The path to aN^{3}LO Parton Distributions

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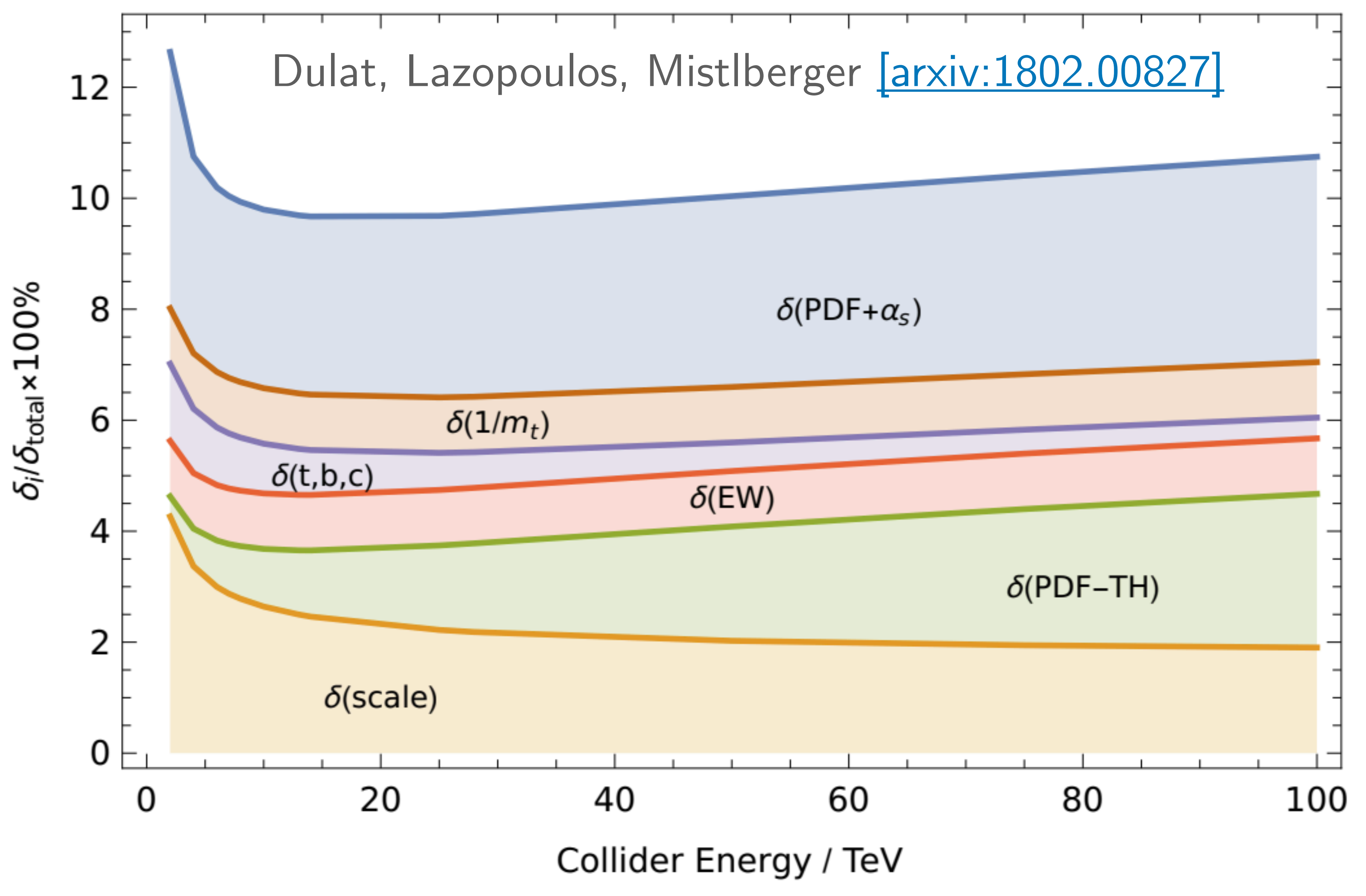
Why do we need N^{3}LO PDFs?

$$\sigma(x,Q^2) = \sum_i \int_x^1 \frac{dz}{z} \mathscr{L}_{ij}(z,\mu^2)\ \hat{\sigma}_{ij}(\frac{x}{z},\frac{Q^2}{\mu^2},\alpha_s) + \mathscr{O}(\frac{1}{Q^2})$$

- Predictions for LHC observables rely on two main ingredients: **Parton Distributions Functions (PDFs)** and partonic **Matrix Elements**.
- In the last years many **2 to 1 processes** have been calculated up to QCD at **N^{3}LO**: $gg \to H$ [arxiv:1503.06056] $qq \to H$ (VBF) [arxiv:1606.00840], [arxiv:1904.09990], [arxiv:2004.04752] $pp \to W^\pm$ [arxiv:2007.13313], [arxiv:2205.11426] $pp \to Z/\gamma$, $pp \to VH$ [arxiv:2209.06138], [arxiv:2107.09085],[arxiv:2207.07056]
- **PDFs uncertainties** are becoming a **bottleneck** for high energy cross sections computations.
- **Combining experimental analysis** with different PDFs sets can be **non trivial.** Theory uncertainties are compatible with experimental systematics.

% Theory Uncertainties in $pp \to H$ (ggF)



ATLAS collaboration [arxiv:2309.12986]

PDF set	$\alpha_s(m_Z)$	PDF uncertainty
MSHT20 [37]	0.11839	0.00040
NNPDF4.0 [84]	0.11779	0.00024
CT18A [29]	0.11982	0.00050
HERAPDF2.0 [65]	0.11890	0.00027

$$\delta_{PDF} = 0.3\ \%$$

$$\alpha_s(\text{NNPDF}) - \alpha_s(\text{CT18A}) = 1.7\ \%$$

Why do we need N^{3}LO PDFs?

- The **interpretation of LHC measurements,** both SM parameters determination ad NP searches **depends** on the the **PDF accuracy and precision**.
- Most widely used **PDFs are at NNLO** and do not include theory uncertainties.

Why do we need N^{3}LO PDFs?

- The **interpretation of LHC measurements,** both SM parameters determination ad NP searches **depend** on the the **PDF accuracy and precision**.
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Approximate N^{3}LO PDFs are now available.

Present results based on:

`NNPDF4.0 aN3LO` [arxiv:2402.1863]

`NNPDF4.0 QED aN3LO` [arxiv:20406:0177]

What impact do they have on LHC cross-sections ?

