Cross-disciplinary studies of nucleon structure & replicability of precision HEP experiments

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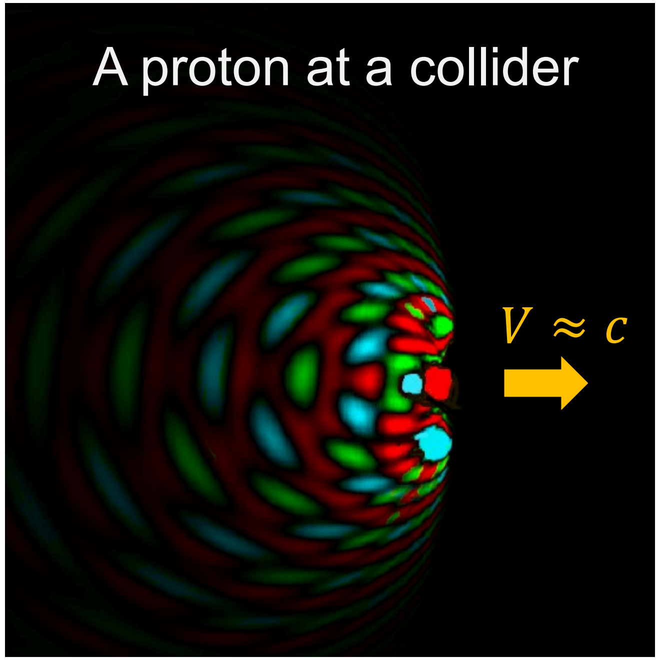
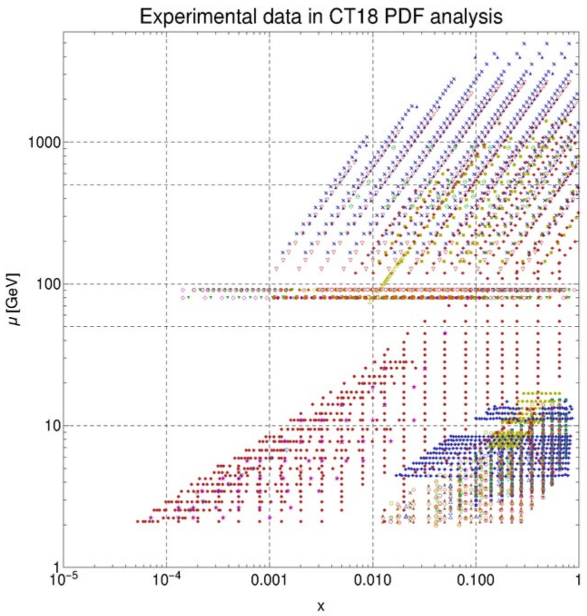
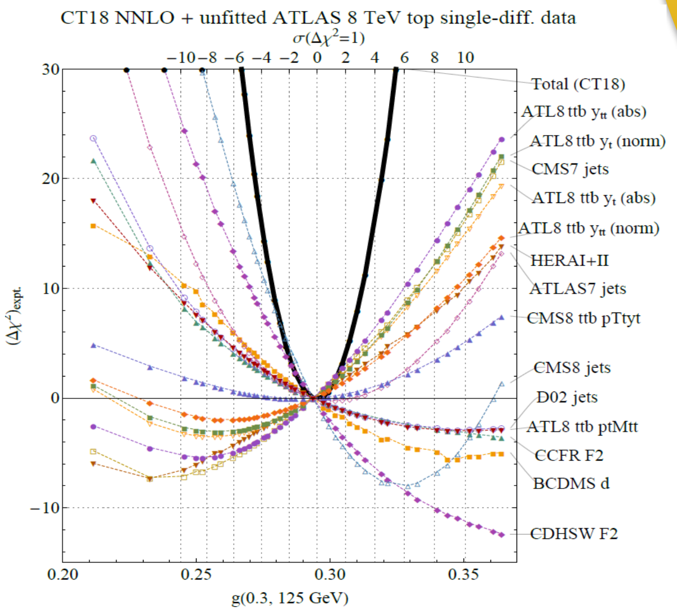
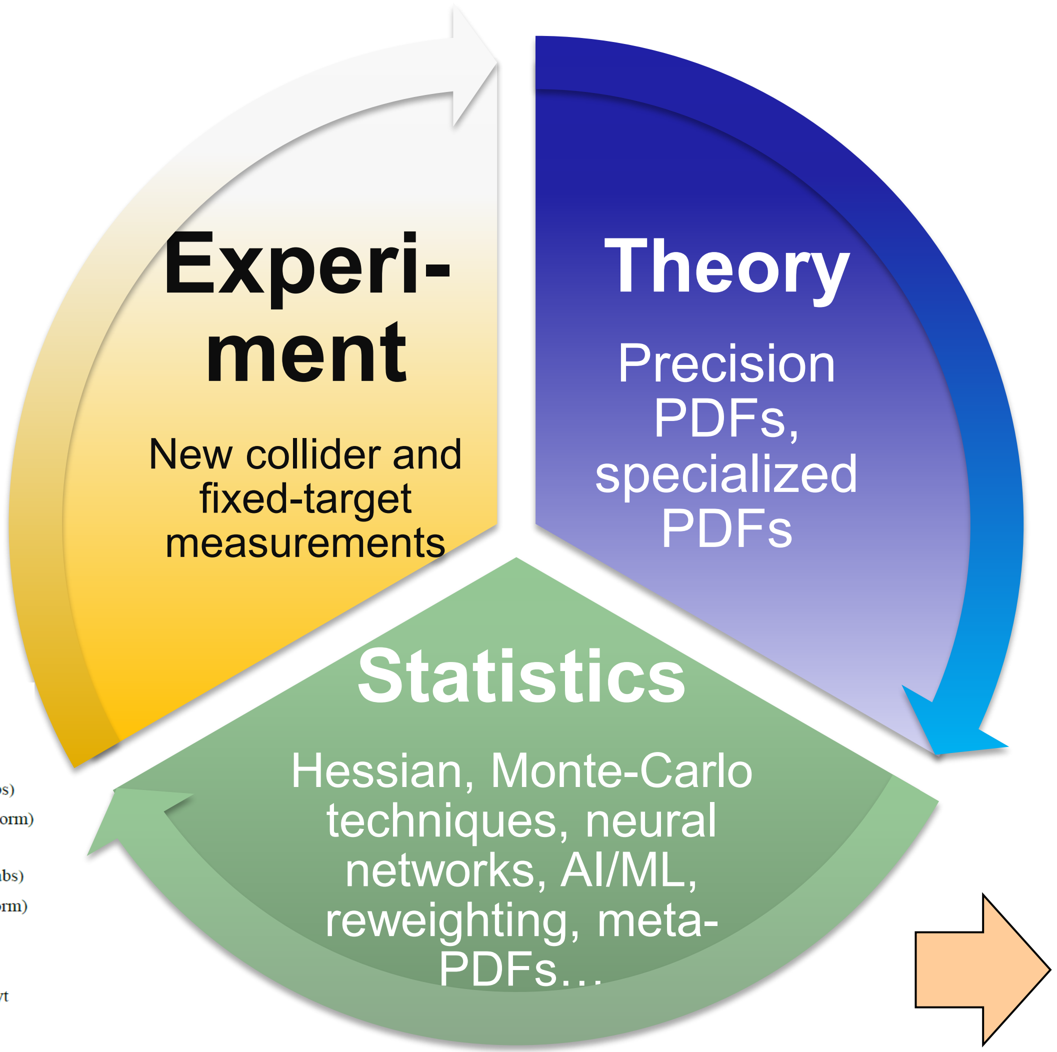
CTEQ-TEA (CT) Global QCD analysis group

