A strong coupling determination from PDFs at aN3LO with theory uncertainties

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LFC24
Trieste, 17 September 2024

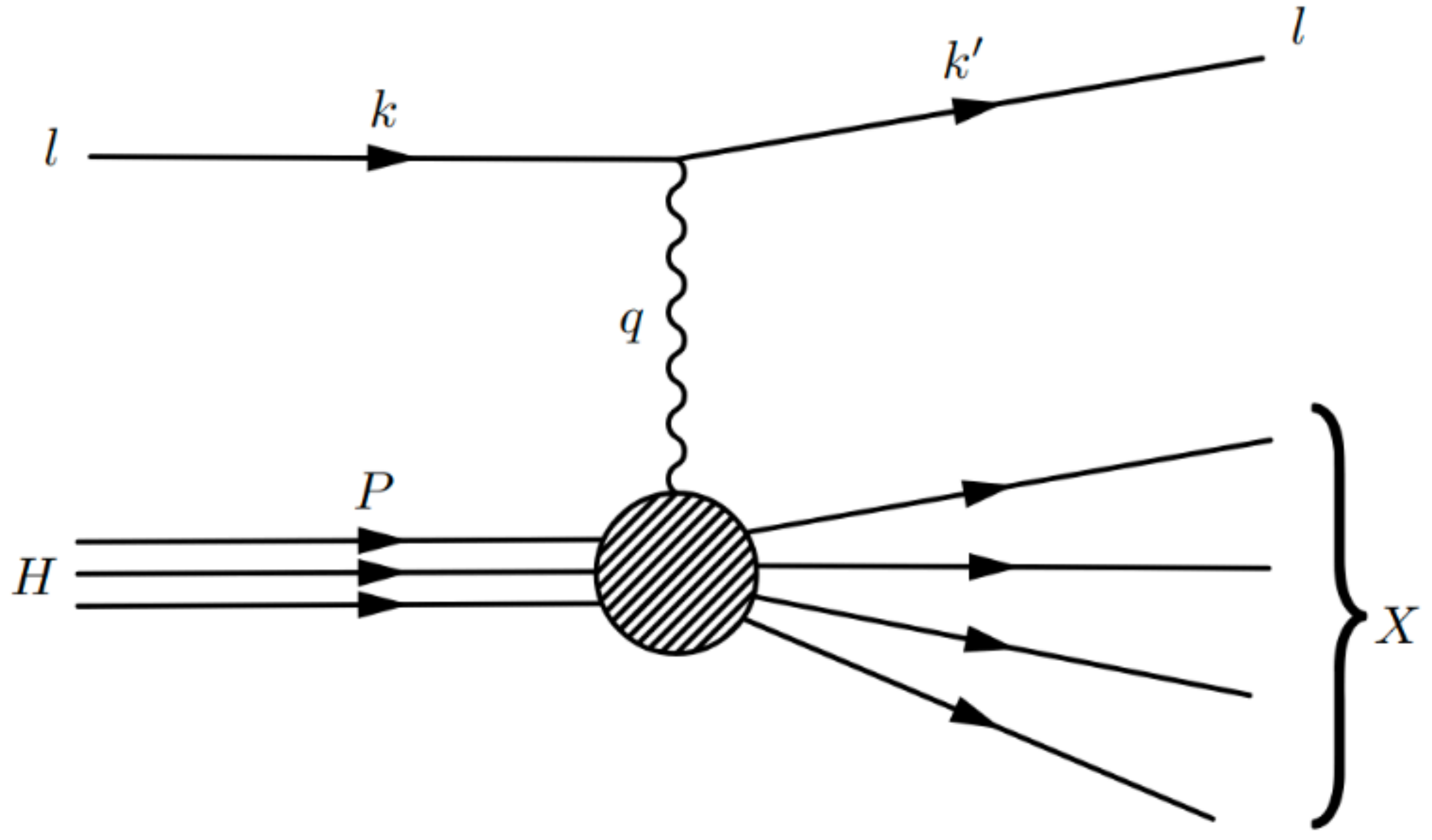
Motivation or why do we need PDFs?

PDFs are a **key ingredient** in collider physics:

non-perturbative

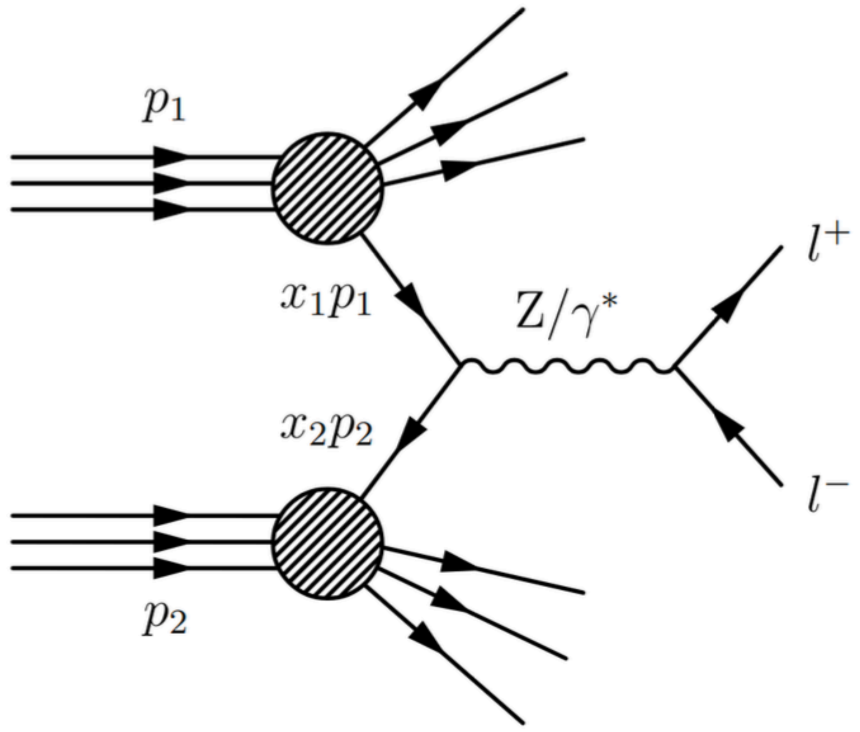
experiment **pQCD**

$$F = \sum_{i \in \{q,\bar{q},g\}} f_i \otimes \hat{\sigma}_i$$



PDFs are **universal**:

$$\sigma = \sum_{i,j \in \{q,\bar{q},g\}} f_i \otimes f_j \otimes \hat{\sigma}_{ij}$$



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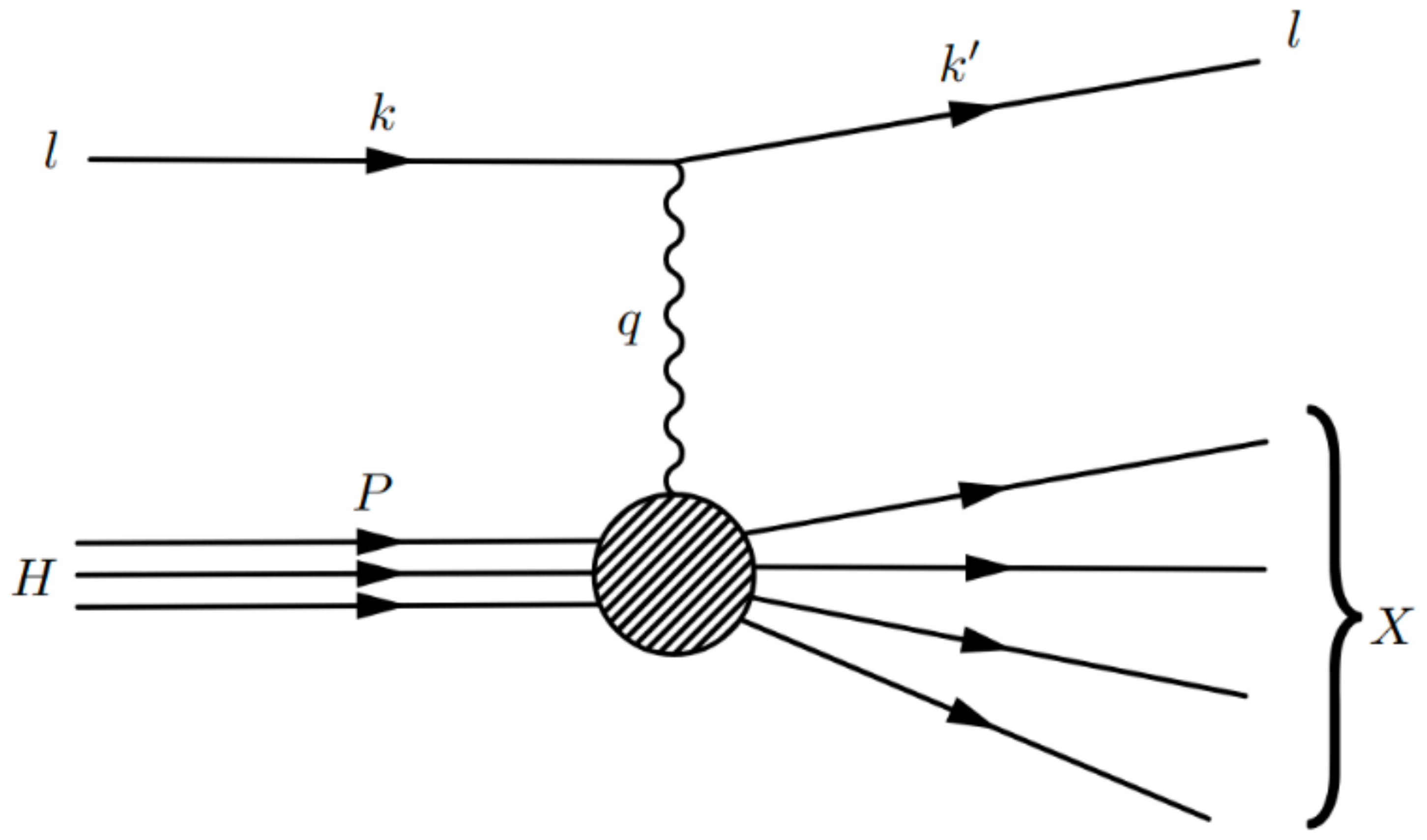
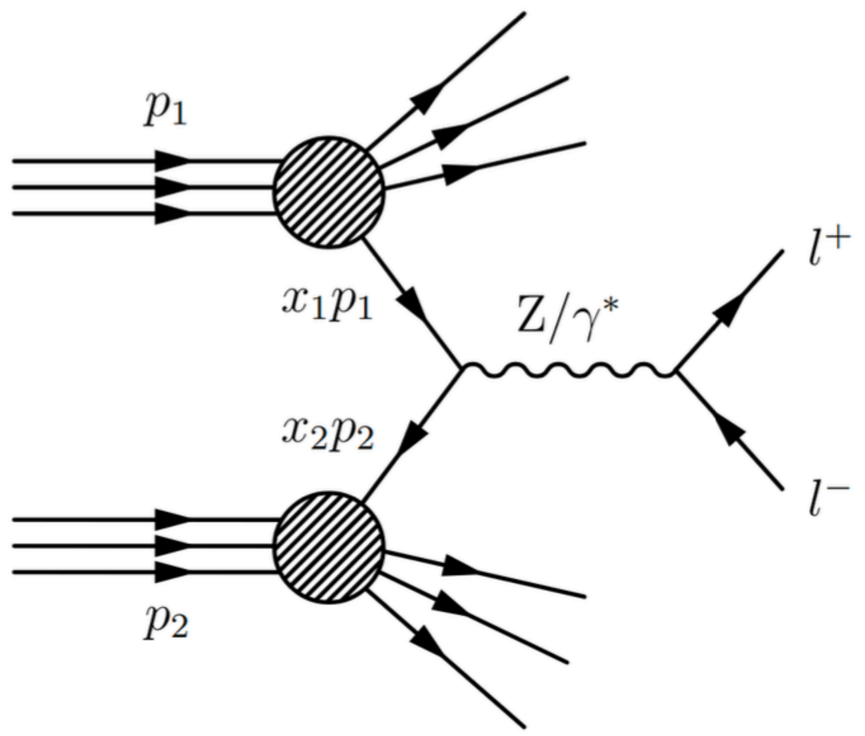