PDFs determination at aN^{3}LO

Theoretical **inputs needed in a PDF fit**:

1. QCD **splitting functions** which controls the DGLAP evolution.

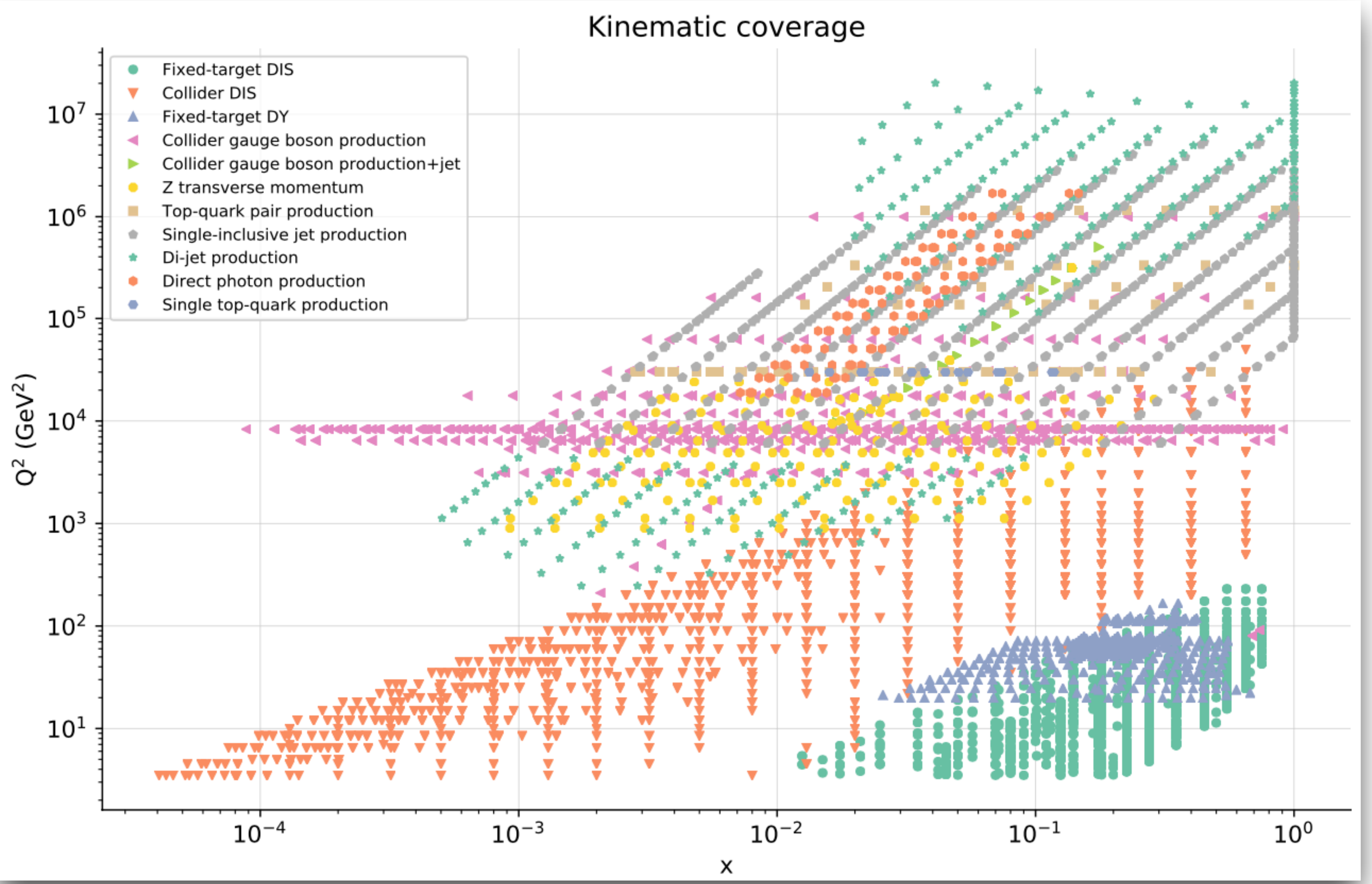
$$Q^2 \frac{df_i}{dQ^2} = P_{ij}(x, \alpha_s) \otimes f_i(x, Q^2)$$

2. **VFNS matching conditions** for each running component.

$$f_i^{(n_f+1)}(x, Q^2) = A_{ij}(x, \alpha_s) f_j^{(n_f)}(x, Q^2)$$

3. Process dependent **Partonic coefficients** functions, both for DIS and hadronic observables.

$$\sigma(x, Q^2) = \sum_{i=0}^{n_f} C_{k,i}(x, \alpha_s) \otimes f_i(x, Q^2)$$



NNPDF4.0 timeline

Sep 2021:
NNPDF4.0 [code & paper]

Jan 2024:
NNPDF4.0 MHOU
NNPDF4.0 QED

Feb 2024:
NNPDF4.0 aN3LO

Jun 2024:
NNPDF4.0 QED aN3LO

aN^{3}LO splitting functions

See G. Falcioni talk

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

Approximation can be constructed from the large number of partial results available.

- **Large-n_f:** $\mathcal{O}(n_f^3)$, $P_{NS}^{(n_f^2)}$ [arxiv:1610.07477]; $P_{qq,PS}^{(n_f^2)}$[arxiv:2308.07958]; $P_{gq}^{(n_f^2)}$ [arxiv:2310.01245]
- **NS small-x** [arxiv:2202.10362]: $$P_{NS}^{(3)} \supset \sum_{k=0}^{6} \ln^k(x)$$
- **Singlet small-x** [arxiv:1805.06460]: $$P_{ij}^{(3)} \supset \sum_{k=0}^{3} \frac{\ln^k(x)}{x}$$
- **Large-x** [arxiv:2205.04493], [arxiv:1911.10174], [arxiv:0912.0369]:

$$P_{ii}^{(3)} \approx A_{4,i} \frac{1}{(1-x)_+} + B_{4,i}\delta(1-x) + C_{4,i}\ln(1-x) + D_{4,i}$$

$$P_{ij}^{(3)} \approx \sum_{k}^{6} \ln^k(1-x)$$

- 5 or 10 lowest **Mellin Moments** [arxiv:1707.08315] [arxiv:2111.15561], [arxiv:2302.07593],[arxiv:2307.04158],[arxiv:2310.05744], ([arxiv:2404.09701], not included)

