Proton structure for precise QCD calculations

Balancing precision and replicability in uncertainty quantification

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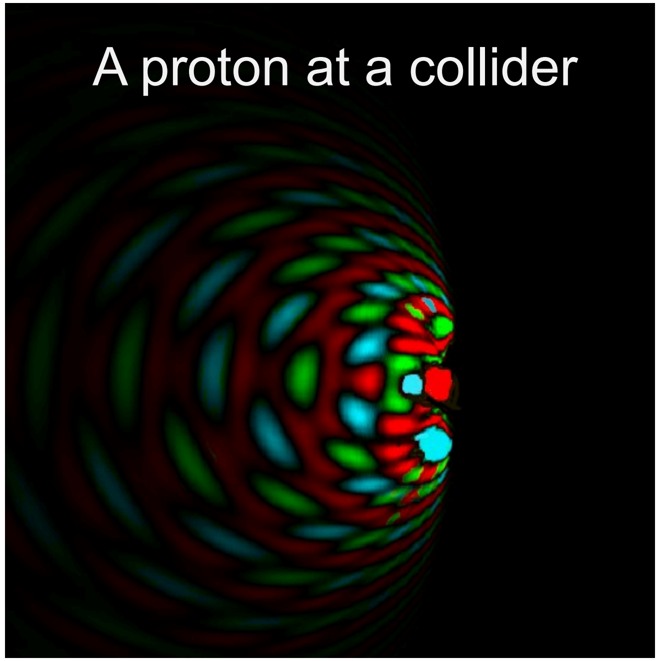
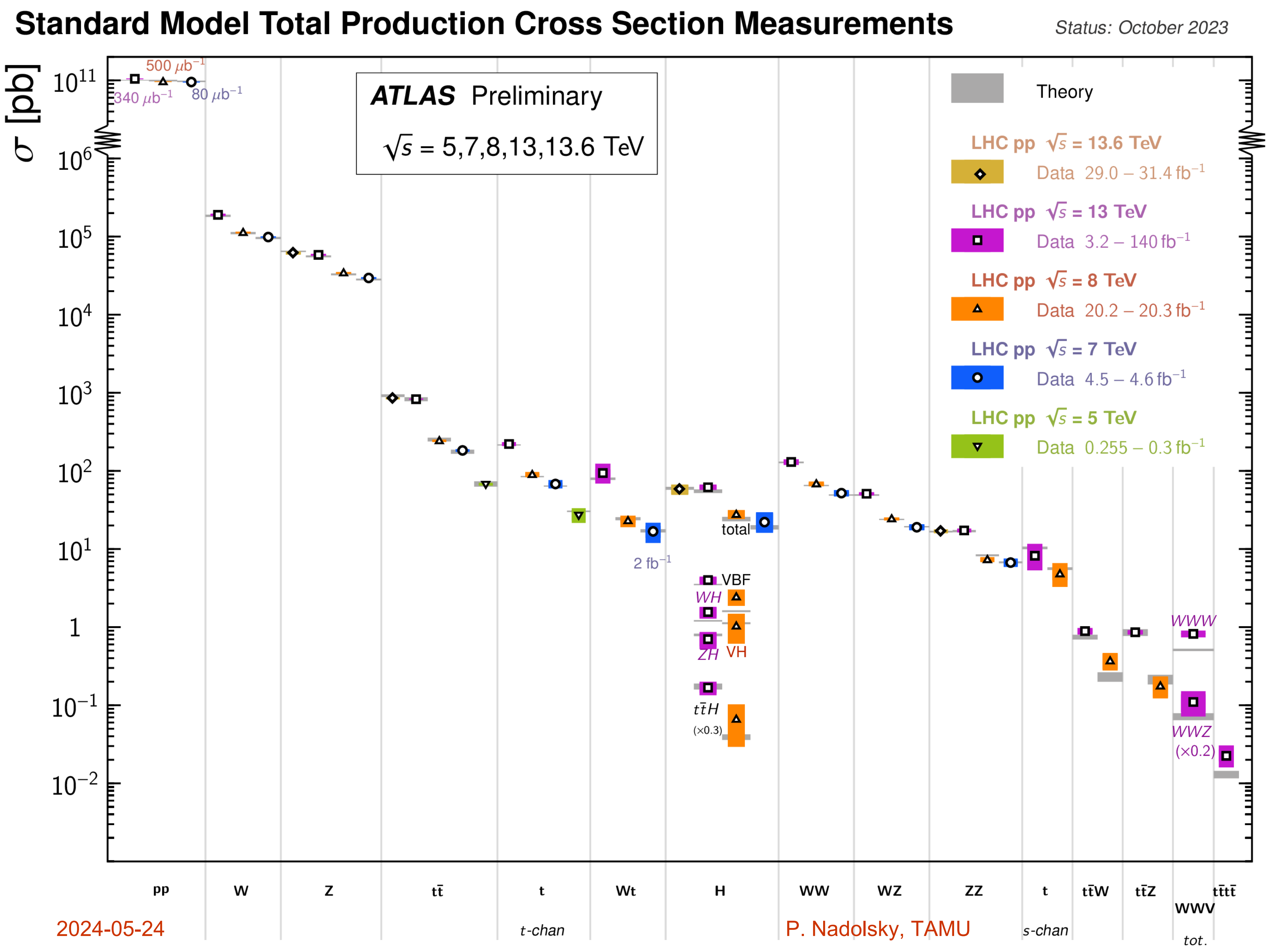
With A. Courtoy, L. Kotz, F. Olness,
and CTEQ-TEA (Tung Et Al.) Global QCD
analysis group

A proton at a collider



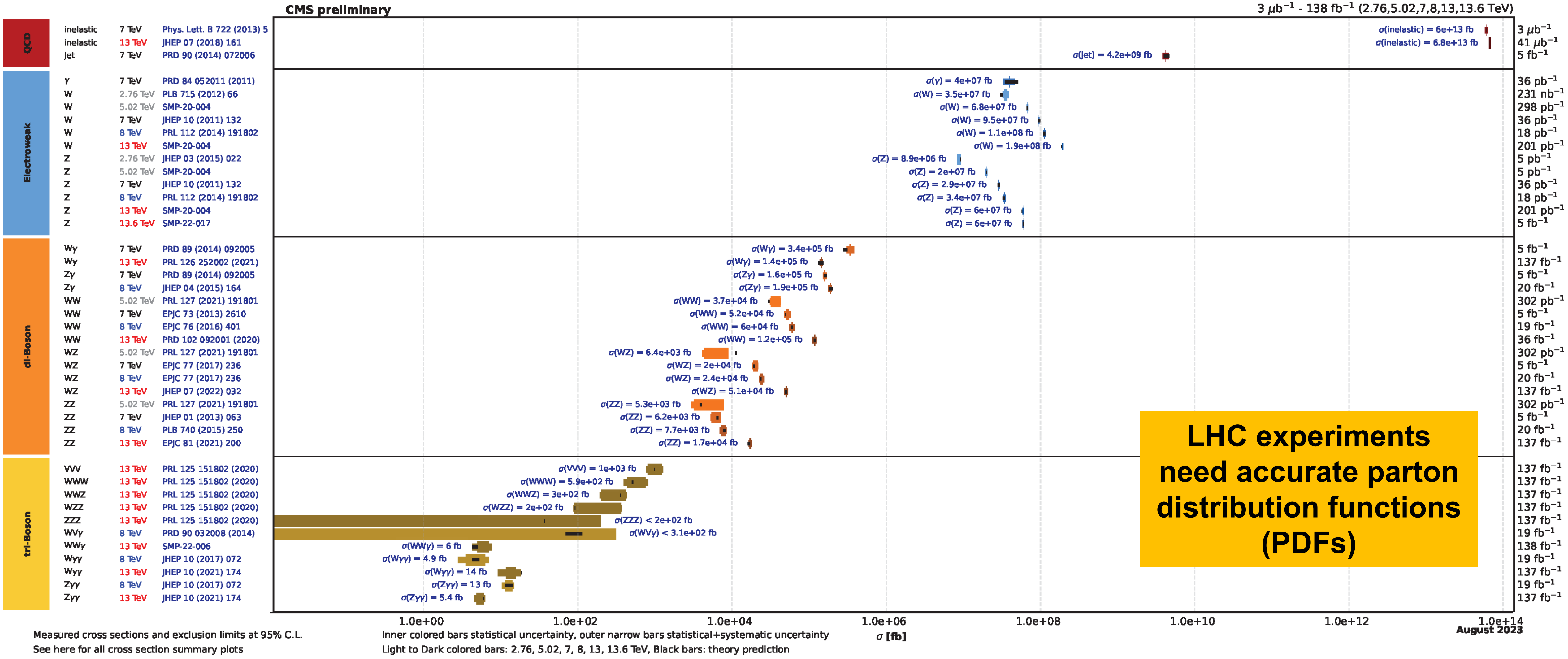
SMU CTEQ

2024-05-24



LHC experiments need accurate parton distribution functions (PDFs)

Overview of CMS cross section measurements I

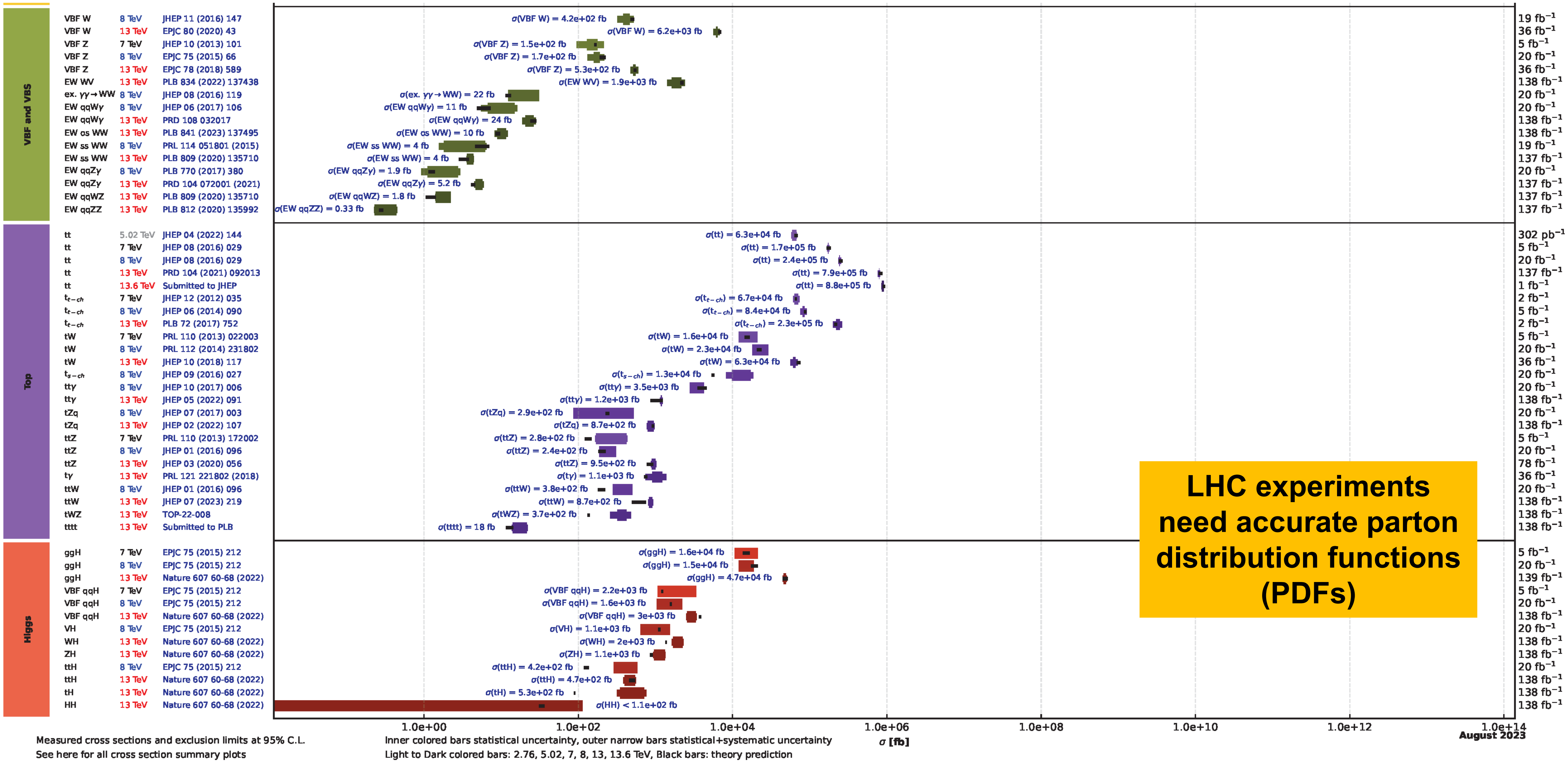


Measured cross sections and exclusion limits at 95% C.L.
See here for all cross section summary plots