PDFs are **universal**:

$$\sigma = \sum_{ij \in \{q,\bar{q},g\}} dx_1 dx_2 f_i(x_1, \mu_F^2) f_j(x_2, \mu_F^2) \hat{\sigma}(x_1, x_2, \alpha_s(\mu_R^2), \frac{Q^2}{\mu_F^2}, \frac{Q^2}{\mu_R^2})$$



splitting function

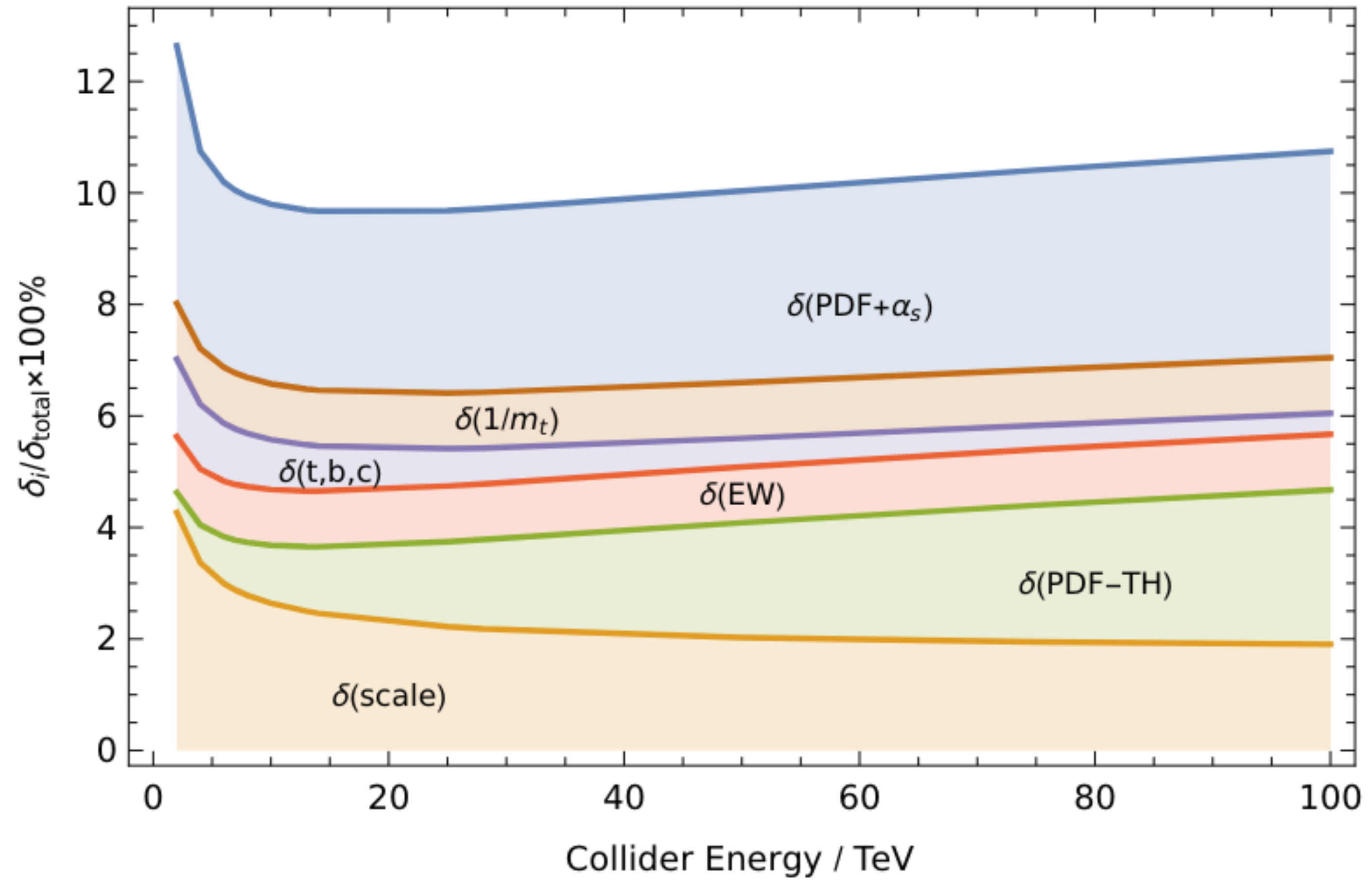
$$\frac{df_i(x, \mu_f^2)}{d\log(\mu_F)} = \sum_j \int_x^1 \frac{dz}{z} P_{ij}\left(\frac{x}{z}, \alpha_s\right) f_j(x, \mu_F)$$

μ_F dependence of PDFs can be computed in pQCD (DGLAP equation)

x dependence of PDFs needs to be fitted to data

Motivation or why do we need N3LO PDFs?

- Predictions at particle colliders such as the LHC use two main ingredients:
  - Matrix elements (MEs)
  - Parton distribution functions (PDFs)
- Much progress has been made in the computation of MEs at N3LO
- **PDF uncertainties are becoming a bottleneck** for many LHC precision calculations
- Most widely used PDF sets are at NNLO and without theory uncertainties



Sources of uncertainty for inclusive Higgs production

Dulat, Lazopoulos, Mistleberger [arXiv:1802.00827]

Since this plot progress in:

- NNLO top quark corrections [arXiv:2105.04436]]
- Mixed QDC-EW corrections [arXiv:2010.09451,2007.09813]

Towards N3LO PDFs

QCD corrections for aN3LO PDFs

A PDF fit requires several theory inputs:

- **DGLAP splitting functions** for PDF evolution
  $$Q^2 \frac{df_i}{dQ^2} = P_{ij} \otimes f_j$$
- **Matching conditions** for variable flavor number schemes
  $$f_i^{(n_f+1)}(x, Q^2) = A_{ij}(x, \alpha_s) f_j^{(n_f)}(x, Q^2)$$
- **Partonic coefficient functions** for the data used in the fit

Splitting Functions (information is partial)

Singlet (P_{qq}, P_{gg}, P_{gq}, P_{qg})
- large-n_f limit [NPB 915 (2017) 335; arXiv:2308.07958]
- small-x limit [JHEP 06 (2018) 145]
- large-x limit [NPB 832 (2010) 152; JHEP 04 (2020) 018; JHEP 09 (2022) 155]
- 5 (10) lowest Mellin moments [PLB 825 (2022) 136853; ibid. 842 (2023) 137944; ibid. 846 (2023) 138215]

Non-singlet ($P_{NS,v}$, $P_{NS,+}$, $P_{NS,-}$)
- large-n_f limit [NPB 915 (2017) 335; arXiv:2308.07958]
- small-x limit [JHEP 08 (2022) 135]
- large-x limit [JHEP 10 (2017) 041]
- 8 lowest Mellin moments [JHEP 06 (2018) 073]

DIS structure functions (F_L, F_2, F_3)
- DIS NC (massless) [NPB 492 (1997) 338; PLB 606 (2005) 123; NPB 724 (2005) 3]
- DIS CC (massless) [Nucl.Phys.B 813 (2009) 220]
- massive from parametrisation combining known limits and damping functions [NPB 864 (2012) 399]

PDF matching conditions
- all known except for $a_{H,g}^3$ [NPB 820 (2009) 417; NPB 886 (2014) 733; JHEP 12 (2022) 134]

Coefficient functions for other processes
- DY (inclusive) [JHEP 11 (2020) 143]; DY (y differential) [PRL 128 (2022) 052001]

E. Nocera, Workshop on Hadron Physics and Opportunities Worldwide
Dalian, China, August 2024

Approximate does not mean poorly-known!

Approximate N3LO splitting functions

$$P_{ij} = \alpha_s P_{ij}^{(0)} + \alpha_s^2 P_{ij}^{(1)} + \alpha_s^3 P_{ij}^{(2)} + \alpha_s^4 P_{ij}^{(3)}, \quad i,j = q,g$$

Complete analytic results for the N3LO splitting functions are not available
Approximations are constructed from partial results

Large-n_f limit: $\mathcal{O}(n_f^3)$, $P_{NS}^{(n_f^2)}$ [arXiv:1610.07477], $P_{qq,PS}^{(n_f^2)}$ [arXiv:2308.07958], $P_{qg}^{(n_f^2)}$ [arXiv:2310.01245]

Small-x limit: Singlet [arXiv:1805.06460], non-singlet [arXiv:2202.10362]

Large-x limit: [arXiv:2205.04493], [arXiv:1911.10174], [arXiv:0912.0369]

Mellin moments: [arXiv:1707.08315] [arXiv:2111.15561], [arXiv:2302.07593], [arXiv:2307.04158],[arXiv:2310.05744], ([arXiv:2404.09701], not included)

How do we use this information?

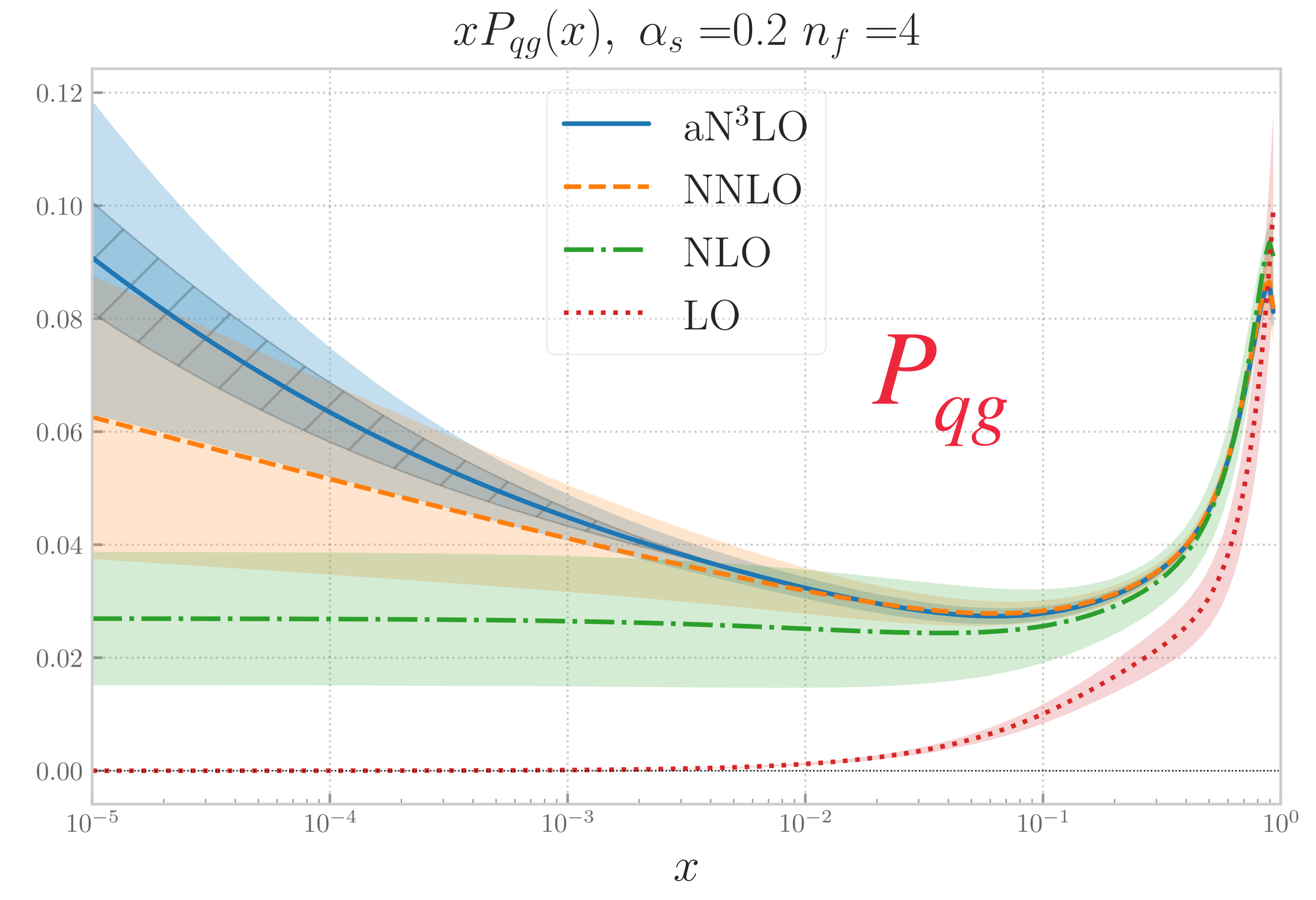
- **Combine small- and large-x** using a basis of different trial functions that reproduces the known moments
- Vary parametrization choices to obtain an ensemble of approximate aN3LO splitting functions
- Determine uncertainty

Approximate N3LO splitting functions

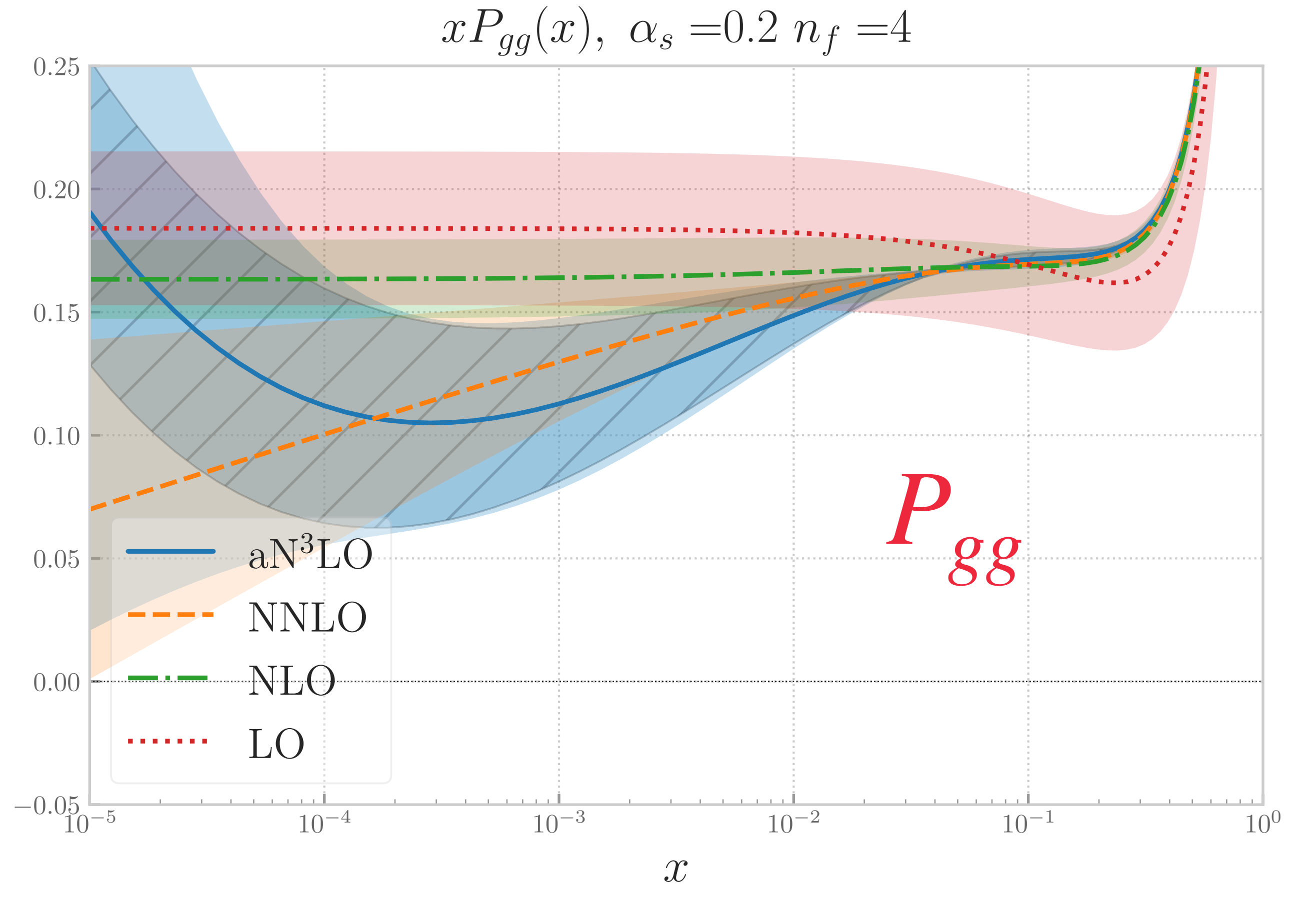
We distinguish two sources of theory uncertainty:

Incomplete Higher Order Uncertainties (IHOUs) due to parametrization of aN3LO contributions (dark band)

Missing Higher Order Uncertainties (MHOUs) due to finite perturbative expansion estimated from scale variations



- For P_{qg}, P_{qq}, and P_{gq} the uncertainty from scale variation is larger than the N3LO approximation uncertainty (IHOU < MHOU)
- For P_{gg} the parametrization uncertainty is significant (dark blue band)
- large-x: good perturbative stability
- small-x: convergence within scale variations fails due to large logs



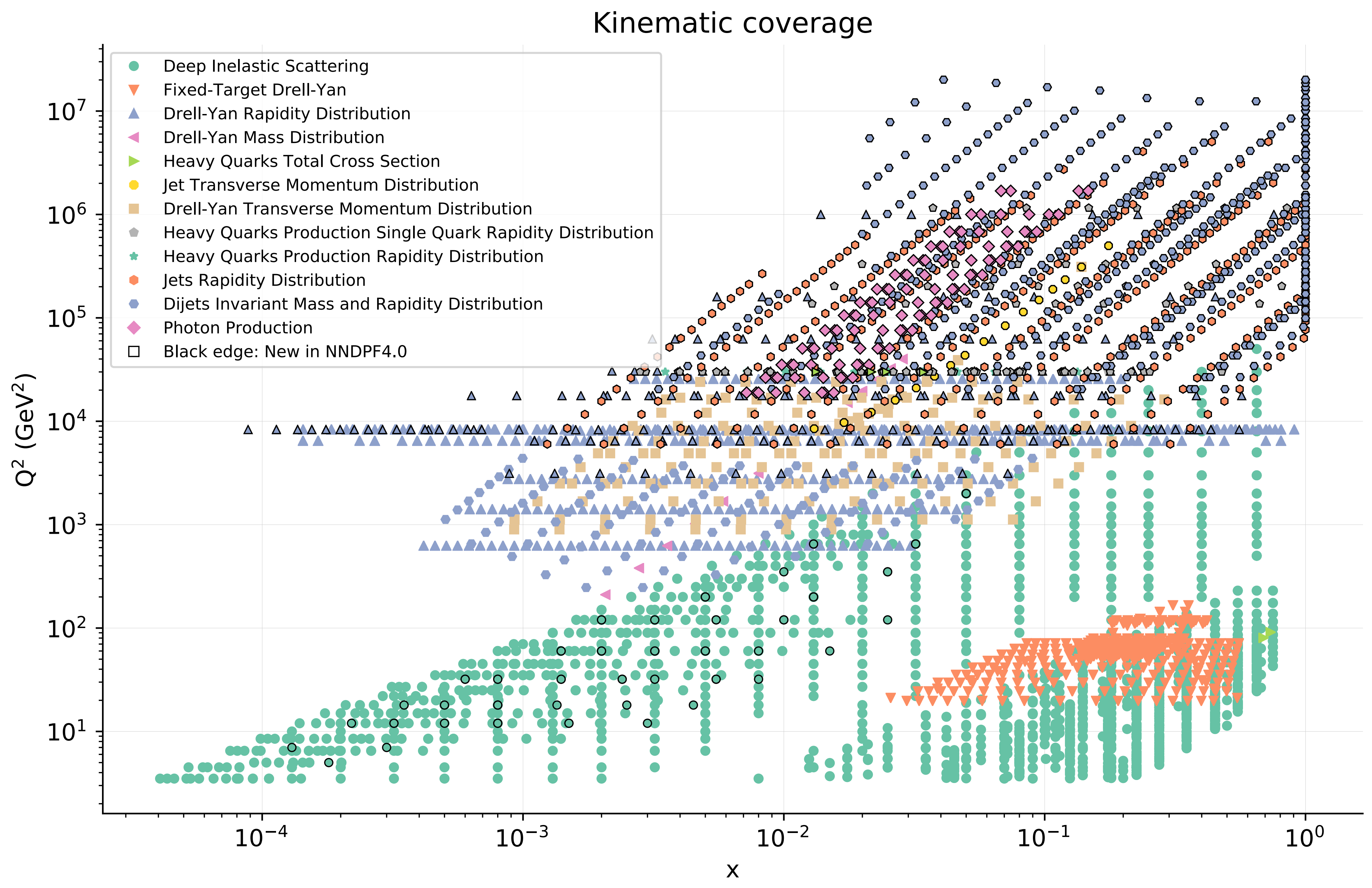
For more info see the Dedicated benchmark ***Les Houches benchmark paper*** *[arXiv:2406.16188]*

The NNPDF4.0 aN3LO PDF set

To produce the N3LO fit, we:

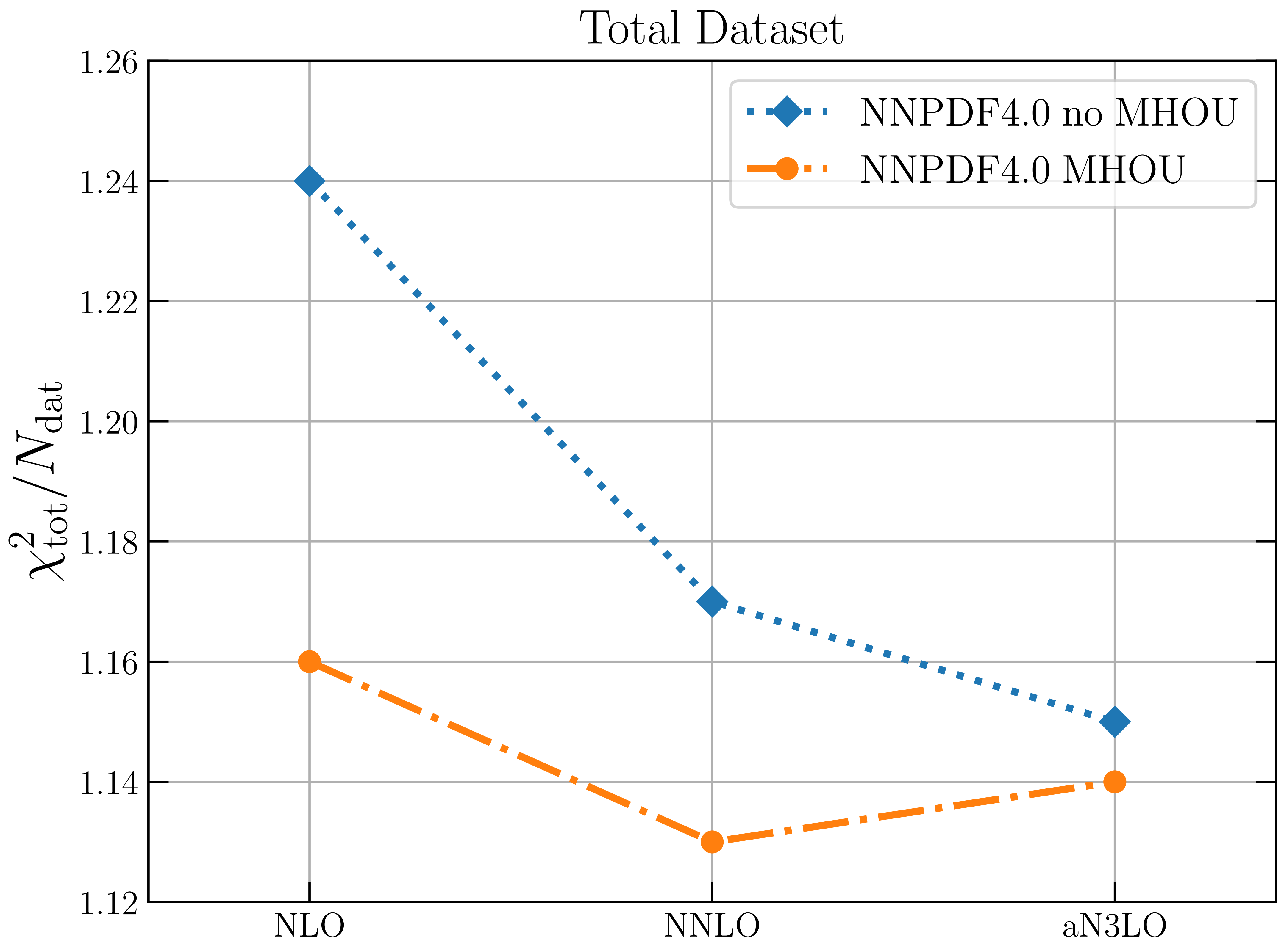
- Use **exact N3LO massless DIS** coefficient functions
- Include **aN3LO contributions in DGLAP massive DIS** and account for IHOUs
- Use NNLO renormalization scale variations to estimate **unknown N3LO terms for hadronic processes**
- Treat **theory uncertainties** on the equal footing with experimental uncertainties:

$$\mathrm{Cov}_{\mathrm{tot}} = \mathrm{Cov}_{\mathrm{exp}} + \mathrm{Cov}_{\mathrm{DGLAP,IHOU}} + \mathrm{Cov}_{\mathrm{DIS,IHOU}} + \mathrm{Cov}_{\mathrm{HAD,MHOU}} + \mathrm{Cov}_{\mathrm{MHOU}}$$



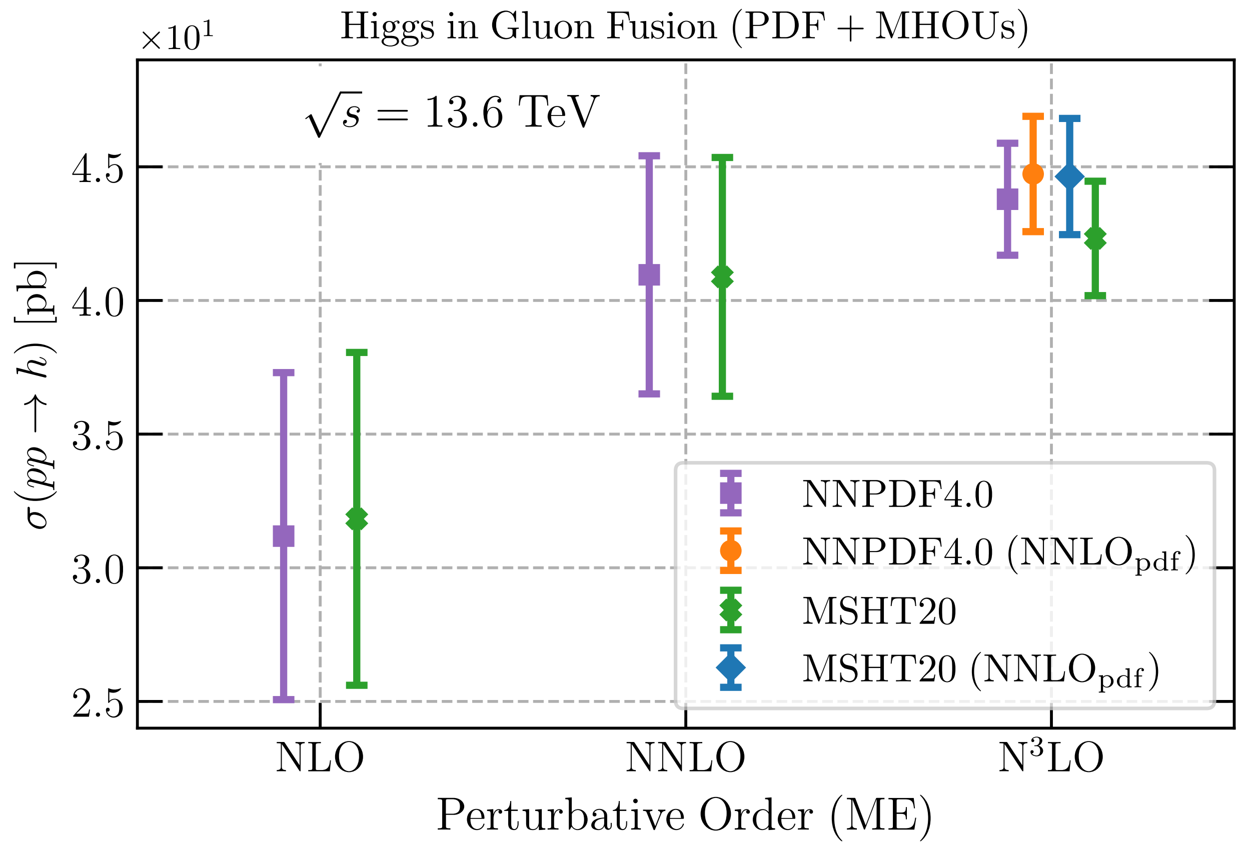
Fit over 4000 datapoints from many processes: DIS, Jets, Top, Drell-Yan, …