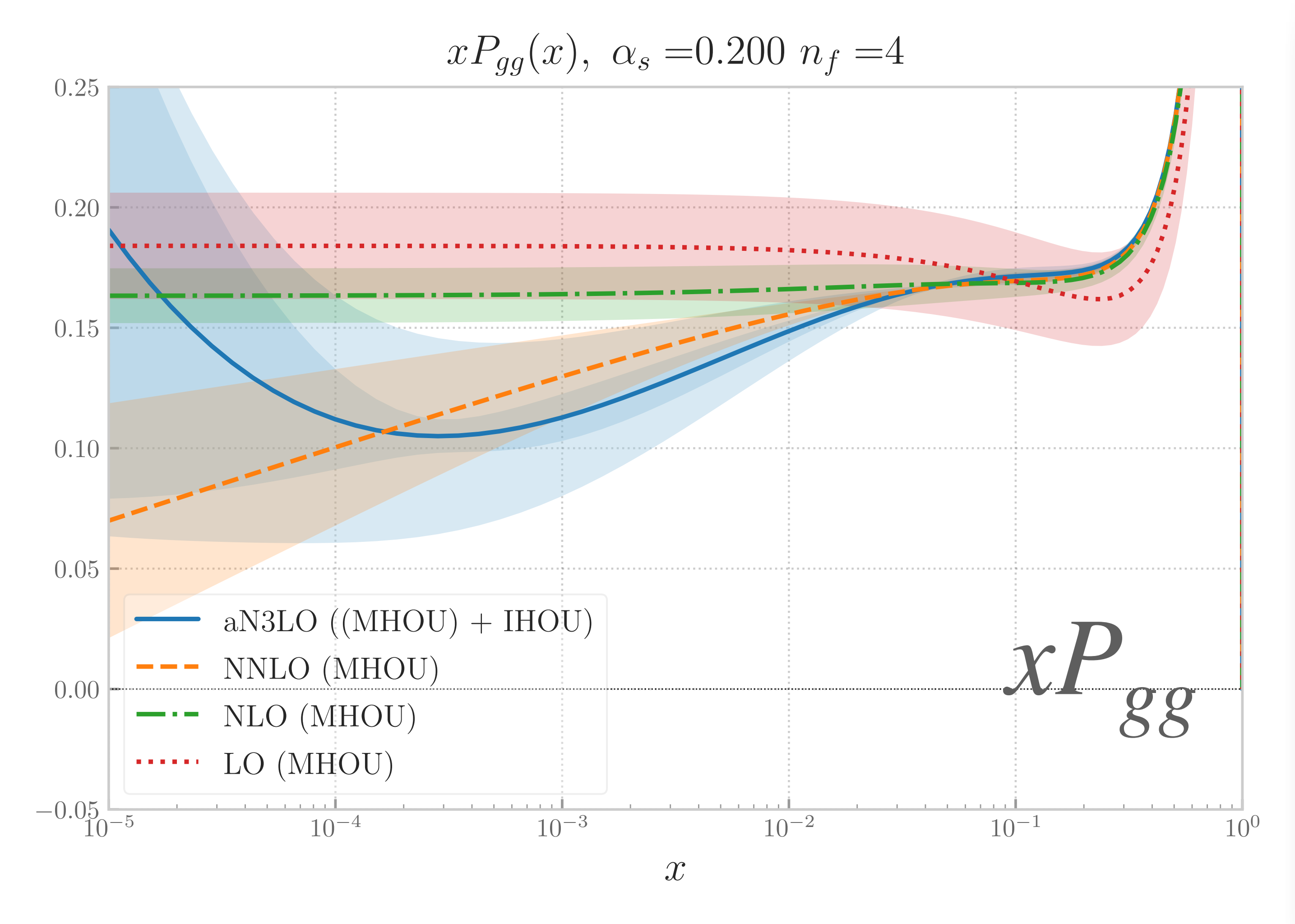
How do we combine the different limits?

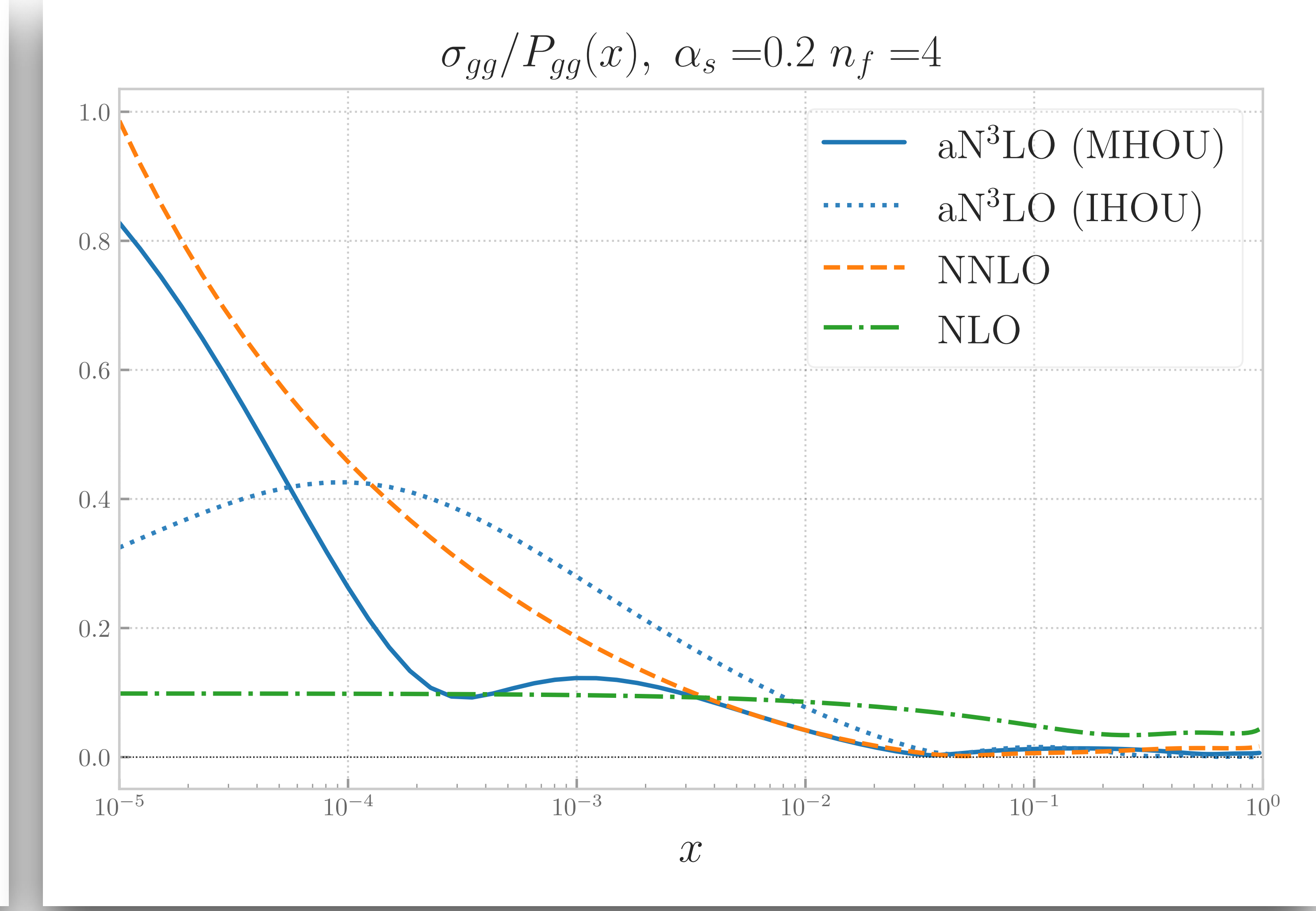
- The approximation procedure is performed in **Mellin space** for each n_f part independently:
- Combine **small-x and large-x** limits to match the Mellin moments, with different possible trial functions.
- Vary the parametrised part to generate a set of approximation and determine **Incomplete Higher Order Uncertainties (IHOU)**
- Determine independently **Missing Higher Order Uncertainties (MHOU)** from scale variation