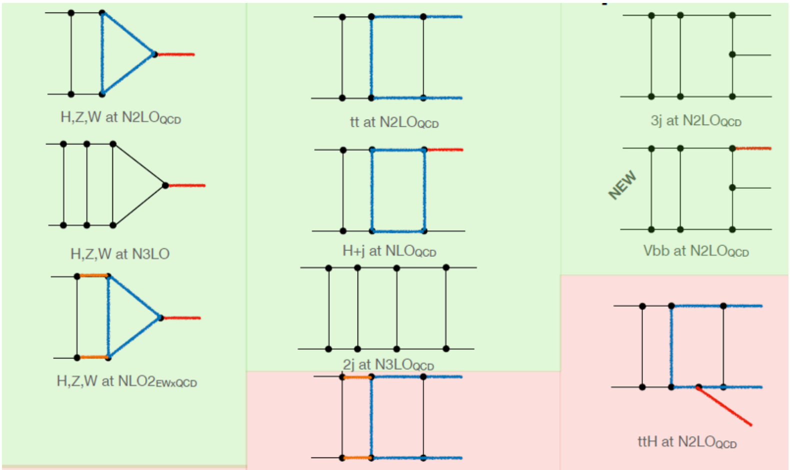


Global fits of proton scattering data at (N)NNLO accuracy

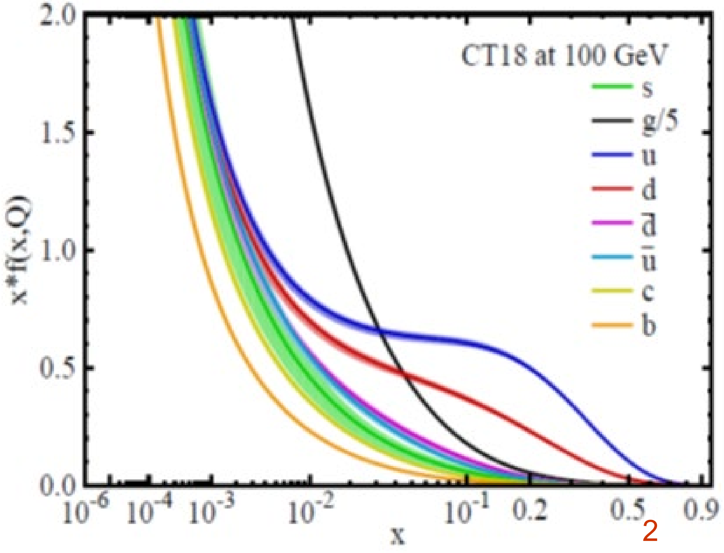








Parton distribution functions with uncertainties



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

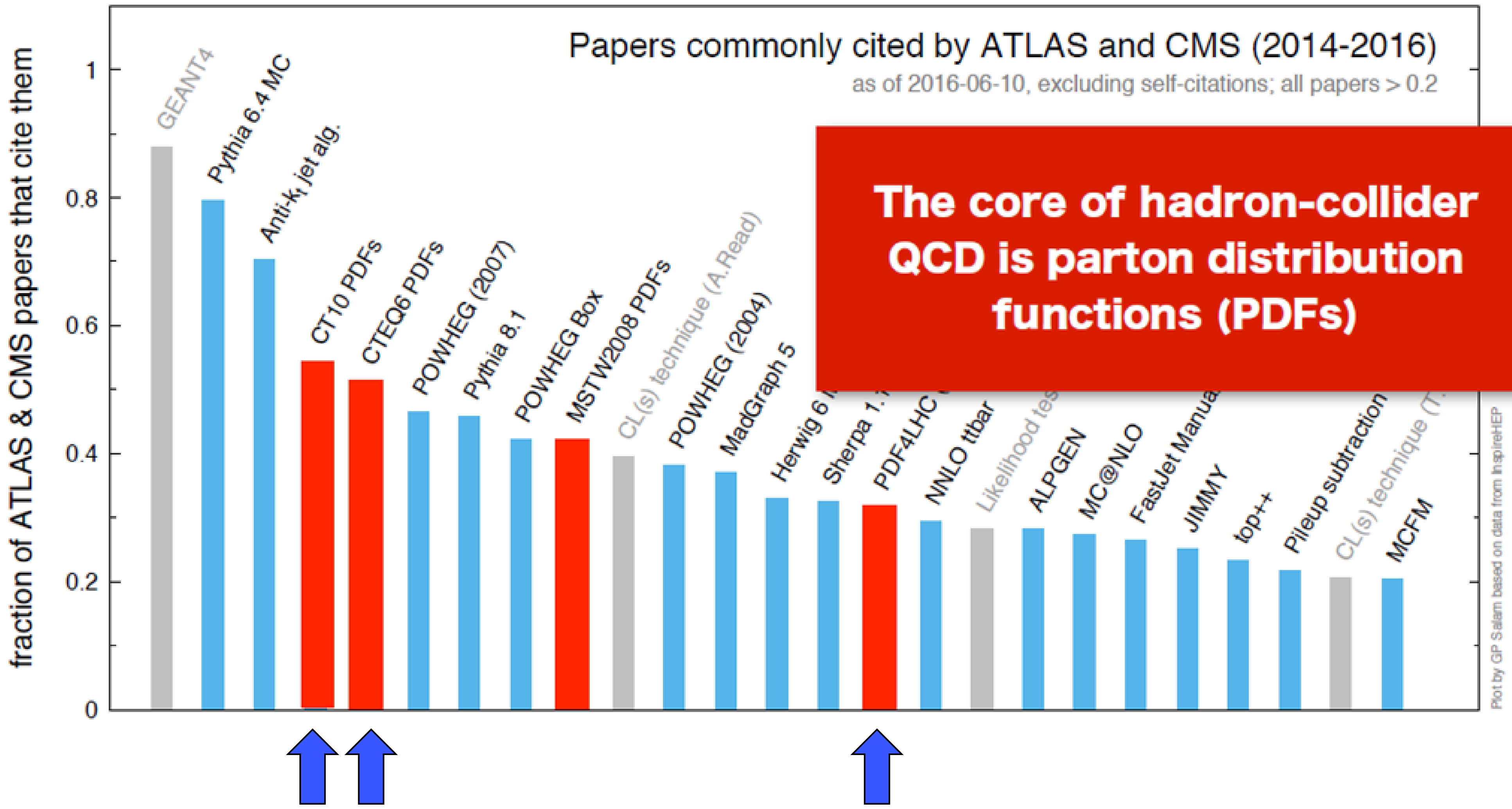
Accurate and fast high-performance computing

Frontier statistical inference in many dimensions

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

Integrated Analysis of Particle Interactions at Hadron Colliders
DOE Early Career Research Award, 2010-2015

- Provide state-of-the-art predictions in QCD to achieve objectives of the LHC studies of electroweak symmetry breaking and new physics searches
- Combine NNLO QCD calculations with precise LHC and legacy experiments measuring PDFs
- Obtain robust estimates of NNLO parton distributions from the multivariate statistical analysis of HEP experimental data
  - **CTEQ-TEA (CT) PDFs**: **CT10 NLO** (2010) and **NNLO** (2012), **CT14 NNLO** (2016),…
- Develop advanced statistical techniques for inference of PDFs from the **big QCD data**
  - **Uncertainty quantification** (UQ) with hundreds of PDF and nuisance parameters
  - Bayesian exploration with Gaussian (**Hessian**) emulation [the main UQ technique]
  - **Monte-Carlo sampling** of the PDF parameter space [auxiliary technique]
  - META PDF method for the combination of PDF ensembles (default in the PDF4LHC21 combination)
- Various QCD calculations: (SI)DIS with massive quarks at NNLO; TMD factorization for LHC Z/W production at approx. NNLO; NNLO production of jets, $t\bar{t}$,…
- 19 journal articles, 18 preprints, computer codes MP4LHC, ResBos-P, MEKS,…



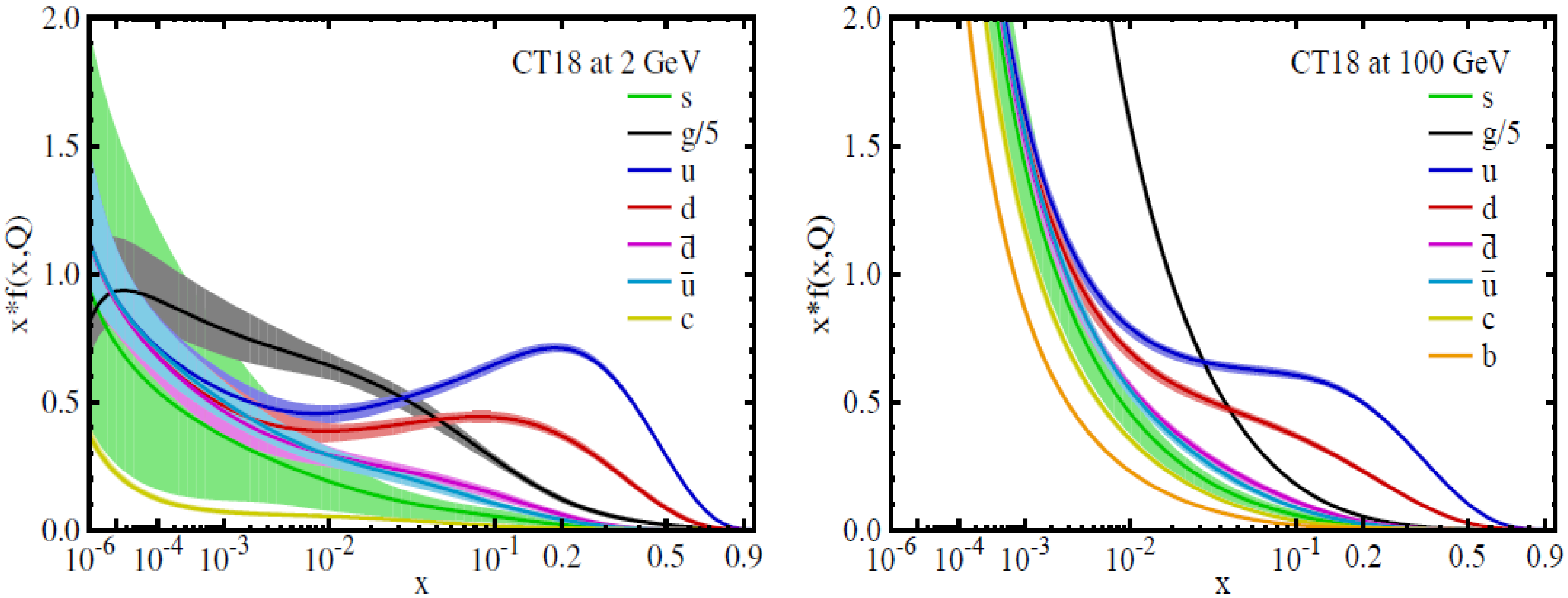
The core of hadron-collider QCD is parton distribution functions (PDFs)