Fit quality

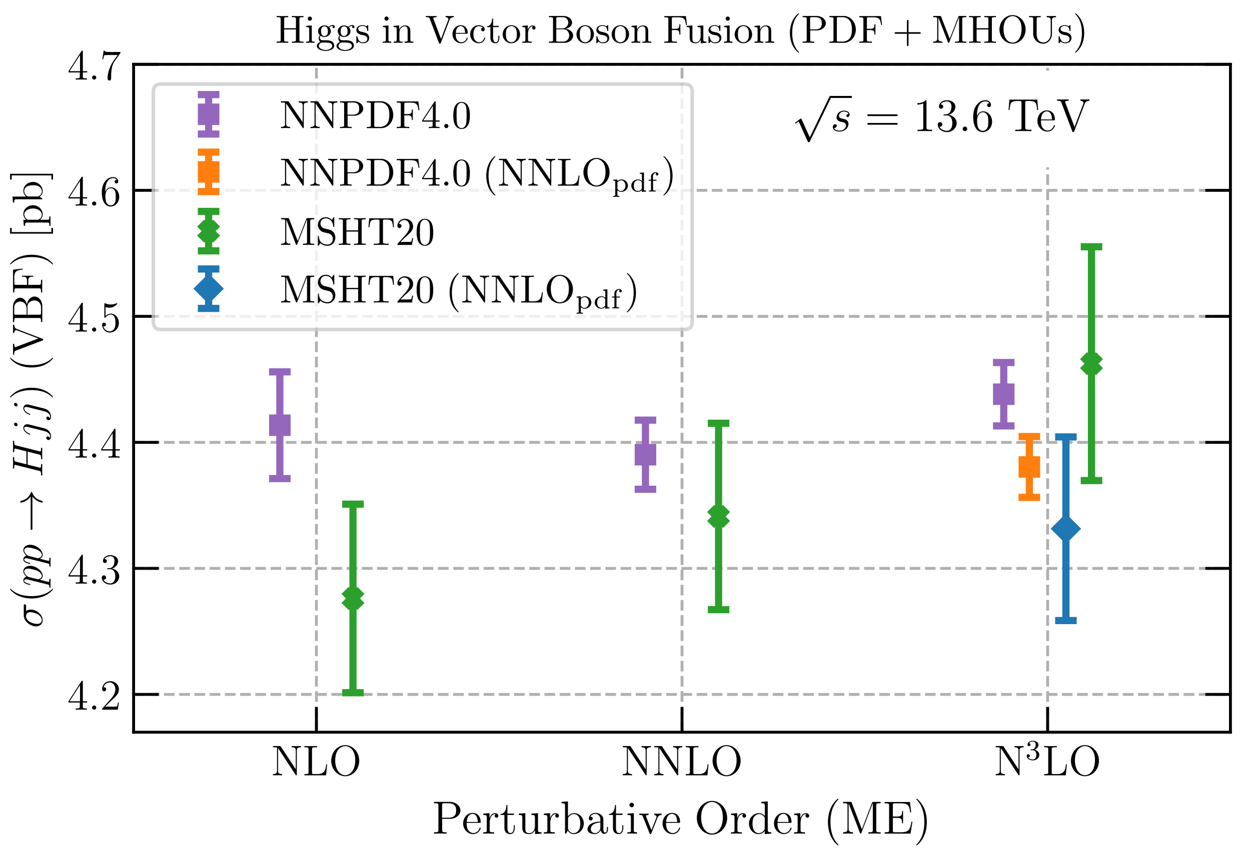


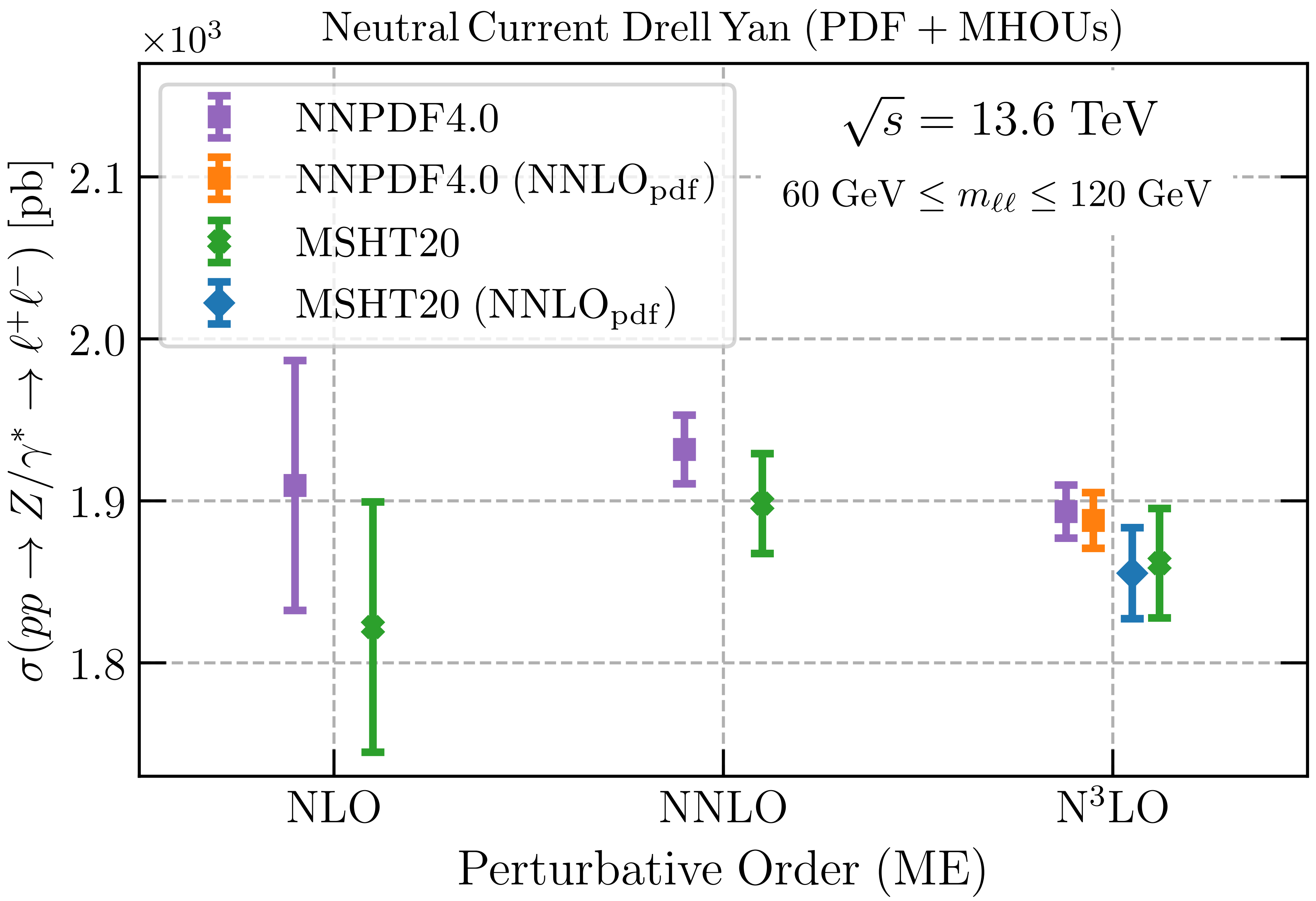
- Without MHOUs the fit improves (lower χ^2) with increasing perturbative order
- With MHOUs the fit depends only weakly on the perturbative order
- At N3LO MHOUs have a small impact on the χ^2

Impact on LHC cross sections



N3LO PDFs result in a small (~2%) suppression of the Higgs gluon fusion cross section compared to **NNLO PDFs**





Generally **good perturbative convergence** for Higgs and DY

N3LO/NNLO ratio is similar for NNPDF and MSHT [arXiv:2406.16188]

NNPDF4.0 QED

[arXiv:2401.08749]

So far we considered only QCD evolution, but $\mathcal{O}(\alpha_s^2) \approx \mathcal{O}(\alpha_{em})$

Also **photon initiated contributions** may be relevant

- Modify the DGLAP running to **account for QED corrections**:

$$P = P_{QCD} + P_{QCD\otimes QED}$$

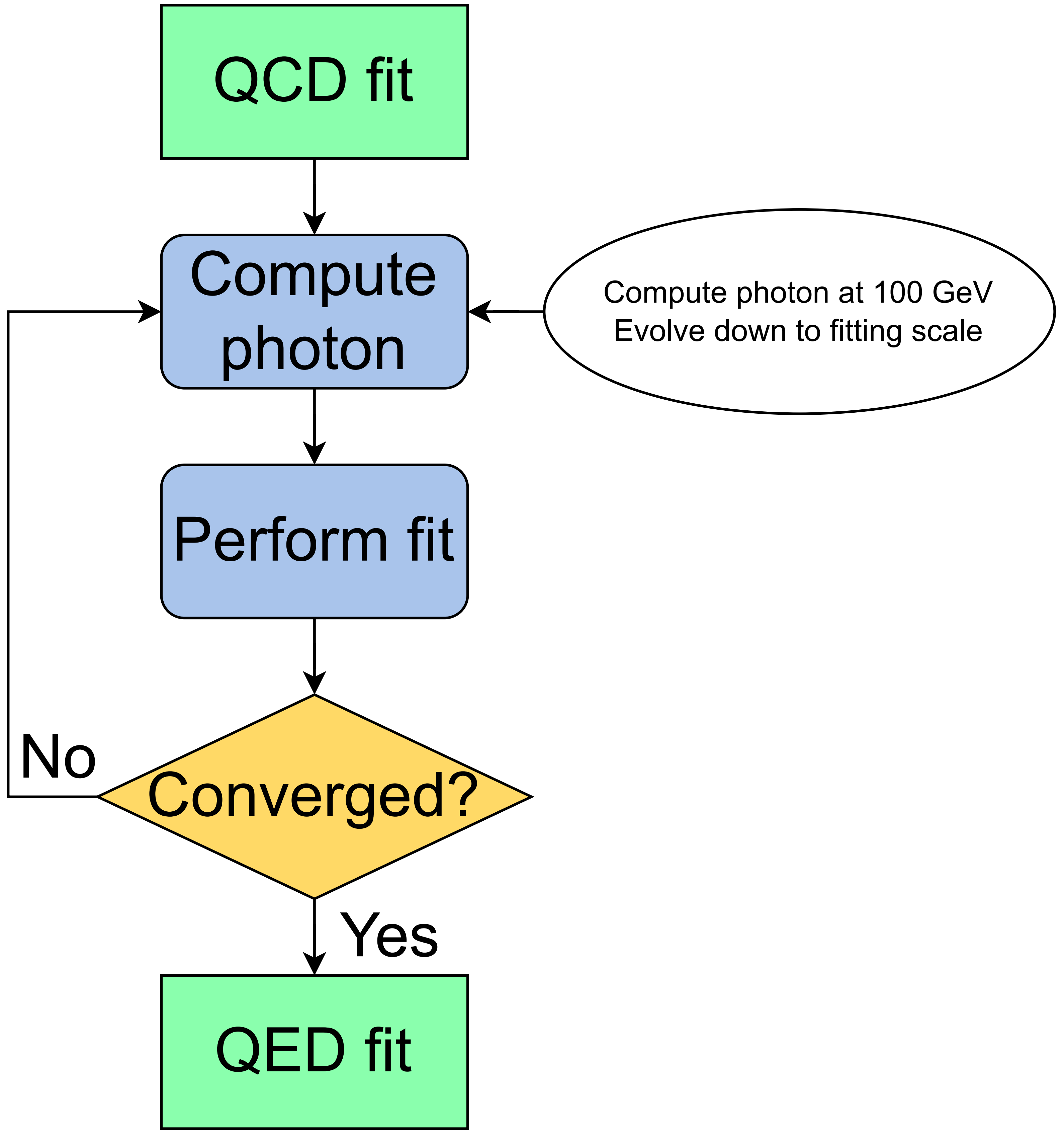
$$P_{QCD\otimes QED} = \alpha_{em} P^{(0,1)} + \alpha_{em}\alpha_s P^{(1,1)} + \alpha_{em}^2 P^{(0,2)}$$

- Data does not provide strong constraints on the photon, but the **photon PDF can be computed from DIS structure functions:** Manohar, Nason, Salam, Zanderighi, [arXiv:1607.04266], [arXiv:1708.01256]

$$x\gamma(x,\mu^2) = \frac{2}{\alpha(\mu^2)} \int_x^1 \frac{dz}{z} \left\{ \int_{\frac{m_p^2 x^2}{1-z}}^{\frac{\mu^2}{1-z}} \frac{dQ^2}{Q^2} \alpha^2(Q^2) \left[-z^2 F_L(x/z, Q^2) + \left(z P_{\gamma q}(z) + \frac{2x^2 m_p^2}{Q^2} \right) F_2(x/z, Q^2) \right] - \alpha^2(\mu^2) z^2 F_2(x/z, \mu^2) \right\}$$

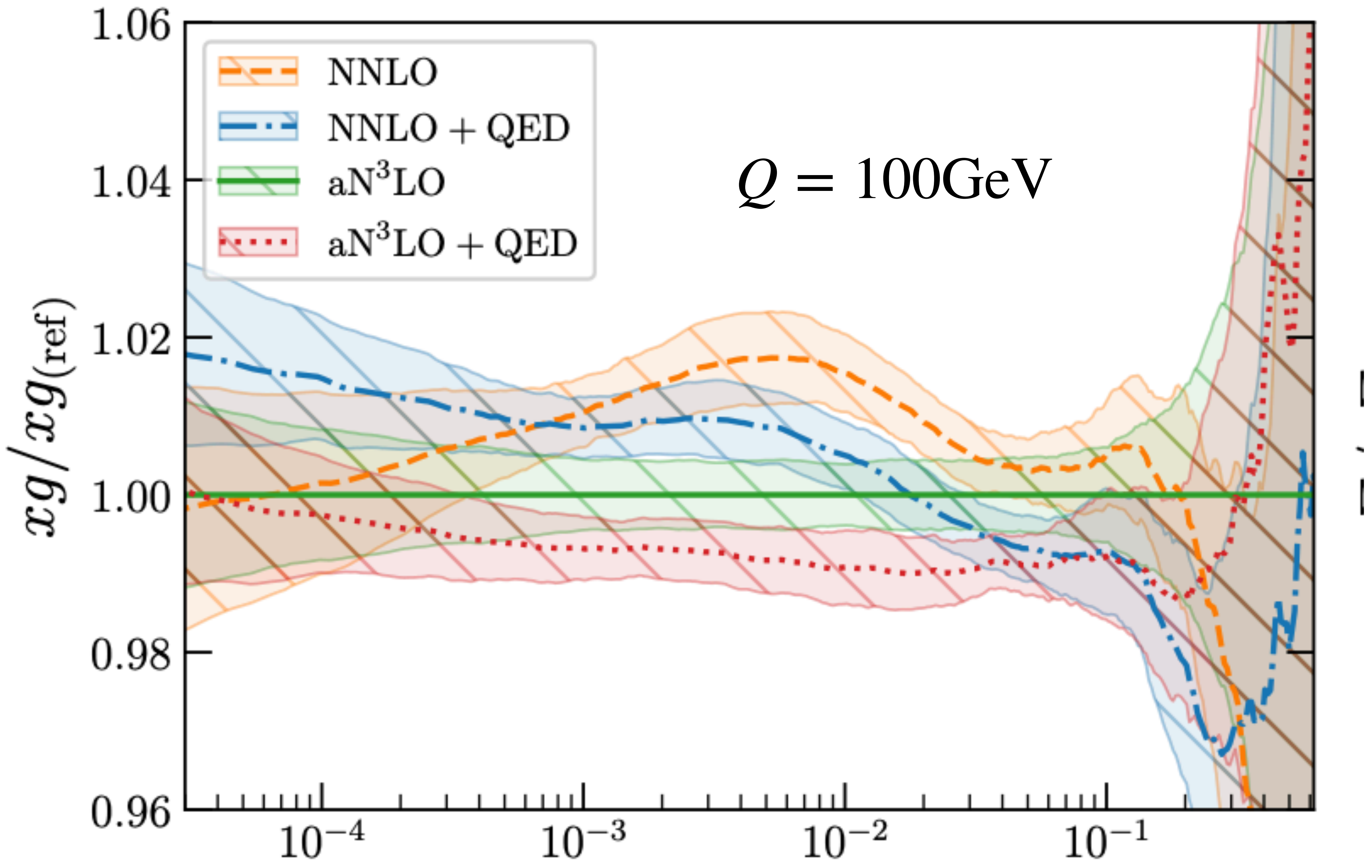
- An iterative procedure is used to address the **interplay between the photon and other PDFs due to the momentum sum rule:**

$$\sum_{i=q,\bar{q},g,\gamma} \int_0^1 dx x f_i(x, Q^2) = 1.$$



NNPDF4.0 aN3LO QED

[arXiv:2406.01779]