aN^{3}LO splitting functions

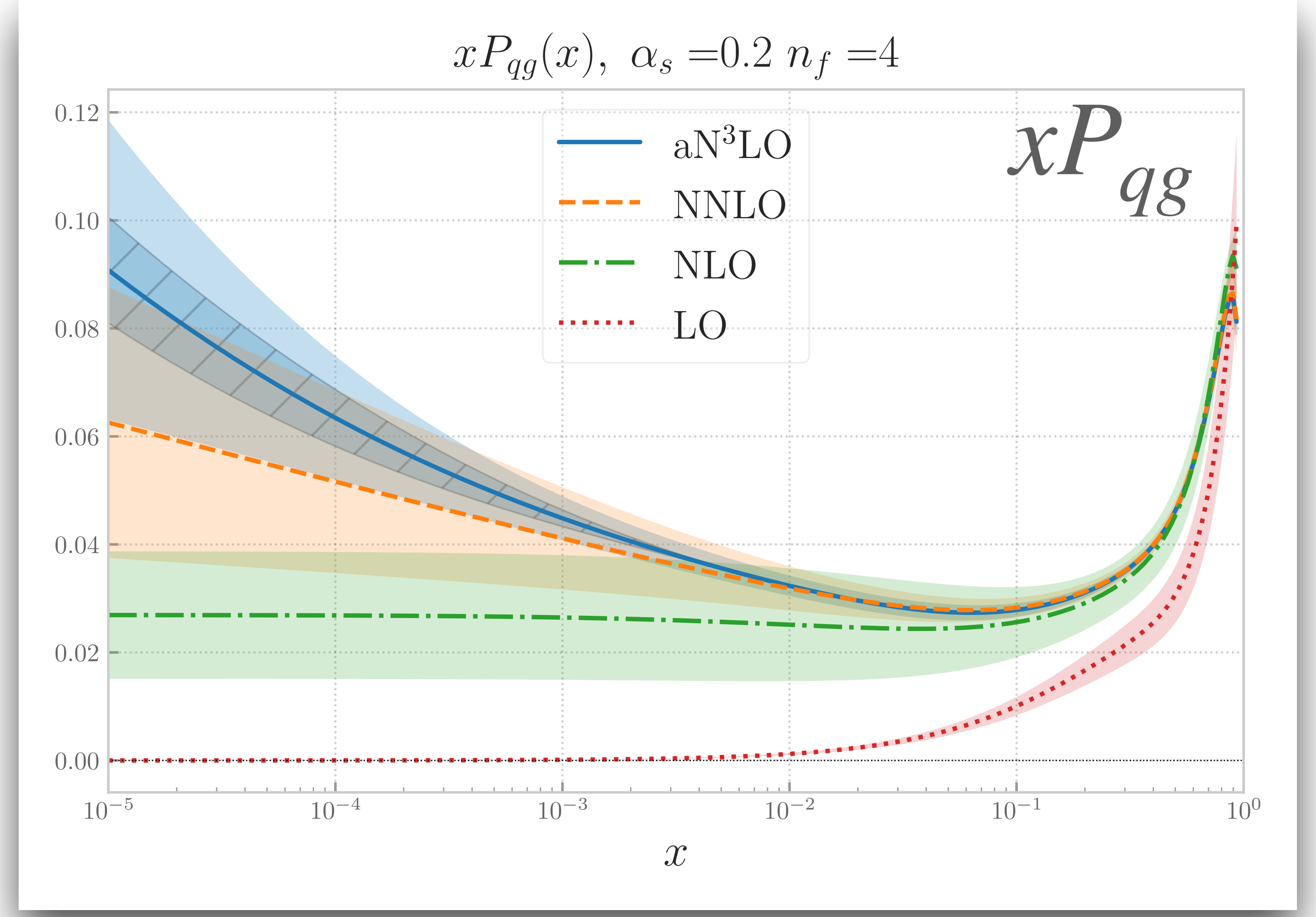
- **Large-x**: good perturbative stability,
- **Small-x**: effect of BFKL logarithms spoils the convergence $[1/x\ln^3(x),\ 1/x\ln^2(x)]$.
- For P_{qg}, P_{qq}, P_{gq} the N^{3}LO **approximation uncertainty is negligible** [IHOU < MHOU].
- In P_{gg} the **N^{3}LO approximation uncertainty is significant** [IHOU > MHOU for $x \geq 10^{-4}$]. Having 10 moments is enough for phenomenological applications.

