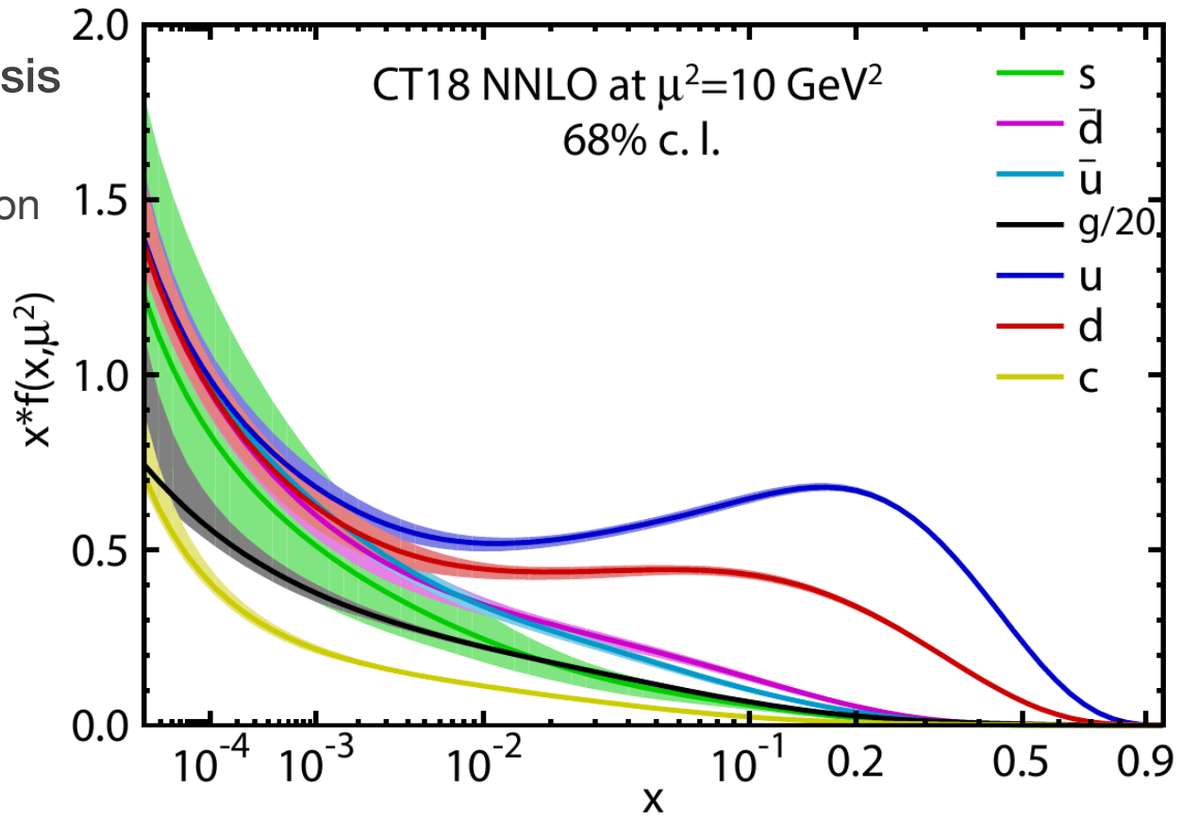




[Hou et al, Phys.Rev.D 103 (2021)]

Epistemic uncertainty is central to the CT fitting's philosophy.

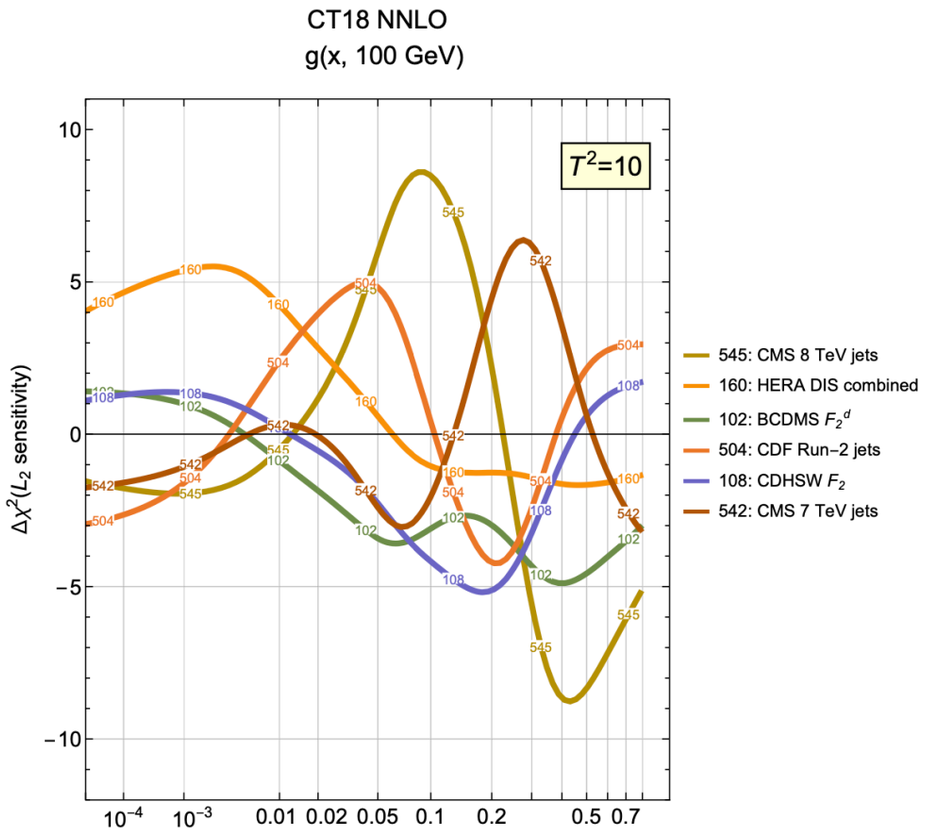
Tools to explore and understand the spread of uncertainties in PDF analyses

- The Hessian formalism allows for unique tools to visualize pulls from various experiments.

[Wang et al, PRD98]
[Hobbs et al., PRD100]

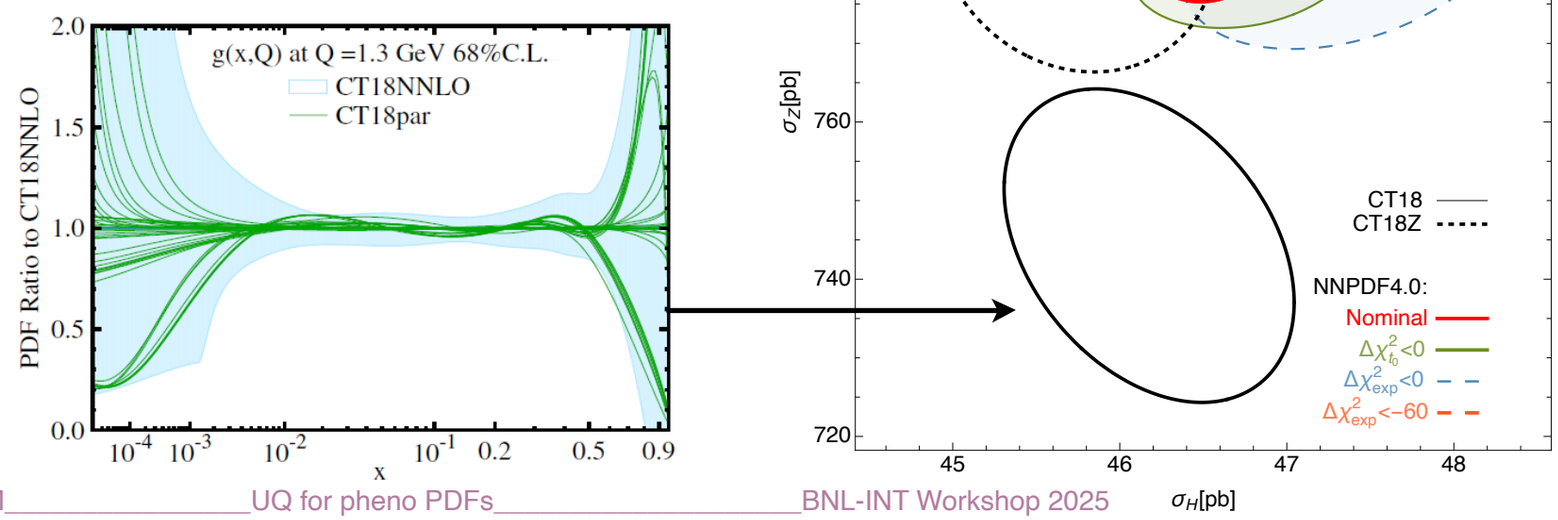
Comparative analysis for ATLASpdfs, CT18 and MSHT20 (+aN3LO)

[Jing et al., PRD108]



- The CT formalism also allows to explore the space of PDF solutions and **reliably estimate PDF uncertainties.**

[Courtoy et al, PRD107]



Parametrizations to tackle inverse problems

Two main approaches to parametrization in global analyses:

I. use an explicit functional form — 20-50 parameters ← e.g., CT
II. use neural networks —20-50 hyperparameters ← e.g., NNPDF

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The rôle of parametrization form in global analyses can be quantified

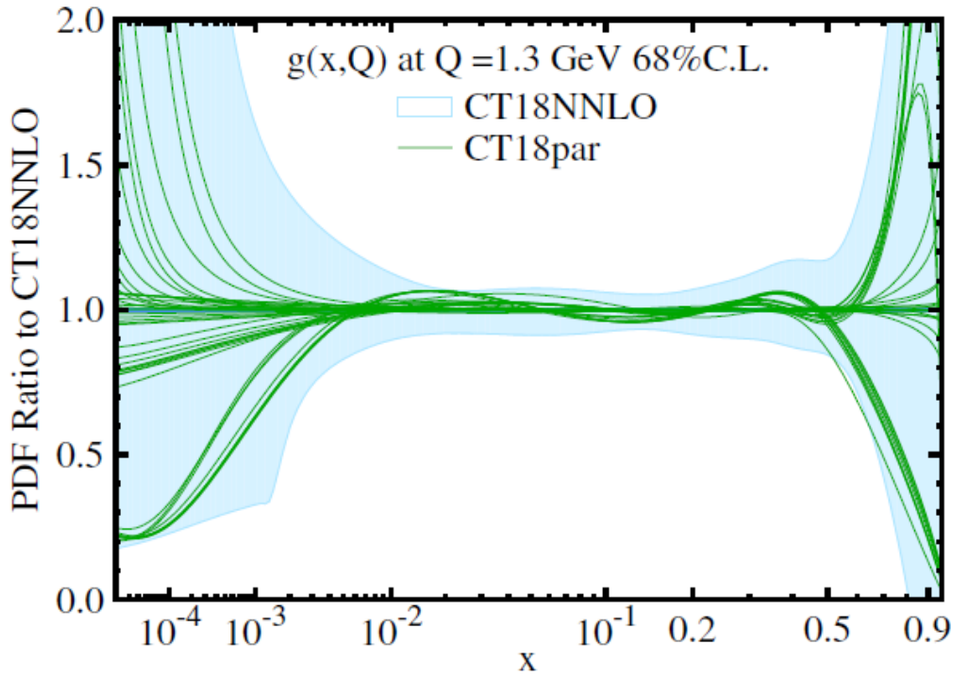
Fantômas4QCD

A new `c++` code automates series of fits using multiple functional forms, called `metamorph`.

