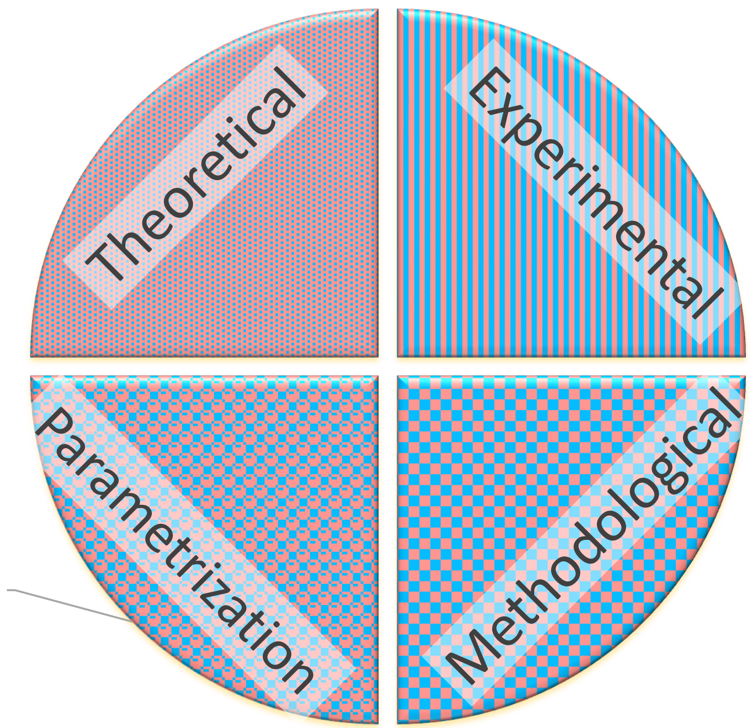
Argonne Mini-Workshop on Monte Carlo Methods

Components of uncertainty in parton distributions for the LHC



In each category, one must maximize

PDF determination accuracy (accuracy of experimental, theoretical and other inputs)

PDF sampling accuracy (adequacy of sampling in space of possible solutions)

MC integration and sampling errors are an important part of the total uncertainty

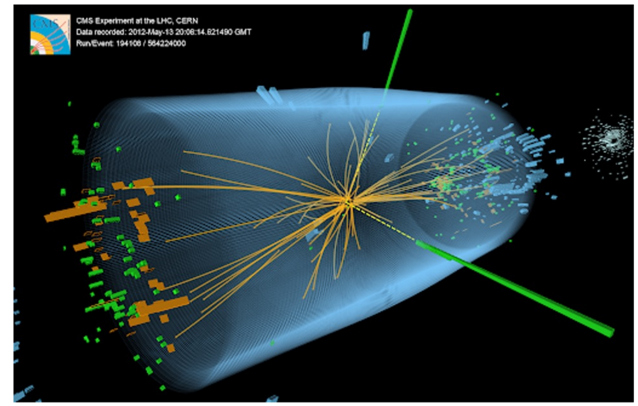
Parton distributions and Inverse Problems in High-Energy Physics

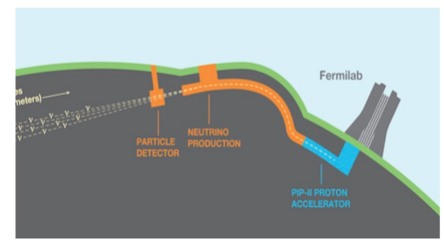
physics motivation for MC studies

Tim Hobbs, Argonne National Lab

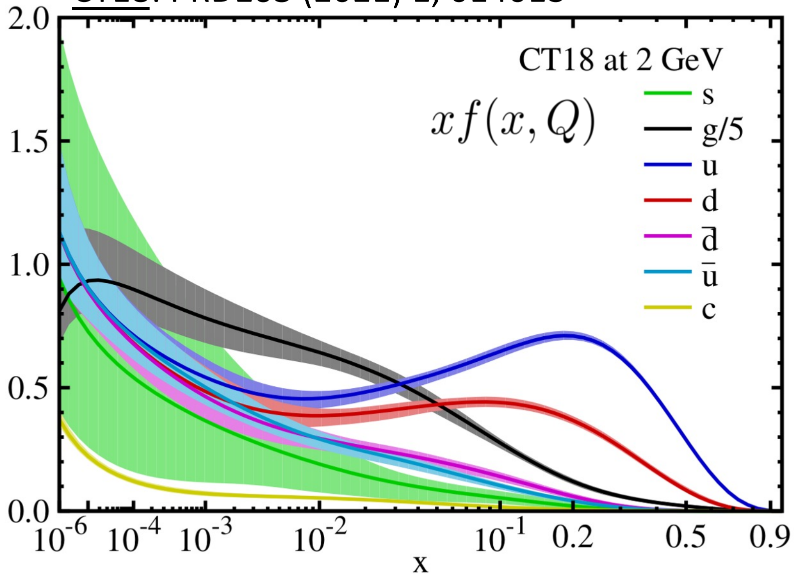
18th May 2023

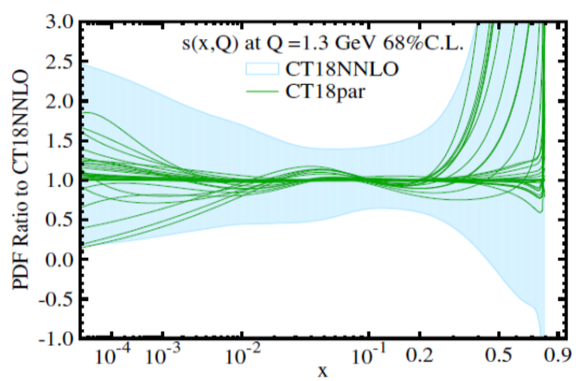
Argonne NATIONAL LABORATORY





CT18: PRD**103** (2021) 1, 014013





Welcome!

Monte Carlo (MC) methods are now ubiquitous

→ active area in mathematics, statistics, computational science

→ extensive applications throughout HEP, nuclear physics (both theory and expt)

today: hear a mix of <u>informal</u> talks and <u>discussions</u> on open issues

→ joint HEP/MCS seminar, Fred Hickernell of IIT

→ morning/afternoon sessions on computation and physics applications

https://indico.fnal.gov/event/59808/

computation ⟷ physics

computation

- low-discrepancy MC sampling (Hickernell)
- AI, Gaussian processes (Rao)
- MC sampling and lattice QCD (Jin)

physics

- MC in HEP
  - theory, event generation (Isaacson)
  - experiment (Chekanov)
- nuclear theory and simulation (Lovato)
- PDF uncertainty quantification (Courtoy)

possible outcomes

complementary developments in computation and physics

→ math/stat. and comp. sci.: formal MC progress, novel algorithms

→ physics: use cases to motivate and sharpen MC methods

discussion on needs and collaborative opportunities

→ forum this afternoon; draft summary document (?)

https://indico.fnal.gov/event/59808/

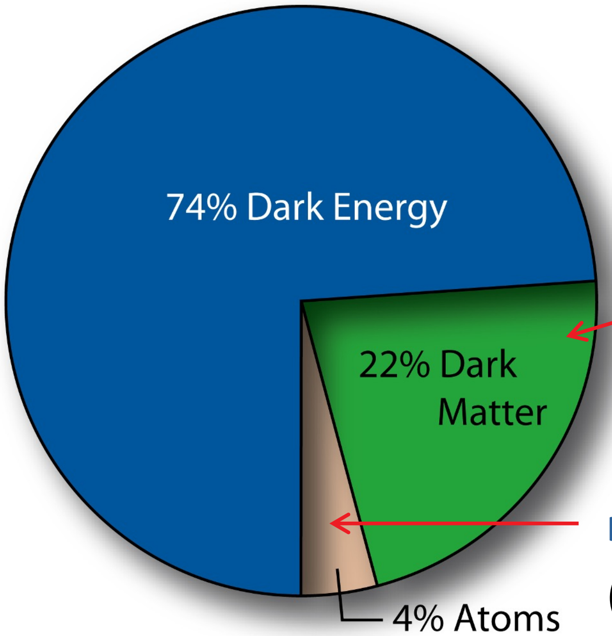
this talk, physics motivation from HEP: PDFs as MC-relevant inverse problem

→ illustrate why particle physicists care deeply about PDF precision

→ next talk, Aurore Courtoy on MC sampling and uncertainty quantification (UQ)