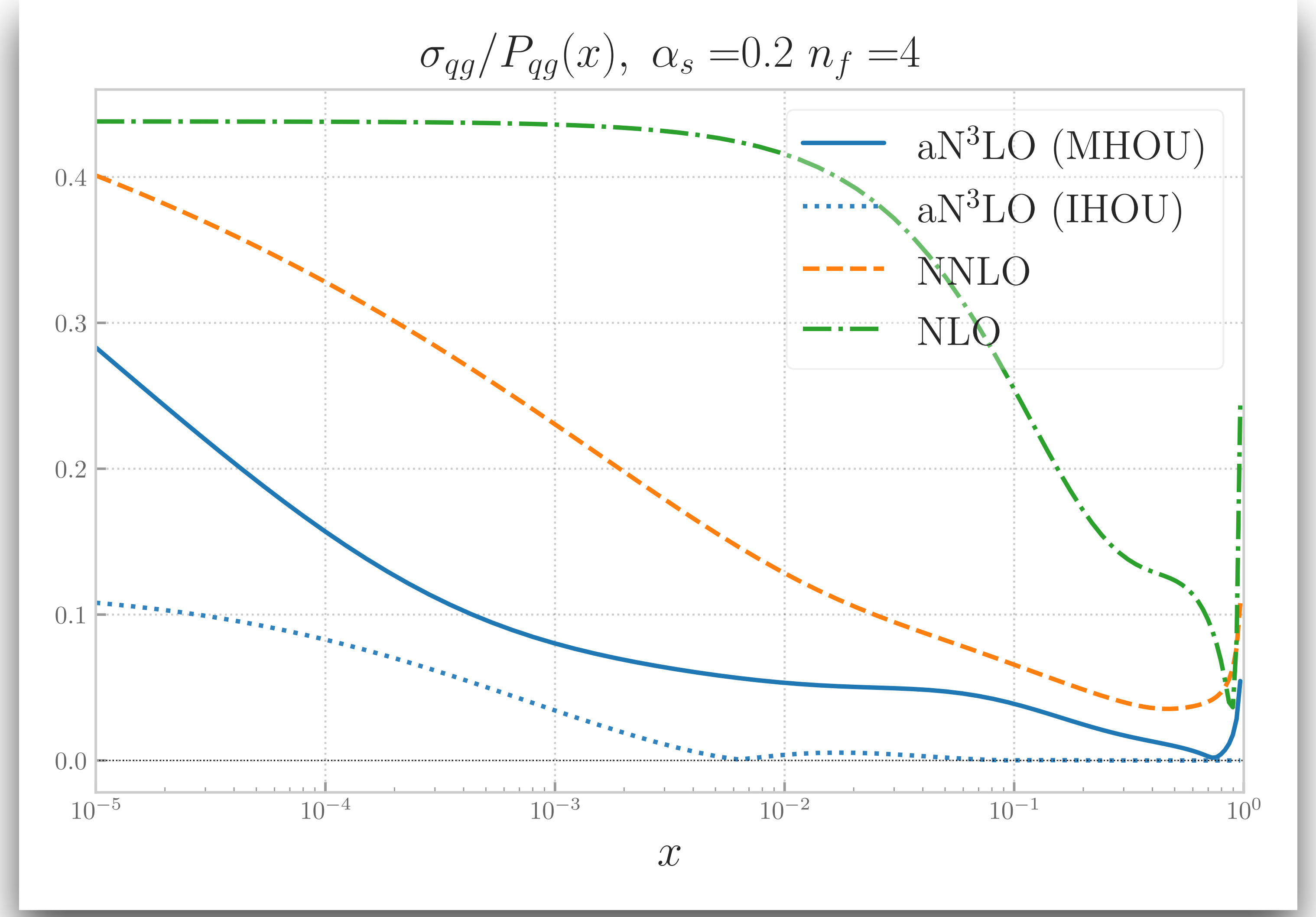
Gluon sector





Quark sector





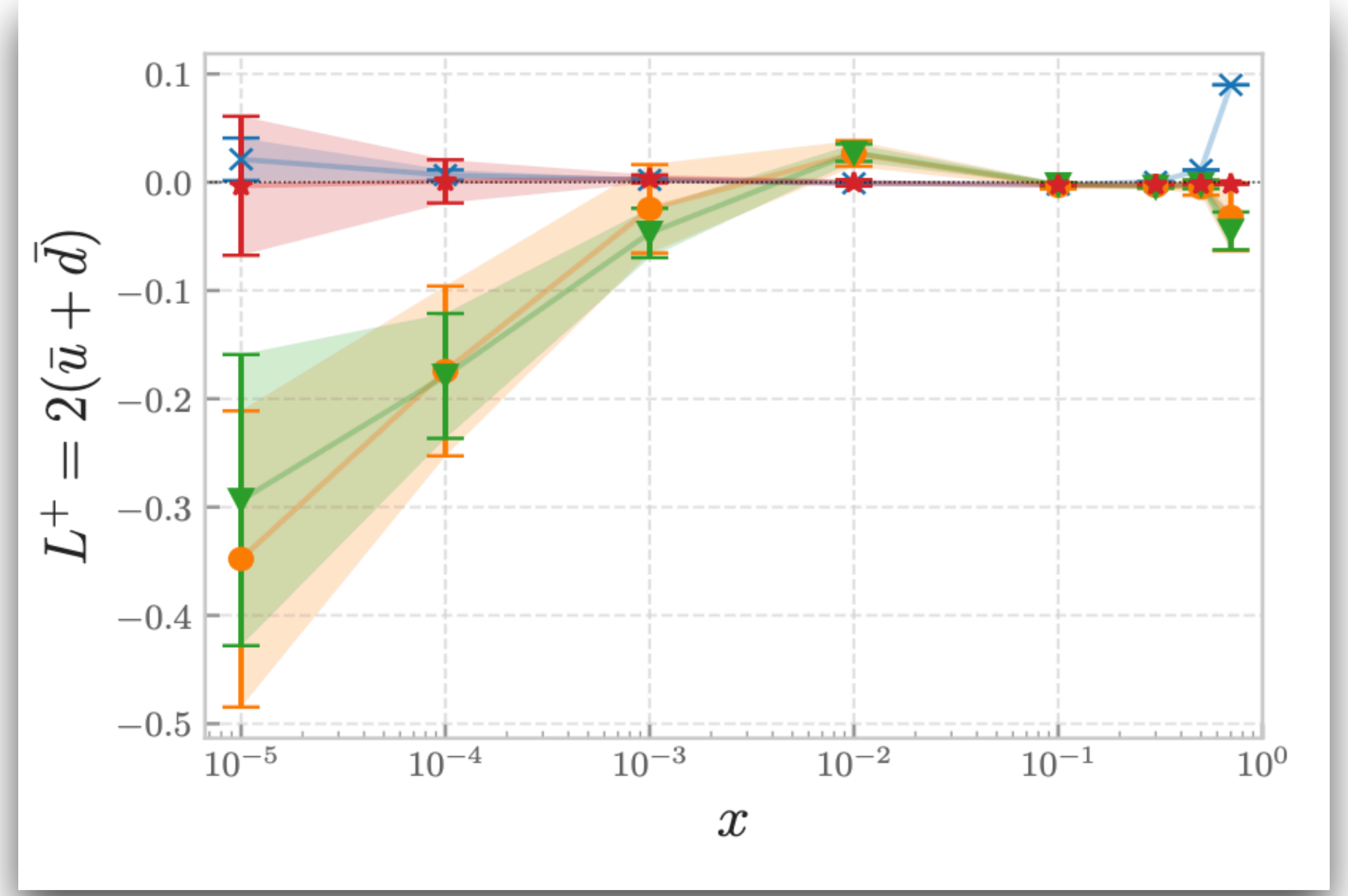
- **IHOU** = incomplete higher order uncertainties [only for aN^{3}LO].
- **MHOU** = missing higher order uncertainties.