Just like *neural networks*,
these polynomial functional forms can approximate any arbitrary PDF shape.

[Kotz, AC, Nadolsky, Olness, Ponce-Chavez, PRD109]
[Kotz, AC, Nadolsky, Ponce-Chavez, 2505.13594]
[Kotz, AC, Hobbs, Nadolsky, Olness, Ponce-Chavez, Purohit, in progress]

Tolerance and parametrization studies



Uncertainty band reproduced, in part, by the spread of possible solutions

→ epistemic uncertainty
→ builds the $T^2 = \Delta\chi^2 > 1$ criterion

We (CT) are looking into information criteria to quantify the tolerance encompassing multiple sources of uncertainties.

Fantômas unlocks the concept of tolerance:

- multiple parametrizations with respective $\Delta\chi^2 = 1$ uncertainty can be bundled into a $\Delta\chi^2 > 1$ error band.
- separation of constraints'contributions

Regression for data-based analyses

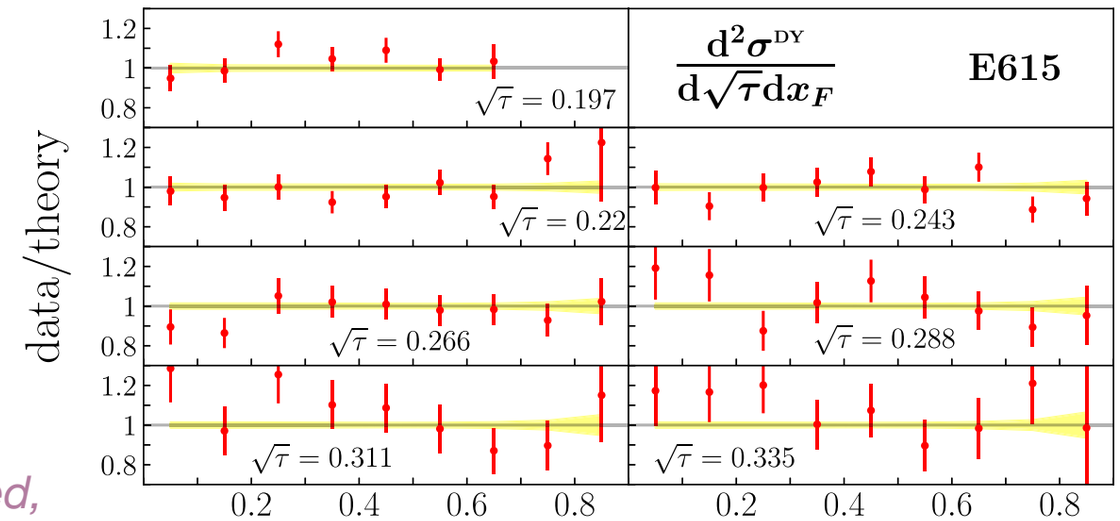
Global analyses involve searching for extrema of a (log-)likelihood function. *[JAM21]*

(Very) simplified:

$$\chi^2 = \sum_i^{N_{\rm exp}} \frac{\left(D_i - \langle T(\{\mathbf{x},\mathbf{a}\})\rangle_i\right)^2}{\sigma_i^2} + \text{penalty terms}$$

discrete data point

*theory prediction averaged, as a function of the variables {**x**} and free parameters {**a**}*



The theory input depends on the PDFs, whose parametrization is an input to the minimization procedure. The comparison to data for various parametrizations can lead to equally good χ^2 values.

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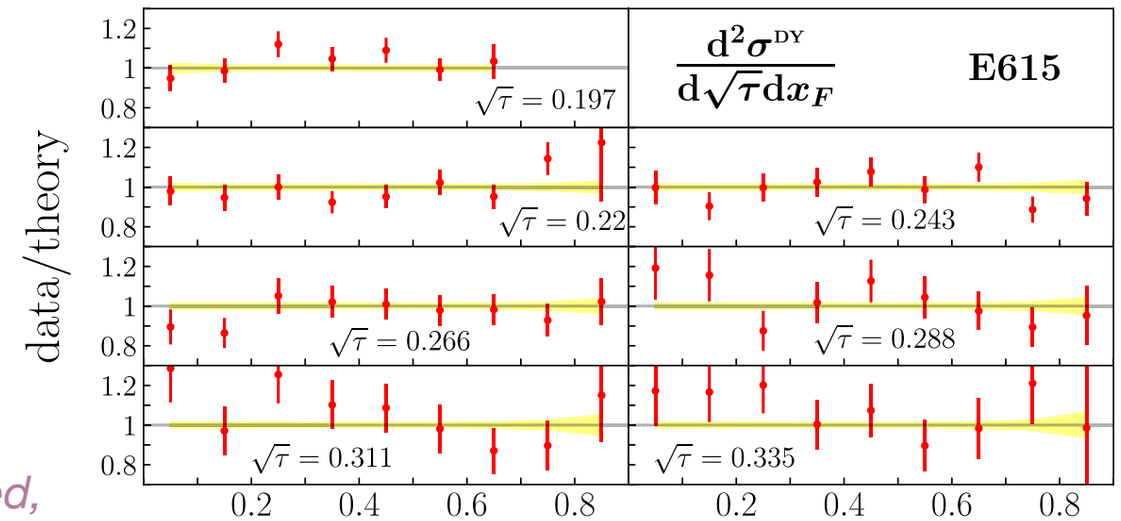

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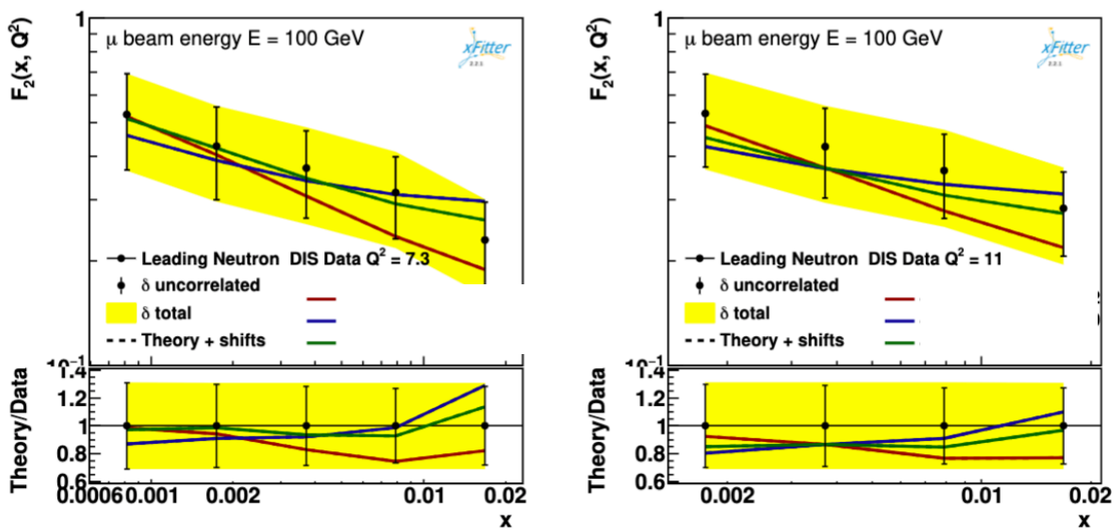
That's fine in the data region,
but the results may vary greatly outside
— extrapolation region.

Why not adopt more than one form?



Generation of parametrizations

`metamorph` is based on Bézier curves — polynomial on a Bernstein basis

$$\mathcal{B}^{(n)}(x) = \sum_{l=0}^{n} c_l \; B_{n,l}(x)$$

$$B_{n,l}(x) \equiv \binom{n}{l} x^l (1-x)^{n-l}$$

The Bézier curve can be expressed as a product of matrices:

$$\mathcal{B} = \underline{T} \cdot \underline{\underline{M}} \cdot \underline{C}$$

vector of coefficients c_l

vector of x^l

matrix of binomial coefficients

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vector of x^l matrix of binomial coefficients

Bézier curve characterized by **control points**, vector of $\mathcal{B} \to \underline{P}$:

$$\underline{P} = \underline{T} \cdot \underline{\underline{M}} \cdot \underline{C}$$

matrix of x^l at $\{x_{\rm CP}\}$

[AC & Nadolsky, PRD103]

[Kotz, et al. PRD109]

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$\underline{\underline{T}}$: matrix of x^l at $\{x_{\rm CP}\}$

[AC & Nadolsky, PRD103]

[Kotz, et al. PRD109]

PDF shape:

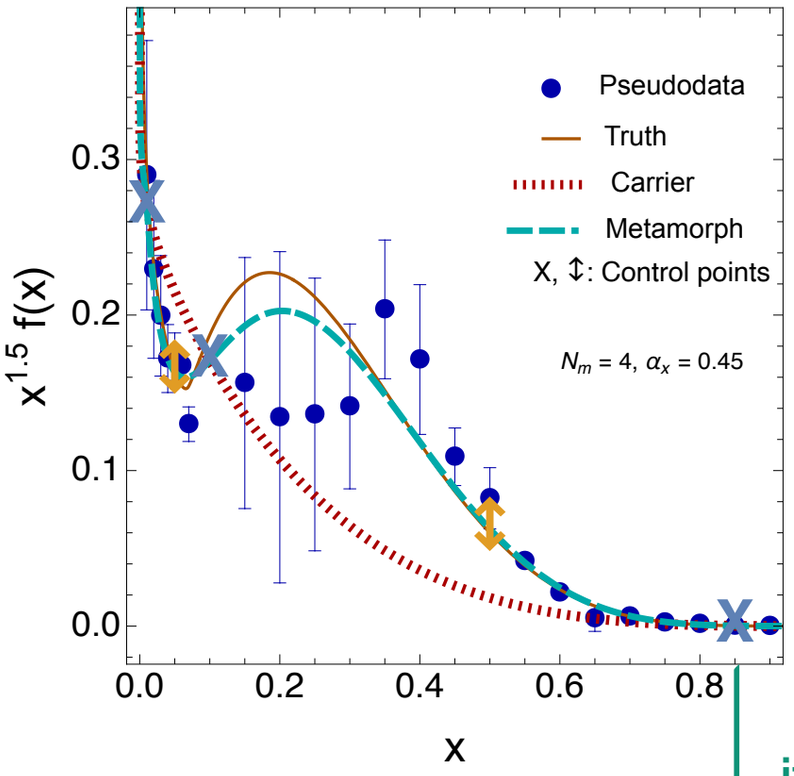
⟹ asymptotics usually ensured by a *carrier function*