HEP: quest for "new physics" (e.g., dark matter) → Standard Model tests

→ activity at numerous facilities using many approaches



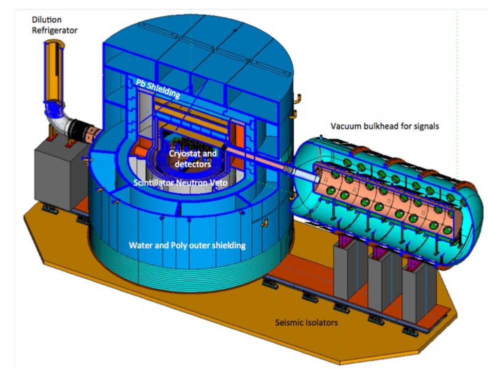
to find this

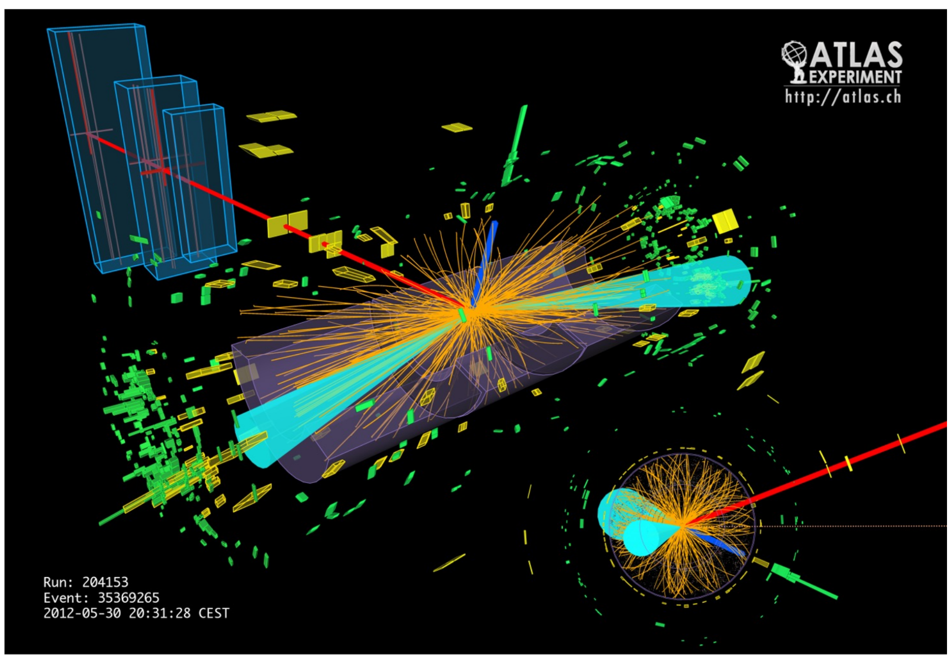
must understand this

(Baryonic matter)

"indirect detection," *e.g.*, AMS

"direct detection," *e.g.*, SuperCDMS





...look for the unexpected in Standard Model processes

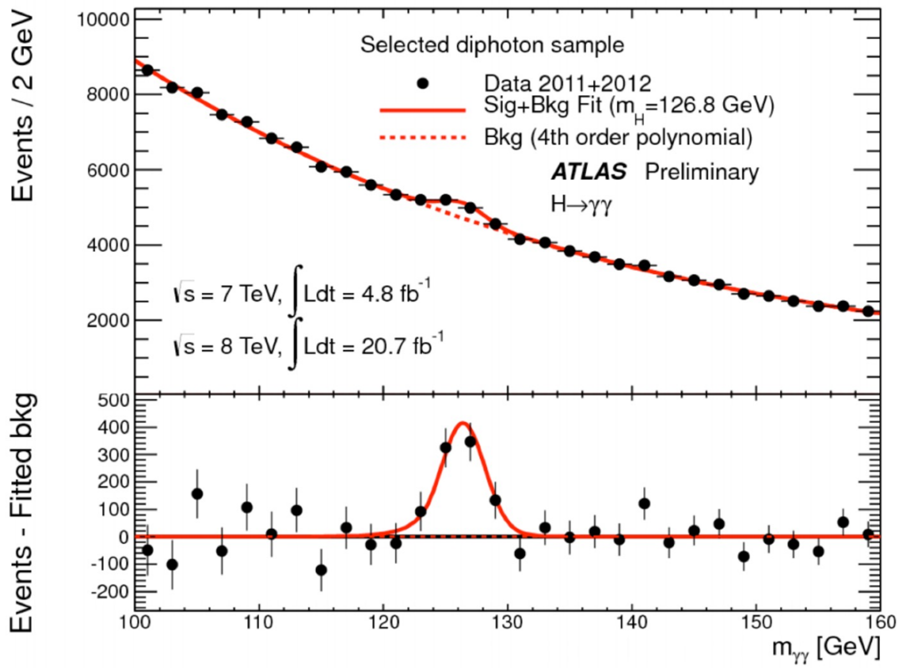
this talk: collider searches;
proton-proton scattering at the LHC, ...

searching for physics beyond the Standard Model (BSM) at colliders

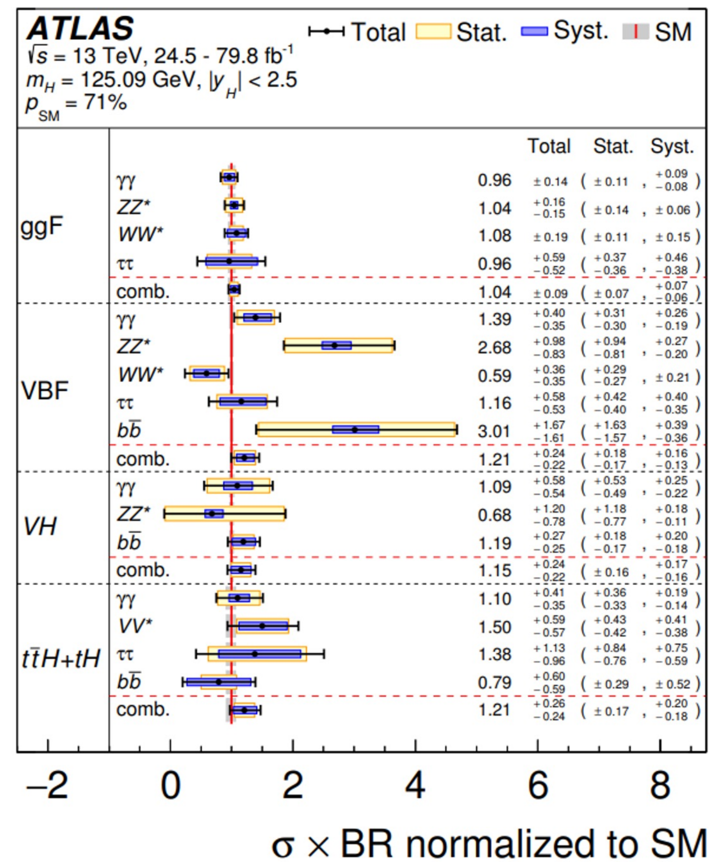
→ "discovery" searches

e.g., examining cross sections, etc., in previously unprobed kinematical regions

Higgs discovery, 2012



Higgs prod·decay/SM (PDG)



→ "precision" searches ★

or, testing the Standard Model through extremely fine measurements...

(deviations could reveal presence of new particles/interactions!)

HEP measurements depend on parton distributions

MANY measurements to test the SM involve colliding protons (and nuclei – talk, A. Lovato)

→ protons scatter through parton-level interactions: quark-quark, quark-gluon, …

→ precision needs accurate theory + **parton distribution functions (PDFs)**

[extracted from data…]

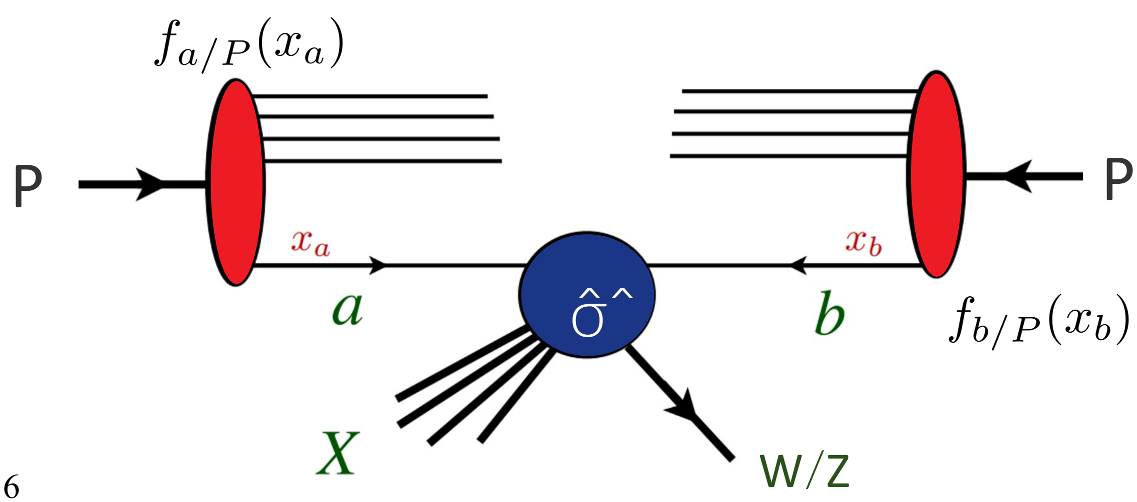
for gauge-boson *pp* production

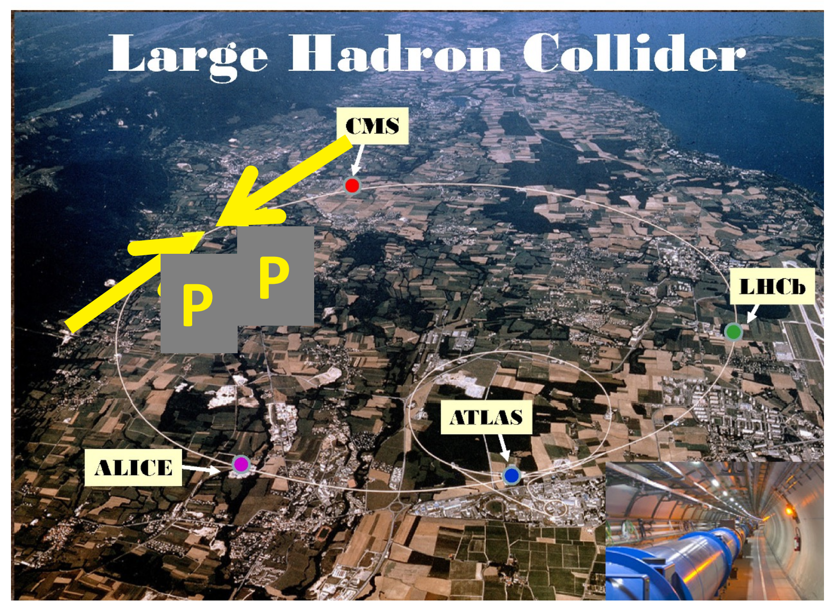
$$\sigma(PP \to W/Z+X) = \sum_n \alpha_s^n \sum_{a,b} \int dx_a dx_b$$