Inner colored bars statistical uncertainty, outer narrow bars statistical+systematic uncertainty
Light to Dark colored bars: 2.76, 5.02, 7, 8, 13, 13.6 TeV, Black bars: theory prediction

LHC experiments need accurate parton distribution functions (PDFs)

Overview of CMS cross section measurements II



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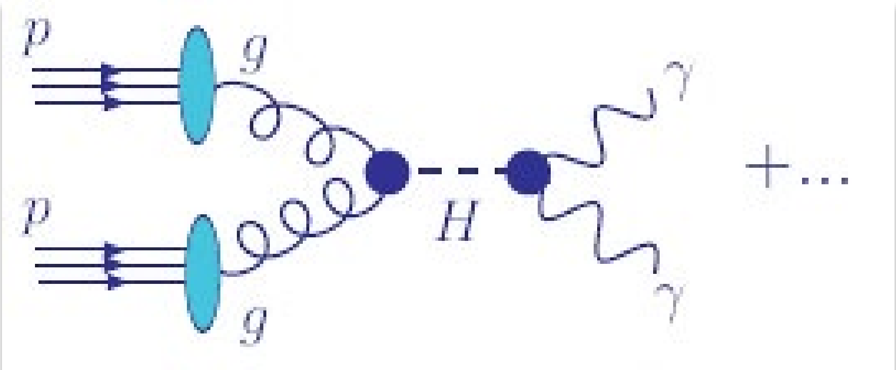
LHC experiments need accurate parton distribution functions (PDFs)

Parton distributions describe long-distance dynamics in high-energy collisions

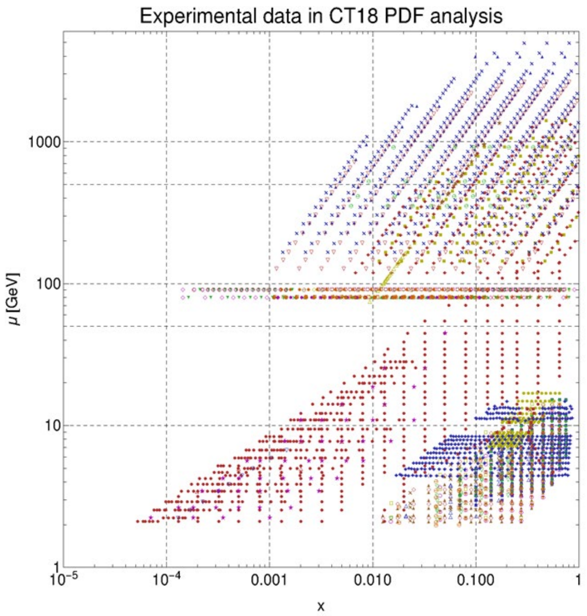


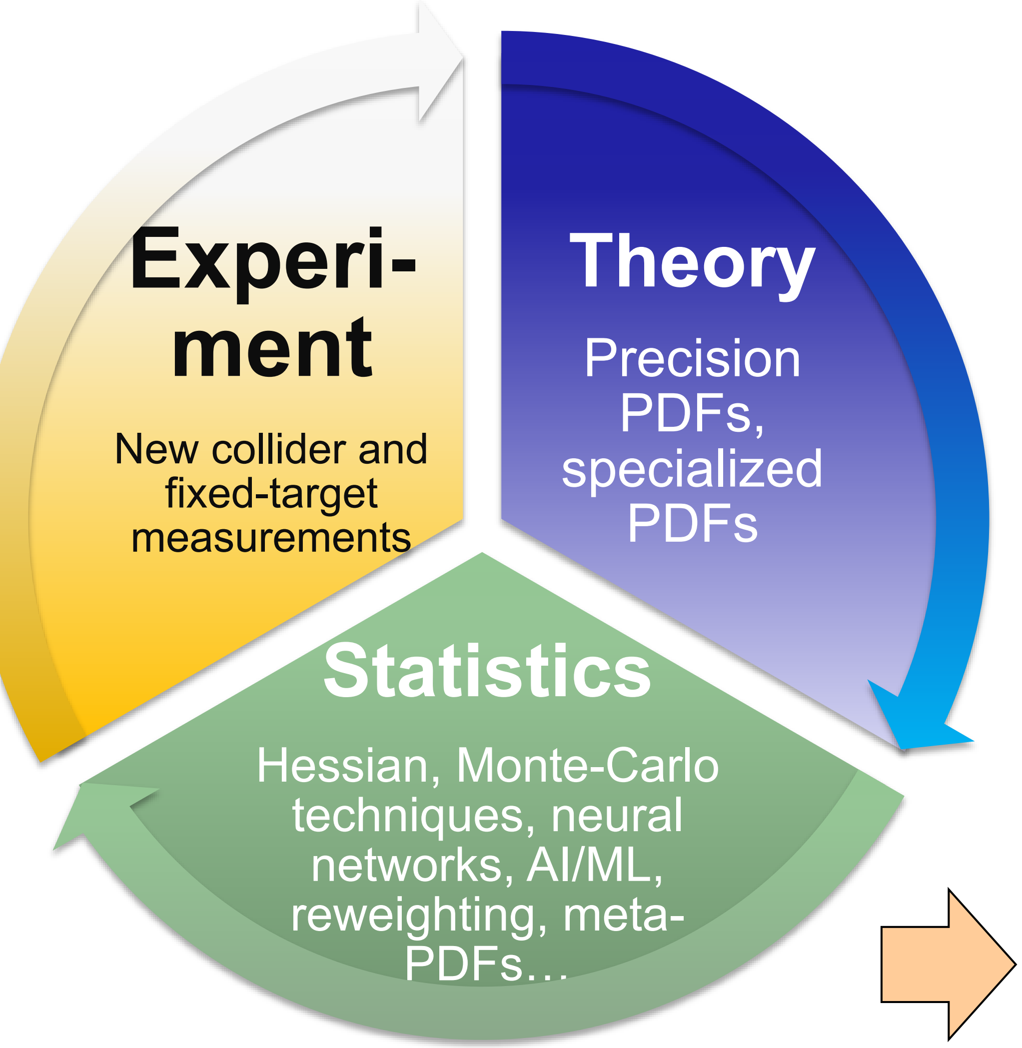
$$\sigma_{pp\to H\to\gamma\gamma X}(Q)=\sum_{a,b=g,q,\bar{q}}\int_0^1 d\xi_a\int_0^1 d\xi_b\hat{\sigma}_{ab\to H\to\gamma\gamma}\left(\frac{x_a}{\xi_a},\frac{x_b}{\xi_b},\frac{Q}{\mu_R},\frac{Q}{\mu_F};\alpha_s(\mu_R)\right)$$
$$\times f_a(\xi_a,\mu_F)f_b(\xi_b,\mu_F)+O\left(\frac{\Lambda_{QCD}^2}{Q^2}\right)$$

$\hat{\sigma}$ is the hard cross section; computed order-by-order in $\alpha_s(\mu_R)$

$f_a(x,\mu_F)$ is the distribution for parton a with momentum fraction x, at scale μ_F

Global fits of proton scattering data at (N)NNLO accuracy





Experi-ment

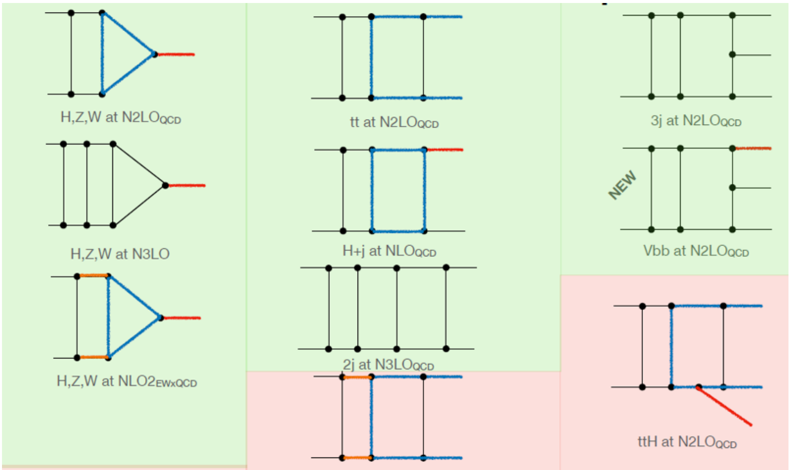
New collider and fixed-target measurements

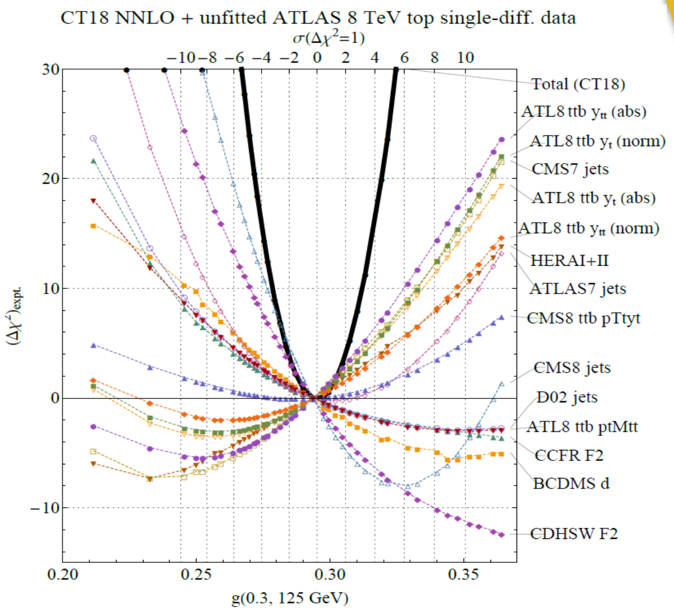
Theory

Precision PDFs, specialized PDFs

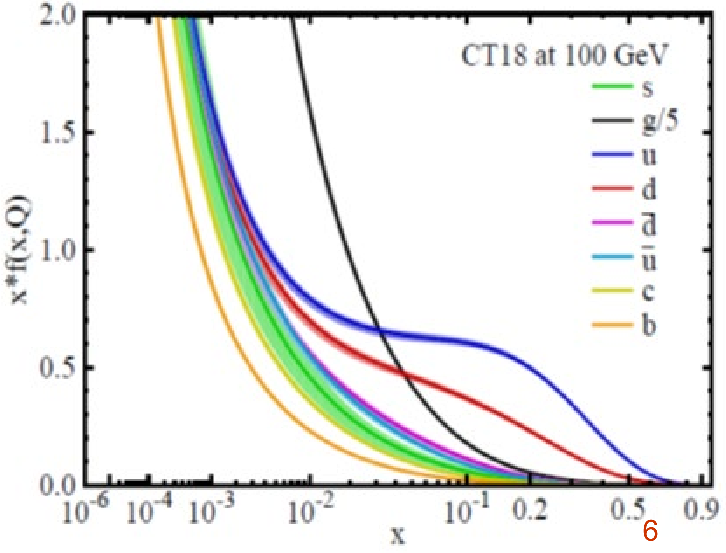
Statistics

Hessian, Monte-Carlo techniques, neural networks, AI/ML, reweighting, meta-PDFs…





Parton distribution functions with uncertainties



Global fits of proton scattering data at (N)NNLO accuracy

A rich domain of SM phenomenology!