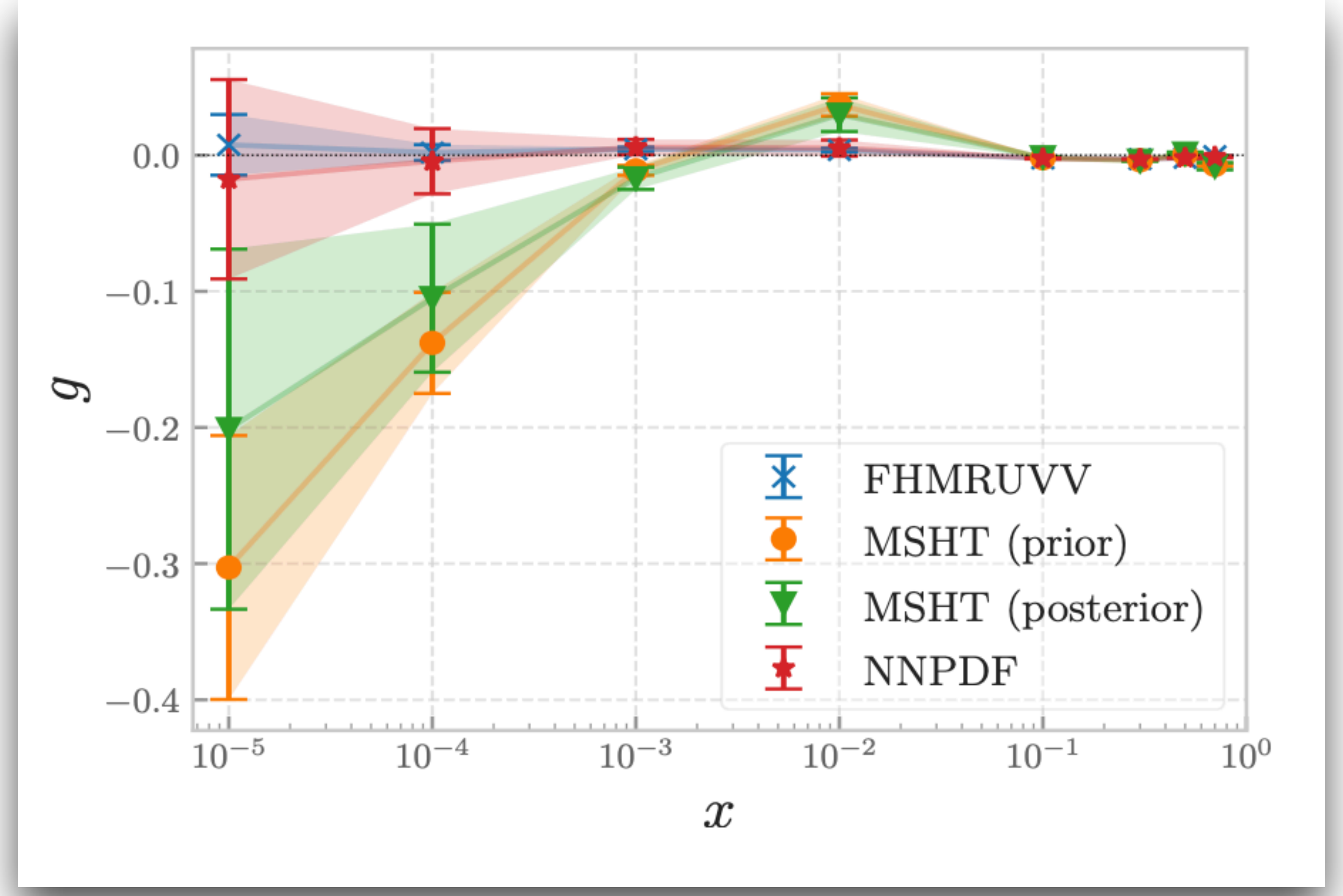
aN^3LO DGLAP evolution benchmark

Cooper-Sarkar, Cridge, Giuli, Harland-Lang, Hekhorn, Huston, GM, Moch, Thorne
[arxiv:2406.16188]

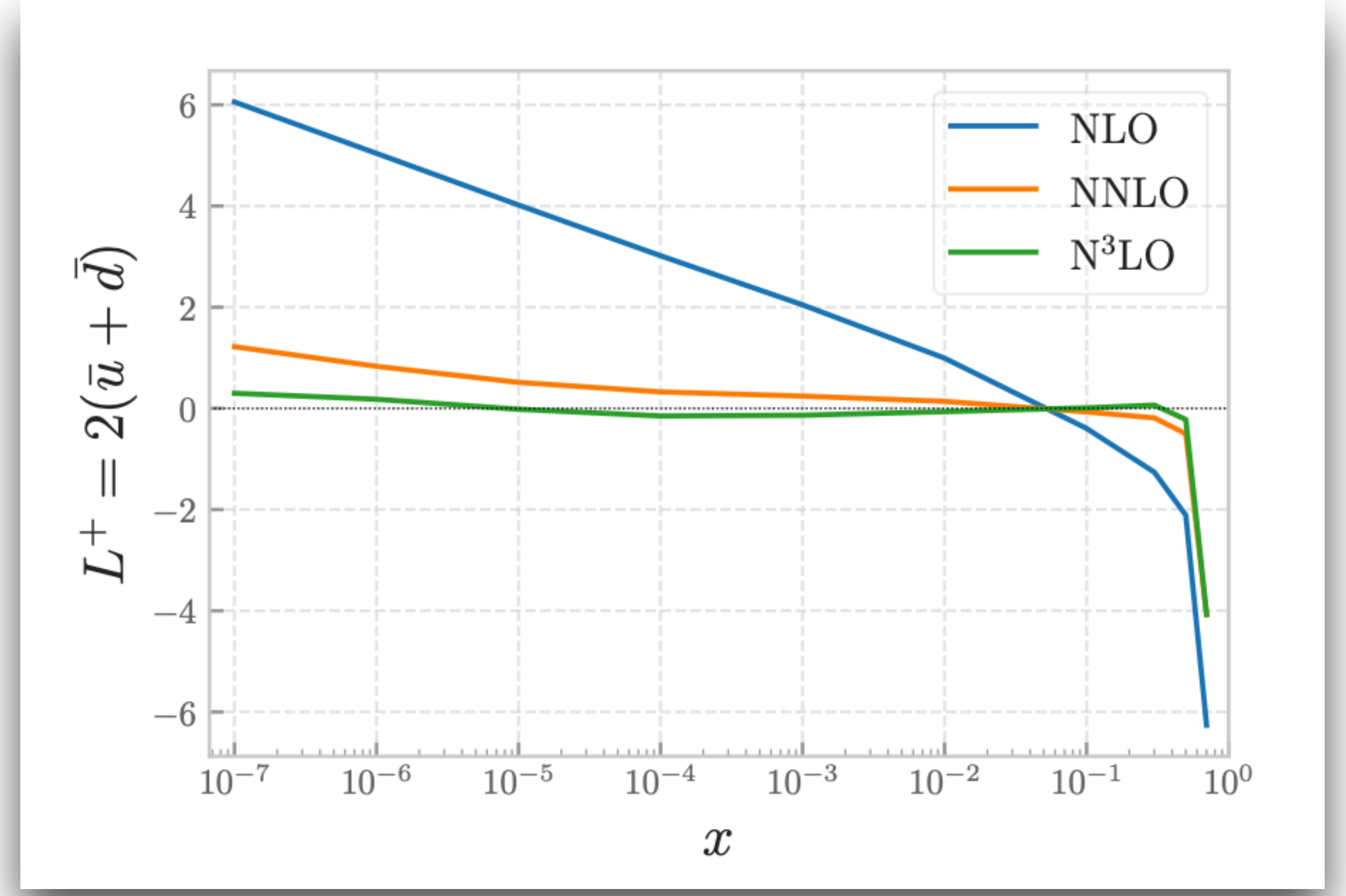
- **Benchmark**: comparison of aN^3LO DGLAP evolution **using different splitting function** approximation, and different evolution codes: MSHT [arxiv:2207.04739], FHMRUVV [arxiv:1707.08315] [arxiv:2111.15561], [arxiv:2302.07593],[arxiv:2307.04158], [arxiv:2310.05744] ([arxiv:2404.09701])
- Effect of aN^3LO is within the 2%, except for small and large-x regions.
- Good agreement of our in-house approximations and FHMRUVV.
- Stability of different DGLAP solution methods has also been checked.