$$\times\, f_{a/P}(x_a)\, \hat{\sigma}^{(n)}_{ab\to W/Z+X}(\hat{s})\, f_{b/P}(x_b)$$

proton **PDFs**

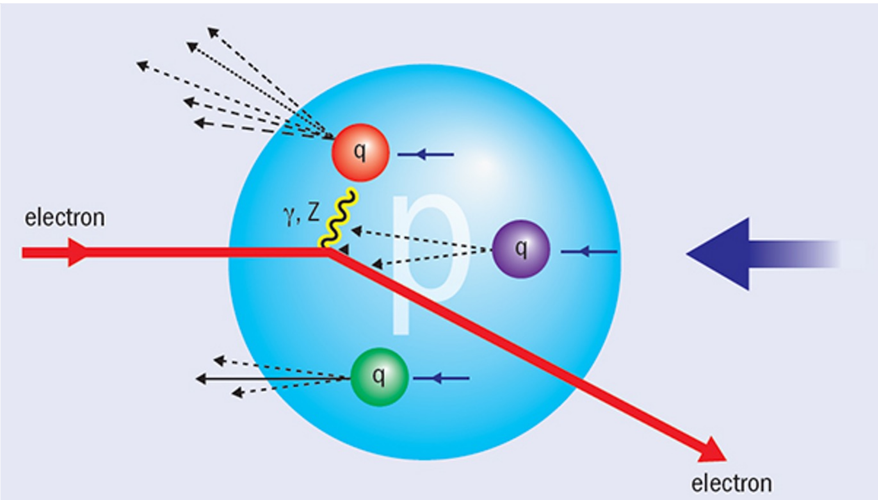
perturbative QCD matrix elements





PDFs and imaging (internal) proton structure: Deeply-Inelastic Scattering (DIS)

high-energy electron-proton scattering can provide "clean" access to proton's **quark** and **gluon** (force carrier) constituents



→ electroweak probe resolves spatial correlations of quark fields

$$\sigma^{ep \to e' X}(x, Q^2) \sim$$

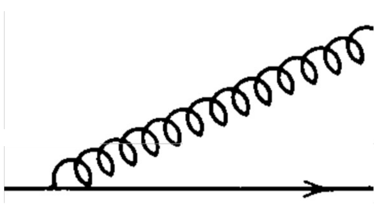
$$F_2(x, Q^2) = x \sum_q e_q^2 \, (f_q + f_{\bar{q}})[x, Q^2]$$

↓

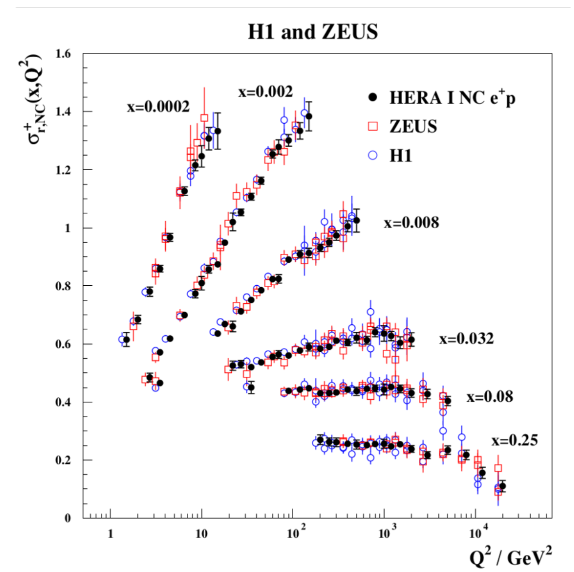
parton distribution functions (PDFs)

$f_q(x,Q^2)$: probability for quark of 'flavor' q (up, down, strange, …) carrying a fraction x of proton's momentum at energy Q

DIS data at different momentum scales constrain gluon



(quark fields exchange momentum through gluon radiation)



why does this work? ...the remarkable properties of QCD

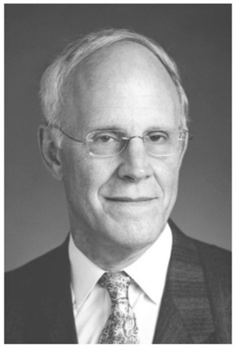


Photo from the Nobel Foundation archive.
David J. Gross
Prize share: 1/3

Photo from the Nobel Foundation archive.
H. David Politzer
Prize share: 1/3

Photo from the Nobel Foundation archive.
Frank Wilczek
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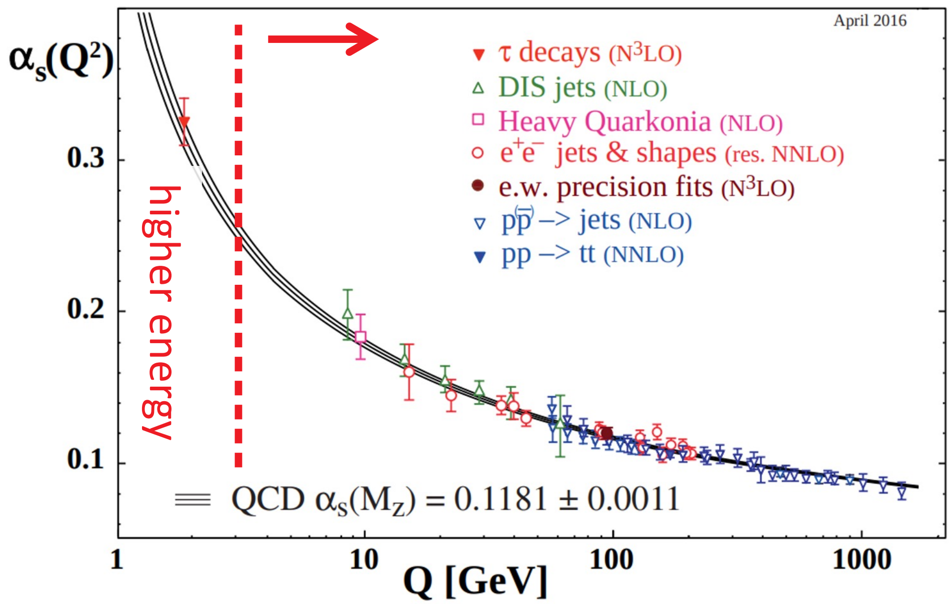
the **β**-function of QCD is negative-definite,

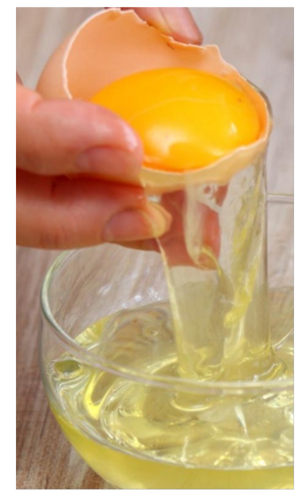
$$\beta(\alpha_s) = \mu_R^2 \frac{d\alpha_s}{d\mu_R^2} = -(b_0 \alpha_s^2 + \dots) < 0$$

→ quark-gluon interactions weak at high energies; **use perturbation theory**



↕ **QCD factorization**

at low energies interactions strong (nonperturbative); **extract PDFs**



<u>fundamental question</u>: how does QCD, which so successfully describes high-energy processes, give rise to the emergent properties of low-energy bound states?

→ *a chief motivation* for QCD as a field

PDF determination as a large inverse problem

in principle, PDFs calculable via nonperturbative techniques (lattice QCD), but extremely challenging

[talk, X. Jin]

$$f_{q/p}(x, Q^2) = \int \frac{d\xi^-}{4\pi} e^{-i\xi^- k^+} \langle p \,|\overline{\psi}(\xi^-)\gamma^+ \mathcal{U}(\xi^-, 0)\psi(0)\,|p\rangle$$