Impact on a wide range of HEP and NP studies

Multiloop QCD and EW computations

Exploration of most complex experimental data sets

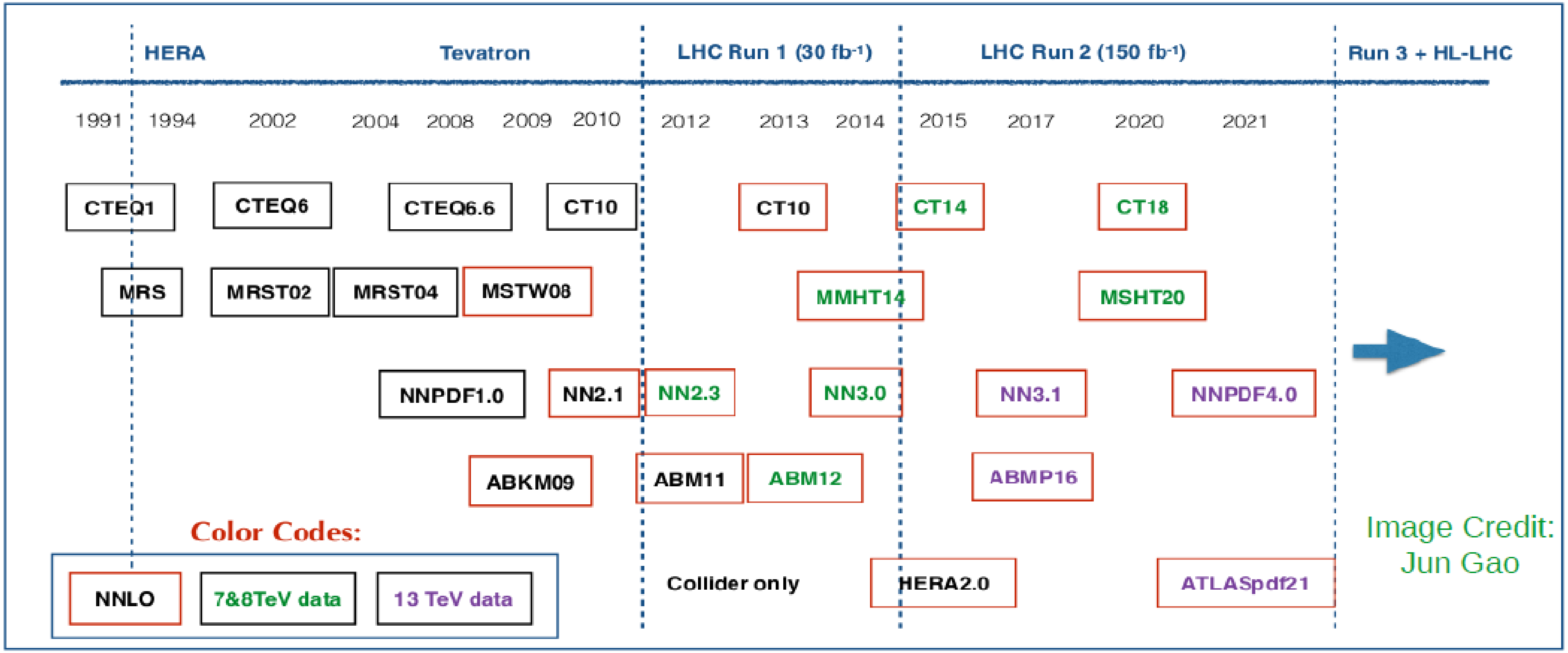
Accurate and fast high-performance computing

Frontier statistical inference in many dimensions

A testing bed for multidimensional uncertainty quantification, ML/AI, …

} opportunities for conceptual breakthroughs

Phenomenological PDF analyses for a nucleon



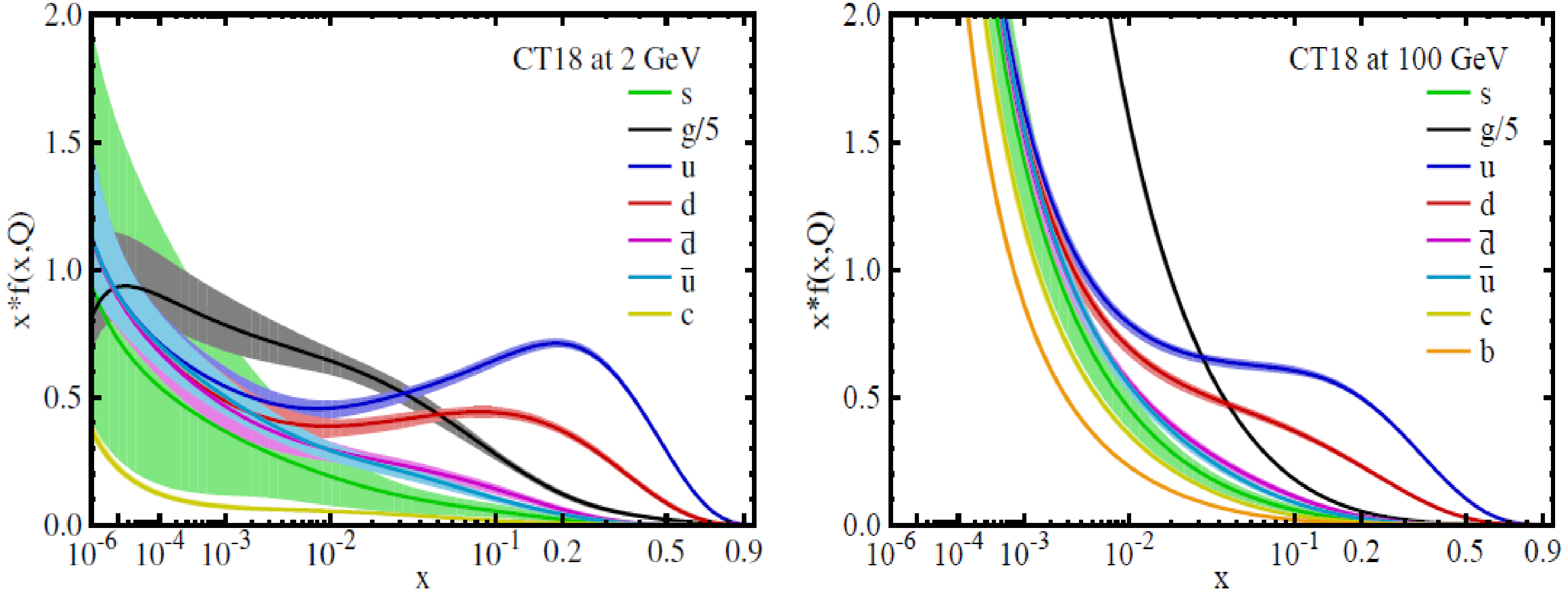
Pursued by several groups – ABM, ATLAS, **CTEQ-TEA (CT)**, CTEQ-Jlab, MSHT, NNPDF, JAM, …

Precision state-of-the art: NNLO QCD + NLO EW; partial N3LO results (NNPDF and MSHT groups)

Data from fixed-target experiments and colliders (HERA, Tevatron, LHC, …)

CT18 parton distributions

Recent PDFs from the CTEQ-TEA group arXiv:1912.10053 [hep-ph]



- Precise experimental data sets from ep collider HERA, LHC, Tevatron, fixed-target experiments
- Next-to-next-to-leading order (NNLO) accuracy in QCD coupling α_s
- Flexible parametric forms
- Central PDFs and bands of estimated uncertainty
- Four PDF ensembles, to account for tensions between data sets

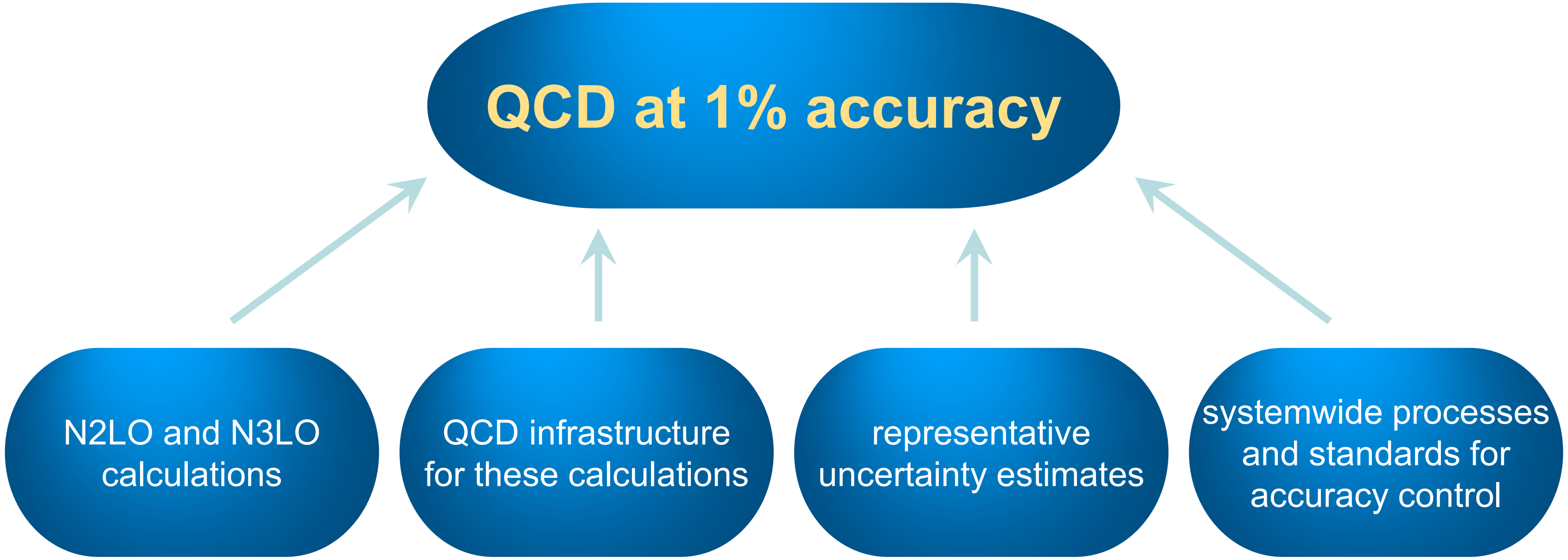
Toward a new generation of CT202X PDFs

1. Multiple preliminary NNLO fits with LHC Run-2 (di)jet, vector boson, $t\bar{t}$ data
   - based on the selections of experiments recommended in 2305.10733, 2307.11153
2. Work on implementation of N3LO contributions
3. Physics applications
   a. QCD+QED PDFs for a proton and neutron
   b. PDF dependence of forward-backward asymmetry
   c. Fast tools for PDF profiling and examination of data tensions
   d. Pion PDFs
   e. …
4. Next-generation PDF uncertainty quantification: Bézier curves, META combination, ML stress-testing, multi-Gaussian approaches, …