Publications based on work of SMU authors

Figure credit: G. Salam

CT18 parton distributions

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

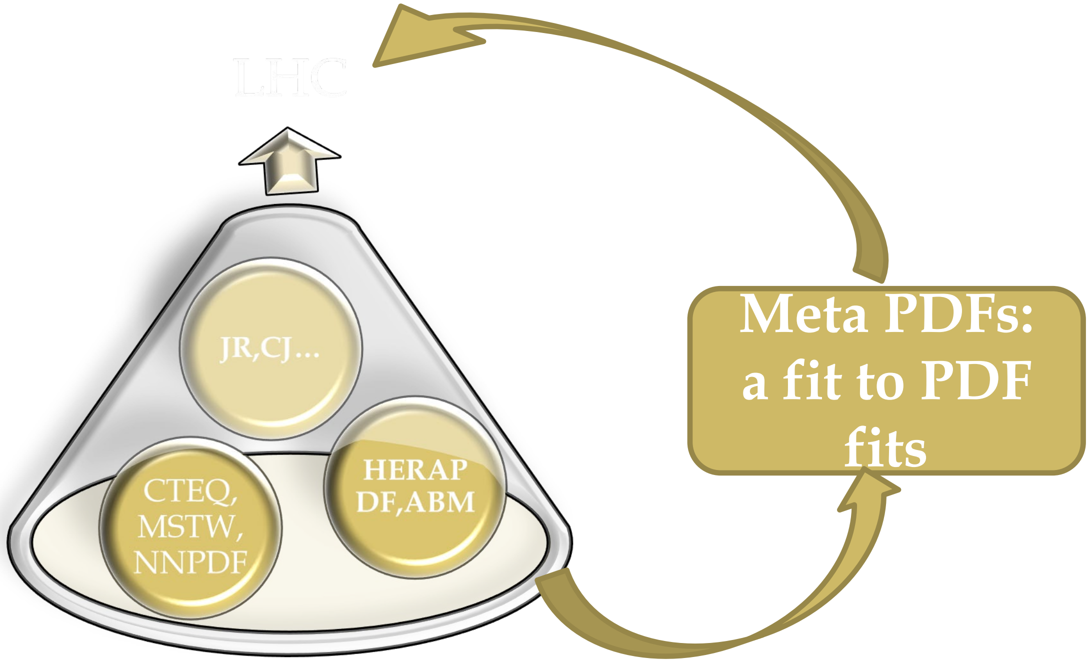


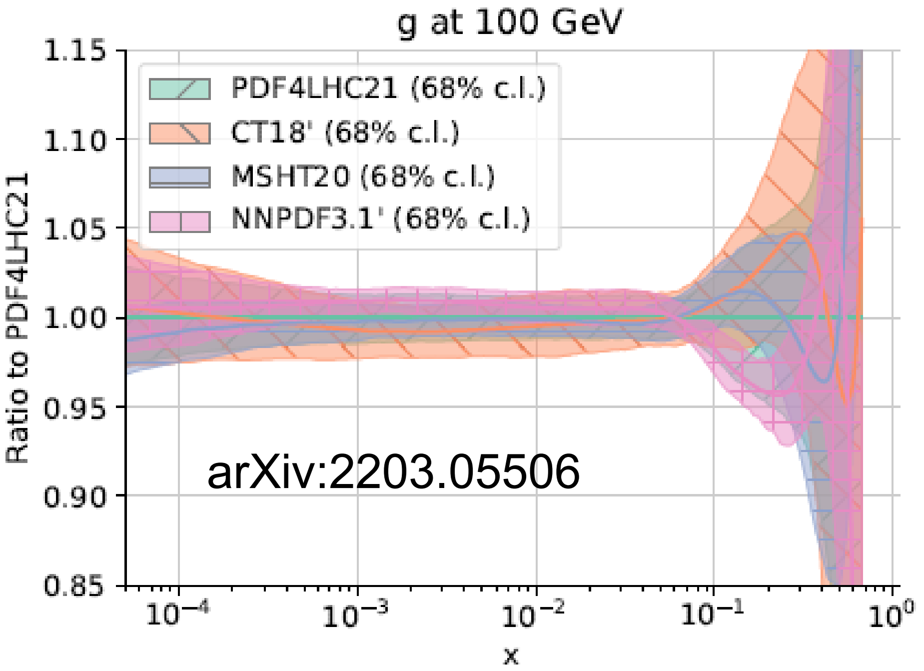
- Precise experimental data sets from ep collider HERA, LHC, Tevatron, fixed-target experiments
- Next-to-next-to-leading order (NNLO) accuracy in QCD coupling α_s
- Flexible parametric forms
- Central PDFs and bands of estimated uncertainty
- Four PDF ensembles, to account for tensions between data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

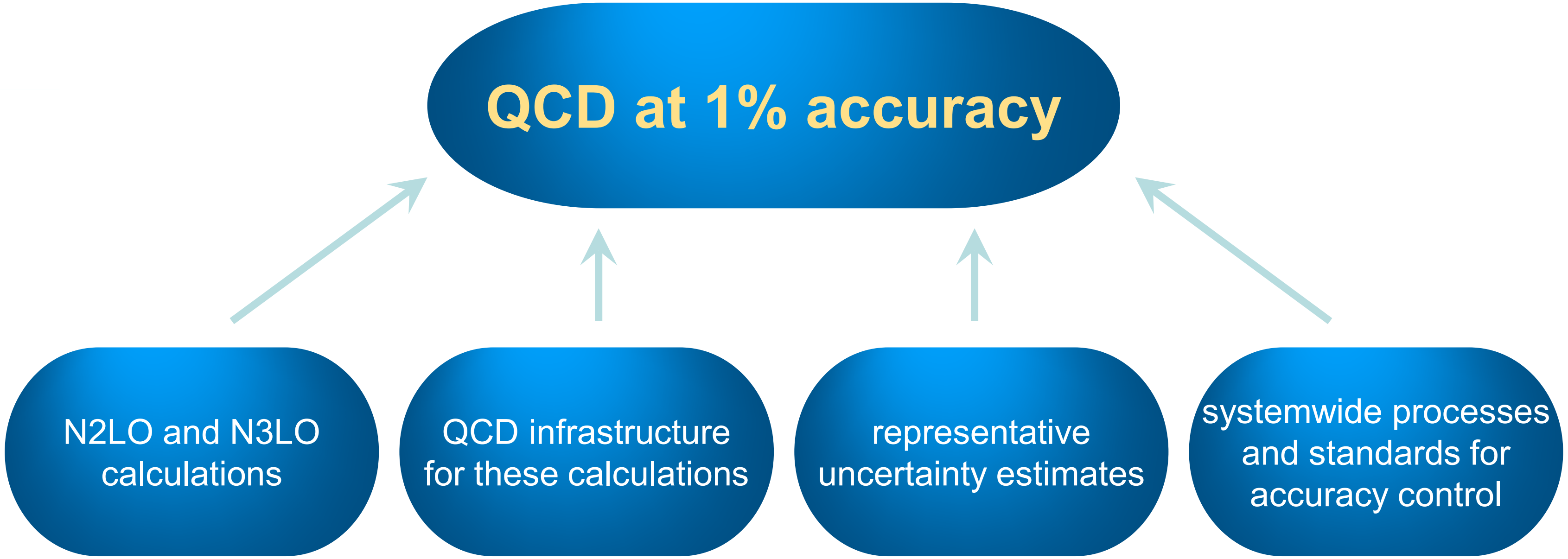
A META combination of parton distributions

J. Gao, P. Nadolsky, JHEP 07 (2014) 035

- A technique to compare and combine PDF ensembles from various groups
- Relies on the Hessian→MC→Hessian conversion using multi-dimensional sampling and PCA from 150 to 30-40 PDF parameters
- Combines CT, MSHT, NNPDF sets in the PDF4LHC 2015 and 2021 combinations







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)