⟹ sum rules imposed through normalization

for q = PDF type (flavor, combination or gluon)

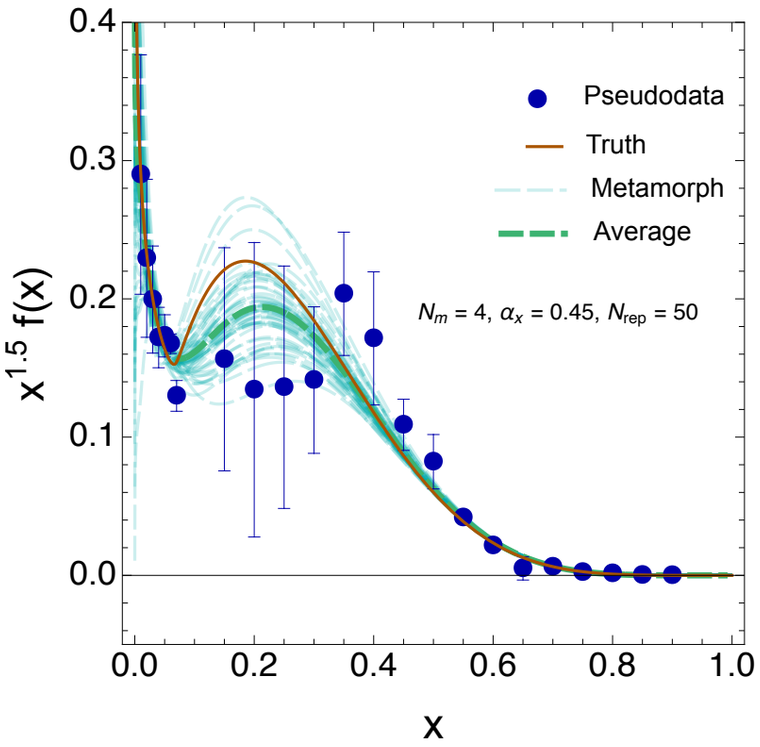
$$x\,q(x,Q_0^2) = \underline{A'_q}\; x^{B_q}(1-x)^{C_q} \times \left(1 + \mathcal{B}^{(N_m)}(x^{\alpha_x}, Q_0^2; \underline{v})\right)$$

Bézier-curve methodology— toy model



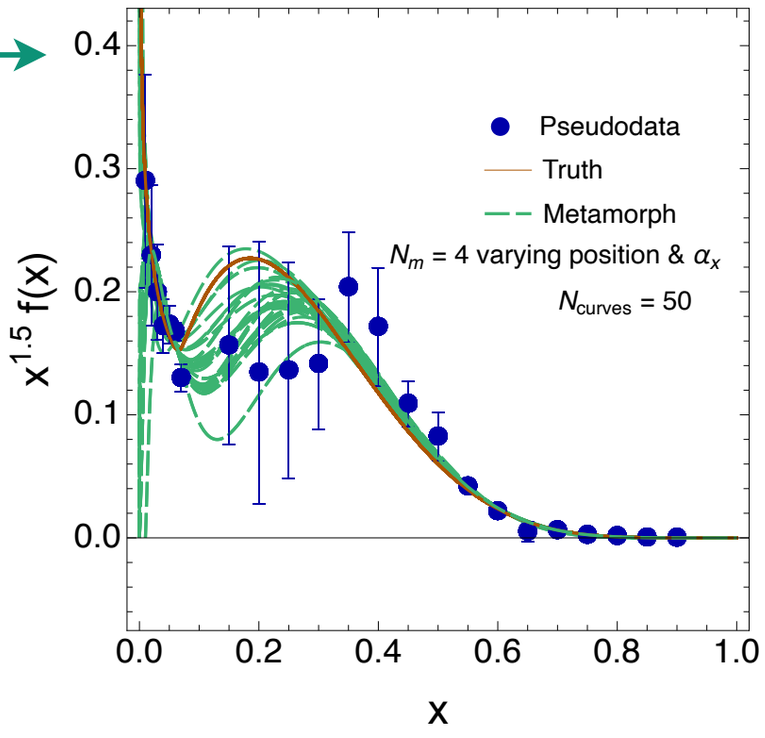
if bootstrapped

sampling on the distribution of data uncertainties



if sampled over `metamorph` settings

sampling over parametrizations



Main idea behind Fantômas4QCD:

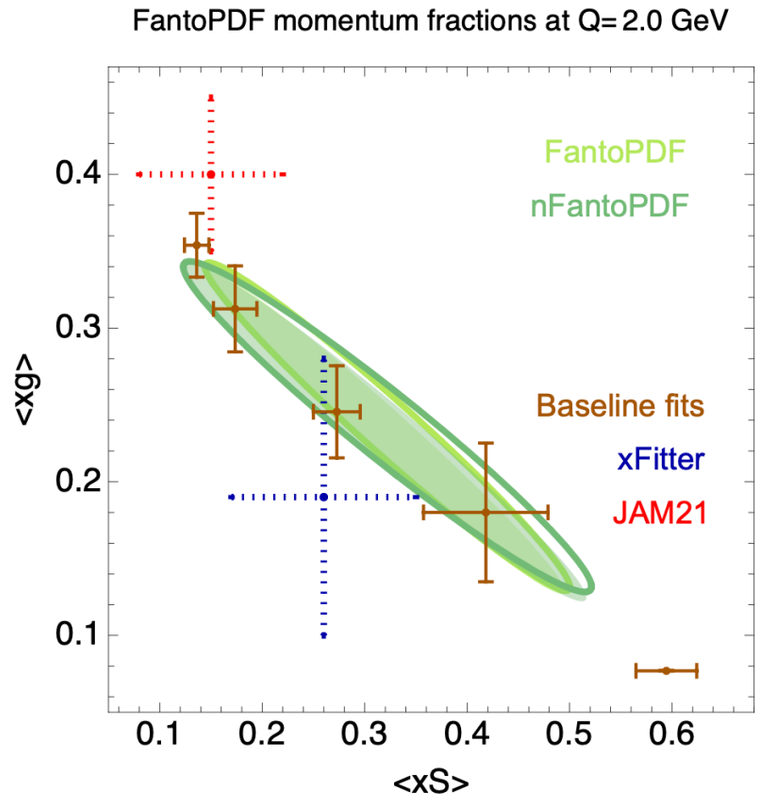
to facilitate unbiased estimates of parametrization dependence.

Sandbox studies

….with awesome physics!

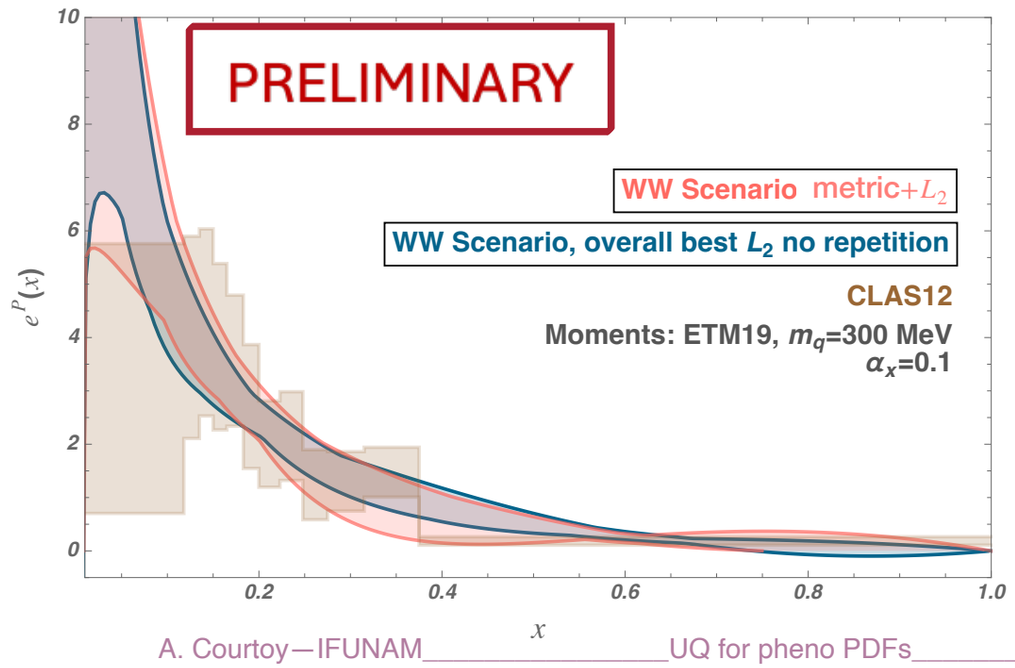
Small(er) scale problems to develop and test the methodology, and learn more physics

- pion PDFs: Fantoπ PDFs — including model combination and UQ from nPDFs
  - **now released**: *Fantômas1.0 PDFs* — soon on LHAPDF
  - **developping**: beta-testing the code for release
  - **developping**: information-ish criteria for model selection



[Kotz, et al., 2505.13594]

- twist-3 collinear PDF — integral constraints and interpolation
  - **developping**: information-ish criteria for model selection



[E. López-Rosa. et al, in progress]