Relative difference w.r.t NNLO evolution, VFNS $Q = 2 \to 100$ GeV





Relative difference Truncated vs Exact DGLAP evolution



aN^3LO QCD corrections to DIS

DIS cross sections (NC and CC) can be written in terms of structure functions: F_2, F_L, xF_3 which are expanded as:

$$\sigma_{DIS} \propto \sum_{i=2,L,3} k_i F_i \propto \sum_{i=2,L,3} k_i \left[C_{i,g}(x,\alpha_s) \otimes g(x,Q^2) + \sum_q C_{i,q}(x,\alpha_s) \otimes q(x,Q^2) \right]$$

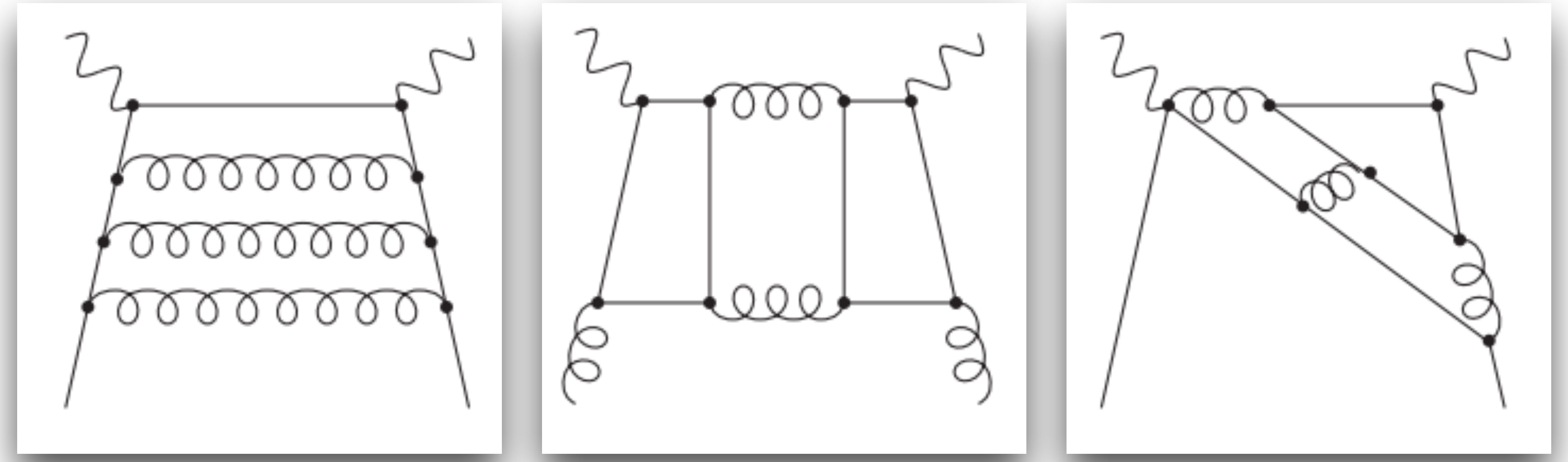
$$C_{i,j} = \alpha_s^0 C_{i,j}^{(0)} + \alpha_s^1 C_{i,j}^{(1)} + \alpha_s^2 C_{i,j}^{(2)} + \alpha_s^3 C_{i,j}^{(3)}, \quad j = q, g$$

- DIS coefficient functions are known at N^3LO in the **massless limit**.
- **Massive N^3LO coefficients** $\mathcal{O}(a_s^3)$ can be **approximated** joining the known limits ($Q \to m_h^2$ $Q^2 \gg m_h^2$ and $x \to 0$) with proper damping functions [arxiv:2401.12139].

$$C_{g,h}^{(3,0)} = C_{g,h}^{thr}(z, \frac{m_h}{Q})\, f_1(z) + C_{g,h}^{asy}(z, \frac{m_h}{Q})\, f_2(z)$$