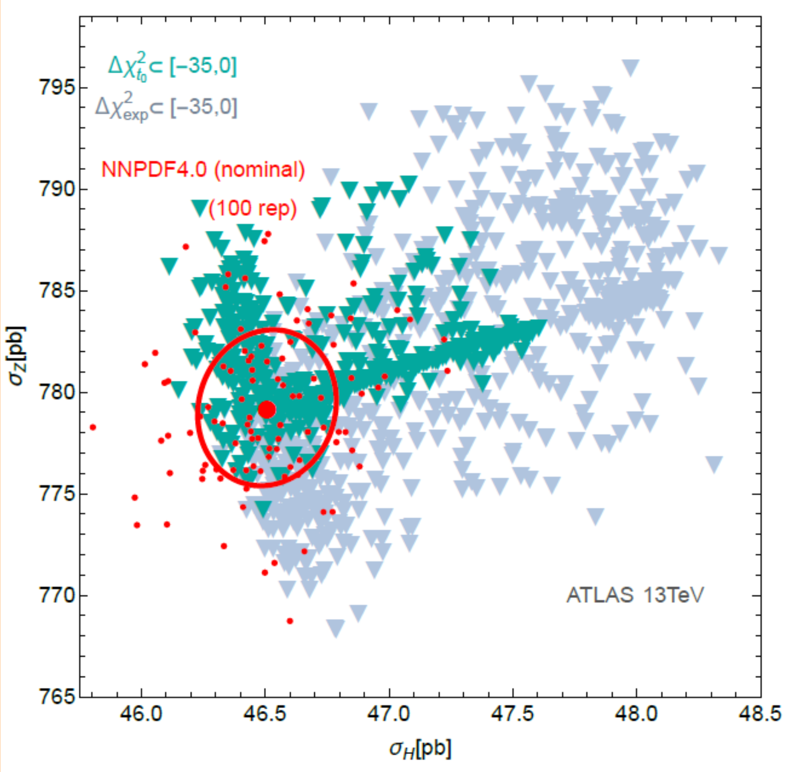
This must be a part of the precision-focused community culture

Ongoing focus at SMU

Figure from Sec. 9 "Cross-Cutting QCD" in the report of the Snowmass'2021 EF05, 06, 07 Topical Groups, arXiv:2209.14872

Ongoing and future studies

- Precision predictions for the HL-LHC, EIC, FPF, MuIC, …
- CT20X NNLO general-purpose PDFs, CT24 MC PDFs with small-x saturation
- Nonperturbative charm in nucleons
- Confronting pheno and lattice QCD inputs for PDFs
- **Multivariate Uncertainty Quantification for precision HEP**
    - Formal aspects of UQ; taming the curse of dimensionality and big-data paradox; connections to AI/ML
    - Fast visualizations of multidimensional probabilities (L_2 sensitivities)
    - **Epistemic uncertainties on PDFs**
    - **Replicability and reproducibility**



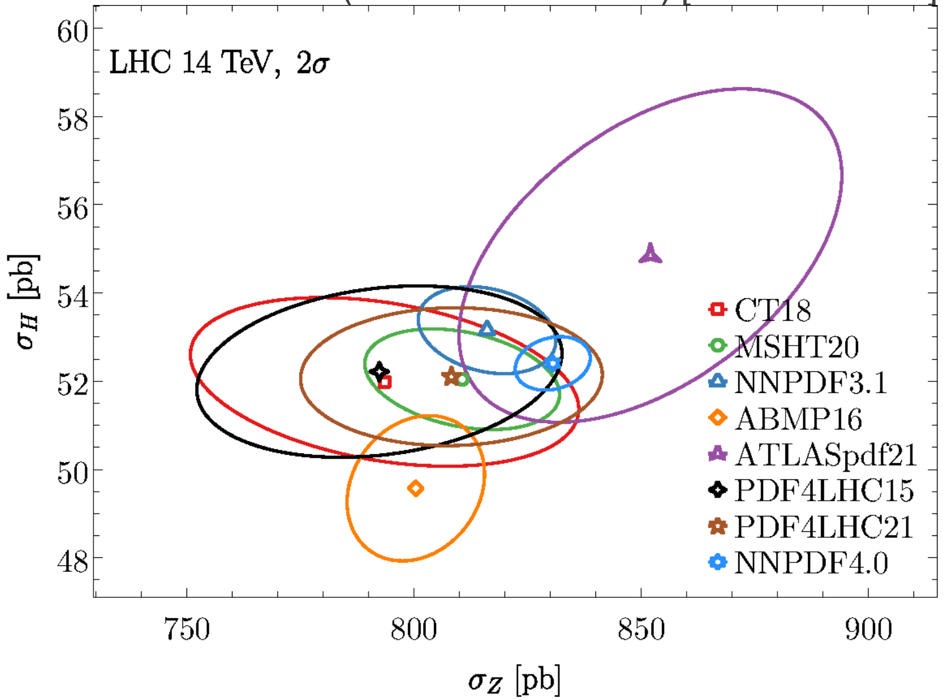
Hopscotch scans: Targeted high-density sampling of 50+ PDF parameter space may increase the nominal PDF uncertainty on key LHC observables
A. Courtoy et al., arXiv:2205.10444

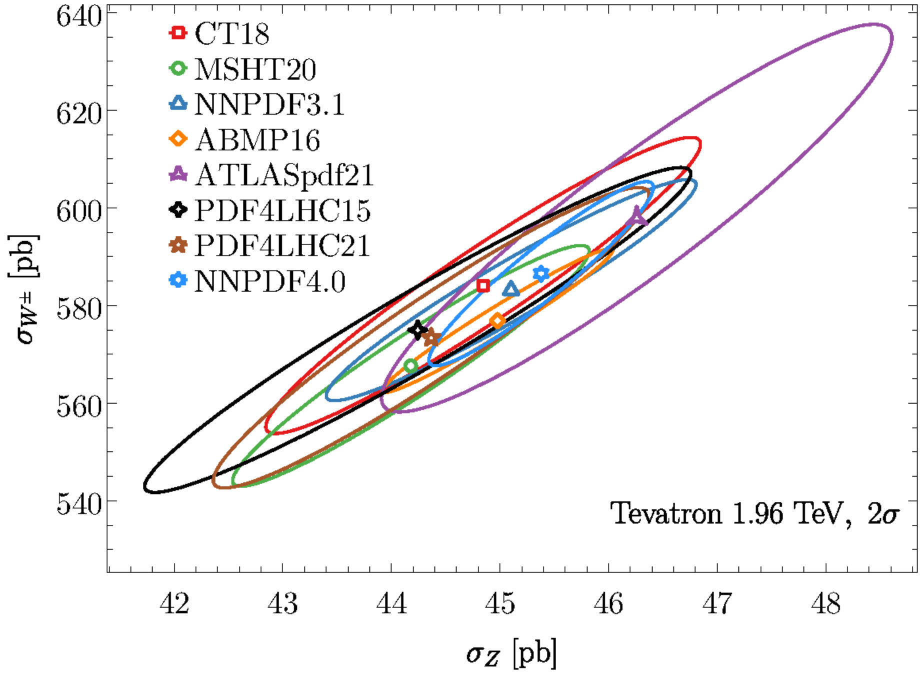
The tolerance puzzle

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

Courtoy, Huston, Nadolsky, Xie, Yan, Yuan, **Phys. Rev. D 107, (2023) 034008** [full comparisons in arXiv: 2205.10444]

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.

Epistemic PDF uncertainty…

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

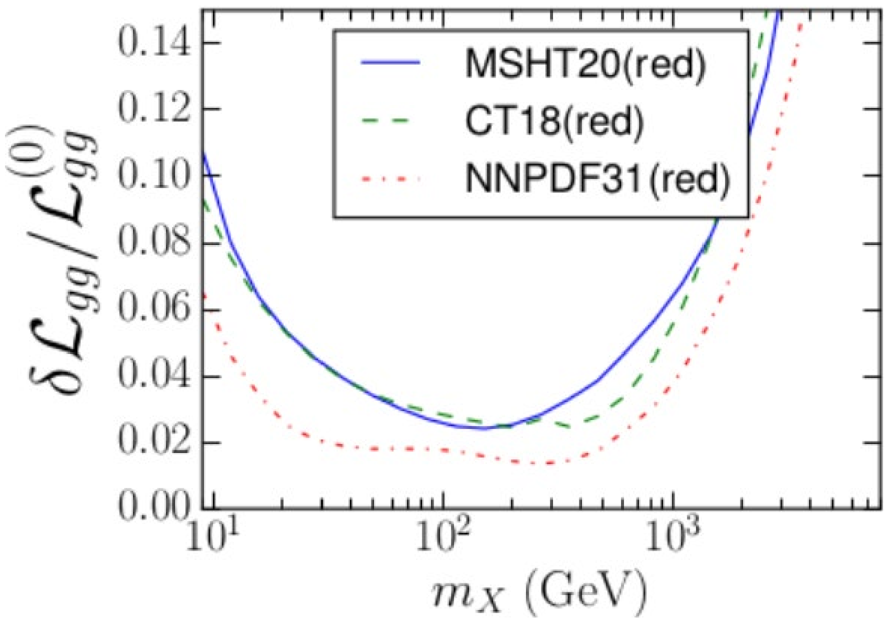
… can dominate the full uncertainty when experimental and theoretical uncertainties are small.