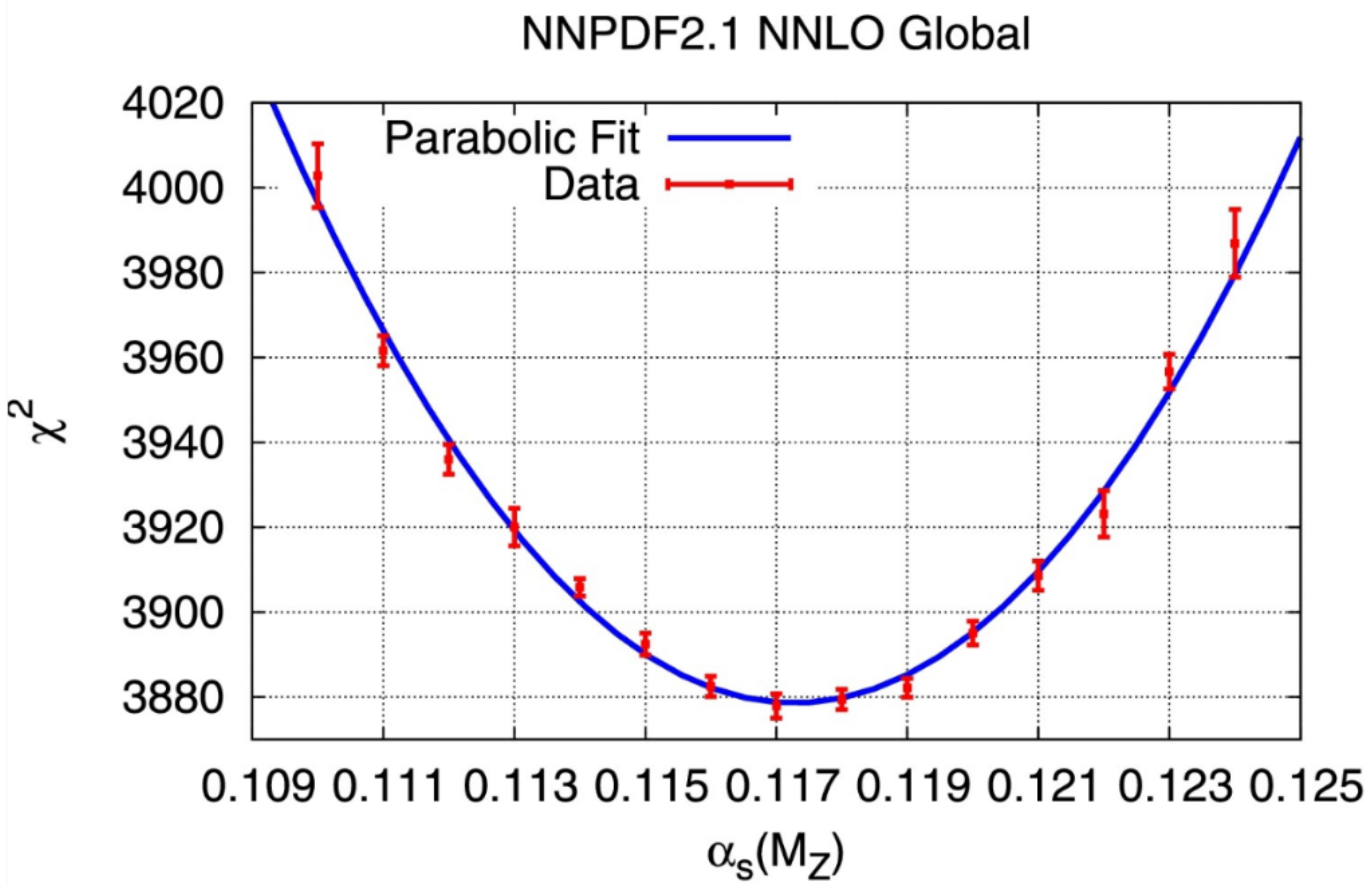
- Photon subtracts momentum from the gluon PDF
- QED effect has a similar magnitude as aN3LO

α_s from NNPDF4.0

In preparation

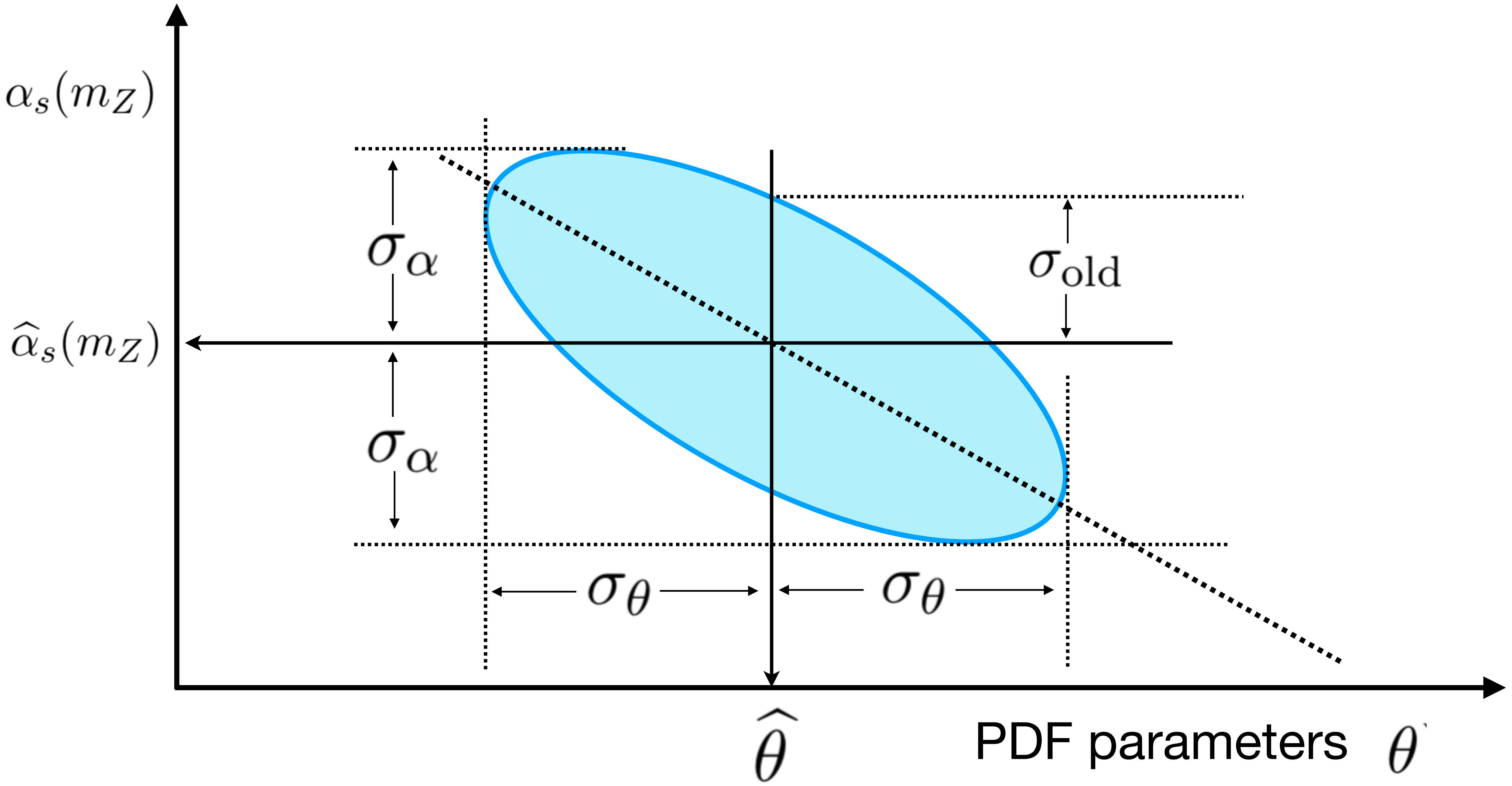
α_s from PDFs

PDFs and α_s are highly correlated so **extracting α_s from collider data requires a simultaneous determination with PDFs**



In most cases α_s is determined by extracting it from a parabolic fit to the χ^2 profile

Uncertainty is determined from $\Delta\chi^2 = 1$



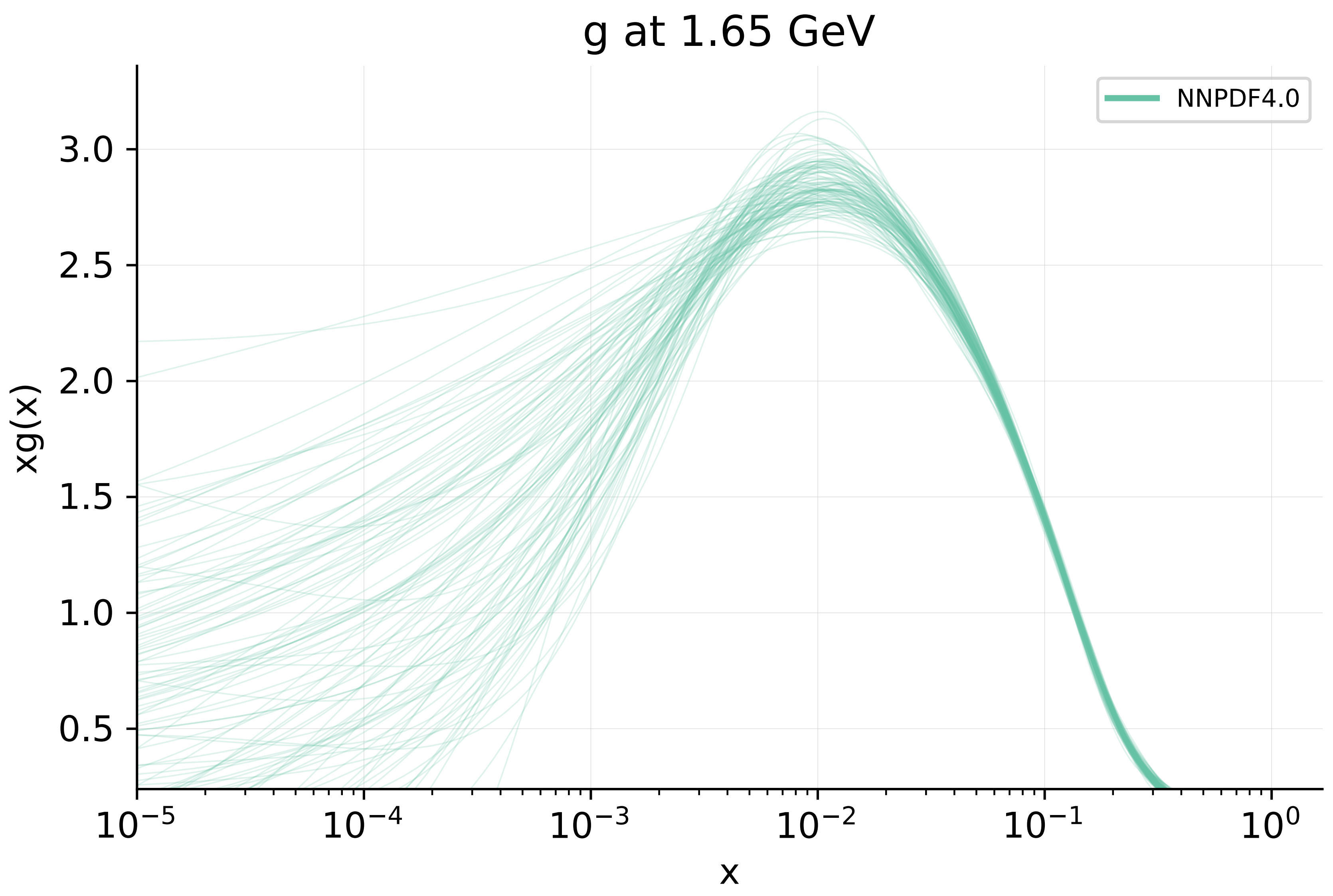
However, the usual methodology neglects correlations between α_s and the PDFs which may lead to underestimated uncertainties