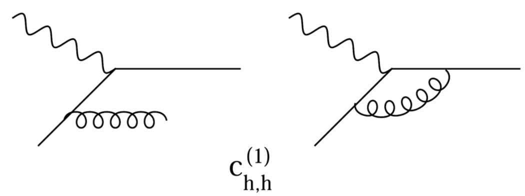
- QCD factorization allows PDFs to be unfolded from data; schematically:

empirical data (cross section)

$$\sigma = C \otimes f_{q/p}$$

→ non-perturbative PDFs: unfold from data

C ↓ calculable in perturbation theory



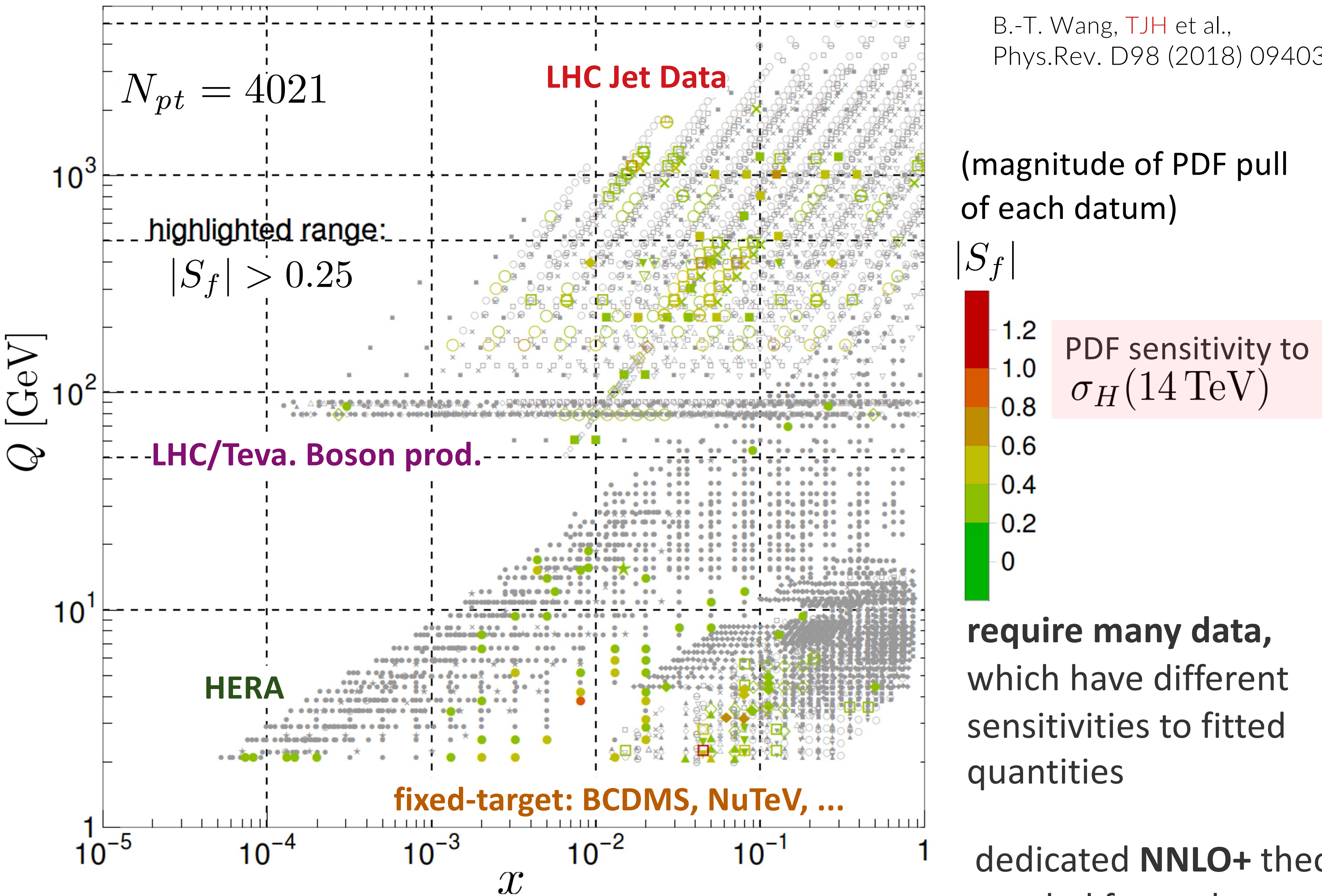
- PDFs are parametrized and fitted at some initial energy scale, $Q_0 \sim M = 1\,\mathrm{GeV}$

  → perturbative *evolution* specifies dependence on $Q^2 > Q_0^2$

- must also unfold complicated flavor and *x* dependence, $x \in [10^{-5}, 0.7]$

fit the world's data from a diverse range of scales and processes

modern PDF analysis: constraints from many data



B.-T. Wang, TJH et al.,
Phys.Rev. D98 (2018) 094030

require many data, which have different sensitivities to fitted quantities

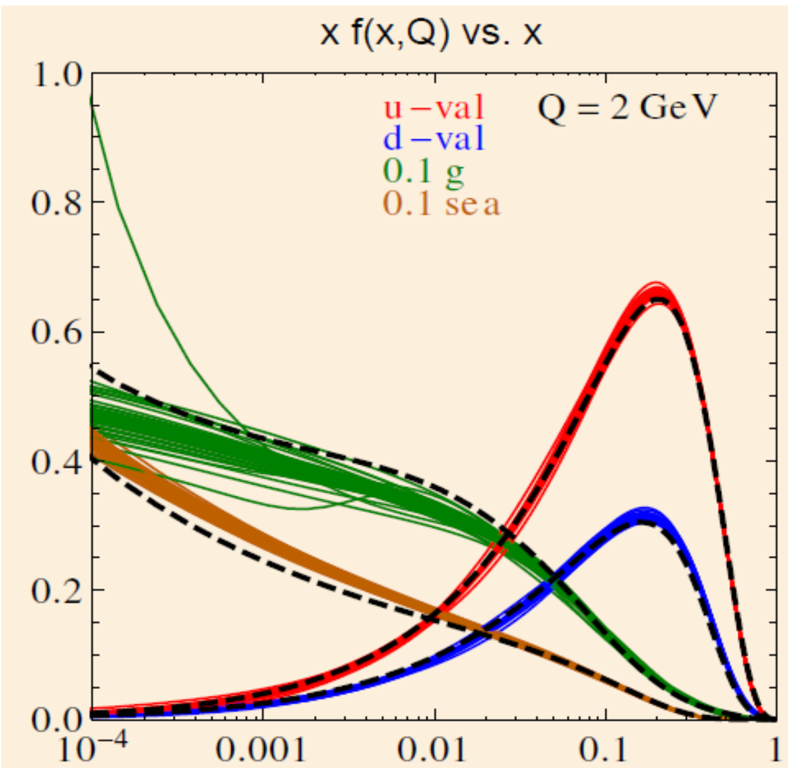
dedicated **NNLO+** theory needed for each

two types of modern PDF analysis approaches

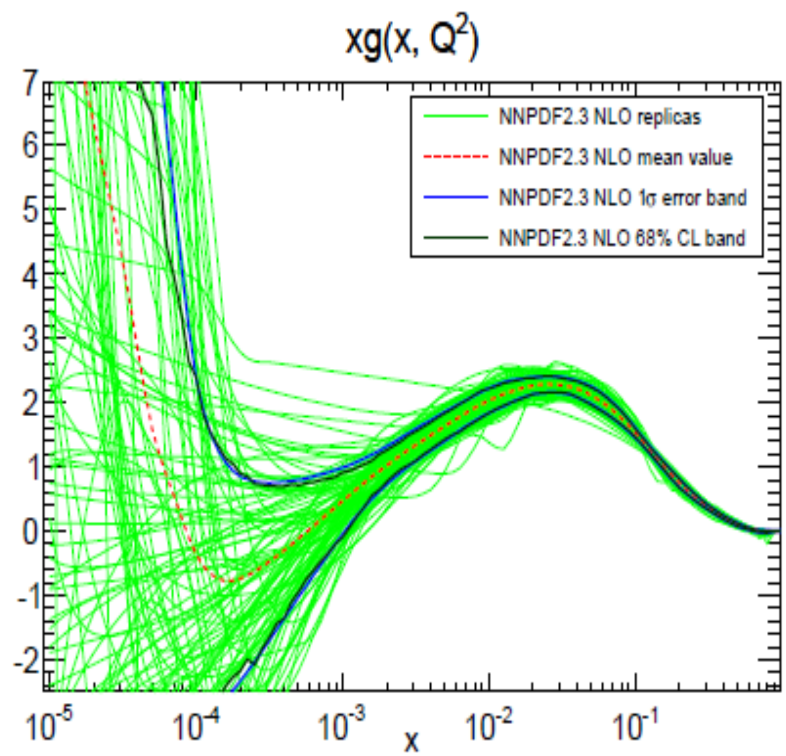
Two powerful, complementary representations.

Analytic parametrizations +

Hessian PDF eigenvector sets
(ABM, CTEQ, HERA, MMHT,…)



Neural network parameterizations +
Monte Carlo PDF replicas **(NNPDF)**



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

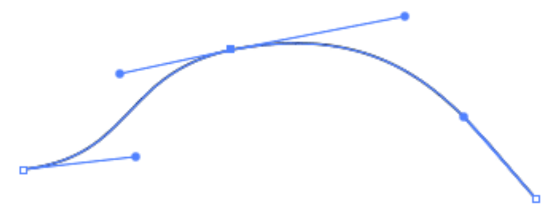
multivariate parametric forms

A typical PDF set may depend on tens to several hundreds of free parameters

CT18 parametrizations: PDF functional forms must be flexible to accommodate a variety of behaviors at initial scale Q_0 are given by

$$f_a(x, Q_0) = A x^{a_1} (1-x)^{a_2} B_a^{(n)}(x; a_3, a_4, \cdots)$$

$\mathrm{B}_{\mathrm{a}}^{(n)}(x) = \sum_{k=0}^{n} a_{k+2} \binom{n}{k} x^k (1-x)^{n-k}$
are **Bézier curves** – flexible polynomials familiar from vector graphics programs