Classification of solutions

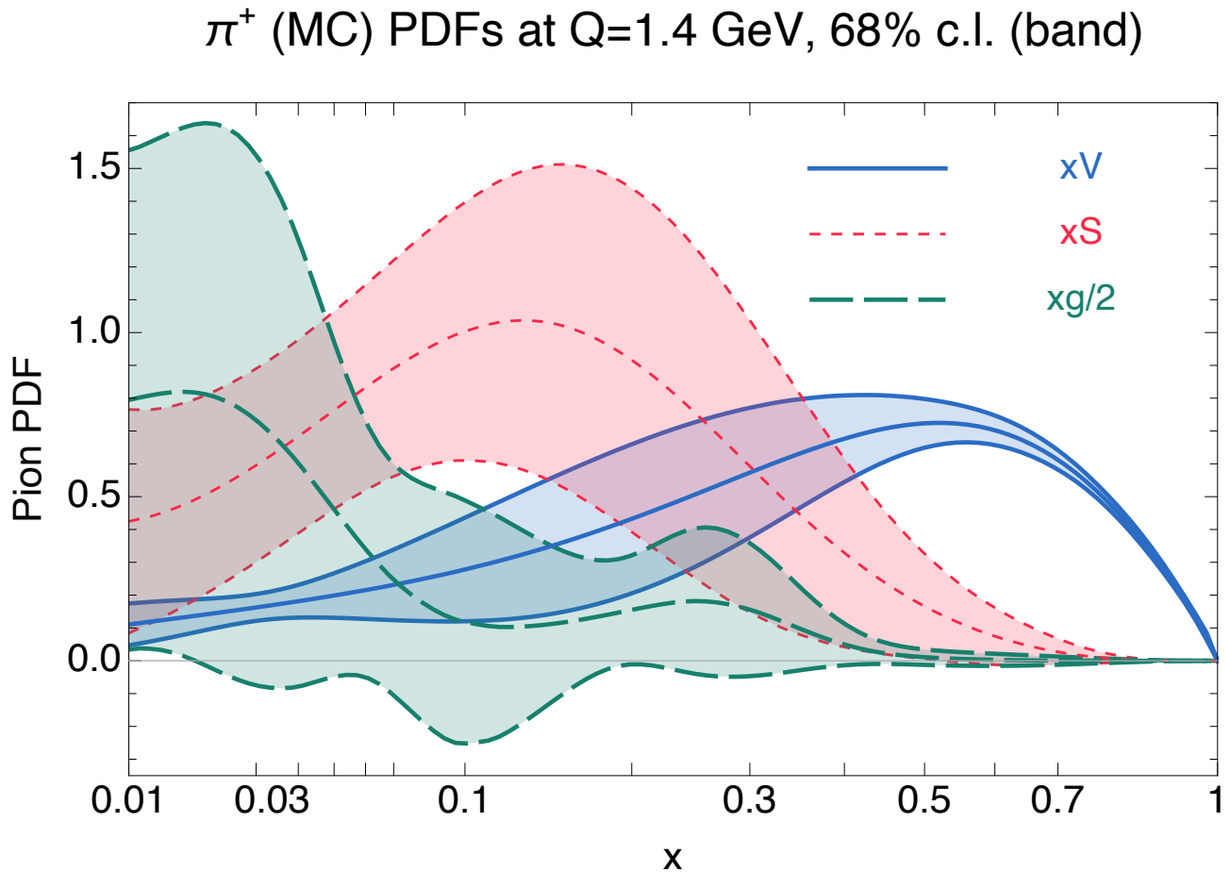
Fantômas πPDFs

⇨ We generated $N \sim 100$ fits corresponding to N sets for $\{N_m, \underline{P}, \alpha_x\}$.

⇨ Well-behaved (convergence + fixed soft constraints) fits are kept.

⇨ Fits within $\chi^2 + \delta\chi^2 = \chi^2 + \sqrt{2(N_{\rm pts} - N_{\rm par})}$ are kept.

The final bundle is generated from the 5 most diverse shapes at Q_0.



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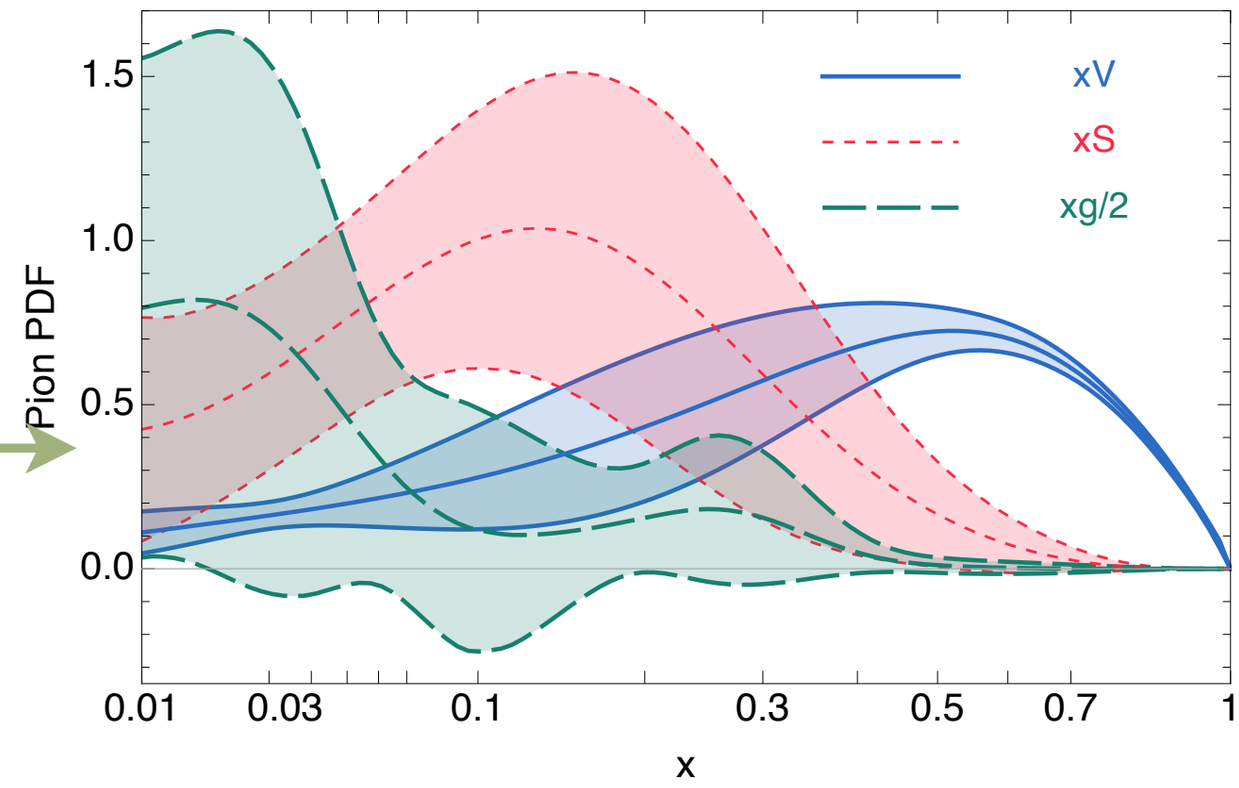
$\tilde{N} = 5$ exchangeable final independent solutions, from which we generate identically distributed MC distributions

— they can be interpreted as being drawn from a common distribution, characterized by a latent parameter θ.

π^+ (MC) PDFs at Q=1.4 GeV, 68% c.l. (band)



Statistical justification of our model combination by de Finetti's theorem.

Likelihood-ratio test

Independent contributions to uncertainty:
the parametrization contributes to the (log)-likelihood but constraints on the parameters, …, contribute to the prior.

$$\chi^2_{\rm tot} = \chi^2 + \chi^2_{\rm prior}$$

$$P(a|D) \propto P(D|a)\, P(a)$$

$$\Leftrightarrow \quad \exp(-\chi^2_{\rm tot}) \propto \exp(-\chi^2)\exp(-\chi^2_{\rm prior})$$

On which basis are PDFs accepted or rejected?

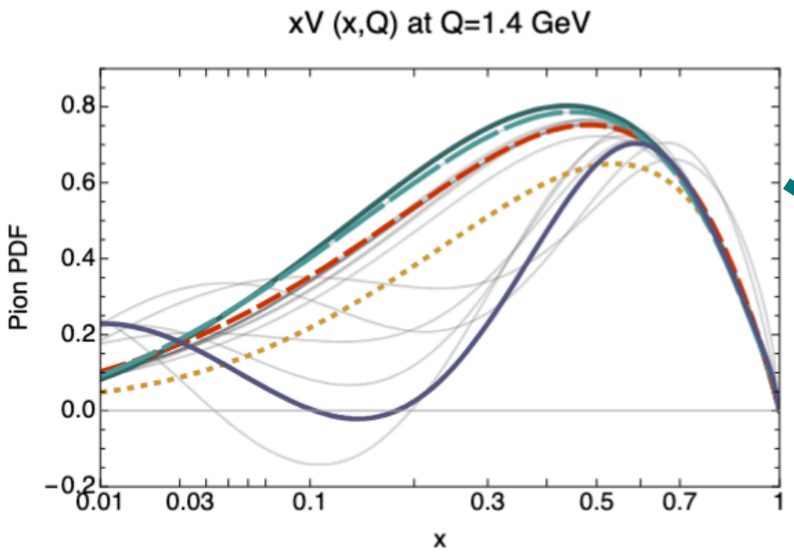
Likelihood ratios:
two replicas can be ordered according to their relative likelihood or relative prior.

$$\frac{P(T_2|D)}{P(T_1|D)} = \frac{P(D|T_2)}{P(D|T_1)} \times \frac{P(T_2)}{P(T_1)}$$

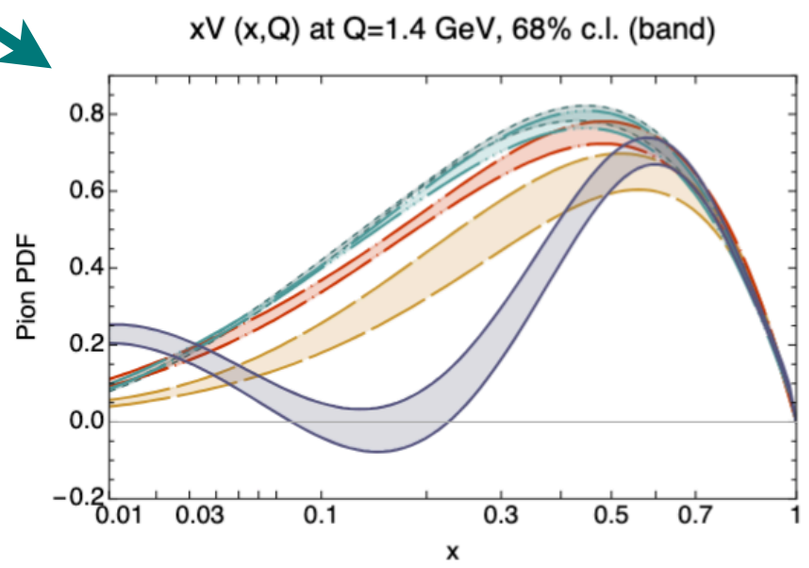
$$\equiv r_{\rm posterior} \qquad \equiv r_{\rm likelihood} \qquad \equiv r_{\rm prior}$$