Multivariate uncertainty quantification in the global PDF fits

- More than 20 years of experience on UQ by CTEQ and other groups
- Essential for statistical analyses of numerous experiments
- Understanding of mathematical foundations for UQ in multivariate and AI frameworks
- Provides guidelines for replicability of precision HEP analyses

Precision
Reproducibility & replicability
Epistemic uncertainty
Big-data paradox
AI applications



QCD at 1% accuracy

N2LO and N3LO calculations

QCD infrastructure for these calculations

representative uncertainty estimates

systemwide processes and standards for accuracy control

Lots of promise in this area

Parton showers, fast NxLO interfaces, PDFs, ... must be comparably accurate

or The Importance of Being Earnest with Systematic Errors (experiment+theory; traditional or AI/ML)

This must be a part of the precision-focused community culture

Publishing statistical models: Getting the most out of particle physics experiments

Kyle Cranmer (New York U.), Sabine Kraml (LPSC, Grenoble), Harrison B. Prosper (Florida State U.), Philip Bechtle (Bonn U.), Florian U. Bernlochner (Bonn U.) Show All(33)

Sep 10, 2021

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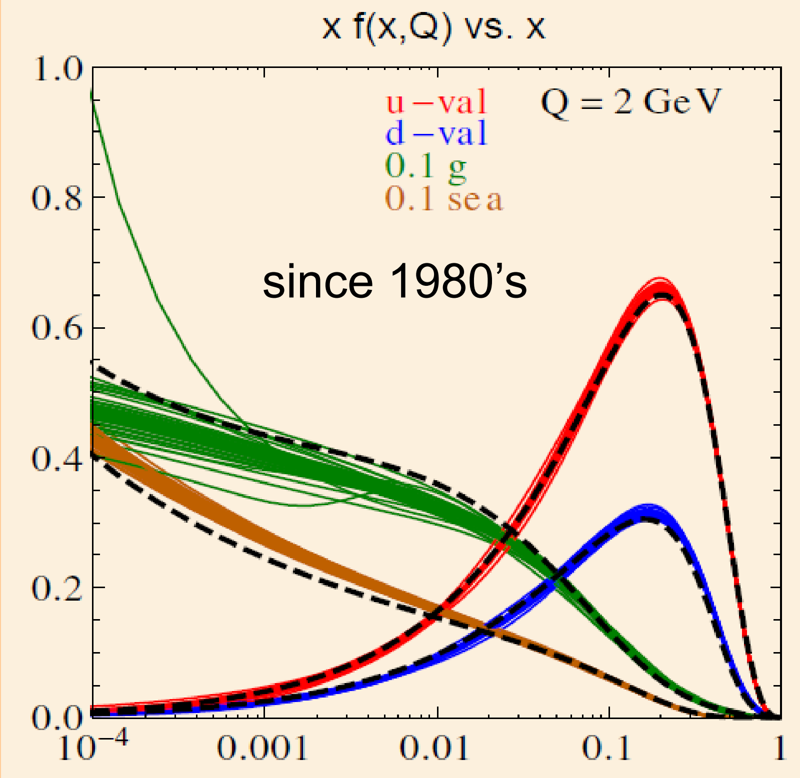
2023 US DOE Funding Opportunity Announcement DE-FOA-0000315

*Advancing **Uncertainty Quantification** in Modeling, Simulation, and Analysis of **Complex Systems***

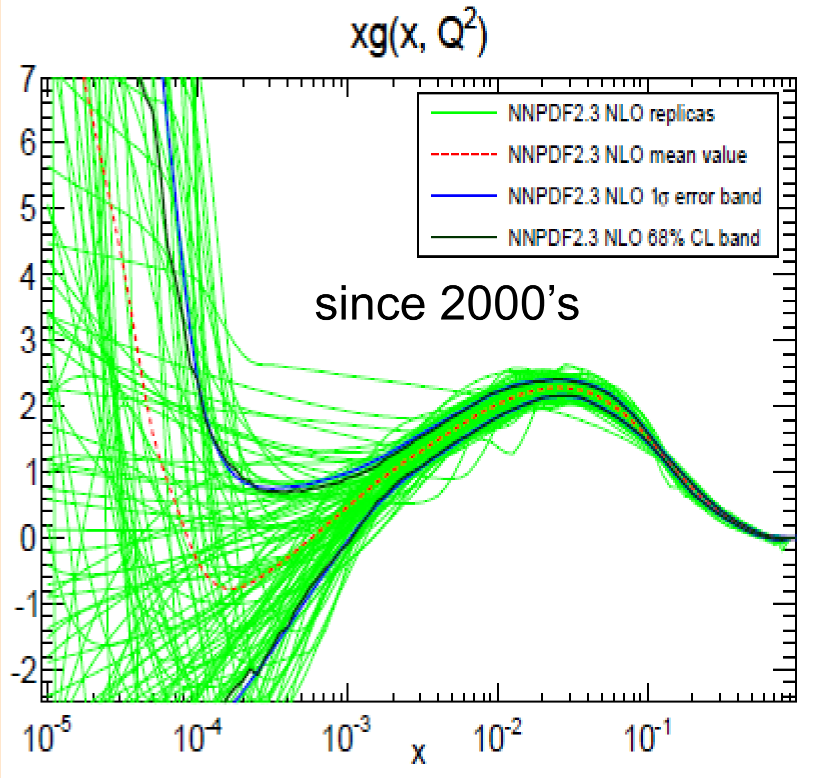
Two complementary approaches to estimate PDF uncertainties

Analytic parametrizations +
Hessian PDF eigenvector sets
(ABM, CTEQ, HERA, MSHT,…)



since 1980's

Neural network parameterizations
+ Monte Carlo PDF replicas
(NNPDF)

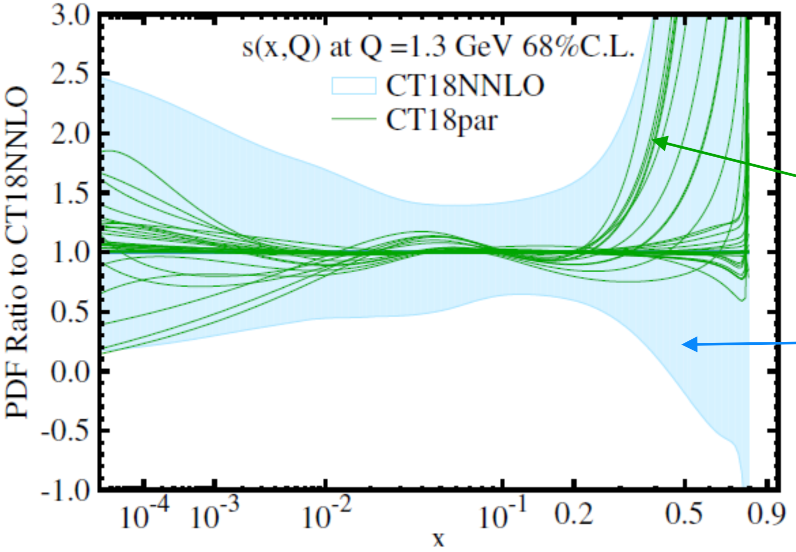


since 2000's

a textbook application of ML in particle physics

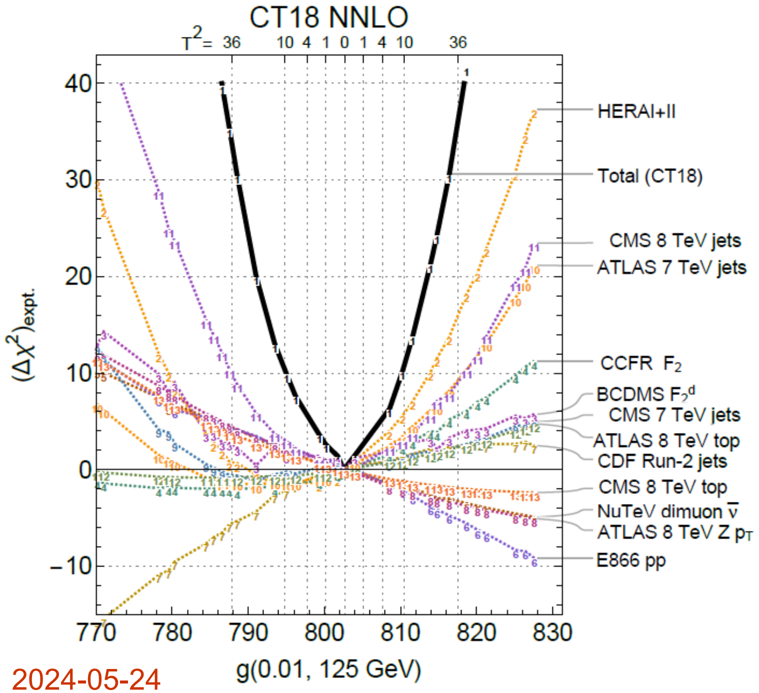
Hessian PDFs can be converted into MC ones, and vice versa.

Hessian PDFs, uncertainties (CT18 PDFs)



preliminary PDFs for alternative parametrizations

final uncertainty with one parametrization



"Bayesian exploration with Gaussian emulation"

Preliminary fits explore experimental, theoretical, parametrization, methodological uncertainties

The final PDFs are released as one quasi-Gaussian (**Hessian**) error set (50-60) that approximates the total uncertainty due to the above factors.

These error sets are constructed with a fixed choice of polynomial parametrization forms. The totality of error sources (not only experimental) is emulated by introducing **tolerance** T: the final 1σ uncertainty corresponds to $\Delta\chi^2 = T^2 \sim 10 - 30$, rather than $T^2 = 1$.

An alternative: Neural-network PDFs

Use **bootstrap** to estimate **aleatory** data fluctuations for a fixed training methodology (called “importance sampling” by NNPDF)

Parametrize PDFs using CNNs with optimized hyperparameters and restricted by prior conditions (positivity of cross sections, etc.)

[The whole fit is based on one “tuned” NN architecture]

All fitting codes, especially the NNPDF one, employ grid techniques for fast integration

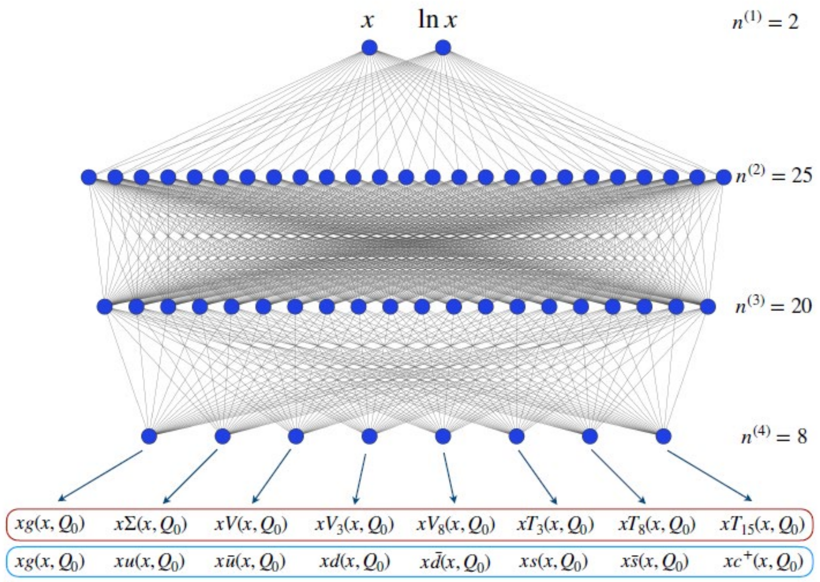


Figure 3.9. The neural network architecture adopted for NNPDF4.0. A single network is used, whose eight output values are the PDFs in the evolution (red) or the flavor basis (blue box). The architecture displayed corresponds to the optimal choice in the evolution basis; the optimal architecture in the flavor basis is different as indicated by Table 3.3).