…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

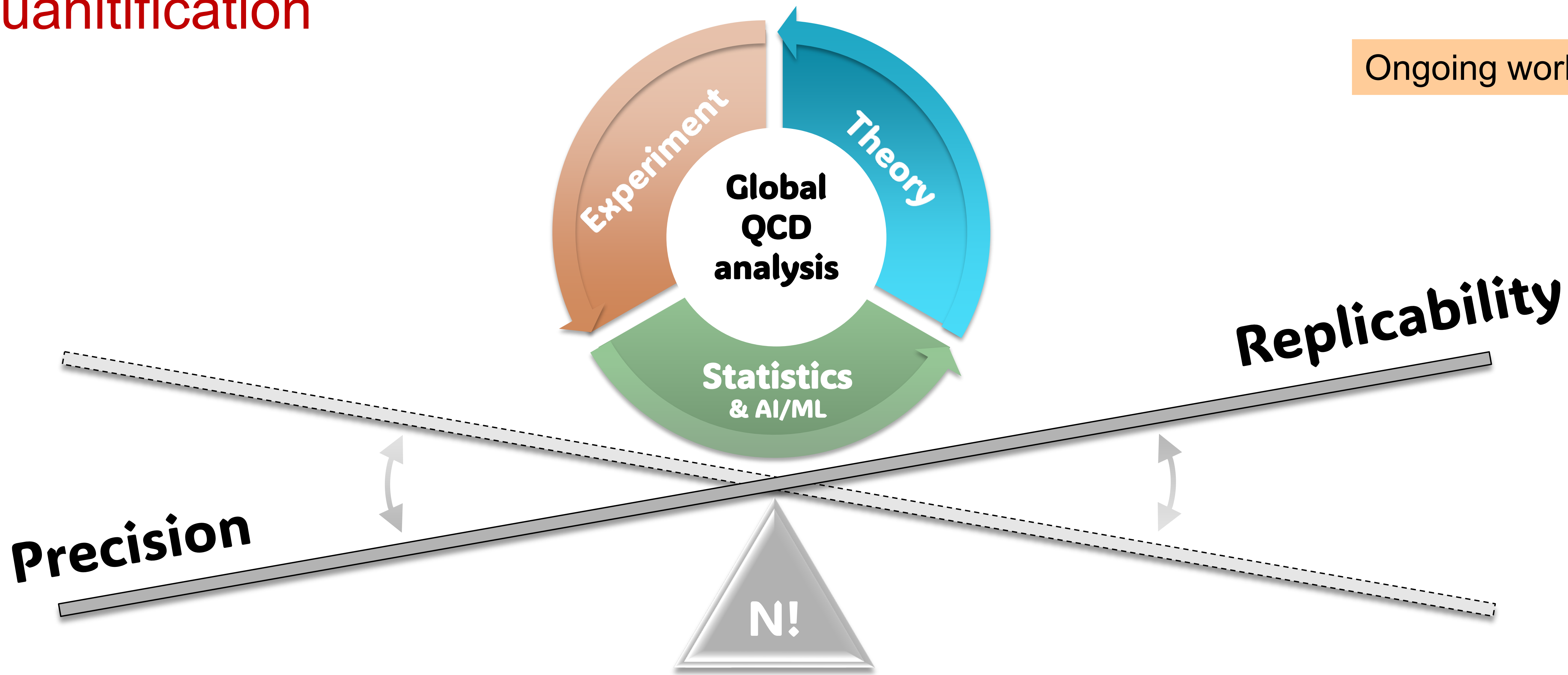


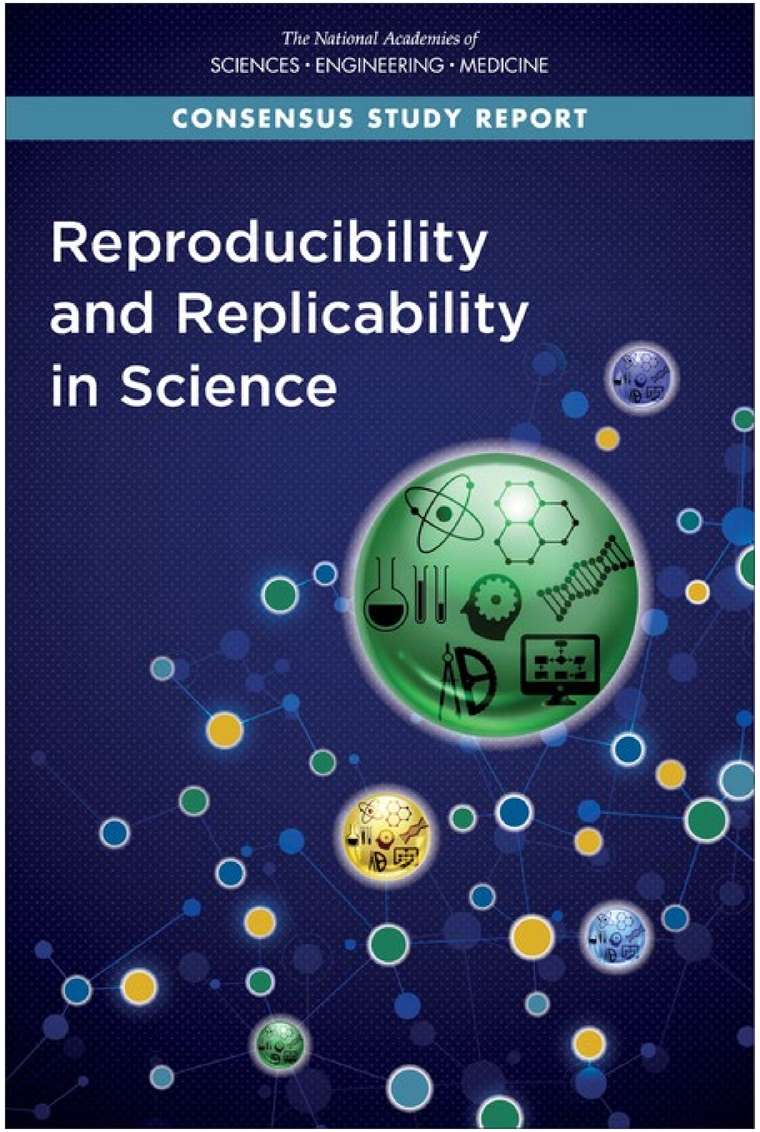
Epistemic uncertainties explain many of the differences among the sizes of PDF uncertainties by CT, MSHT, and NNPDF global fits to the same or similar data

Details in arXiv:2203.05506, arXiv:2205.10444

Balancing precision and replicability in PDF uncertainty quanitification

Ongoing work





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

Adopting the replicability mindset for precision HEP

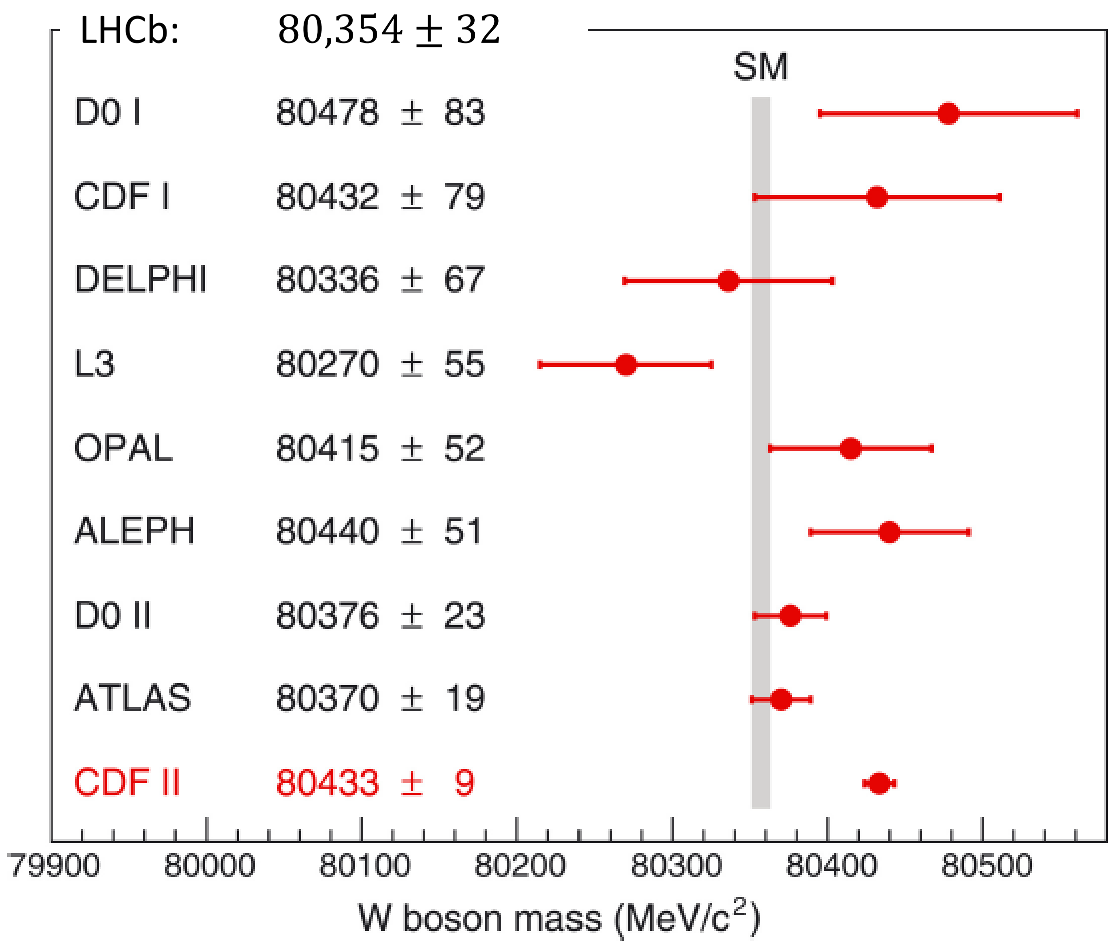


Figure reproduced from CDF-II measurement (Science 376, 170).