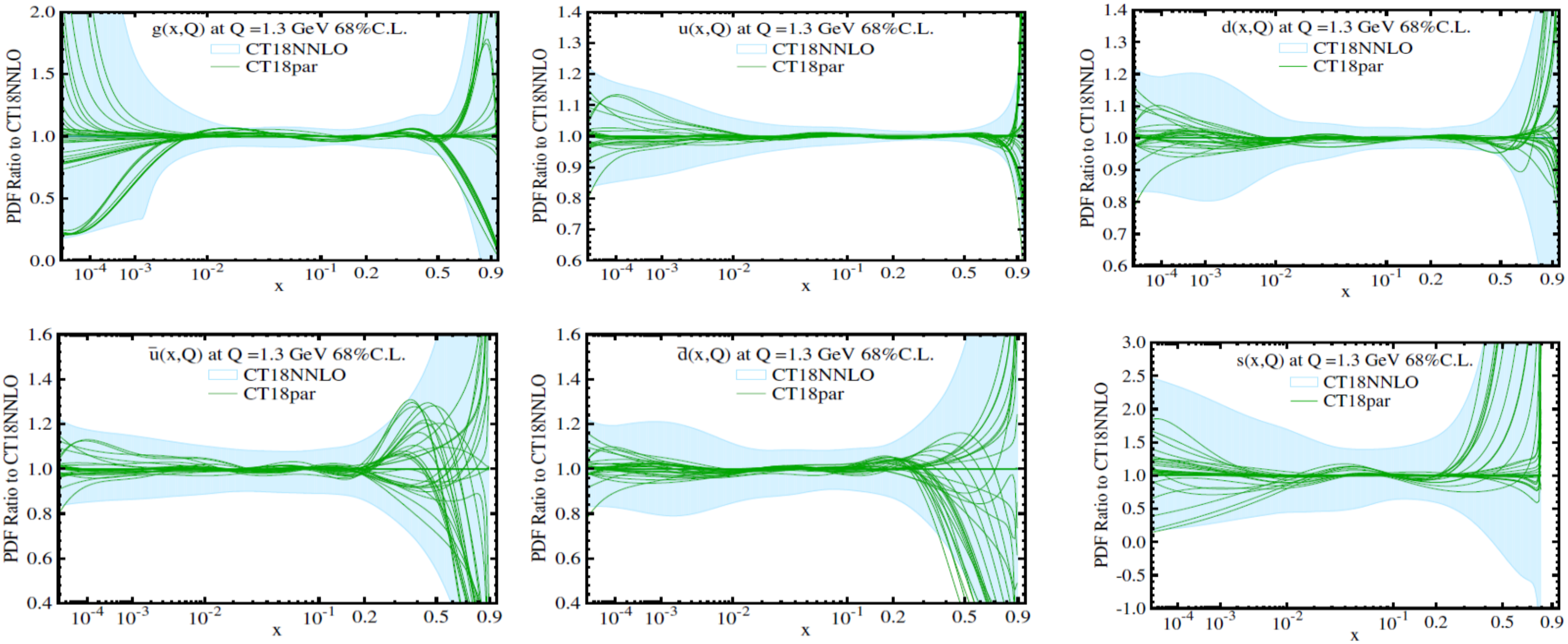


Bézier curves can mimic a variety of behaviors of PDFs and their uncertainties. A powerful alternative to neural networks!

[A. Courtoy, P. N., arXiv: 2011.10078]

- *interpretability*: parametric forms can also more readily map to QCD-based physics models of PDFs ultimately, the “true” underlying parametrization is unknown

250+ candidate nonperturbative parametrization forms of CT18 PDFs



- CT18par – a sample of **some** non-perturbative parametrization forms tried in CT18
- No data constrain very large-x or very small-x regions.

neural-network parametrizations of PDFs

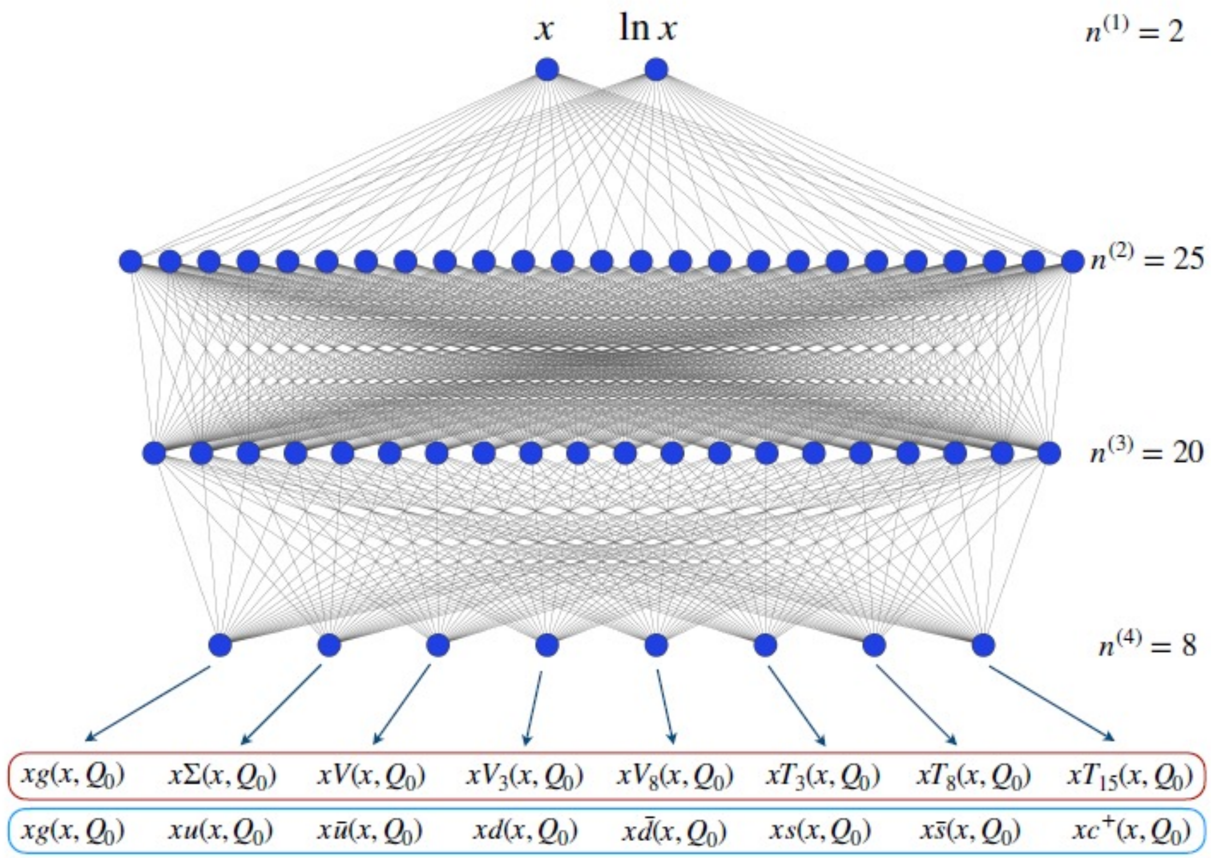


Figure 3.9. The neural network architecture adopted for NNPDF4.0. A single network is used, whose eight output values are the PDFs in the evolution (red) or the flavor basis (blue box). The architecture displayed corresponds to the optimal choice in the evolution basis; the optimal architecture in the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

R. Ball et al. (NNPDF), arXiv:2109.02653

- parametrize PDFs' x dependence through multi-layer perceptron
  - → best fit and error determined from $\mathcal{O}(1000)$ Monte Carlo replicas

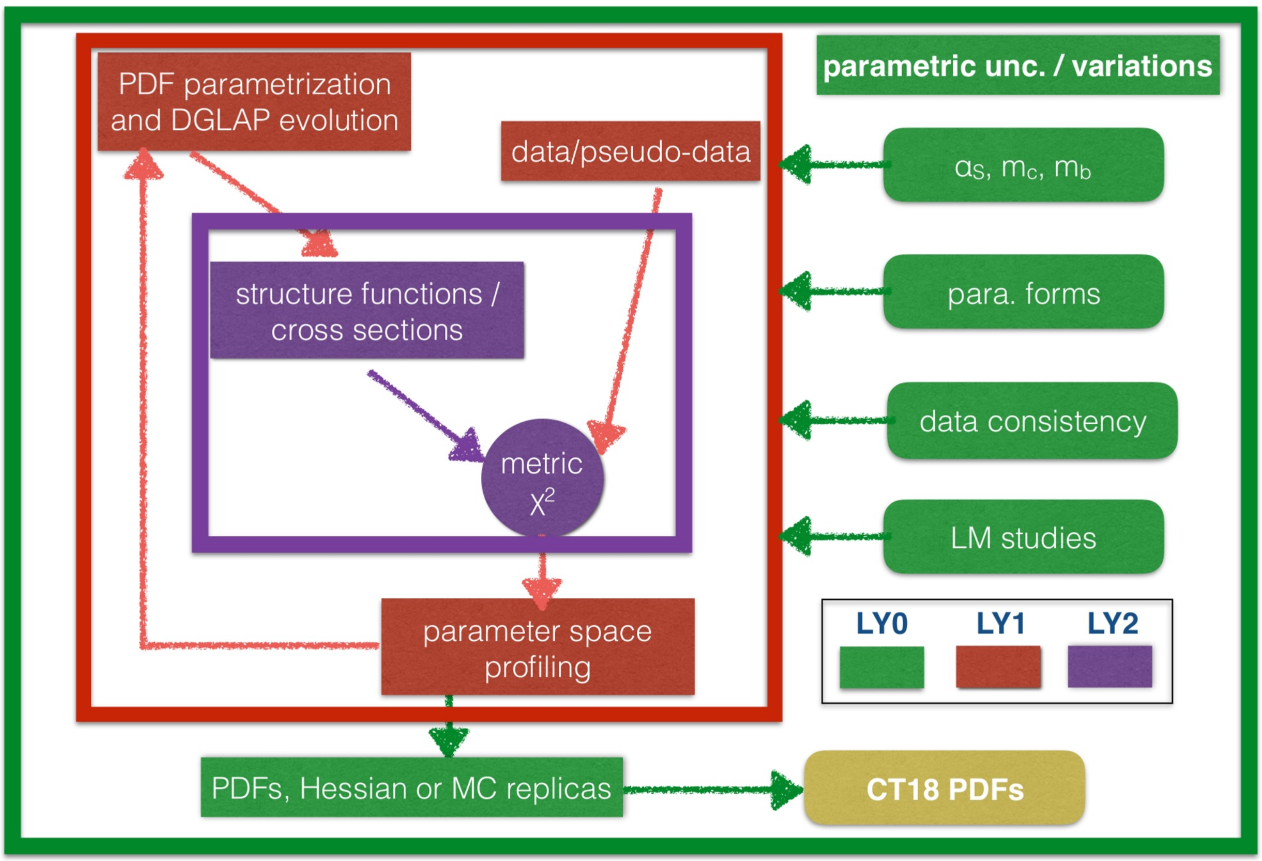
all PDF analyses combine data, theory in global (simultaneous) analyses