NNPDF4.0 PDF ensemble,
R. Ball et al., arXiv:2109.02653

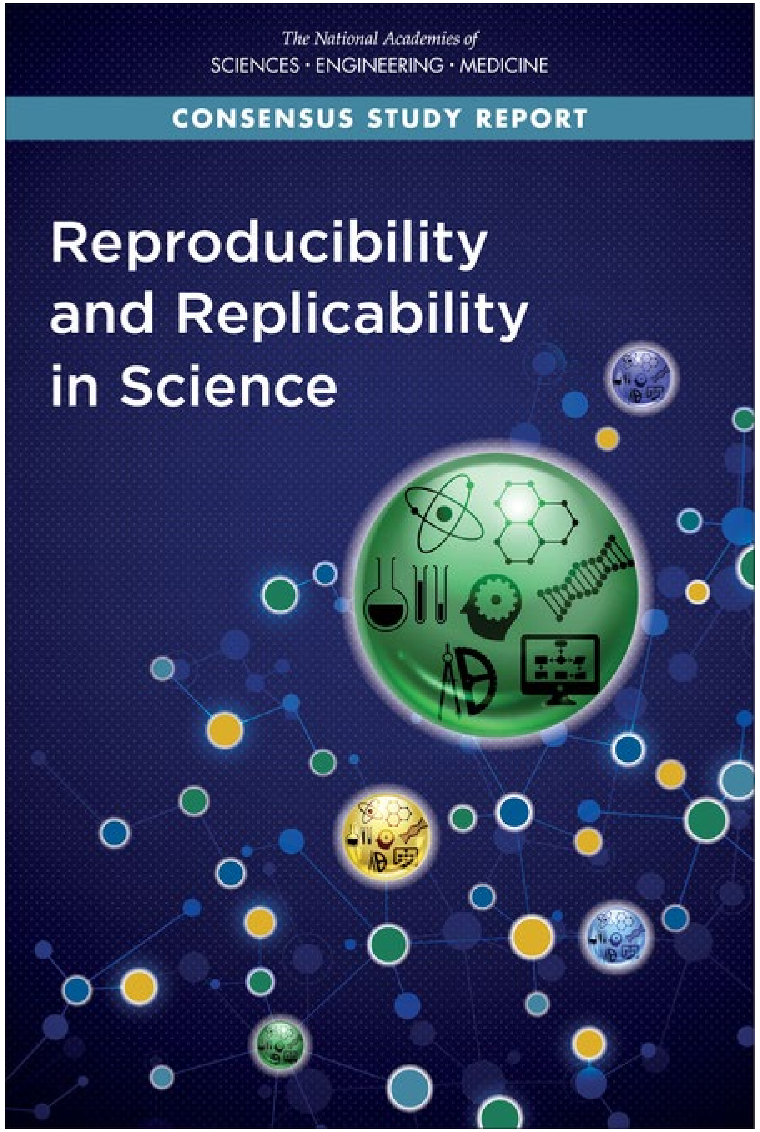
Statistics with many parameters is different!

In many applications, especially AI/ML ones:

1. **There is no single global minimum of** χ^2 (or another cost function)
2. **The law of large numbers may not work**
   - uncertainty may not decrease as $1/\sqrt{N_{rep}}$, leading to the **big-data paradox** [Xiao-Li Meng, 2018]:

The bigger the data, the surer we fool ourselves.

3. **Replication of complex measurements is daunting**



The National Academies of
SCIENCES · ENGINEERING · MEDICINE

CONSENSUS STUDY REPORT

Reproducibility
and Replicability
in Science

US National Academy of Sciences, Engineering, and Medicine, 2019, https://doi.org/10.17226/25303

Are W boson mass measurements replicable?

For instance, W boson mass measurements at the Tevatron and LHC

LHCb: $80{,}354 \pm 32$

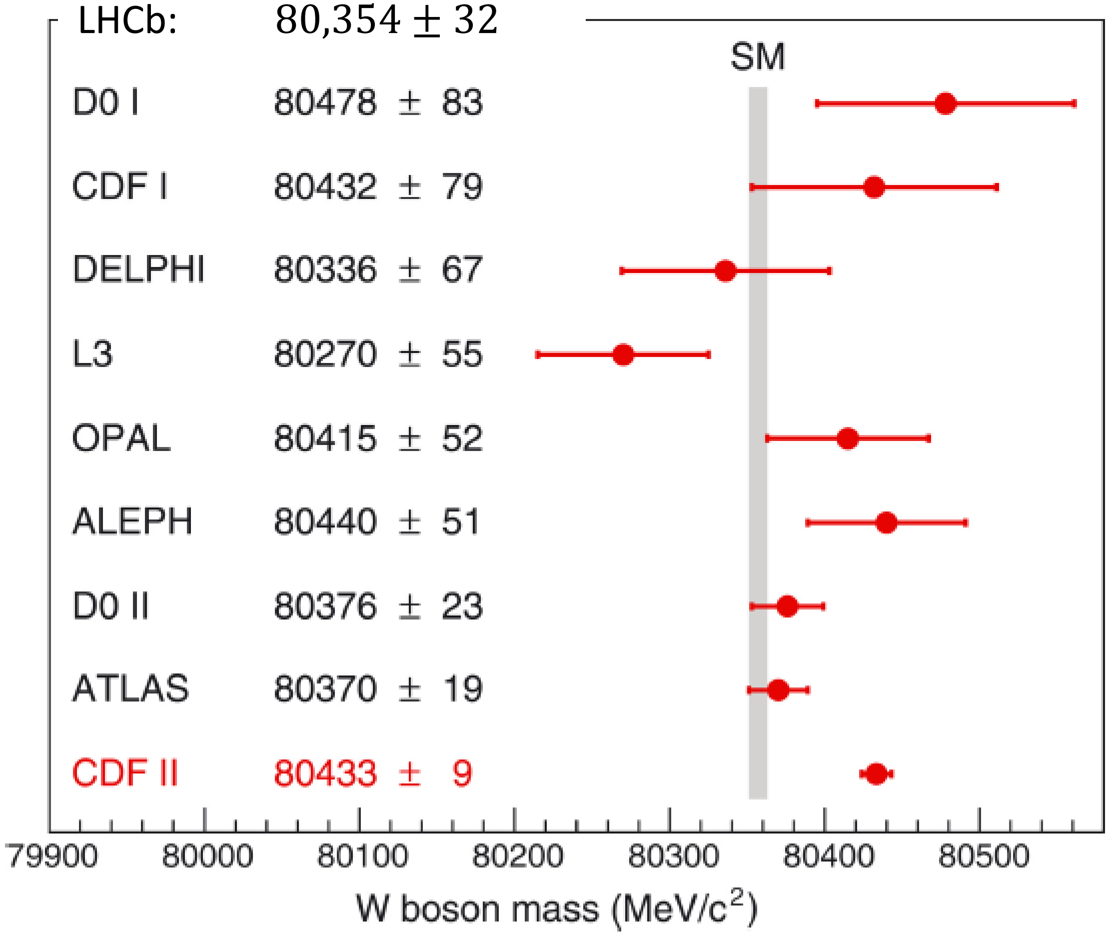
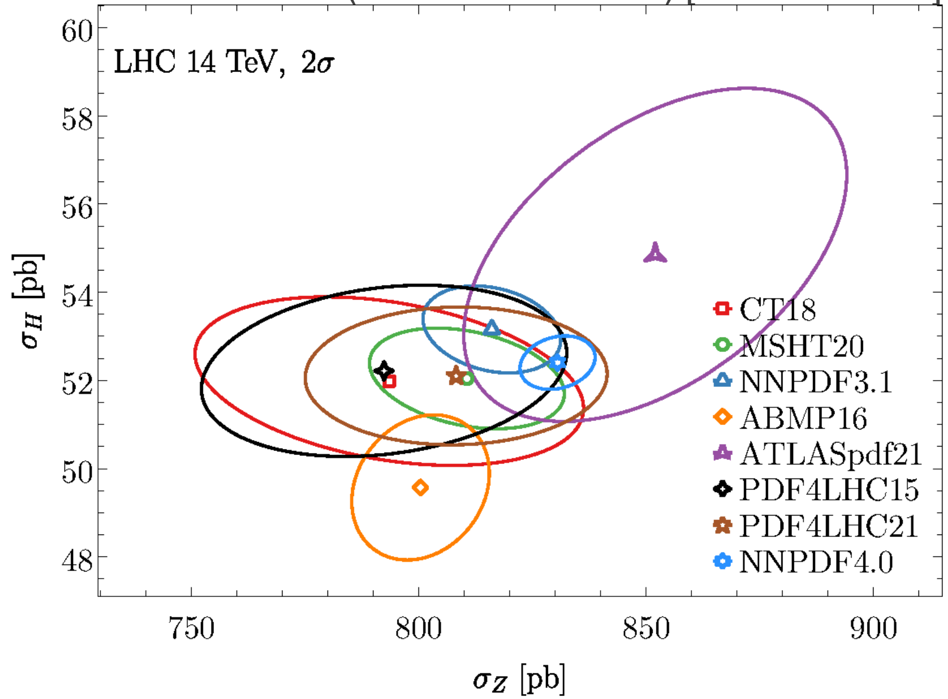


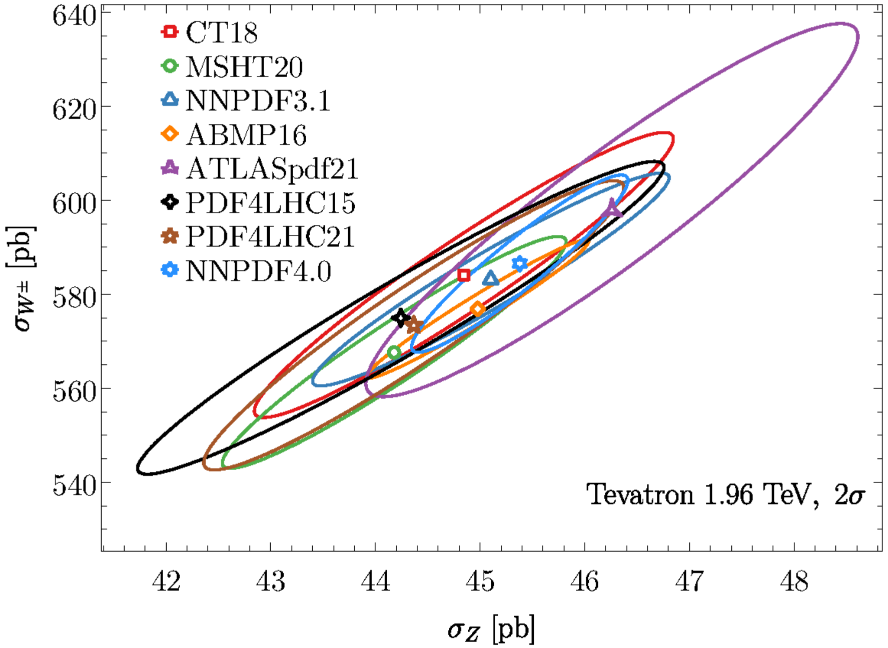
Figure reproduced from CDF-II measurement (Science 376, 170).