Replicability is a requirement of obtaining consistent results across studies aimed at answering the same scientific question, each of which has its own analysis strategy or data.

Complexity and insufficient control of systematic effects, haphazard applications of AI/ML, and social factors increase the risk of non-replicable results

Such risks can be mitigated by adopting known community-wide strategies (**replicability mindset**)

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"

Backup

Replicability across STEM fields

"… AI can help verify what we already know by addressing **science's replicability crisis. Around 70% of scientists report having been unable to reproduce another scientist's experiment—a disheartening figure.** As AI lowers the cost and effort of running experiments, it will in some cases be easier to replicate results or conclude that they can't be replicated, contributing to a greater trust in science."

Eric Schmidt, This is how AI will transform the way science gets done, MIT Technology Review, 2023-07-05

Will AI/AGI hurt or help replicability?

Replicability risks for precision QCD

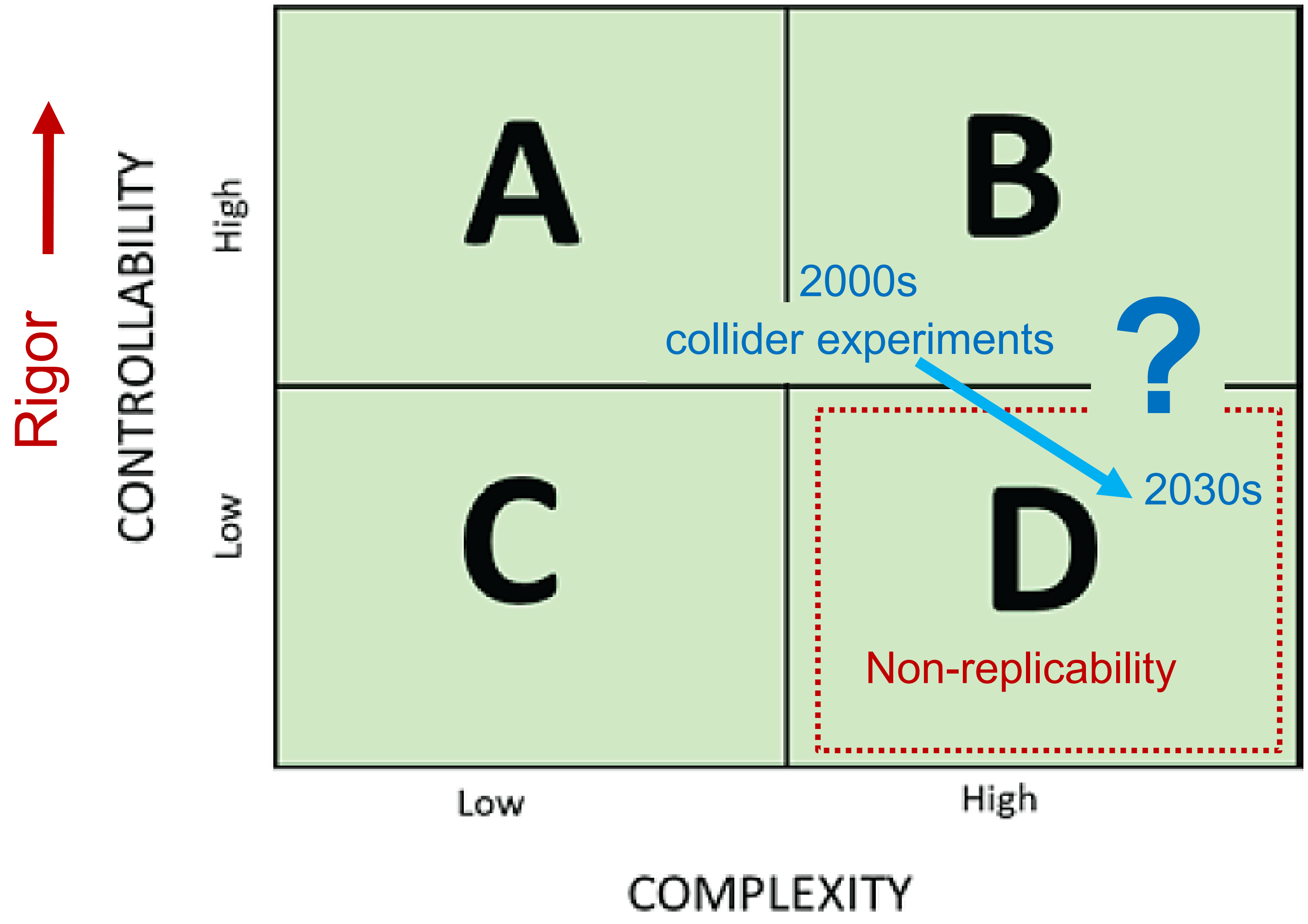
Replicability is a requirement of obtaining consistent results across studies aimed at answering the same scientific question, each of which has its own analysis strategy or data.

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

Future scenarios for QCD precision analysis

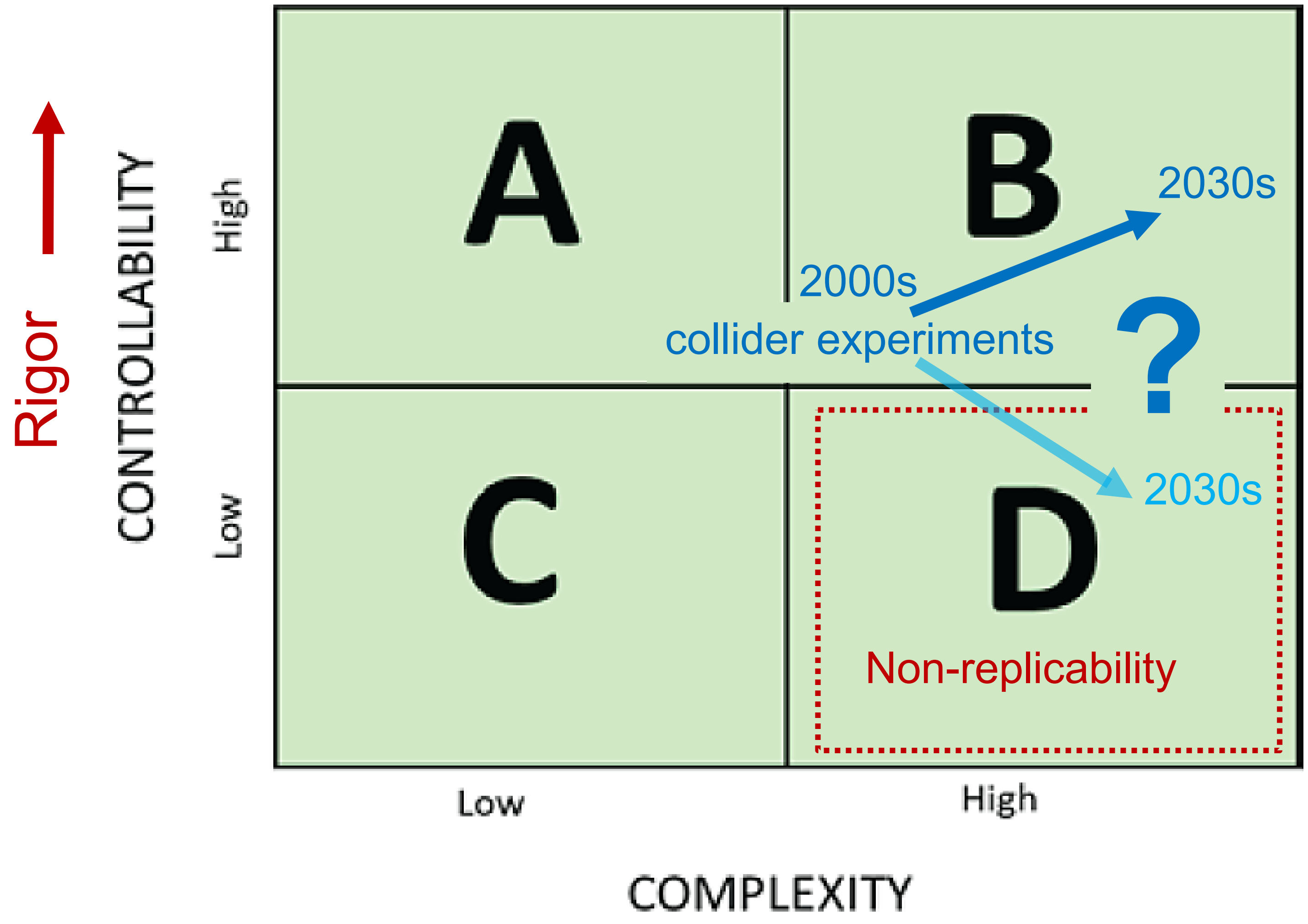


significant risk with current practices

similar to non-replicability issues in other STEM fields

Based on Fig. 5.2 in "REPRODUCIBILITY AND REPLICABILITY IN SCIENCE"