<u>critical point</u>: not enough to blindly fit small models to few high-profile expts

→ correlations may produce systematic biases

→ there may be incompatibilities among incompletely understood theory ingredients

→ tensions may exist among data



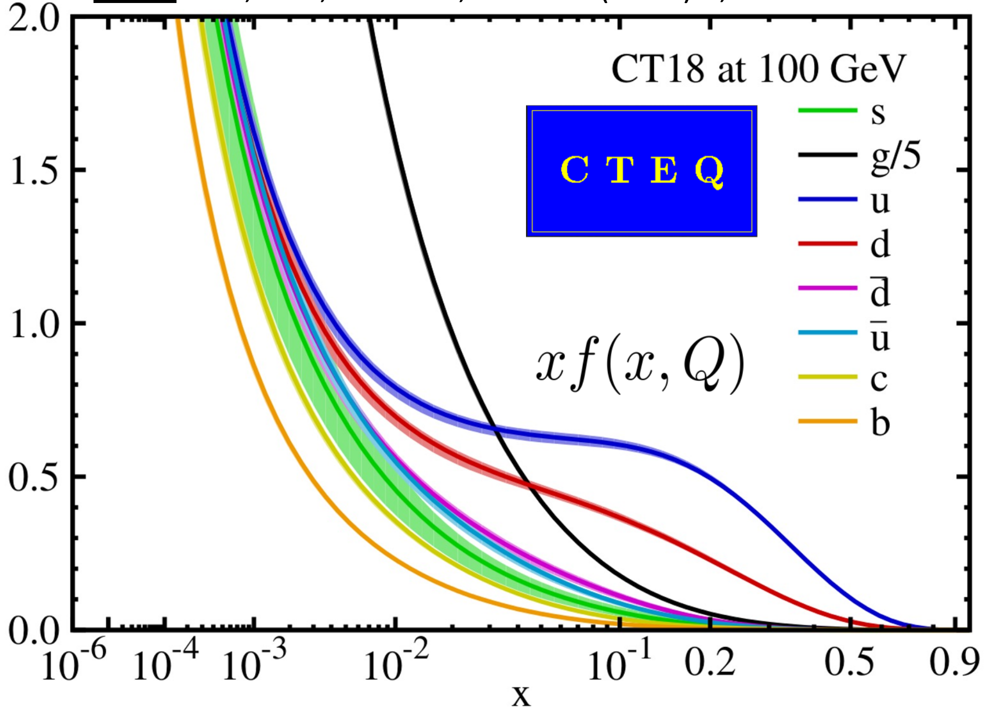
must perform <u>comprehensive</u> **global** analyses

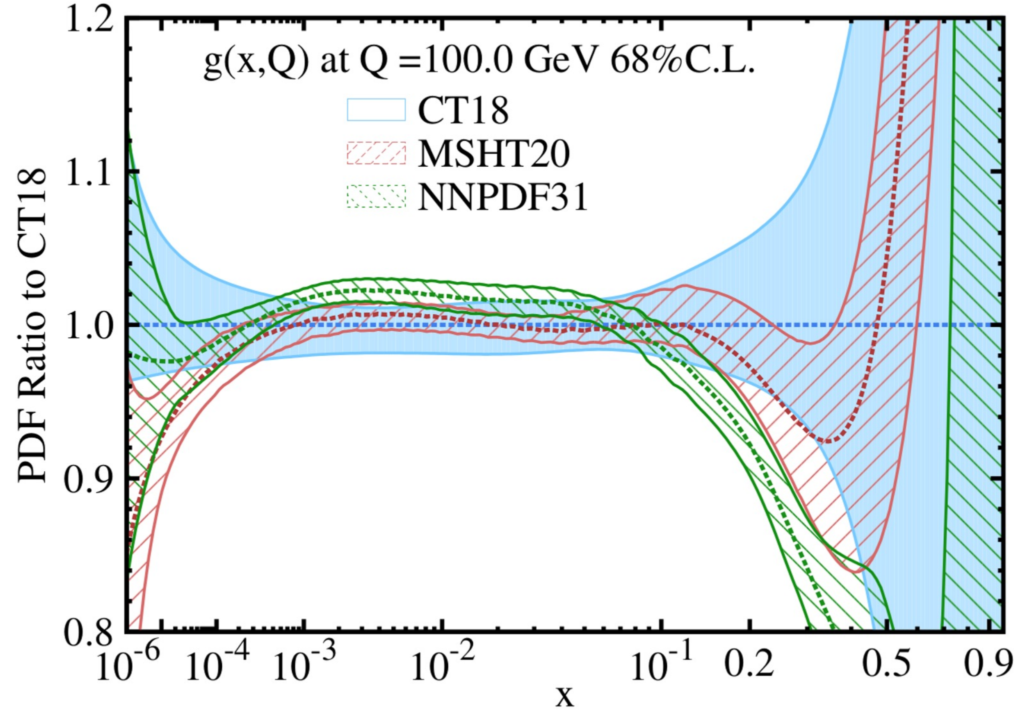
result: QCD global fits – precision for HEP from diverse data