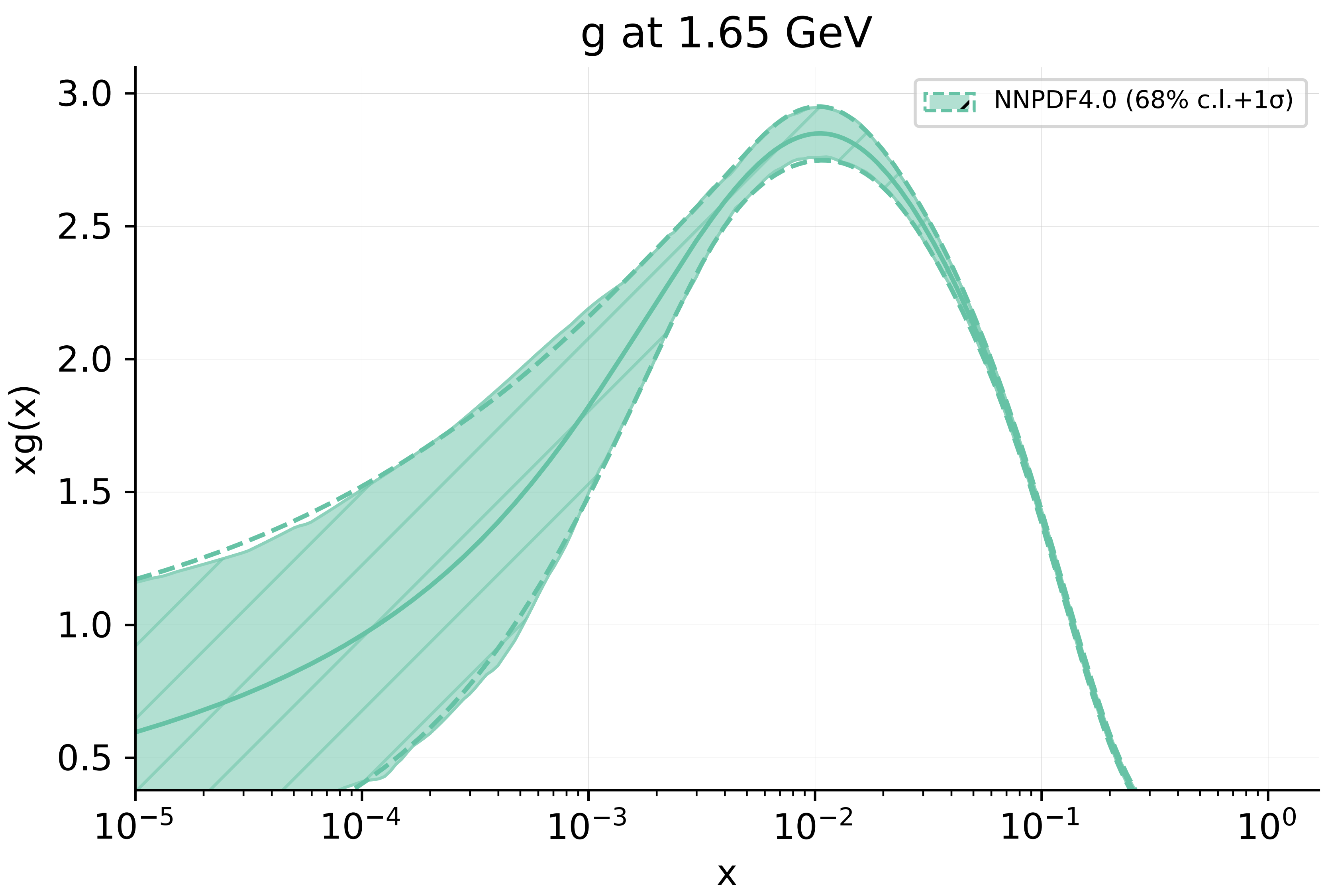
Intermezzo - how to propagate experimental uncertainty to PDFs

An NNPDF set (usually) consists of 100 PDF replicas produced as follows:

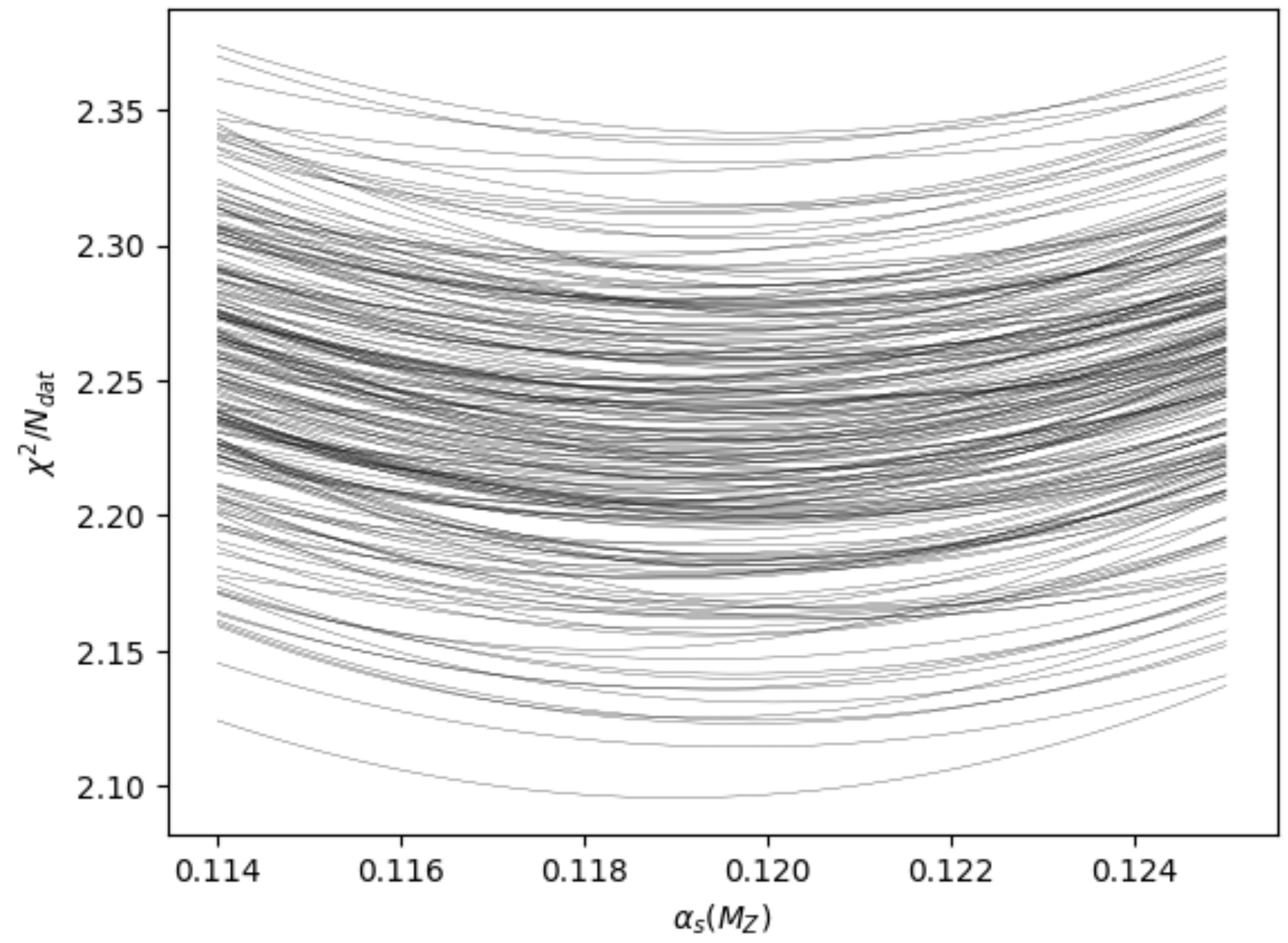
1. Assume experimental data is **defined** by a vector of central values and a covariance matrix
2. Sample this distribution to create 100 Monte Carlo replicas in data space
3. Perform a fit to each of the data replicas

➡A PDF set encoding experimental uncertainties

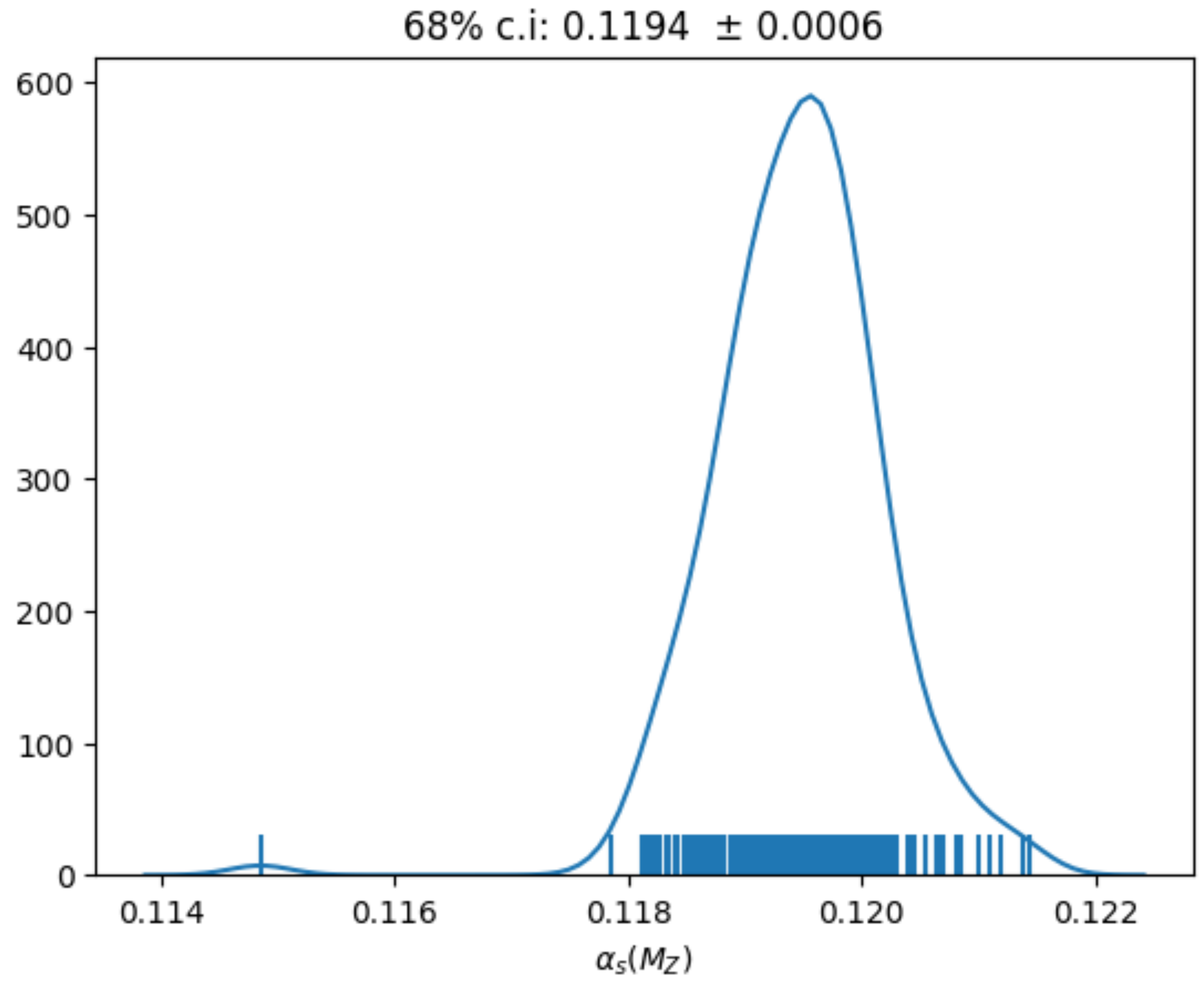




Simultaneous minimization of PDF and α_s



Fit the same data replica at different values of α_s and fit a parabola for each replica …



… then look at the distribution of minima of the parabolas

α_s from correlated theory uncertainties

The "correlated replicas" method is computationally costly and lacks a mathematical framework

Alternatively, α_s can be determined in a Bayesian framework from nuisance parameters: [arXiv:2105.05114]

1. Model the theory uncertainty as a shift correlated for all datapoints

   $T \to T + \Delta\alpha_s \cdot \beta$, for $\beta \equiv \frac{\partial}{\partial \alpha_s} T$

   we can then write

   $$P(T \mid D, \Delta\alpha_s) \propto \exp\left(-\frac{1}{2}(T + \Delta\alpha_s \cdot \beta - D)^T \mathrm{Cov}_{EXP}^{-1}(T + \Delta\alpha_s \cdot \beta - D)\right)$$

2. Choose a prior

   $$P(\Delta\alpha_s) \propto \exp\left(-\frac{1}{2}\Delta\alpha_s^2\right)$$

3. Marginalize over $\Delta\alpha_s$ to get $P\left(T|D\right)$

4. Compute the posterior for $\Delta\alpha_s$ using the ingredients we just wrote down

   $$P(\Delta\alpha_s \mid T, D) = \frac{P(T \mid D, \Delta\alpha_s)P(\Delta\alpha_s)}{P(T \mid D)} \propto \exp\left[-\frac{1}{2}Z^{-1}(\Delta\alpha_s - \overline{\Delta\alpha_s})\right]$$

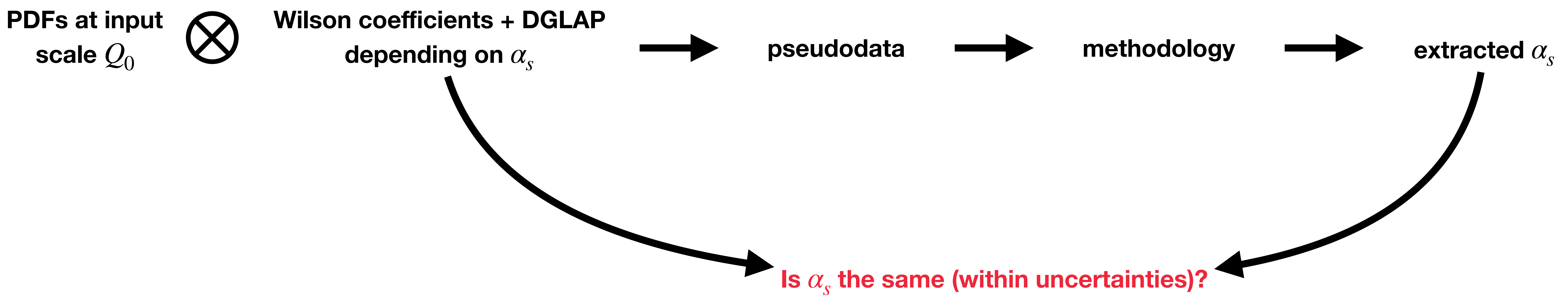
For predictions T computed using α_s^0, **the final value is** $\alpha_s = \alpha_s^0 + \overline{\Delta\alpha_s} \pm Z$

Both methodologies give the same result!

Validating the methodologies

We use closure tests to validate our methodology

Basic idea: generate a global pseudo dataset from theory predictions and extract α_s from this.