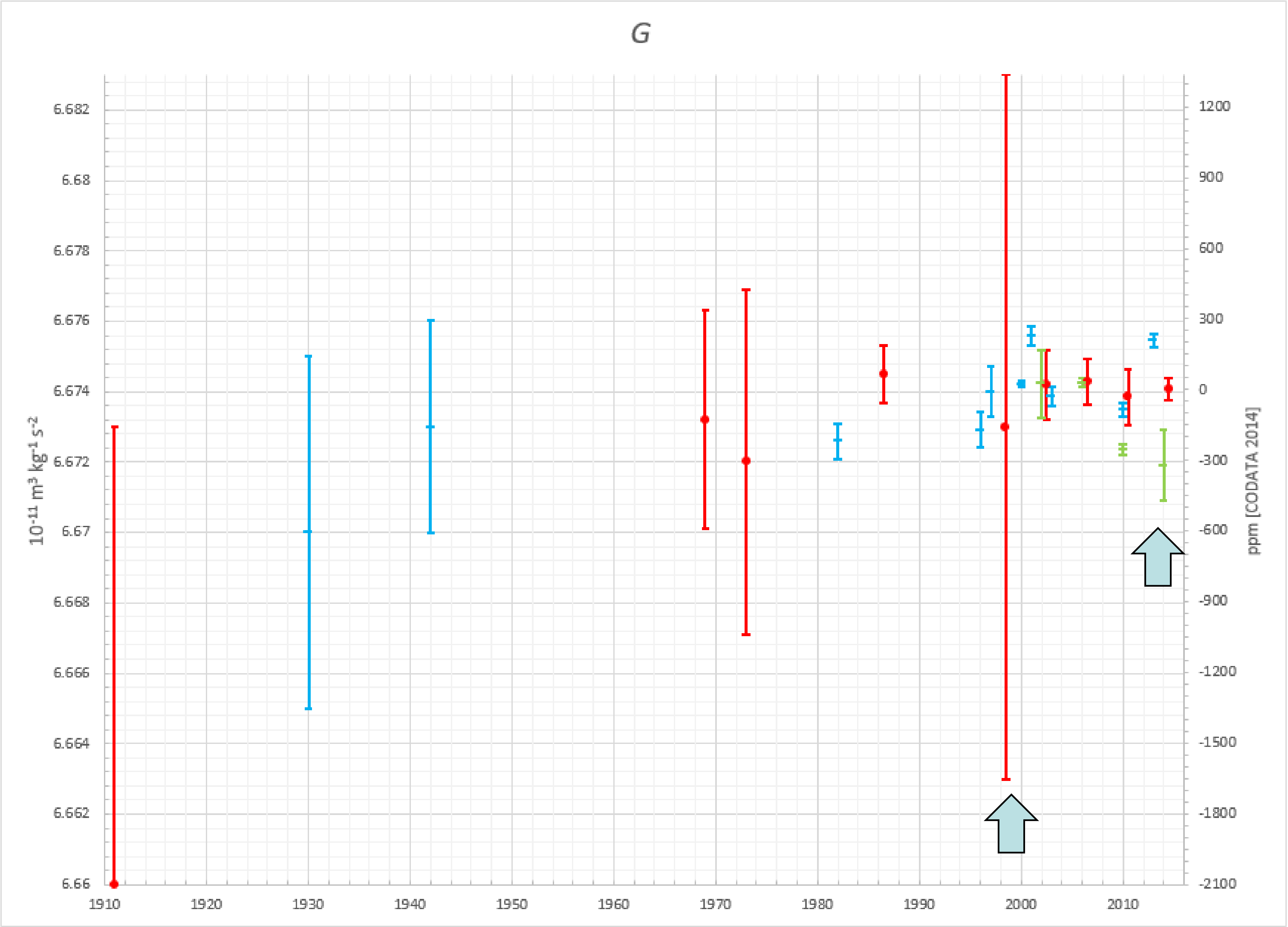
Future scenarios for QCD precision analysis



preferred scenario; requires a coordinated community strategy to adopt the **replicability mindset**

Based on Fig. 5.2 in "REPRODUCIBILITY AND REPLICABILITY IN SCIENCE"

World average for the gravitational constant



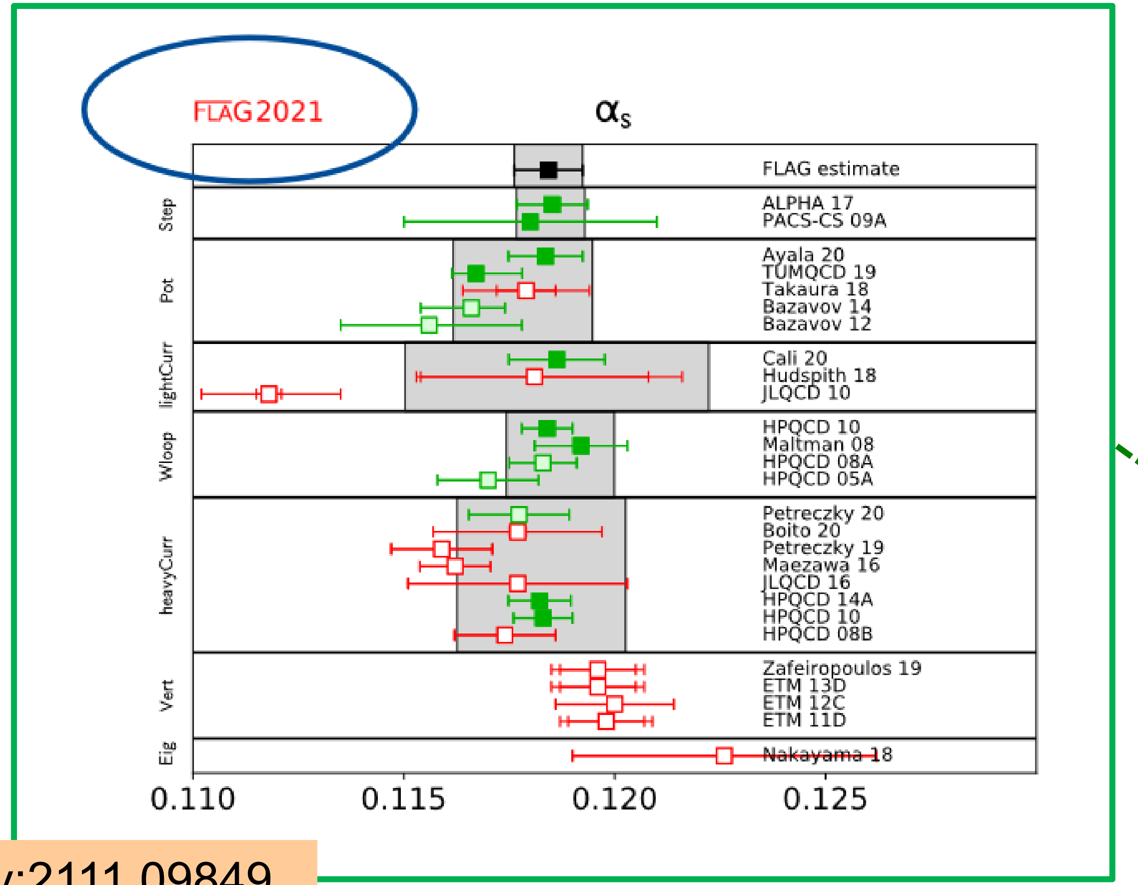
Timeline of measurements and recommended values for *G* since 1900: values recommended based on the NIST combination (red), individual torsion balance experiments (blue), other types of experiments (green).