upcoming programs need high-precision → reductions to PDF uncertainties

→ necessary to extend theory accuracy; MC improvements

CT18: Hou, Gao, TJH et al, PRD**103** (2021) 1, 014013



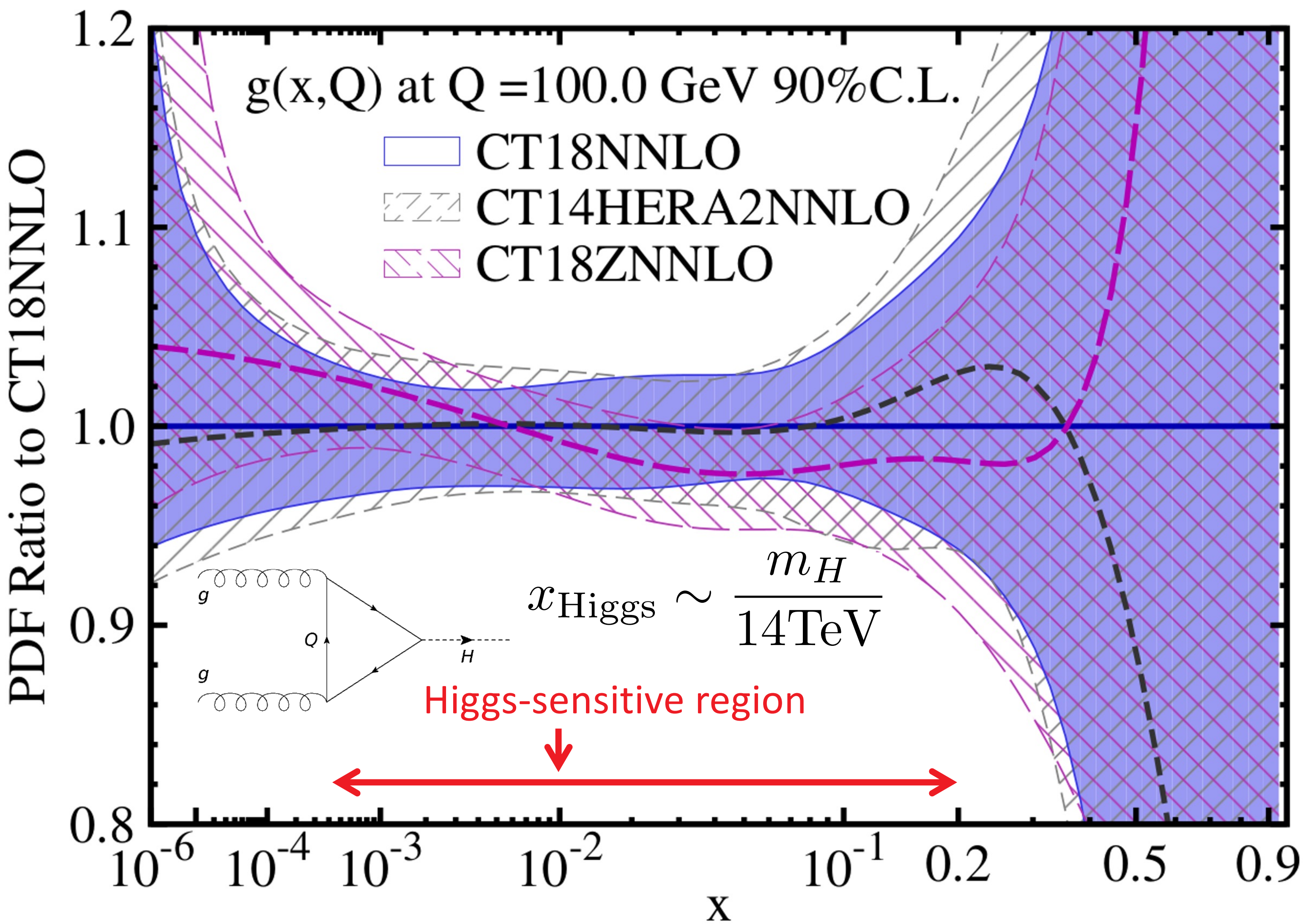


→ NLO EW corrections, especially for LHC data

→ extensive benchmarking for HEP; PDF4LHC21

J. Phys. G 49 (2022) 8, 080501

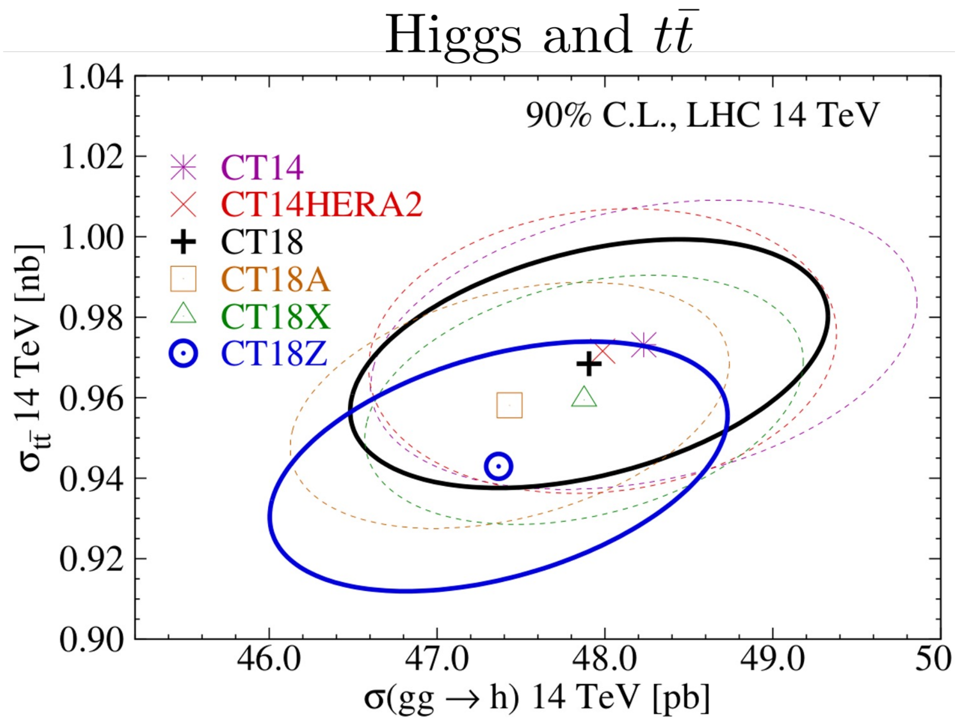
LHC Run-1 gluon PDF impact in CT14 → CT18(Z)



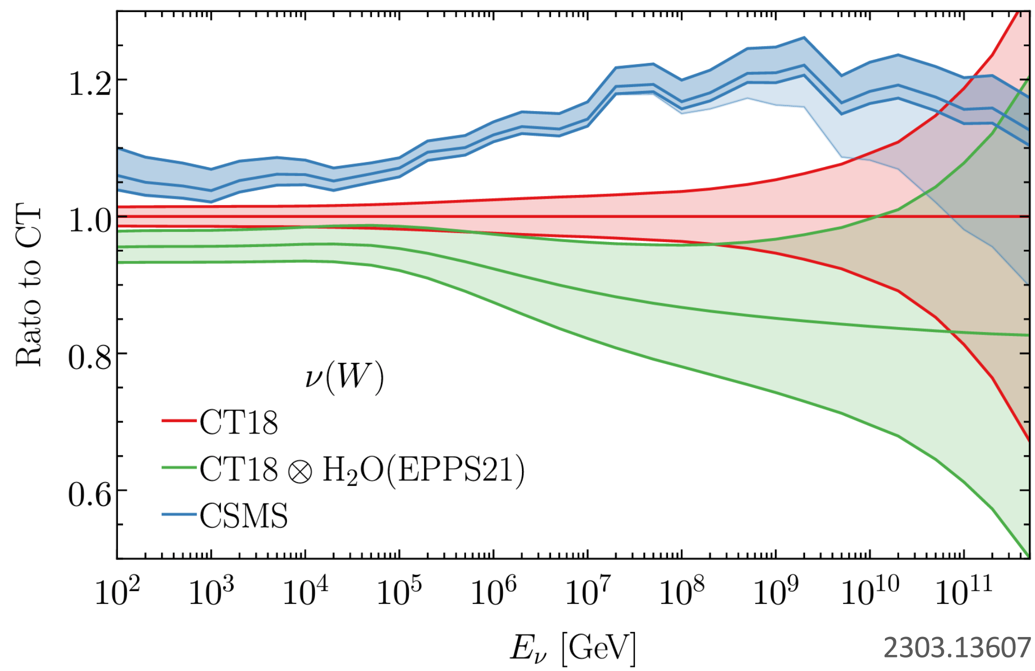
knowledge of the gluon content of the nucleon directly translates into constraints on SM Higgs production

PDF errors translate into phenomenological limitations

- from PDF analysis, state-of-the-art predictions for fundamental LHC observables → *e.g.*, **total cross sections at 14 TeV**



charged-current DIS neutrino cross section



- pervasive issue beyond LHC: neutrino cross sections similarly PDF-limited

…above, for ν telescopes; analogous PDF uncertainties at low energies relevant for DUNE

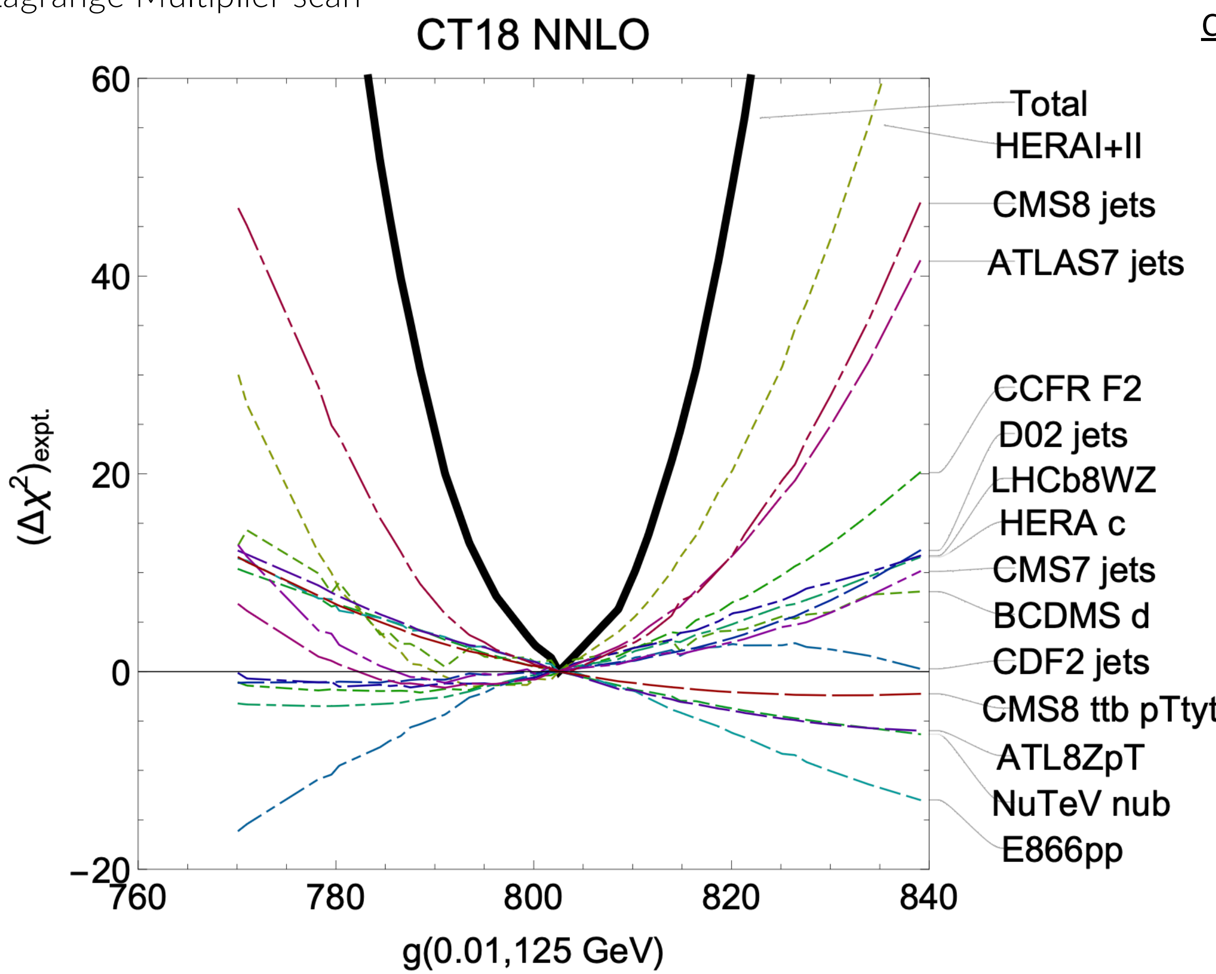
interface with MC event generators, experimental interpretation

[talks, J. Isaacson, S. Chekanov]

compatibility of fitted data sets is a crucial question

tensions among individual fitted experiments drive a larger PDF uncertainty

Lagrange Multiplier scan



<u>CT18:</u> PRD**103** (2021) 1, 014013

examine change in χ^2 as PDF continuously varies away from fitted central value

larger gluon… and Higgs cross section… favored by some expts [like E866pp], but not others [like 8 TeV CMS jets]

serious impediment to higher precision in PDFs and resulting theory predictions

Sources of PDF uncertainty

Kovarik et al., arXiv: 1905.06957

1. **Experimental uncertainties**, e.g., statistical, correlated and uncorrelated systematic uncertainties of each experimental data set;

2. **Theoretical uncertainties** due to the absent radiative contributions, approximations in parton showering simulations

3. **Parameterization uncertainties** associated with the choice of the PDF functional form or AI/ML replica training algorithm
   - contribute at least a half of the CT18 total PDF uncertainty

4. **Methodological uncertainties** associated with the selection of experimental data sets, fitting procedures, and goodness-of-fit criteria.