aleatory — epistemic + aleatory — probabilities

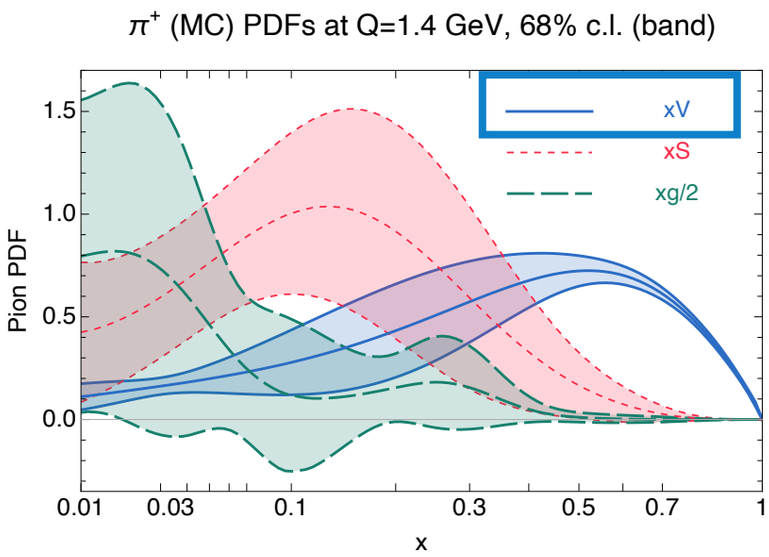
Model combination



$\Delta\chi^2 = 1$ criterion



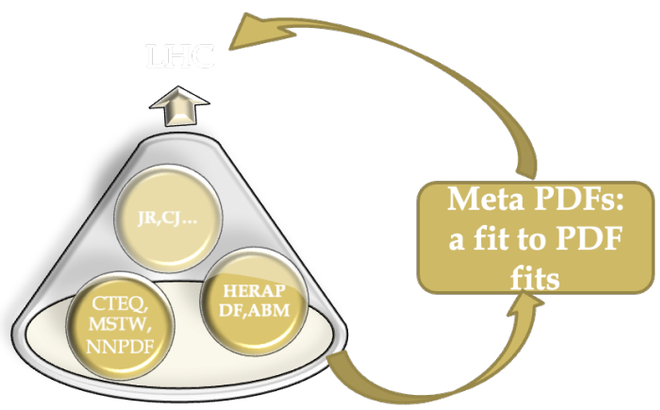
Bundled models



For π^+ PDFs,
$q = V = 2(u - \bar{u})$,

Models combined using METAPDF

Update of the `mp4lhc` and `mcgen` codes in the context of Fantômas
[Kotz et al, very soon]

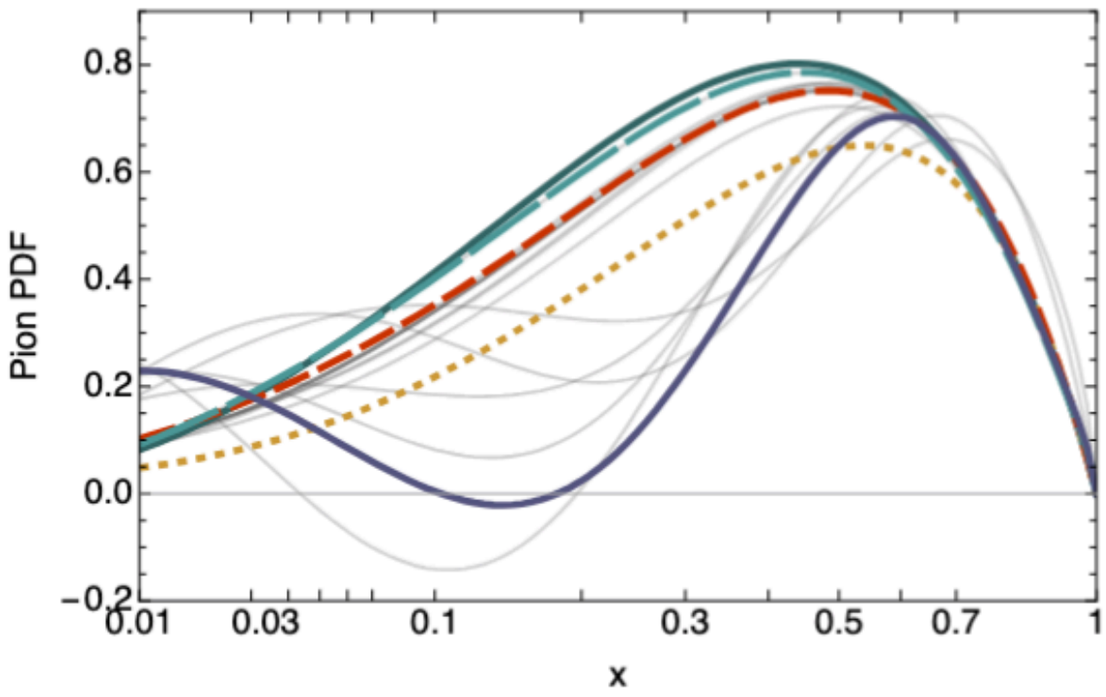


[Gao & Nadolsky, JHEP07]

Criterion for shape selection

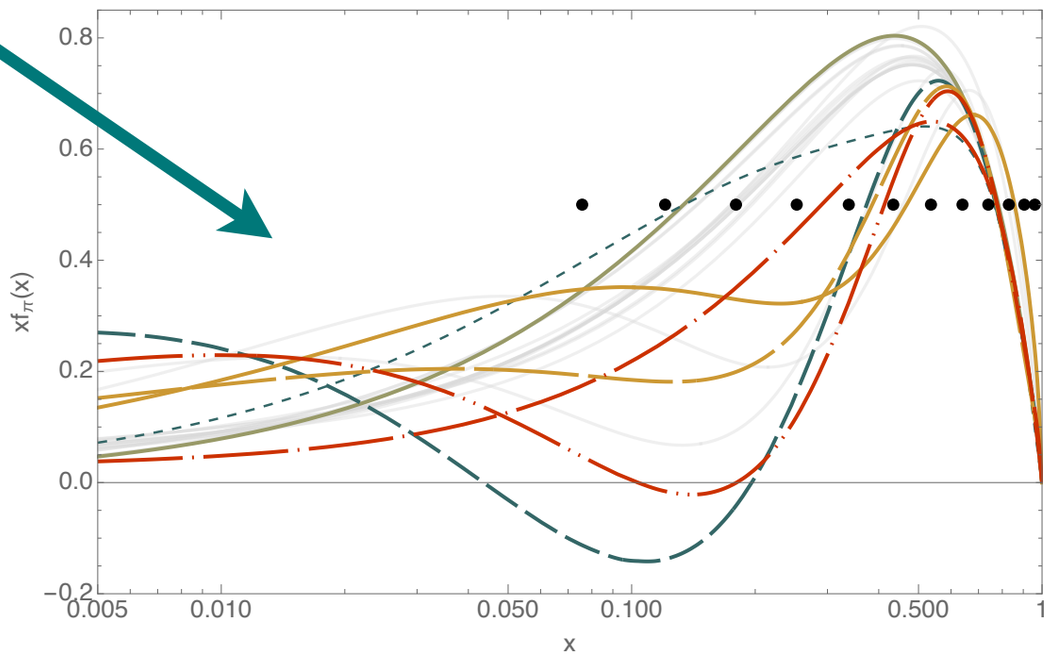
So far, we've used an ad hoc criterion for the selection of the most diverse shapes.

In progress: automatize the selection based on shapes and use of information criteria — likelihood-ratio test and quantititative criteria



Published Fantoπ PDFs

Preliminary one-flavor selection of the Fantoπ solutions based on information criteria



[UNAM's group— AC, A. Vargas-Rosas]

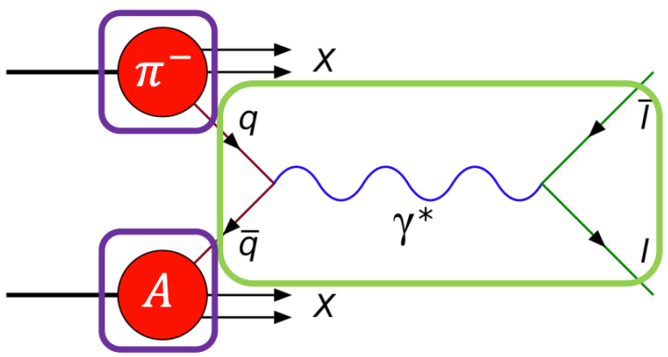
Third-party uncertainty propagation

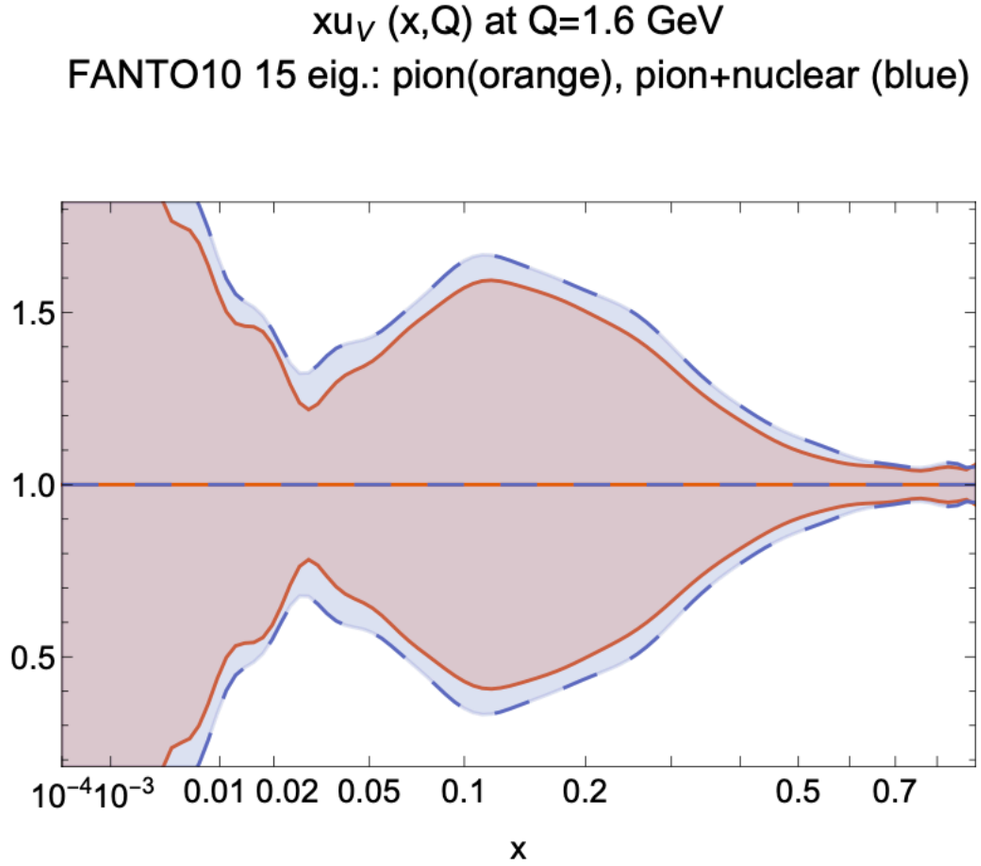
For processes with more than one unknown function:

SIDIS — fragmentation and PDF
Drell-Yan — PDF and nuclear PDF
…

Prescription to propagate the uncertainty for Hessian-based input. It uses mcgen, model combination and selection criteria.

Here:
nCTEQ15 nuclear uncertainties on DY is propagated.
Small effect.