The tolerance puzzle

Why do groups fitting similar data sets obtain different PDF uncertainties?

Precision PDFs (Snowmass 21 WP) [2203.13923v2]





The answer has direct implications for high-stake experiments such as *W* boson mass measurement, tests of nonperturbative QCD models and lattice QCD, high-mass BSM searches, etc.

Comparisons of the latest PDF sets

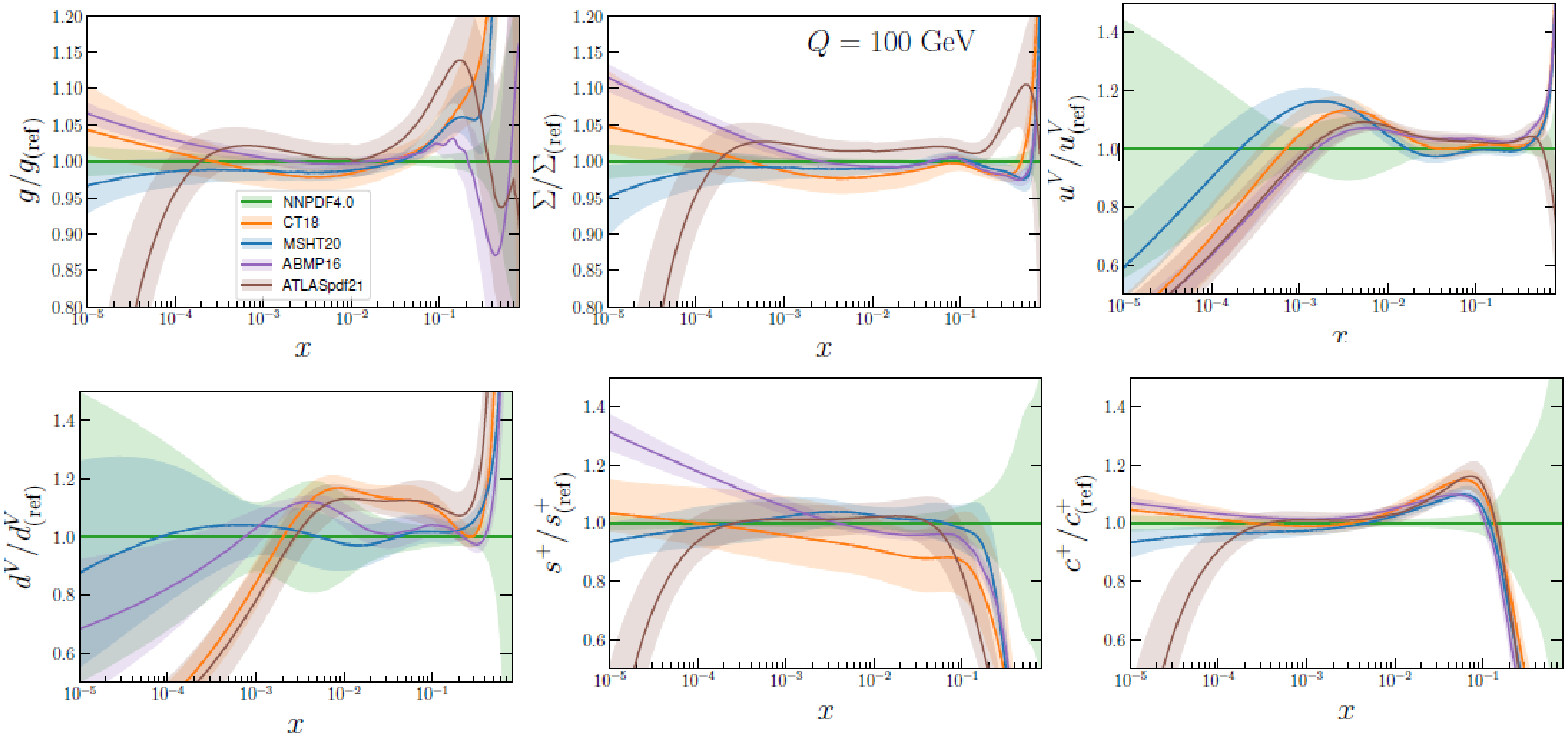


FIG. 2. Comparison of the PDFs at $Q = 100$ GeV. The PDFs shown are the N2LO sets of NNPDF4.0, CT18, MSHT20, ABMP16 with $\alpha_s(M_Z) = 0.118$, and ATLASpdf21. The ratio to the NNPDF4.0 central value and the relative 1σ uncertainty are shown for the gluon g, singlet Σ, total strangeness $s^+ = s + \bar{s}$, total charm $c^+ = c + \bar{c}$, up valence u^V and down valence d^V PDFs.

Replicability risks for precision HEP

Nearly all complex STEM fields encounter replicability challenges.

Modern particle physics is not an exception.

1. It is complex! Is it rigorous enough?
   - Many approaches, especially AI-based ones, increase complexity and are not rigorously understood
2. It often uses wrong prescriptions for estimating epistemic uncertainties
   - Tens to hundreds of systematic uncertainties affect measurements, phenomenology, and lattice QCD

Ongoing studies of systematic uncertainties are essential and still insufficient

- from the experiment side

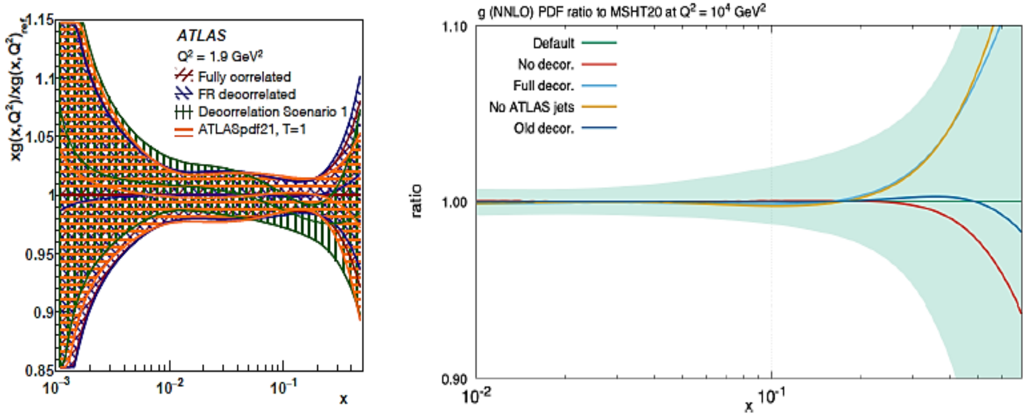


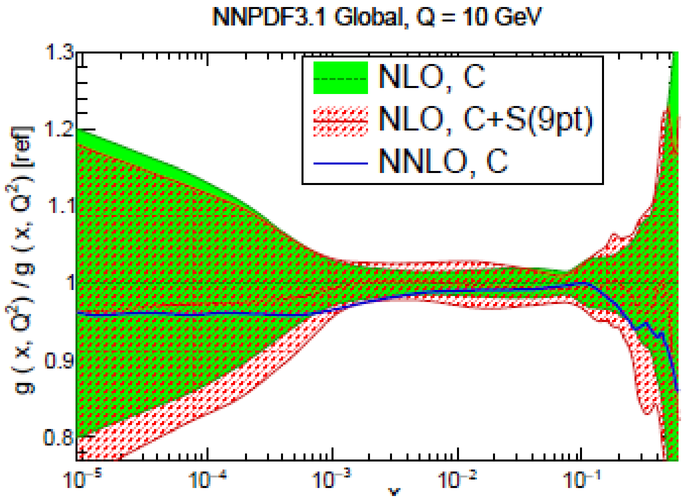
FIG. 9. Difference in the gluon PDF shown in ratio to the ATLASpdf21 (default) gluon(left). This default uses Decorrelation Scenario 2 and this is compared to the use of Full Correlation, Full decorrelation of the flavour response systematic and Decorrelation Scenario 1. The effect of no decorrelation, the default correlation of [9], the decorrelation in [362], and full decorrelation for the MSHT20 gluon (right).

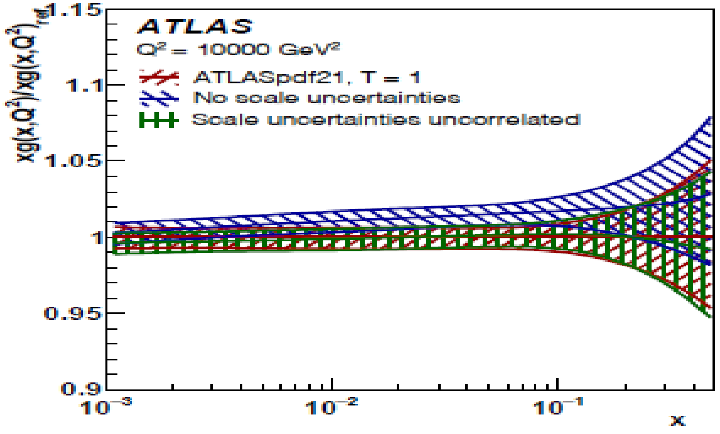
S. Amoroso et al., 2203.13923, Sec. 5.A

Strong dependence on the definition of corr. syst. errors raises a general concern:

Overreliance on Gaussian distributions and covariance matrices for poorly understood effects may produce very wrong uncertainty estimates
[N. Taleb, Black Swan & Antifragile]