This question is answered through the analysis of various statistical estimators

Results

Results are perturbatively stable (also found by MSHT)

NNLO: $\alpha_s(M_Z) = 0.1194 \pm 0.0007$

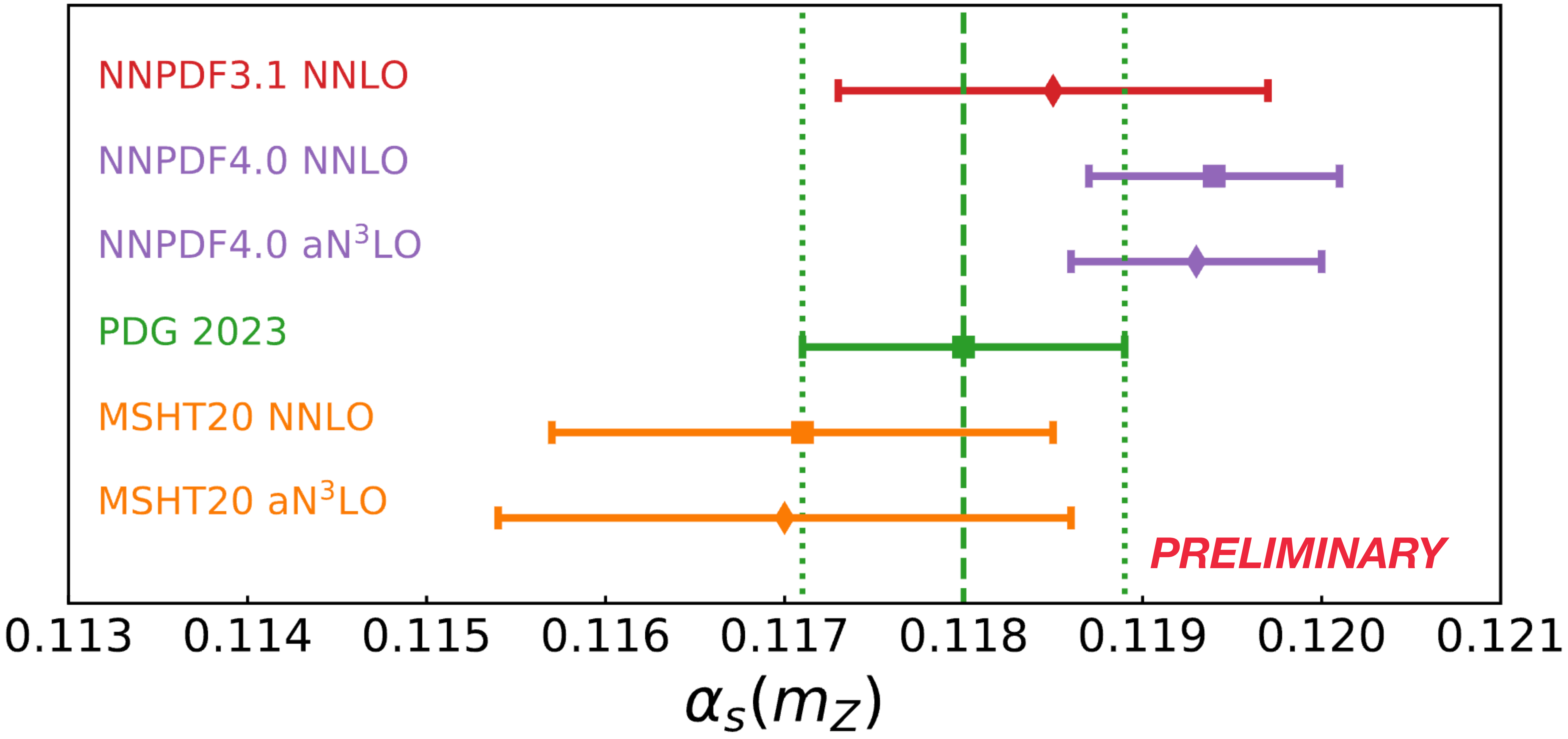
aN3LO: $\alpha_s(M_Z) = 0.1193 \pm 0.0007$

In agreement with NNPDF3.1: $\alpha_s(M_Z) = 0.1185 \pm 0.00012$

w/o MHOUs:

NNLO: $\alpha_s(M_Z) = 0.1204 \pm 0.0004$

aN3LO: $\alpha_s(M_Z) = 0.1200 \pm 0.0003$



Theory uncertainties improve perturbative stability

This determination will also be updated with QED effects

Summary and Outlook

- PDFs are a key ingredient for LHC physics

- aN3LO PDFs allow for a consistent computation of observables at N3LO. Initial results suggest good convergence for Higgs and Drell-Yan production

- SM parameters from collider data require a simultaneous determination with the PDFs

PRELIMINARY

- **The extracted strong coupling constant is perturbatively stable between NNLO and aN3LO:** $\alpha_s(M_Z) = 0.1194 \pm 0.0007$ **and** $\alpha_s(M_Z) = 0.1193 \pm 0.0007$

Towards NNPDF4.1:

- Replace NNLO K-factors with full calculation
- Methodological improvements, e.g. new hyperoptimization metrics
- Extension of the NNPDF dataset

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Thank you for your attention!

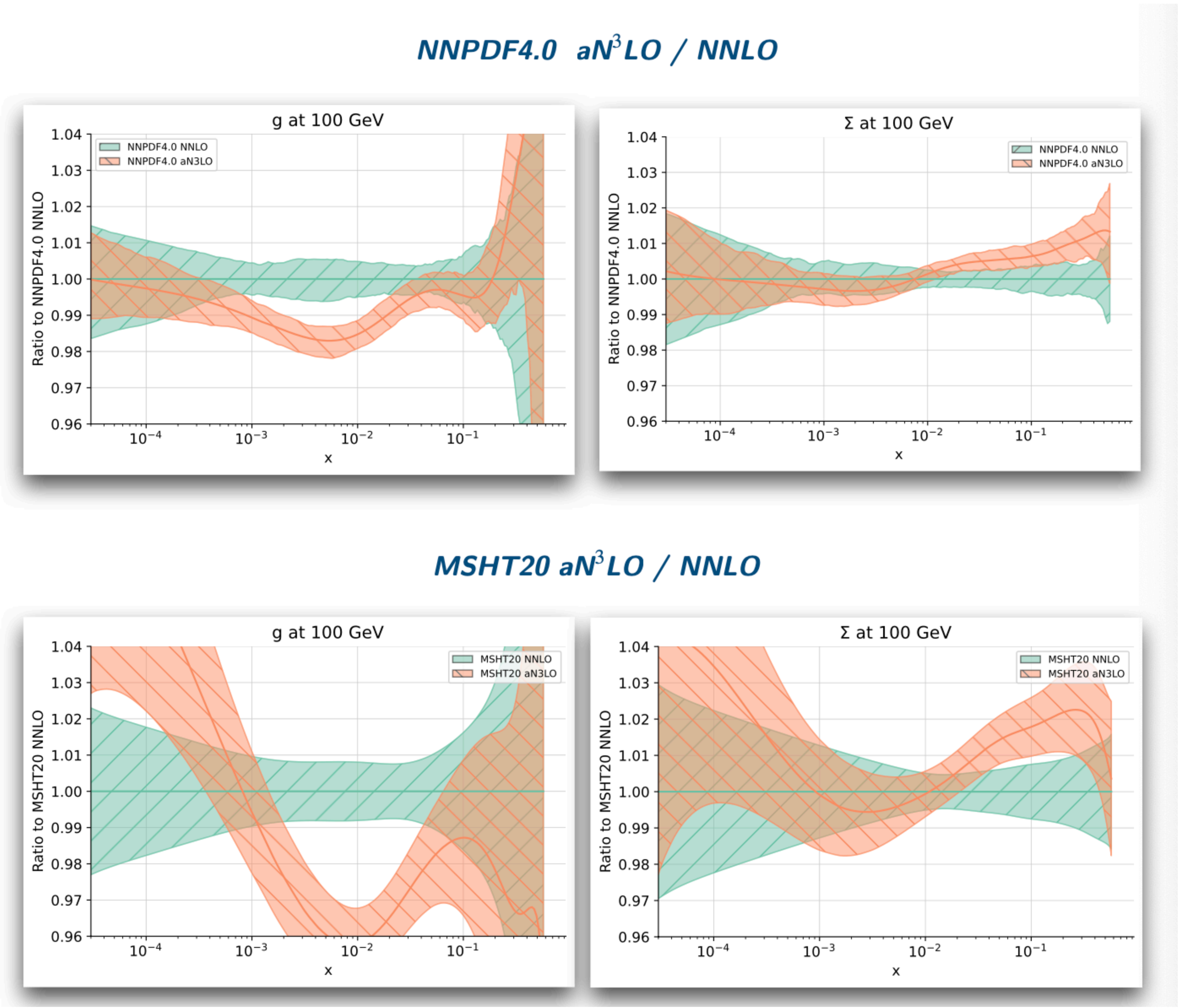
Backup slides

Comparison to MSHT20 aN3LO

[arXiv:2207.04739]

Main differences are due to:

- **Mellin moments** for splitting functions computed in the last two years: MSHT has an earlier cut-off/publication date
- **DGLAP parameterization uncertainty**. NNPDF uses only prior while MSHT extracts posterior from data
- Treatment of **partonic coefficients**: DIS heavy quark schemes, hadronic k-factors
- **Fitting methodology and data**



G. Magni, HP2
Turin, September 2024

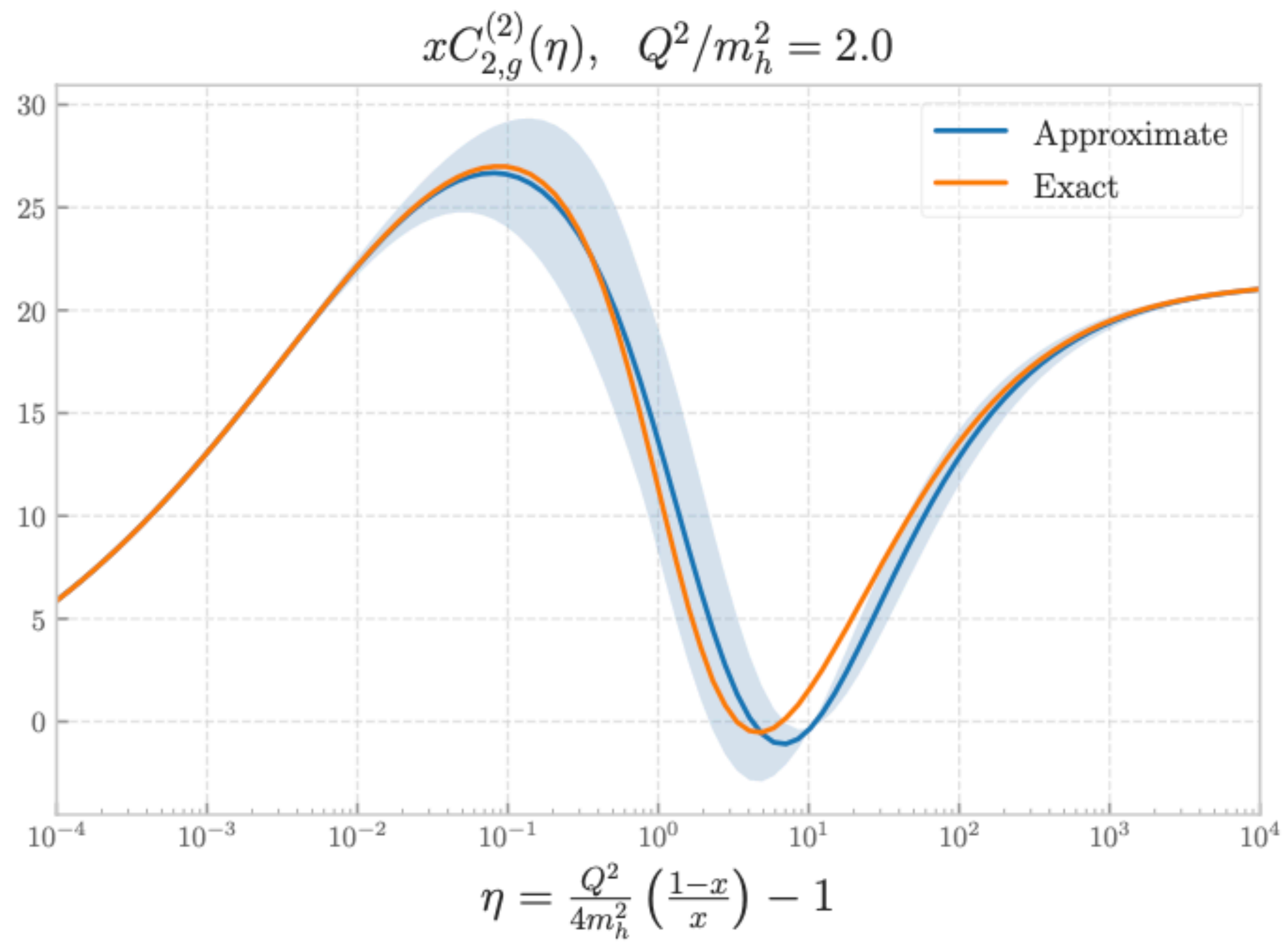
aN3LO DIS coefficients

- DIS coefficient functions are known up to N3LO in the massless limit [Larin, Nogueira, Van Ritbergen, Vermaseren, 9605317], [Moch Vermaseren Vogt, 0411112, 0504242], [Davies, Moch, Vermaseren, Vogt, 0812.4168, 1606.08907]
- Massive coefficient functions can be constructed by smoothly joining the known limits from threshold and high energy resummation, and the massless limit [Barontini, Bonvini, Laurenti, in preparation]

$$C^{(3)}(x, m_h^2/Q^2) = C^{(3),\text{thr}}(x, m_h^2/Q^2) f_1(x) + C^{(3),\text{asy}}(x, m_h^2/Q^2) f_2(x)$$

$$f_1(x) \xrightarrow[x \to x_{\max}]{} 1, \quad f_2(x) \xrightarrow[x \to x_{\max}]{} 0$$