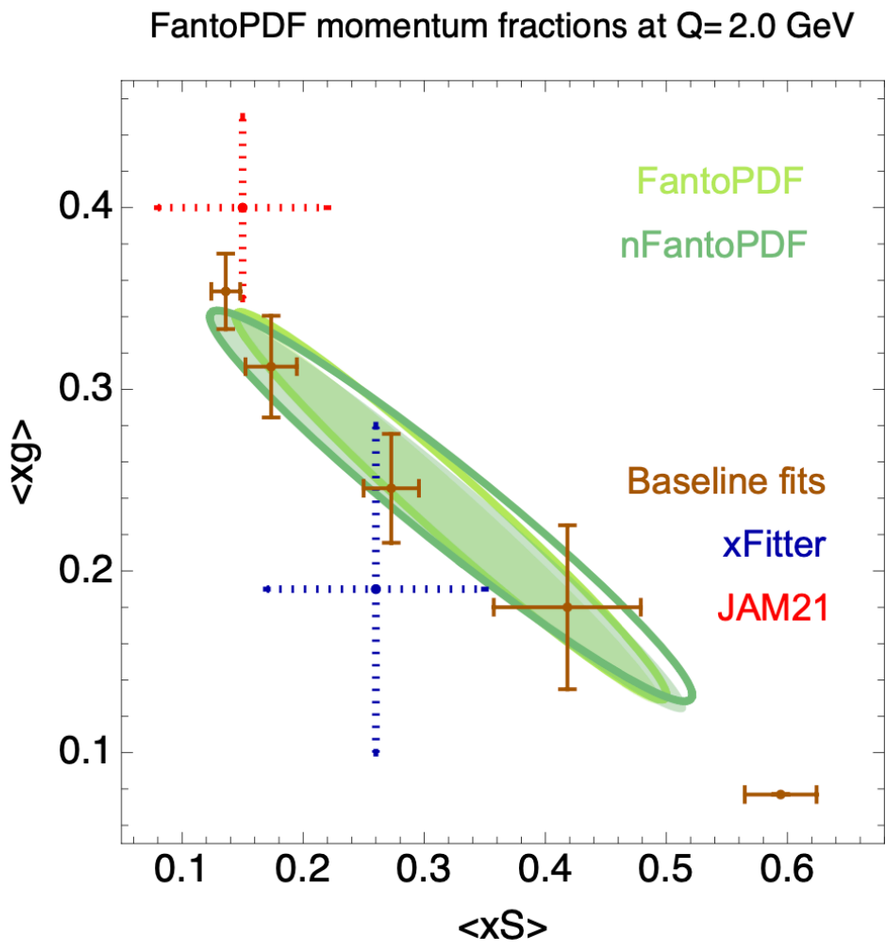


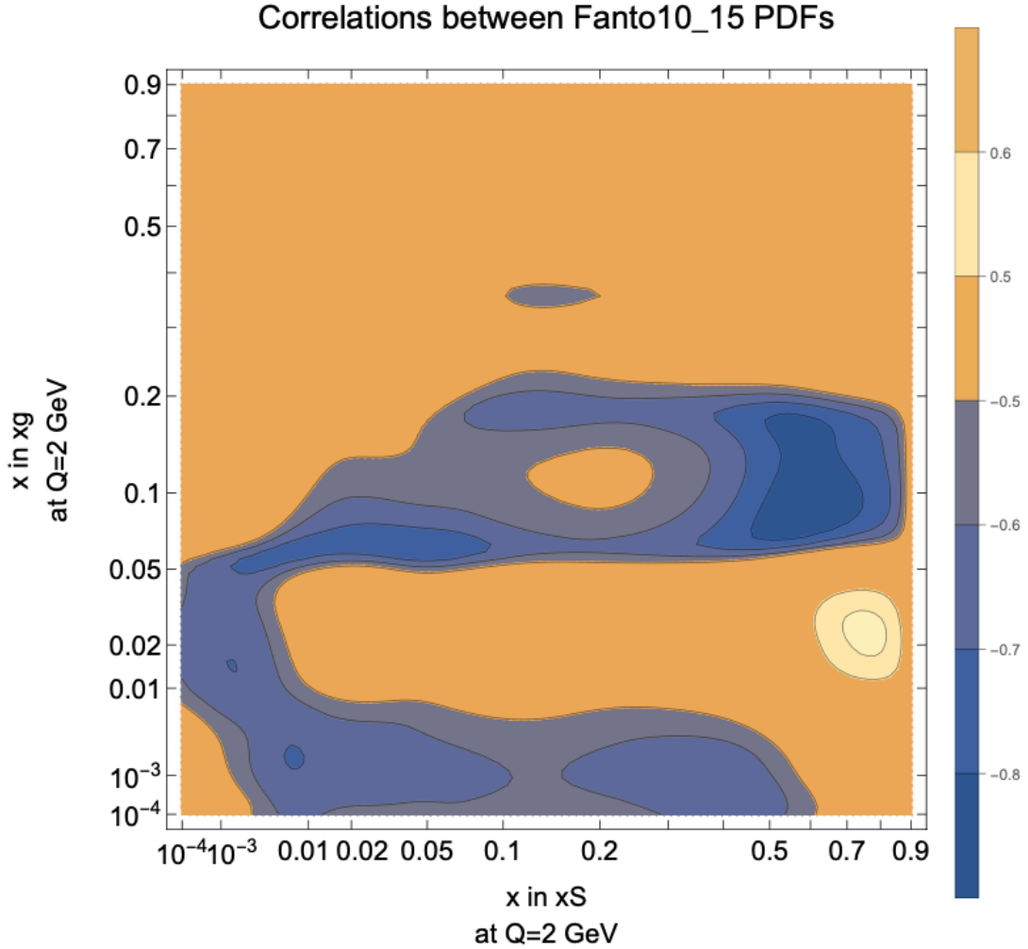


[Kotz, et al., 2505.13594]

Pion momentum fractions

[Kotz, et al., 2505.13594]





"*Our selection of the*" data supports a zero-gluon solution, while it has a hard time finding solutions leading to higher gluon momentum fractions.

Data sets: Drell-Yan (~65%) + prompt-photon (~25%) and leading-neutron DIS (~10%) — entanglement/ anticorrelation between sea and gluon distributions. Differs from JAM's pool.

Moments from the lattice

Name	Q[GeV]	$\langle x(u+\bar{u})_{\pi^+}\rangle$	$\langle xg\rangle$
FantoPDF	2	0.331(25)	0.24(10)
HadStruct [19]	2	0.2541(33)	–
[Gao et al., PRD102]	3.2	0.216(19)(8)	–
ETM [46]	2	0.261(3)(6)	–
ETM [91]	2	$0.601(28)\vert_{u+d}$	0.52(11)
[Meyer et al., PRD77]	2	–	0.37(8)(12)
[Shanahan et al., PRD99]	2	–	0.61(9)
[MSU, 2310.12034]	2	–	0.364(38)(36)
ZeRo Coll. [95]	2	0.245(15)	–
[Martinelli et al., PLB196]	7	0.02	–

Lattice can access either quarks or gluons
— only the recent ETM coll. results have both.

Variations in ensemble settings among lattice results.

[Kotz, et al., PRD109]

Name	Q [GeV]	$\langle xV\rangle$	$\langle xS\rangle$	$\langle xg\rangle$
FantoPDF (DY+γ+LN)	$\sqrt{1.9}$	0.49(8)	0.34(19)	0.18(12)
xFitter [9] (DY+γ)	$\sqrt{1.9}$	0.55(6)	0.26(15)	0.19(16)
xFitter w/o scale variation	$\sqrt{1.9}$	0.55(2)	0.26(9)	0.19(9)
JAM'18 [8] (DY)	1.27	0.60(1)	0.30(5)	0.10(5)
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JAM'21 [11] (DY+LN)	1.27	0.53(2)	0.14(4)	0.34(6)
CT18 NLO (proton)	$\sqrt{1.9}$	0.443(6)	0.160(10)	0.396(10)

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Variations in ensemble settings among lattice results.

Gluon momentum fraction varies greatly!

[Kotz, et al., PRD109]

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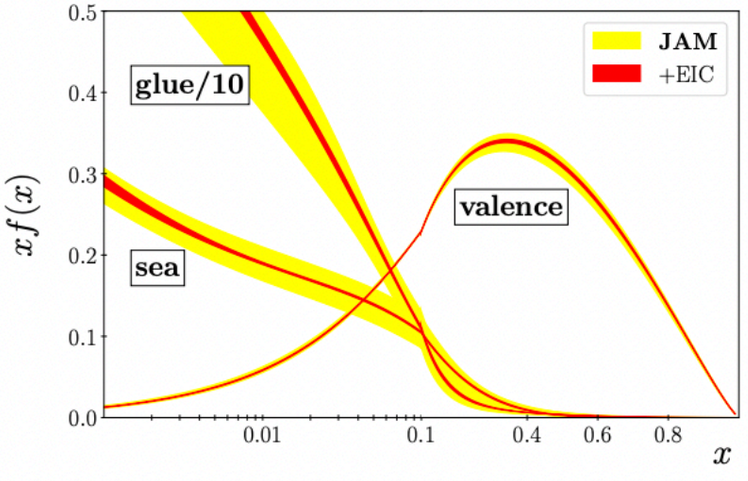
EIC: what is the gluon content of the pion?

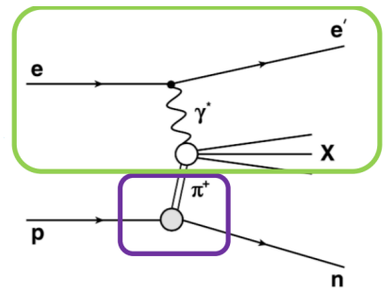
Yellow Report

Science Question	Key Measurement	Key Requirements
What are the quark and gluon energy contributions to the pion mass?	Pion structure function data over a range of x and Q^2.	• Need to uniquely determine $e+p \to e'+X+n$ (low $-t$) • CM energy range ∼10-100 GeV • Charged and neutral currents desirable
Is the pion full or empty of gluons as viewed at large Q^2?	Pion structure function data at large Q^2.	• CM energy ∼100 GeV • Inclusive and open-charm detection
What are the quark and gluon energy contributions to the kaon mass?	Kaon structure function data over a range of x and Q^2.	• Need to uniquely determine $e+p \to e'+X+\Lambda/\Sigma^0$ (low $-t$) • CM energy range ∼10-100 GeV
Are there more or less gluons in kaons than in pions as viewed at large Q^2?	Kaon structure function data at large Q^2.	• CM energy ∼100 GeV • Inclusive and open-charm detection
Can we get quantitative guidance on the emergent pion mass mechanism?	Pion form factor data for Q^2 = 10-40 $(\mathrm{GeV}/c)^2$.	• Need to uniquely determine exclusive process $e+p \to e'+\pi^++n$ (low $-t$) • $e+p$ and $e+D$ at similar energies • CM energy ∼10-75 GeV



[Arrington et al. J. Phys. G 48]

While COMPASS++ is confirming NA10's results, we need the EIC: leading-neutron DIS



- pulls from future data in specific kinematics?
- correlations of PDFs with observables?
- disentaglement of sea and gluon PDF?
- model dependence?