The combination error bars are unstable after 1995

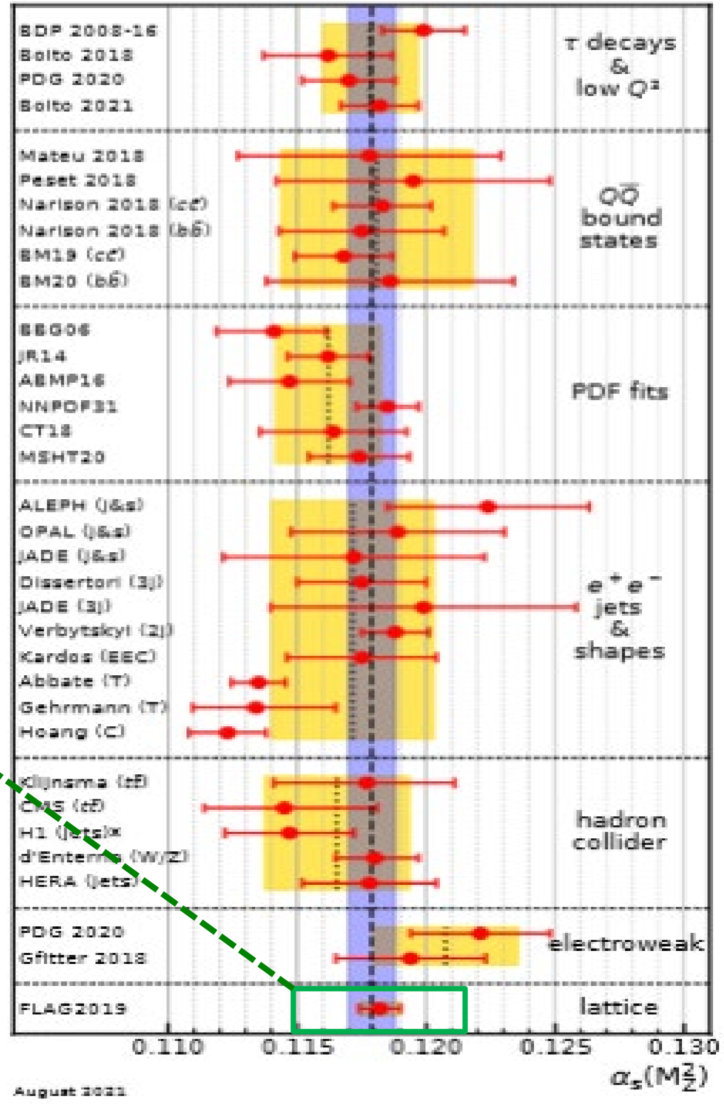
Some precise individual measurements are in a conflict among themselves and post-2014 combination

https://en.wikipedia.org/wiki/Gravitational_constant#Modern_value, retrieved on Oct. 22, 2023

Lattice QCD & world-average α_s combination



arXiv:2111.09849



Lattice determinations of α_s in multiple channels are projected to be [far] more precise than many experiments. Several challenges with combining the eclectic α_s inputs with the current procedure.

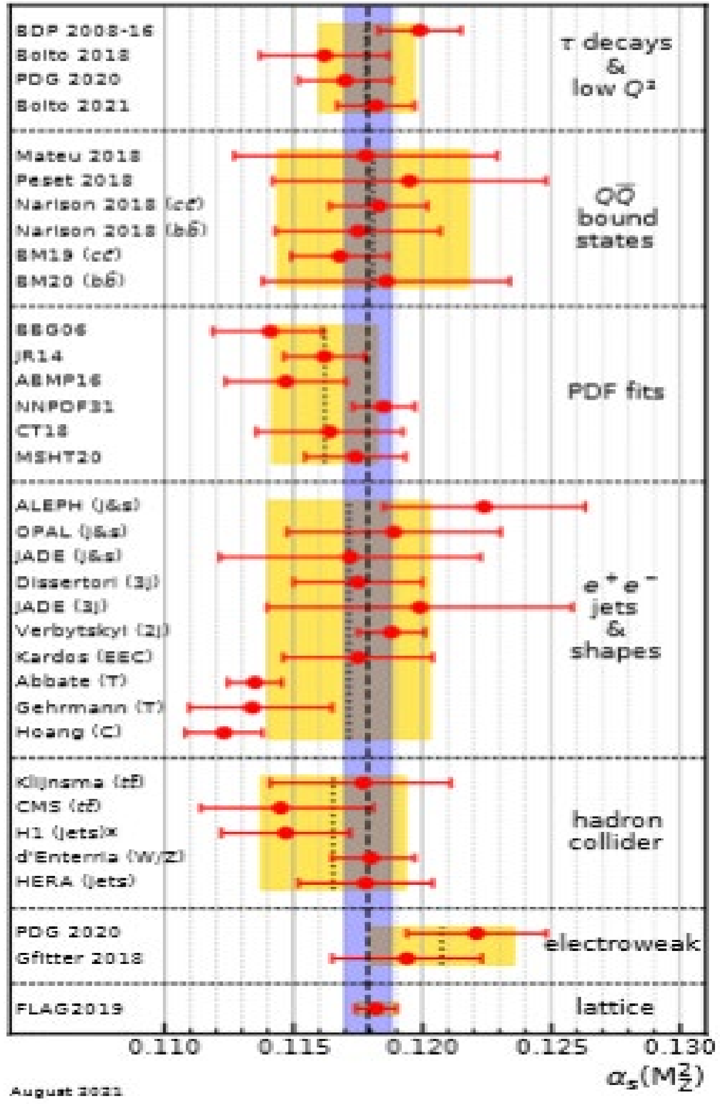
Time to rethink how the world-average α_s combination is performed?

Future measurements of the QCD coupling

individual α_s measurements can reach precision of $\sim 0.1\%$

and symbols: CIPT='contour-improved perturbation theory', FOPT='fixed-order perturbation theory', NP='nonperturbative QCD', SF='structure functions', PS='Monte Carlo parton shower'.

Method	Relative $\alpha_s m Z$ uncertainty: Current theory & exp. uncertainties sources	Relative $\alpha_s m Z$ uncertainty: Near (long-term) future theory & experimental progress
(1) Lattice	0.7% Finite lattice spacing & stats. $N^{2,3}$LO pQCD truncation	$\approx$ 0.3% (0.1%) Reduced latt. spacing. Add more observables Add $N^{3,4}$LO, active charm (QED effects) Higher renorm. scale via step-scaling to more observ.
(2) τ decays	1.6% N^3LO CIPT vs. FOPT diffs. Limited τ spectral data	$<$ 1.% Add N^4LO terms. Solve CIPT–FOPT diffs. Improved τ spectral functions at Belle II
(3) $Q\bar{Q}$ bound states	3.3% $N^{2,3}$LO pQCD truncation $m_{c,b}$ uncertainties	$\approx$ 1.5% Add $N^{3,4}$LO & more ($c\bar{c}$), ($b\bar{b}$) bound states Combined $m_{c,b} + \alpha_s$ fits
(4) DIS & PDF fits	1.7% $N^{2,(3)}$LO PDF (SF) fits Span of PDF-based results	$\approx$ 1% (0.2%) N^3LO fits. Add new SF fits: $F_2^{p,d}$, g_i (EIC) Better corr. matrices, sampling of PDF solutions. More PDF data (EIC/LHeC/FCC-eh)
(5) e^+e^- jets & evt shapes	2.6% NNLO+$N^{(1,2,3)}$LL truncation Different NP analytical & PS corrs. Limited datasets w/ old detectors	$\approx$ 1.5% ($<$ 1%) Add $N^{2,3}$LO+N^3LL, power corrections Improved NP corrs. via: NNLL PS, grooming New improved data at B factories (FCC-ee)
(6) Electroweak fits	2.3% N^3LO truncation Small LEP+SLD datasets	($\approx$ 0.1%) N^4LO, reduced param. uncerts. ($m_{W,Z}$, α, CKM) Add W boson. Tera-Z, Oku-W datasets (FCC-ee)
(7) Hadron colliders	2.4% NNLO(+NNLL) truncation, PDF uncerts. Limited data sets ($t\bar{t}$, W, Z, e-p jets)	$\approx$ 1.5% N^3LO+NNLL (for color-singlets), improved PDFs Add more datasets: Z p_T, p-p jets, σ_i/σ_j ratios,...
World average	0.8%	$\approx$ 0.4% (0.1%)



D. d'Enterria et al., EF QCD, arXiv:2203.08271

Tips for improving replicability

1. With $O(10-1000)$ free parameters, including nuisance parameters, the $\Delta\chi^2 = 1$ criterion for 1σ PDF uncertainties is almost certainly incomplete. Stop using it “as is”. There are strong mathematical reasons.

2. Current practices for estimating systematic uncertainties are likely insufficient.

3. Thoroughly estimate the dependence on PDF parametrization forms, NN hyperparameters, and analysis settings when other uncertainties are small.

    - Public tools for this are increasingly available: xFitter, NNPDF code, ePump, Fantômas, MP4LHC,…