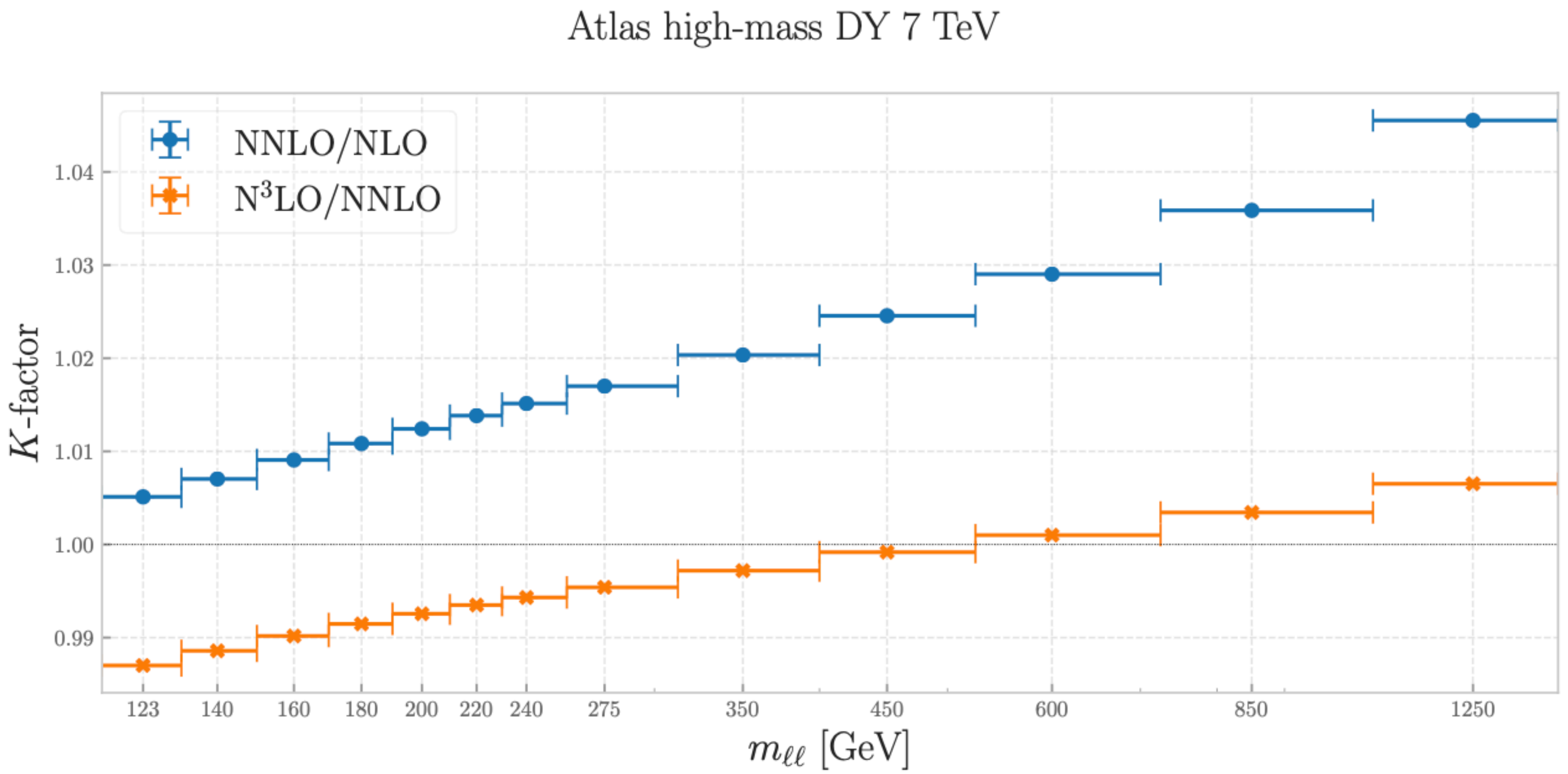
$$f_1(x) \xrightarrow[x \to 0]{} 0, \quad f_2(x) \xrightarrow[x \to 0]{} 1$$



Validate the procedure at NNLO
Uncertainty band is obtained by varying interpolation functions

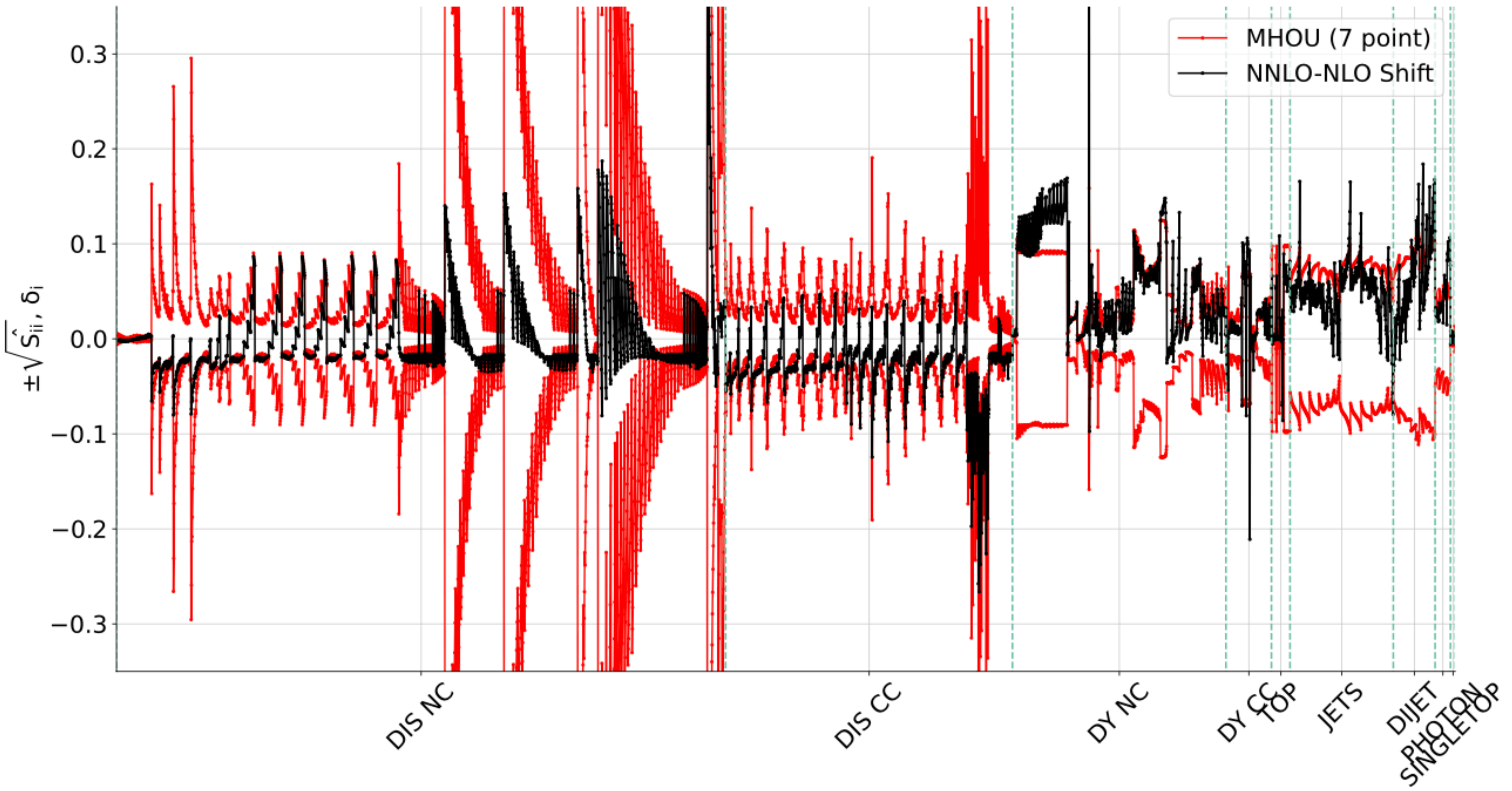
Hadronic processes

- Corrections to collider DY and W production can be included through k-factors
- N3LO effects around 1 to 2% for LHC observables
- For many processes N3LO corrections are not available, for those we introduce account for MHOU through μ_r variations



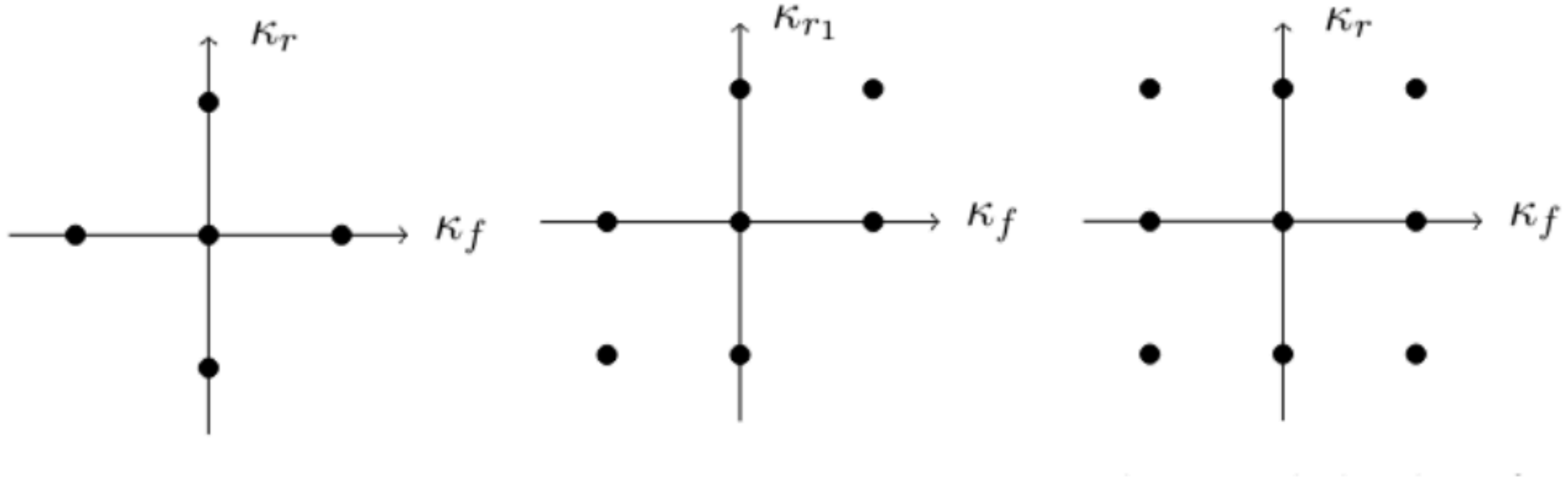
Validating the MHOU covmat

Validate the MHOU procedure by comparing the NLO covmat with estimated MHOUs to the known NNLO-NLO shifts



Theory uncertainties in PDFs

- MHOUs are estimated through 7 point factorization and renormalization scale variations



5,7,9 point prescription

- In a fit we minimize the χ^2:

$$P(T|D) \propto \exp\left[-\frac{1}{2}(T-D)\,C^{-1}\,(T-D)\right] = \exp\left[-\frac{1}{2}\chi^2\right]$$

- Include theory covmat C_{MHOU} at same footing as exp covmat $C = C_{\mathrm{exp}} + C_{\mathrm{MHOU}}$

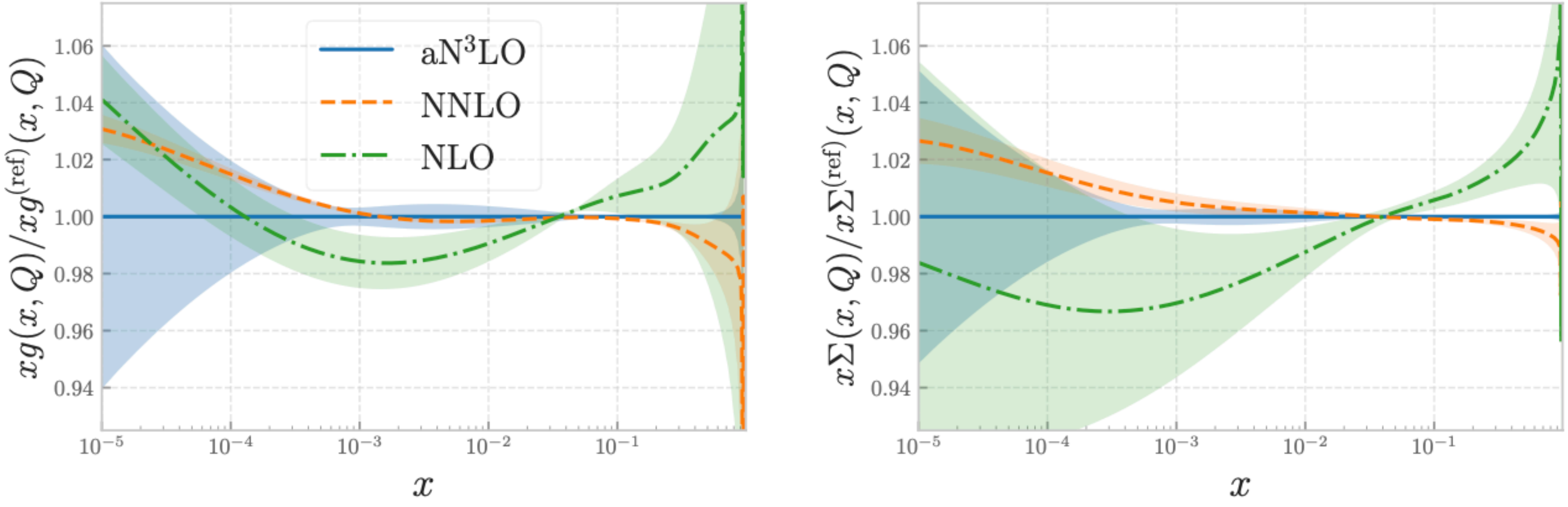
$$C_{\mathrm{MHOU},ij} = n_m \sum_{V_m} \left(T_i(\kappa_f,\kappa_r) - T_i(0,0)\right)\left(T_j(\kappa_f,\kappa_r) - T_j(0,0)\right)$$

- Incomplete higher order uncertainties on the approximation of the DGLAP splitting kernels are independent and added in quadrature:

$$C = C_{\mathrm{exp}} + C_{\mathrm{MHOU}} + C_{\mathrm{IHOU}}$$

aN3LO DGLAP evolution

NNPDF4.0 evolved from $Q = 1.65$ GeV to $Q = 100$ GeV



- Effects of N3LO corrections to DGLAP evolution at most percent level, except at small-x and large-x
- Good perturbative convergence