Interpolation with constraints — scalar PDF

Set-up:

Decomposition of the scalar PDF $$e^q(x) = e^q_{\rm loc}(x) + e^q_{\rm gen}(x) + e^q_{\rm mass}(x)$$

$e^q_{\rm loc}$: σ terms

$e^q_{\rm mass}$: quark mass

↓ = Mellin moment

CLAS12 data on beam-spin asymmetry

Point-by-point extraction through DiFF at LO *[AC et al., PRD106]*

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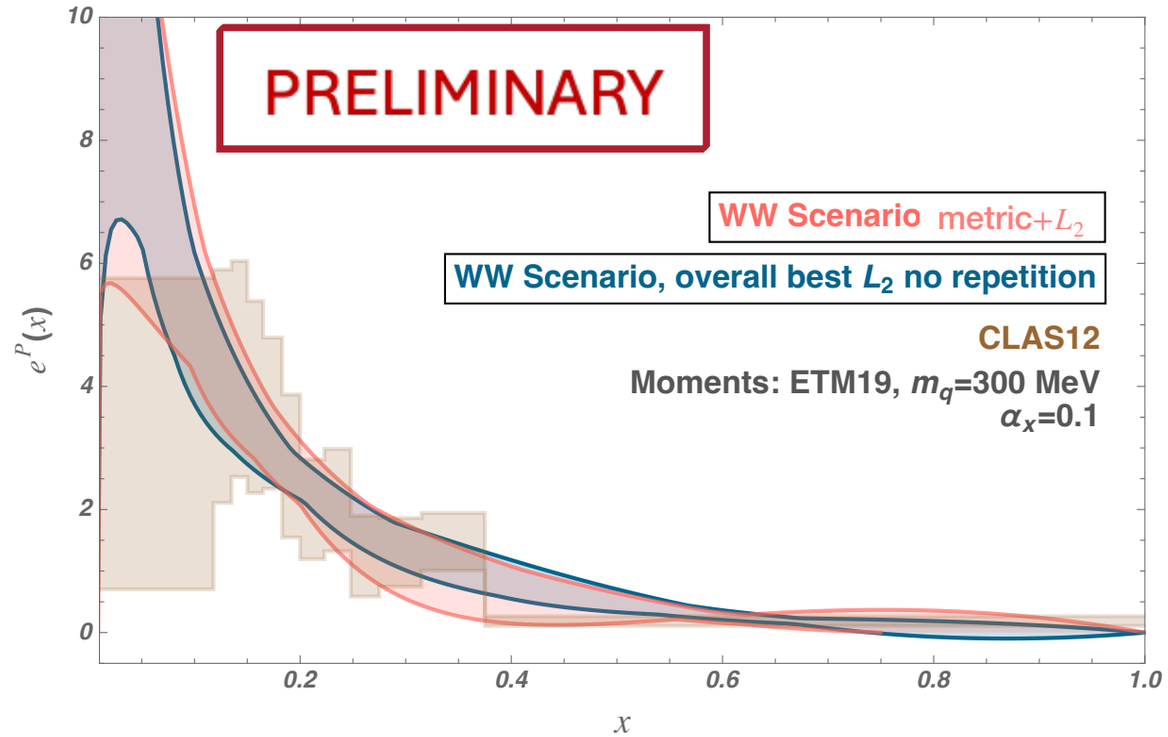
CLAS12 data on beam-spin asymmetry

Point-by-point extraction through DiFF at LO *[AC et al., PRD106]*

Problem that would allow a unique solution, were it not for integral constraints.

The Bézier curve system can be solved exactly for specific dimensions in interpolation mode.

⟹ *developing methodologies to impose moments.*



Caveats: the method leads to a large number of models!

⟹ *developing metrics to be used in penalties in loss function.*

[E. López Rosa, Master thesis, UNAM]
[E. López-Rosa. et al, in progress]

EIC: studies of multiparton dynamics

Yellow Report

Large range of Q^2 values, includes smallish x regions

Sandbox for factorization and evolution studies

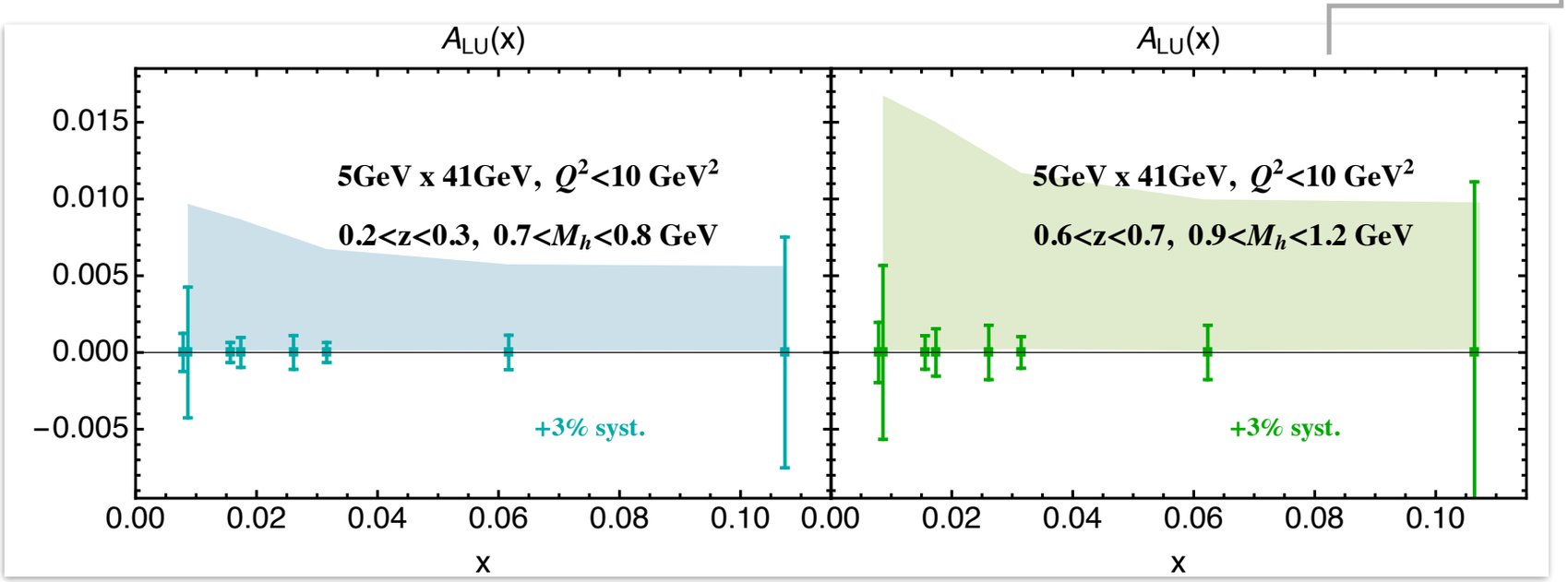
Complementary to fixed-target experiments (HERMES, CLAS,…)

Golden channel

fully inclusive DIS, access to g_T

Silver channel

semi-inclusive DIS, access to e(x)



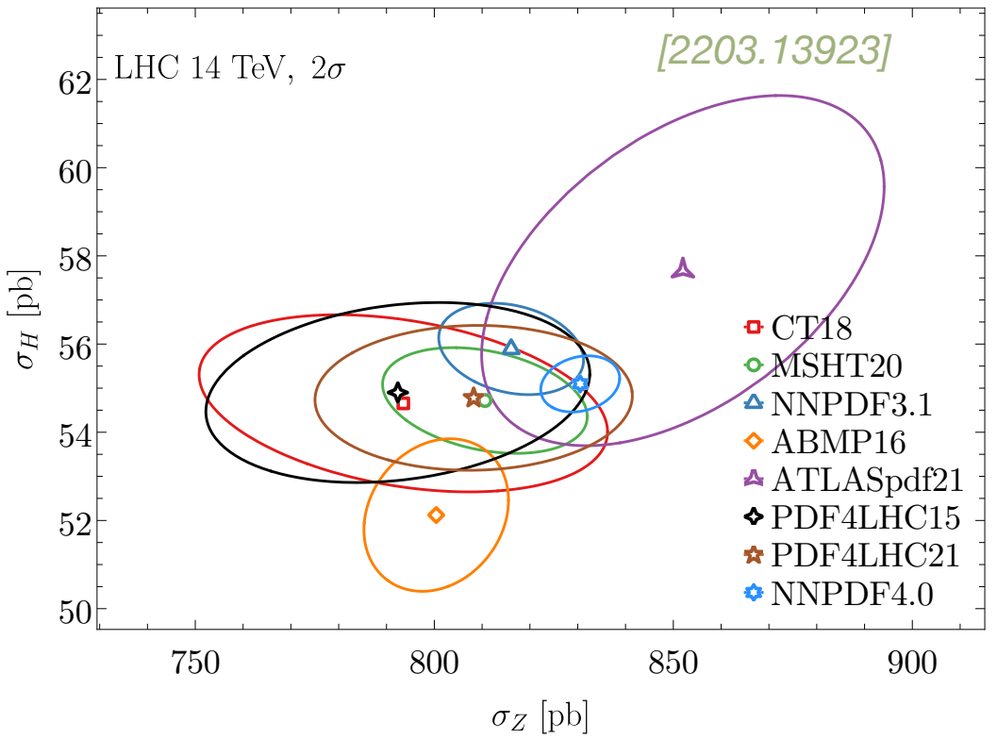
CTEQ (Wu-Ki Tung Et Al.) group

Thanks to the sandbox studies, we can move on to our main goal:

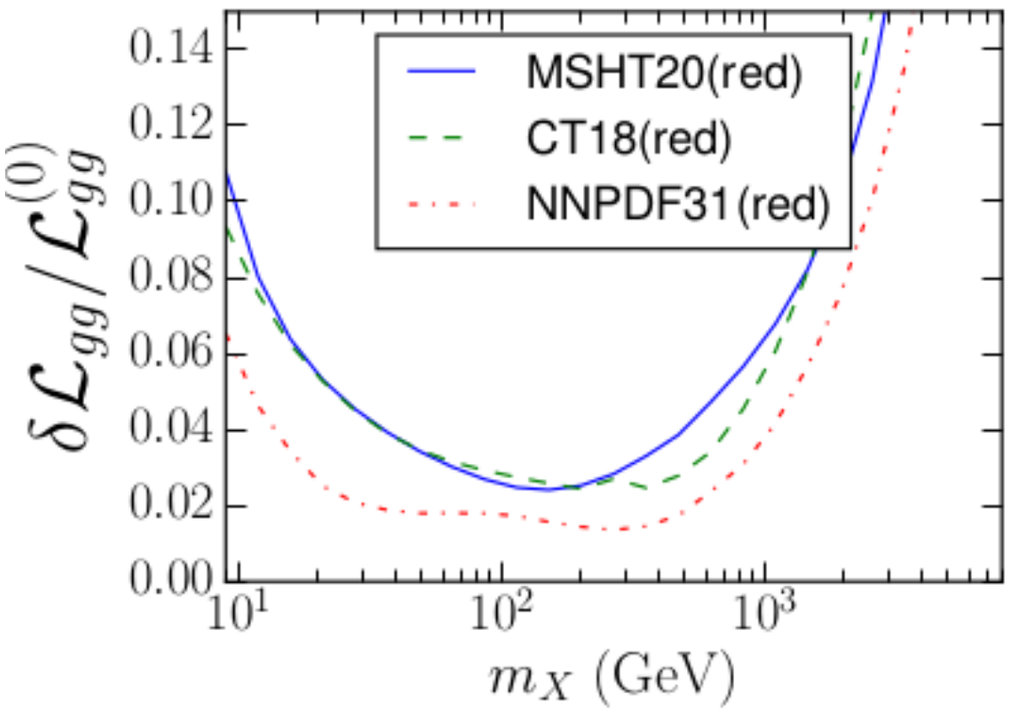
sampling bias and model combination for the unpolarized PDF.