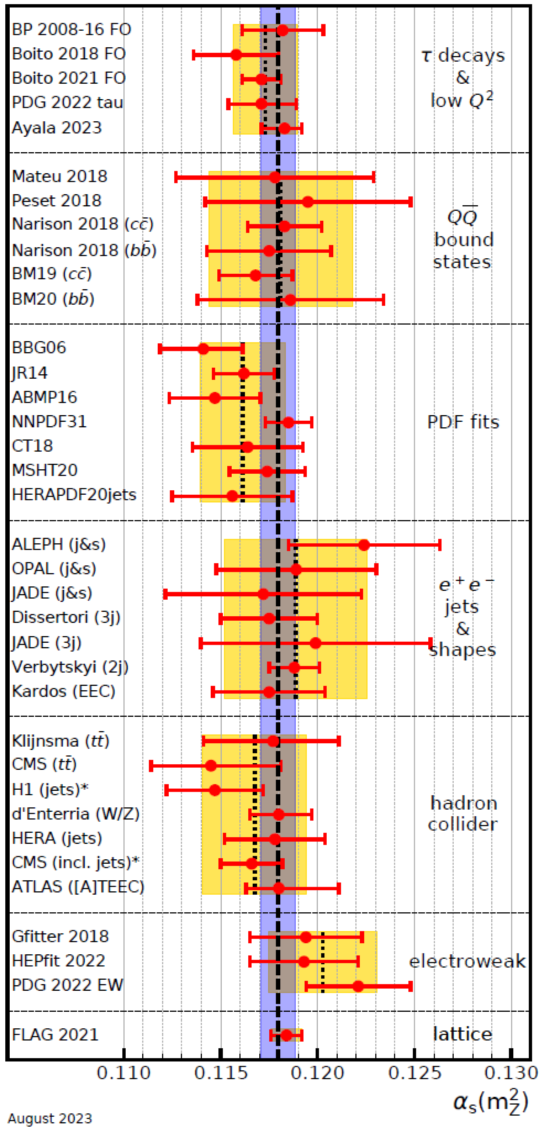
- from the theory side

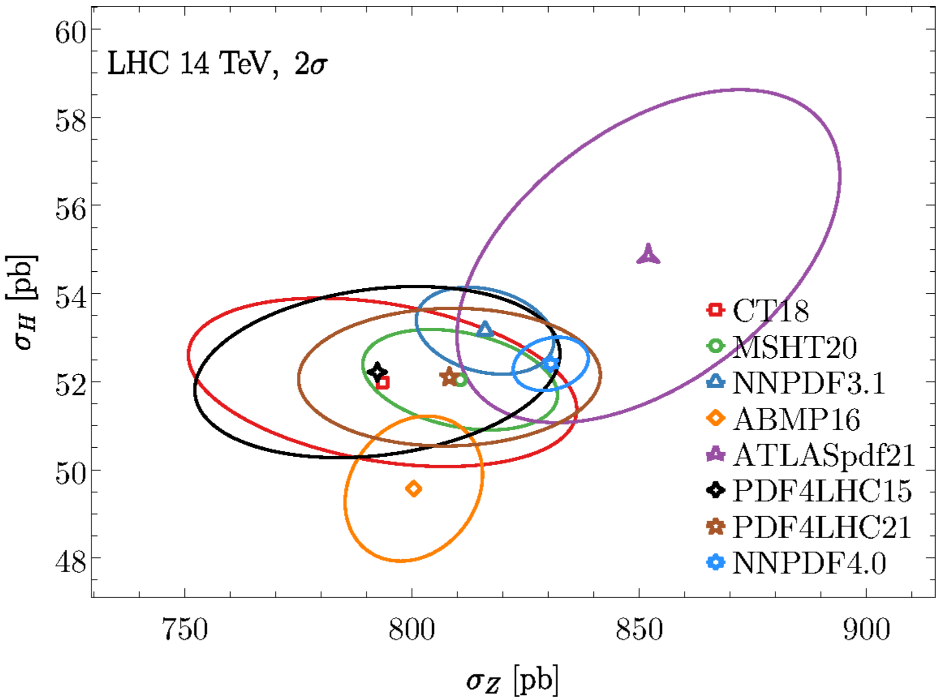




Examples: studies of theory uncertainties in the PDFs by NNPDF3.1 and ATLAS21

Replicability and PDF uncertainties



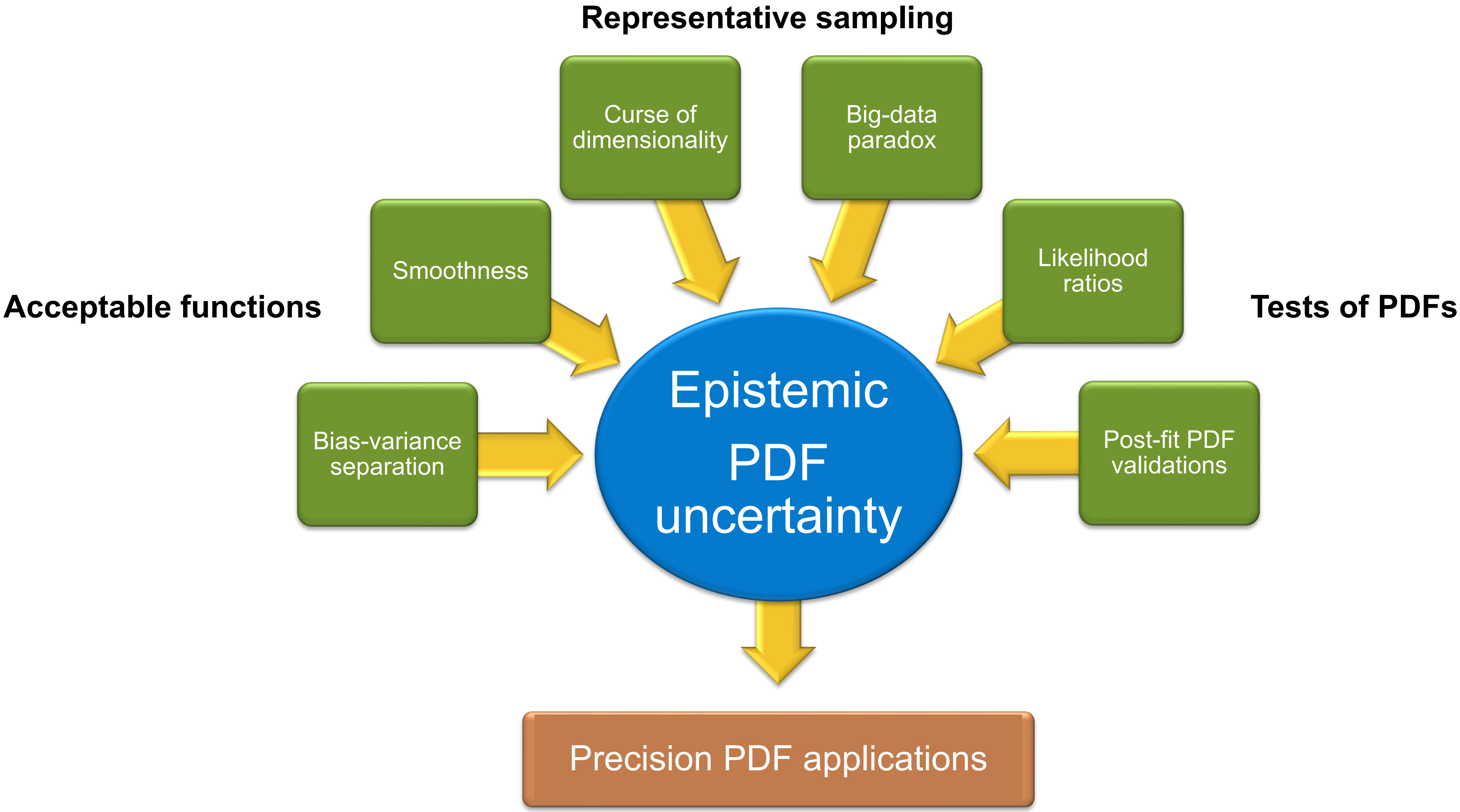


Quantification of **epistemic** PDF uncertainties is a central factor affecting **replicability** of upcoming determinations of the QCD coupling constant α_s , Higgs couplings, mass of weak bosons.

aleatory vs. **epistemic** uncertainties

Uncertainty due to lack of knowledge or incomplete models —bias (may be reduced by analysis improvements)

Statistical uncertainty propagated from experiments — reduced by increasing data size



Representative sampling

Curse of dimensionality

Big-data paradox

Acceptable functions

Smoothness

Bias-variance separation

Tests of PDFs

Likelihood ratios

Post-fit PDF validations

Epistemic PDF uncertainty

Precision PDF applications

Epistemic PDF uncertainty…

…reflects **methodological choices** such as PDF functional forms, NN architecture and hyperparameters, or model for systematic uncertainties

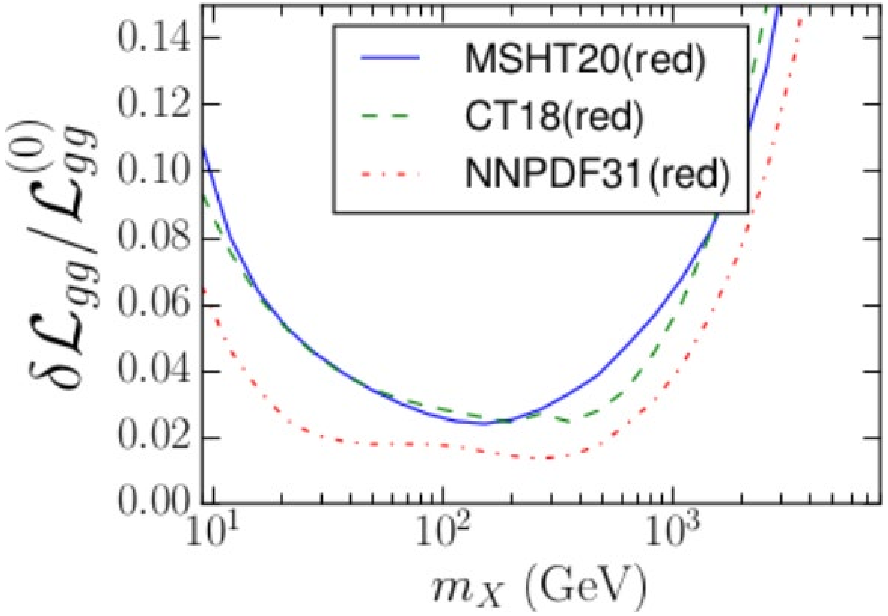
… can dominate the full uncertainty when experimental and theoretical uncertainties are small.

…is associated with the **prior probability**.

… can be estimated by **representative sampling** of the PDF solutions obtained with acceptable methodologies.

⇒ sampling over choices of experiments, PDF/NN functional space, models of correlated uncertainties…

⇒ in addition to sampling over data fluctuations

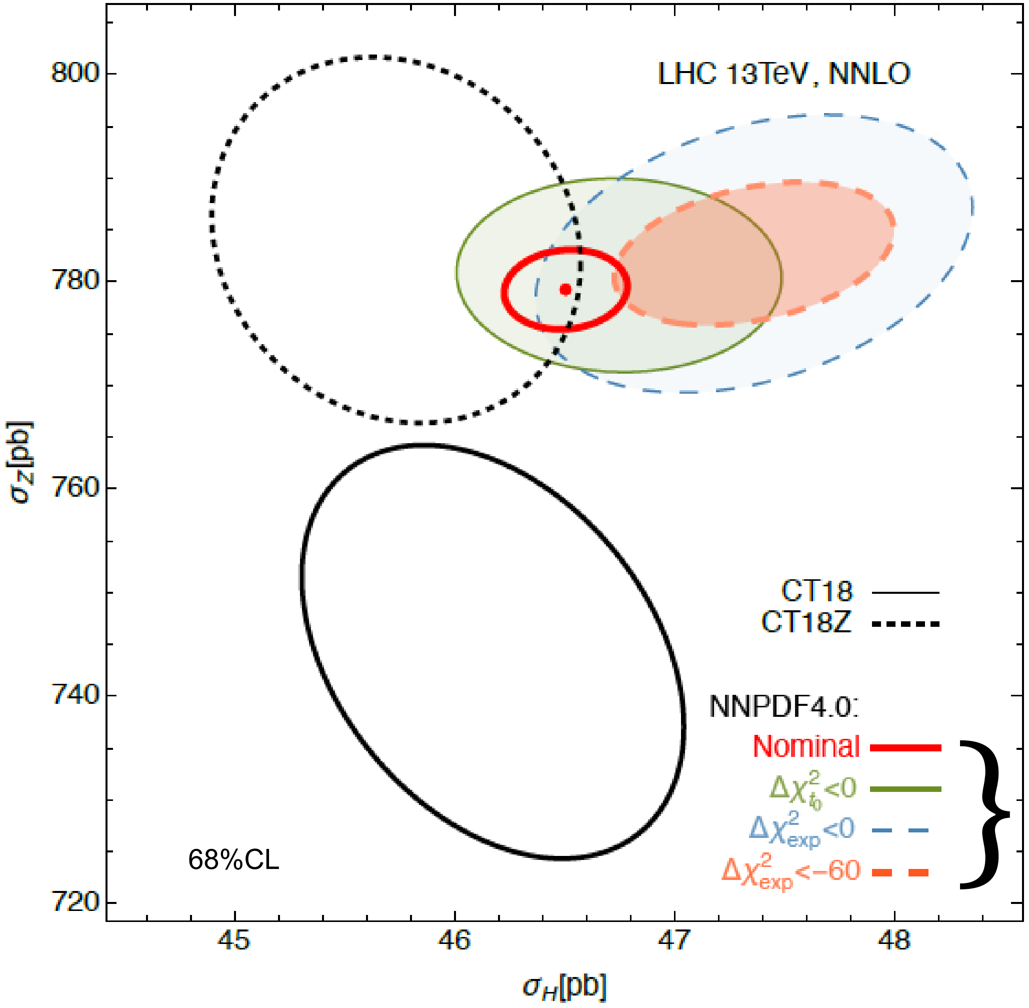


Epistemic uncertainties explain many of the differences among the sizes of PDF uncertainties by CT, MSHT, and NNPDF global fits to the same or similar data