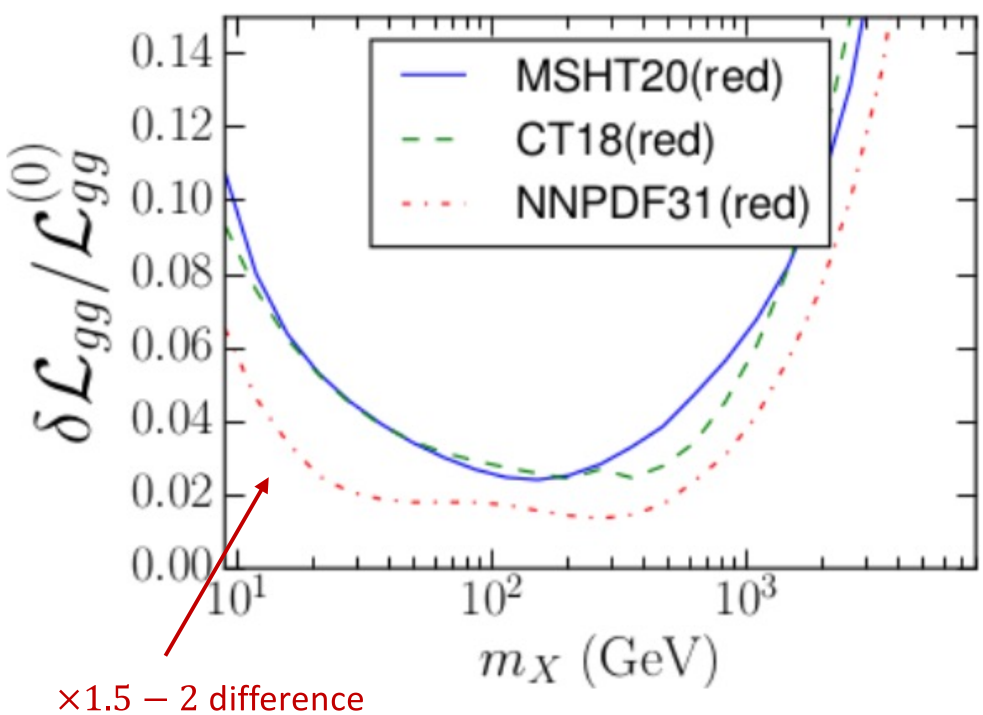
The uncertainty of published CT18 PDFs estimates the sum of four contributions

→ **in practice, each of these may contribute to tensions among fitted data sets**

the tolerance puzzle

Relative PDF uncertainties on the gg luminosity at 14 TeV in three PDF4LHC21 fits to the **identical** reduced global data set

arXiv:2203.05506

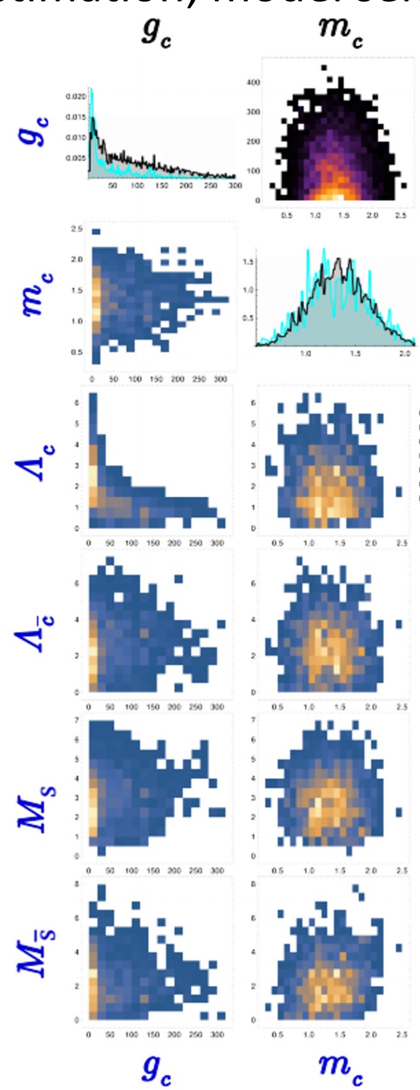


While the fitted data sets are identical or similar in several such analyses, the resulting PDF sets may differ because of methodological choices adopted by the PDF fitting groups.

NNPDF3.1' and especially 4.0 (based on the NN's+ MC technique) tend to give smaller uncertainties in data-constrained regions

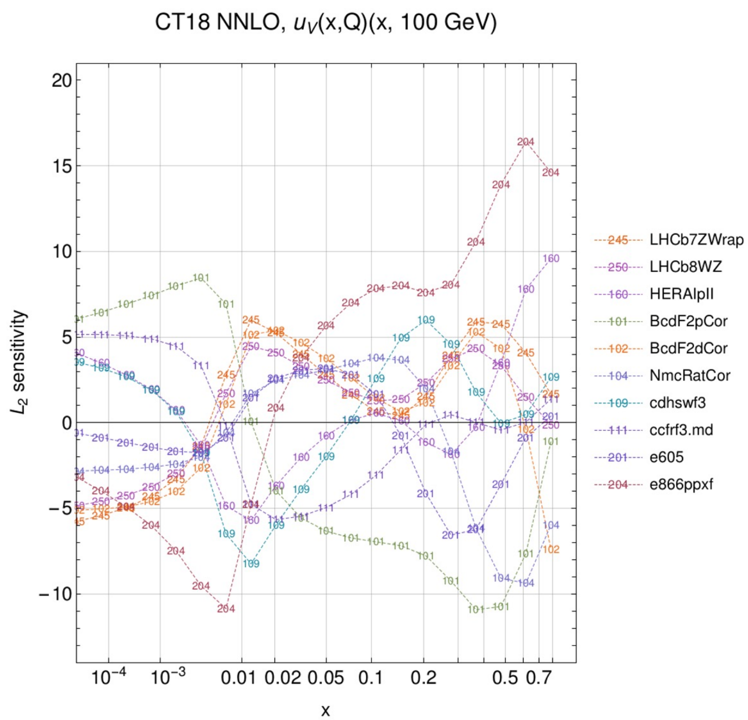
negotiating this landscape: ‘big data’ tools are needed

advanced parameter estimation; model selection



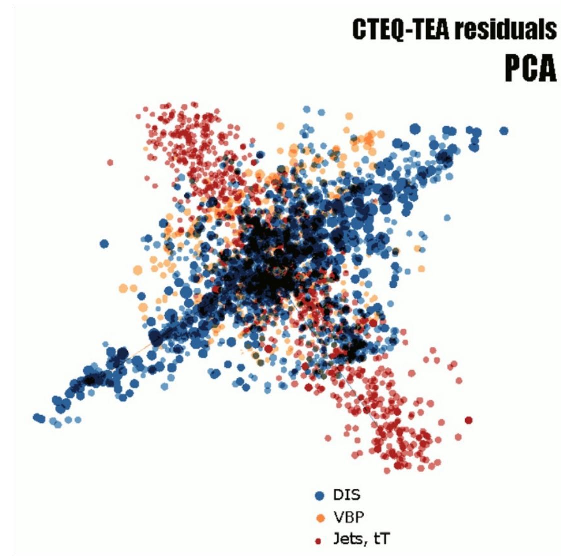
MCMC

fast statistical methods



data embedding

[**p**rincipal-**c**omponent **a**nalyses]



TensorFlow

[AIML MC opportunities, V. Rao]

→ techniques might interface computationally-intensive analyses; scale on computational clusters

deploy to resolve tensions, understand theory space

conclusion: PDFs for greater HEP 'discovery potential'

PDF determination is a highly multi-dimensional inverse problem

→ subtleties in parameter estimation and error quantification

[next talk, A. Courtoy]

→ frontier area in precision for HEP

→ advances in parameter space exploration can influence many HEP fields

[main seminar, F. Hickernell]

critical for understanding QCD; **necessary for precision HEP measurements**

→ limit sensitivity of BSM searches at LHC, neutrino programs, …

computationally, not a 'static' problem

→ interplay of statistical methods and QCD theory, expt. implementation

(constantly evolving…)

→ lessons from adjacent fields (nuclear, lattice, …) likely valuable

supplementary material