Unpolarized PDFs, EIC and precision physics

Uncertainties differ among various global analyses collaborations



PDF4LHC21 [J.Phys.G 49]

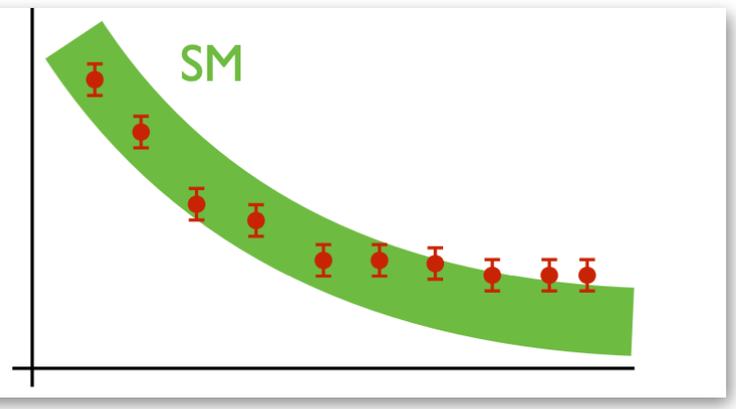


Near future:
study of the building of the tolerance criterion for CT25, enhanced parametrization study,…

Not-so-near future:
complementarity of data, especially at large-x values and for the sea sector, will matter ⇒ EIC?

Unpolarized PDFs, EIC and precision physics

- Most likely look for "new interactions"
- Small deviations from SM : PRECISION
- EFT description / BSM model



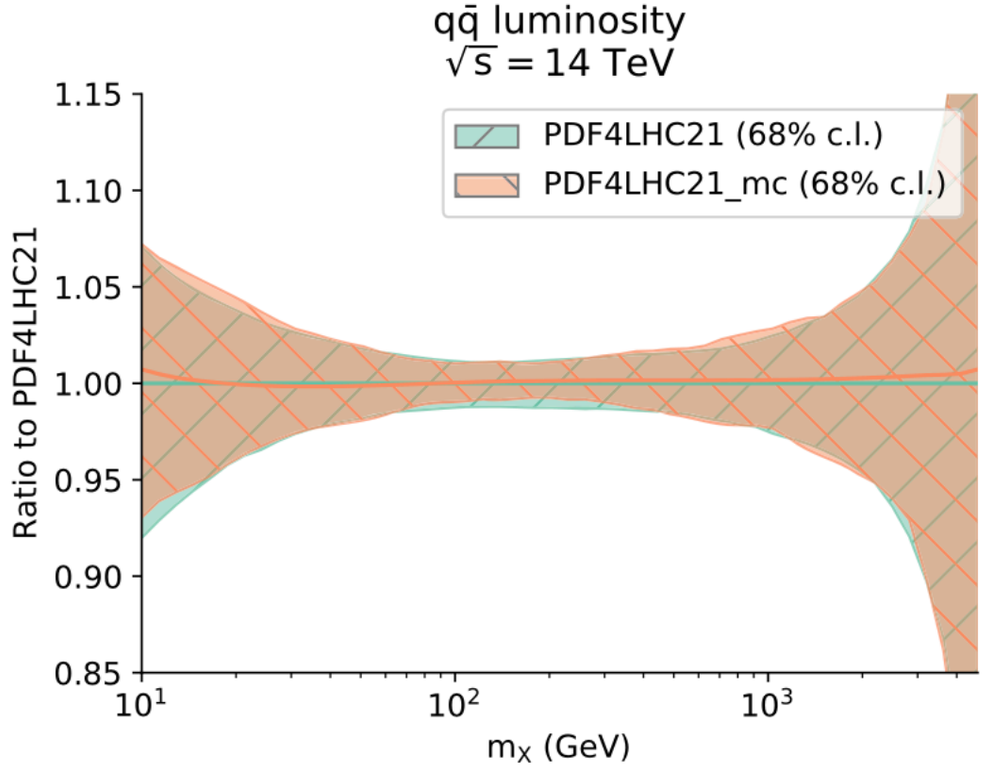
Credit:
Daniel de Florian (DIS2023)

Large invariant mass in parton luminosity related to large-x values. Precision on LHC observables may rely on our knowledge of large-x PDFs.

Uncertainties on large-x PDFs hamper the searches for new physics.

Looking for New Physics in the tails of Drell-Yan like processes involves PDFs at large x and Q : $(x_1 x_2 \geq 0.3, Q = 8\,\mathrm{TeV})$.

[Fu et al., PhysRevD109,
Ball et al., EPJC82]



[PDF4LHC21, J.Phys.G 49]

Conclusions

Global QCD analyses are important to access hadron-structure information.
Inverse problems, which sets of solutions are evolving.

Our take today: moving towards epistemic PDF uncertainties with polynomial approximators — Bézier curves.

Rôle of the parametrization in the sampling accuracy: we make use of **Bézier-curve methodology**

⟹ the EIC will contribute to learning PDFs in complementary kinematical ranges

⟹ Uncertainty quantifcation requires going beyond the $\Delta\chi^2 = 1$ prescription

⟹ Posterior means likelihood + priors — use of information-like criteria to select solutions

⟹ The model combination also stems from a distribution — de Finetti

⟹ Sandbox studies

Pion PDFs: Fantomas1.0 available
`metamorph` can be used to study many functions
Reliable uncertainty on the PDF analysis (to NLO)
re: larger where no data constrains $q^{\pi}(x, Q^2)$

Collinear twist-3 PDF
Playground for my group
Integration of constraints from moments
Development of metrics for shape selection

Fantômas standalone code

Fantômas Unconfined: global QCD fits with Bézier parameterizations

Lucas Kotz[a,1], Aurore Courtoy[b,2,*], Tim Hobbs[c,3], Pavel Nadolsky[d,4,**], Fredrick Olness[a,5], Maximiliano Ponce-Chavez[d], Varada Purohit[a]

xFitter embedded in "PDF Parametrization"

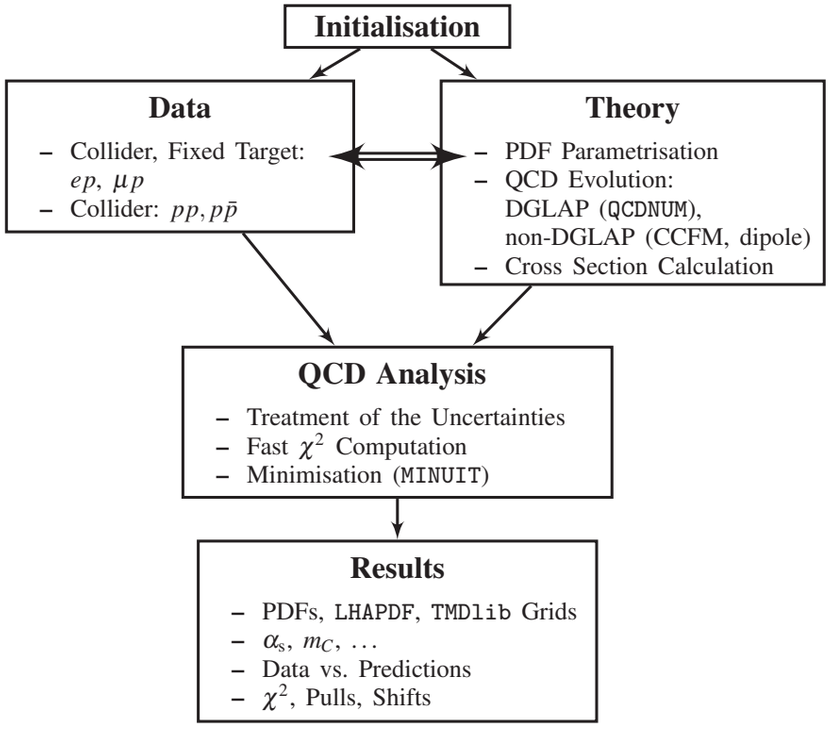


Figure 1: Schematic structure of the `xFitter` program.

Companion standalone to be plugged wherever the user decides to

- C++ module
- MetamorphCollection class object
- reads steering cards
- check sum rules
- shuffles

Fantomas1.0:
https://cteq-tea.gitlab.io/project/00pdfs/#mesonPDFs

Latin American contribution to the EIC

LASF4RI

Latin American Strategy Forum for Research Infrastructure

Developing a strategy to strengthen Latin American Scientific Collaborations and their impact.

Brazilian Journal of Physics (2025) 55:145
https://doi.org/10.1007/s13538-025-01778-x

Check for updates

Latin American Strategy Forum for Research Infrastructure (III LASF4RI Contribution)

The Glue That Binds Us All—Latin America and the Electron-Ion Collider

A. C. Aguilar[1] · A. Bashir[2] · J. J. Cobos-Martínez[3] · A. Courtoy[4] · B. El-Bennich[5] · D. de Florian[6] · T. Frederico[7] · V. P. Gonçalves[8] · M. Hentschinski[9] · R. J. Hernández-Pinto[10] · G. Krein[11] · M. V. T. Machado[12] · J. P. B. C. de Melo[13] · W. de Paula[7] · R. Sassot[14] · F. E. Serna[15] · Supporting authors outside Latin America: L. Albino[16] · I. Borsa[17] · L. Cieri[18] · I. M. Higuera-Angulo[19] · J. Mazzitelli[20] · Á. Miramontes[18] · K. Raya[21] · F. Salazar[22] · G. Sborlini[23] · P. Zurita[24]

✉ A. Courtoy
aurore@fisica.unam.mx

✉ B. El-Bennich
bennich@unifesp.br

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EN

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