Details in **arXiv:2203.05506**, **arXiv:2205.10444**

Example: the impact of epistemic uncertainty on NNLO Higgs and Z cross sections

Details in
A. Courtoy et al.,
arXiv:2205.10444

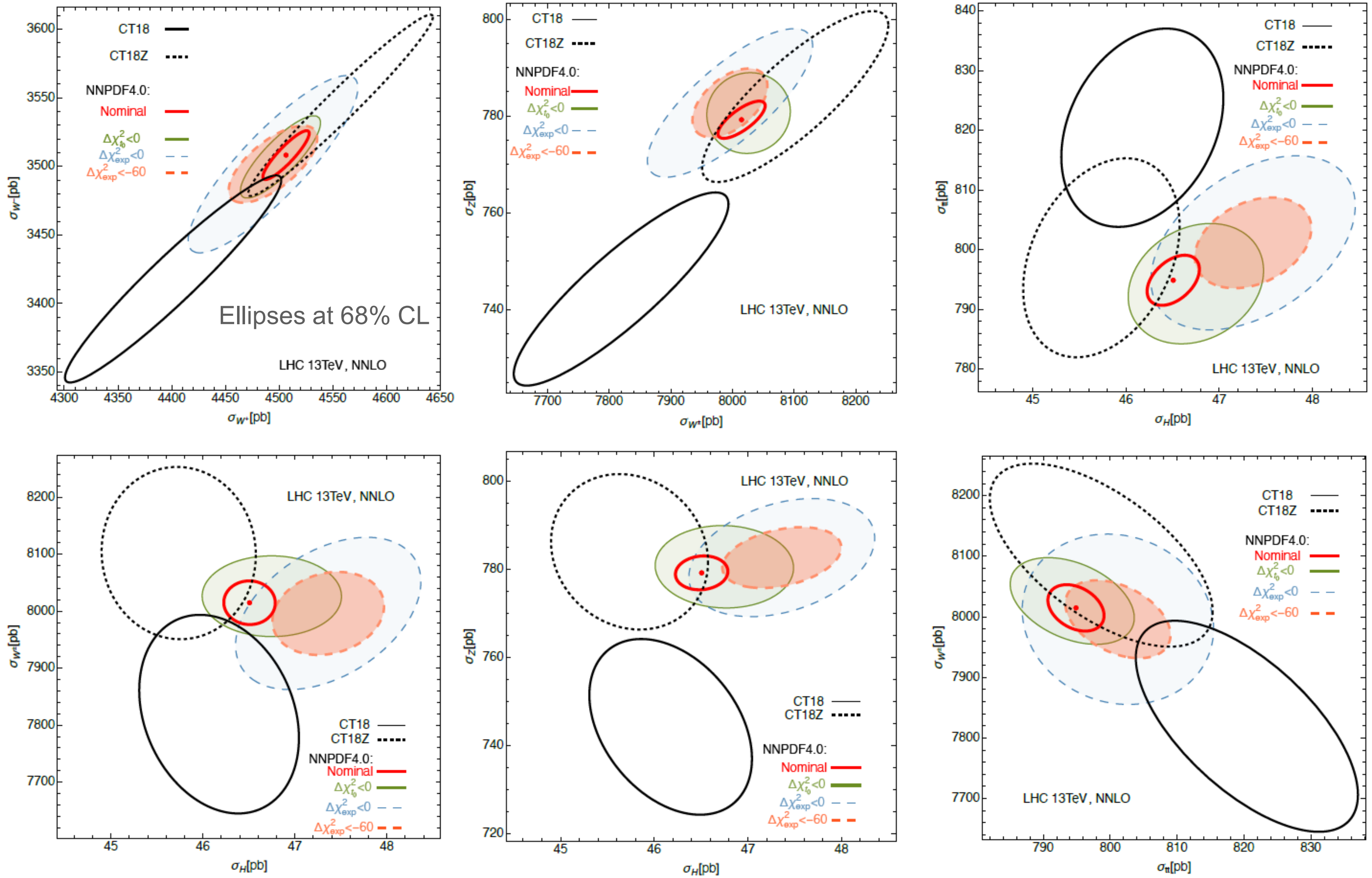


} obtained with the same NNPDF4.0 fitting code using a “**hopscotch scan**” of the PDF param. space

all ellipses contain acceptable predictions according to the likelihood-ratio test
Nominal NN4.0 uncertainty is too small!

arXiv:2205.10444

Impact of epistemic uncertainties on other cross sections



The ellipses are projections of 68% c.l. ellipsoids in N_{par}-dim. spaces

$N_{par} = 28$ and 50 for CT18 and NNPDF4.0 Hessian PDFs

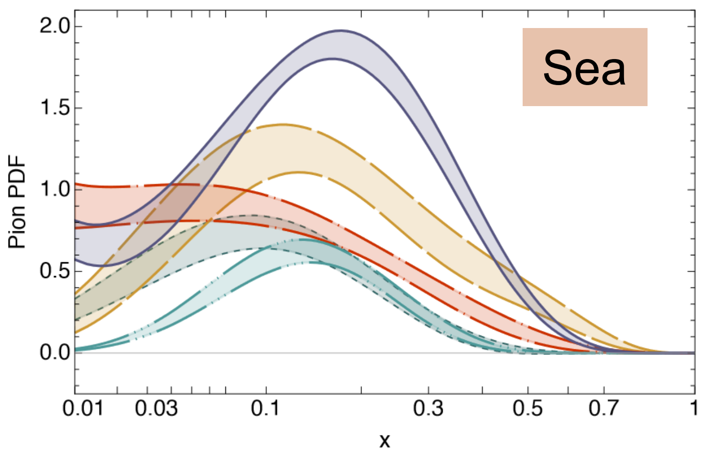
New approaches to determine the PDF tolerance

On the example of Fantômas pion PDFs

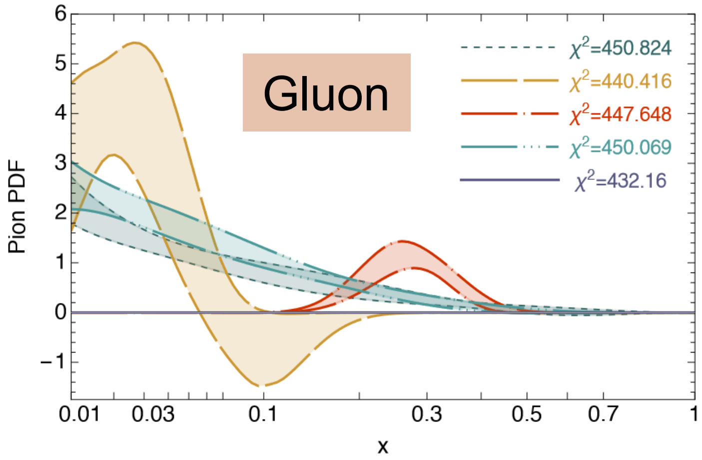
$\pi^{\pm}$

L. Kotz, A. Courtoy, M. Chavez, P. N., F. Olness, arXiv:2311.08447

xS (x,Q) at Q=1.4 GeV, 68% c.l. (band)

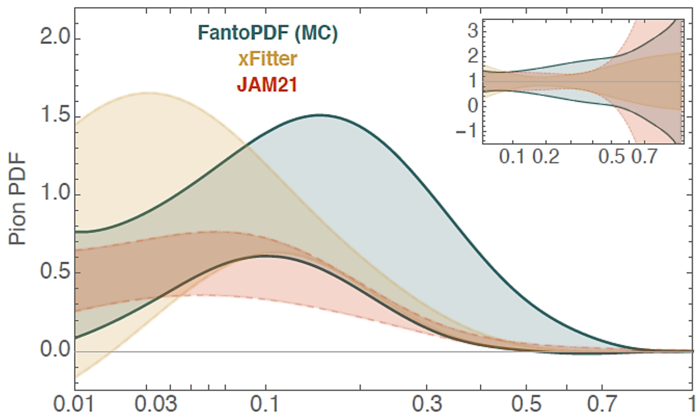


xg (x,Q) at Q=1.4 GeV, 68% c.l. (band)

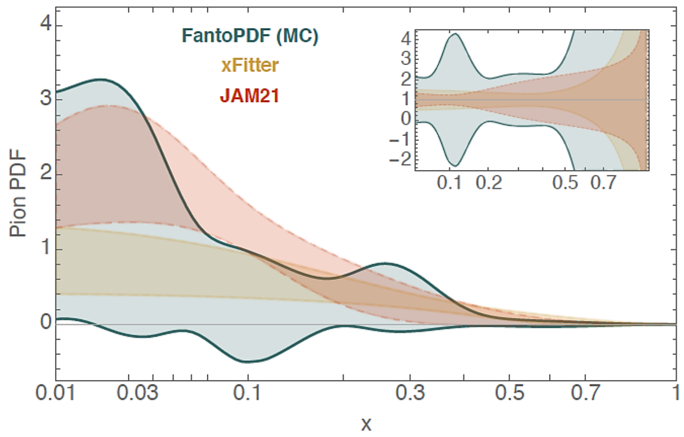


META PDF technique combines aleatory error bands for multiple parametrization forms

xS (x,Q) at Q=1.4 GeV, 68% c.l. (band)



xg (x,Q) at Q=1.4 GeV, 68% c.l. (band)



Final remarks

Epistemic uncertainty (due to parametrization, methodology, parametrization/NN architecture, smoothness, data tensions, model for syst. errors, ...) is increasingly important in (N)NNLO global fits as experimental and theoretical uncertainties decrease

Nominal PDF uncertainties in high-stake measurements (ATLAS W mass, Higgs cross sections…) thus should be tested for *control of tensions* and *robustness of sampling over acceptable methodologies.*

Smoothness of Hessian and NN PDFs is another such aspect associated with the prior that should be explored.

Tools for such studies already exist, e.g. hopscotch scans.

This is also necessary for combination of PDFs including data correlations
[LHC EW, Jet & Vector boson WGs, https://tinyurl.com/4wcnd8xn; https://tinyurl.com/2p8d8ba3; https://tinyurl.com/2p8tcn5b; Ball, Forte, Stegeman, arXiv:2110.08274].

Better control of the epistemic uncertainties is central for replicability of upcoming QCD measurements.

Strategies for improving replicability and reproducibility

Preselection of planned studies based on their likely replicability

Detailed documentation of methods and uncertainty quantification in the publications

Training of researchers in relevant statistical methods

Journal policies that encourage replicability

Support from the funding agencies for the research infrastructure and collaborations focusing on replicability

Support for open publication of the analysis codes and key data, using agreed-upon formats

“Skin-in-the-game” incentives for researchers to produce replicable results

Based on “REPRODUCIBILITY AND REPLICABILITY IN SCIENCE”