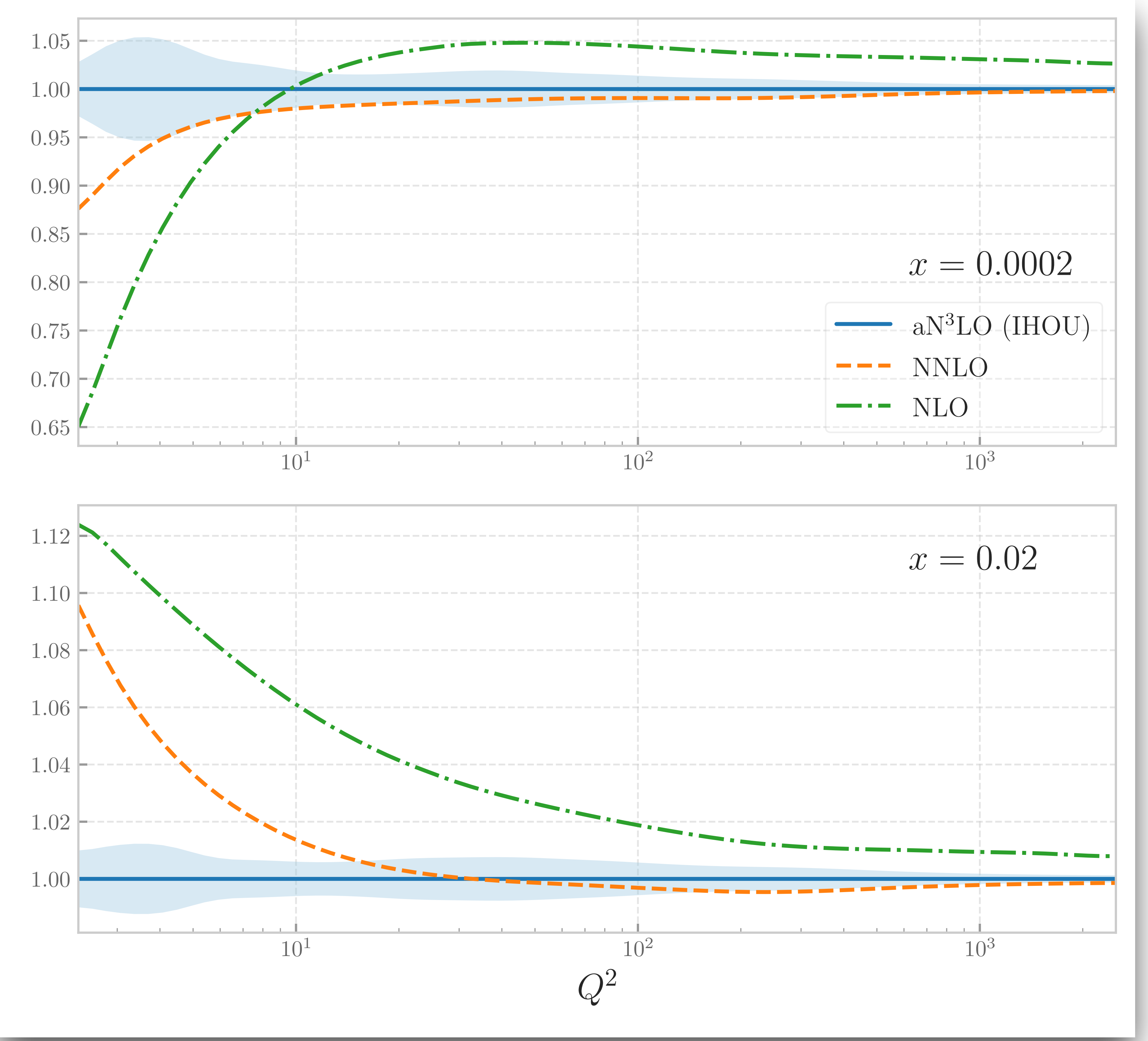
- IHOU from massive coefficient are also taken into account.

Representative N^3LO QCD corrections to DIS



γ/Z: [arxiv:9605317] [arxiv:0411112] [arxiv:2208.14325], $W^{\pm}$: [arxiv:1606.08907]

$F_2(Q^2)$ at different pQCD orders

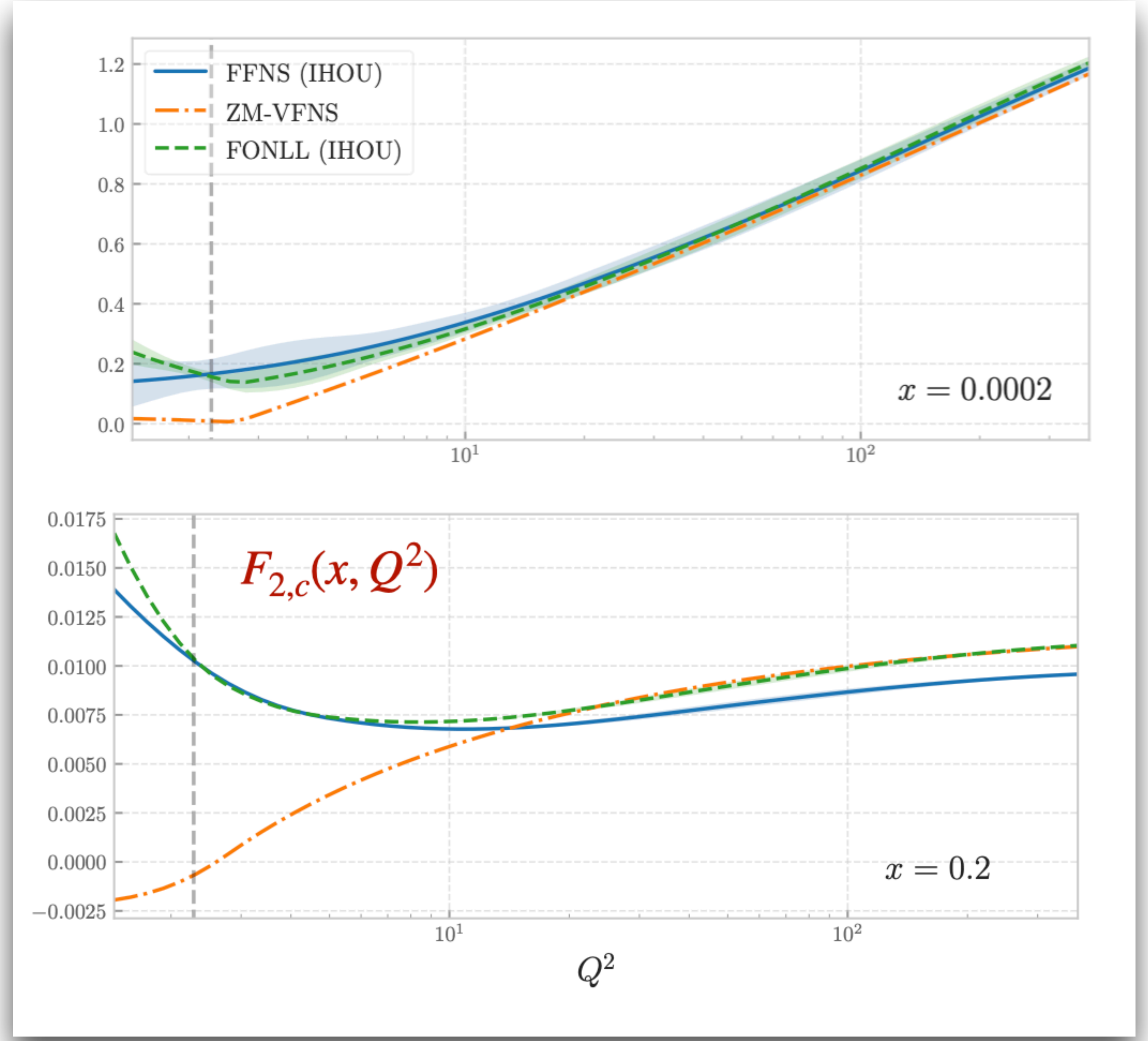


VFNS at aN^{3}LO

To properly describe DIS data, we must treat heavy quarks consistently during a PDF fit and adopt a **Variable Flavor Number Scheme.**

$$\begin{pmatrix} g \\ \Sigma \\ h^+ \end{pmatrix}^{n_f+1} (\mu_h^2) = \mathbf{A}^{(n_f)}_{S,h^+}(\mu_h^2) \cdot \begin{pmatrix} g \\ \Sigma \\ h^+ \end{pmatrix}^{n_f} (\mu_h^2)$$

PDFs matching conditions included at N^{3}LO almost completely [arxiv:0904.3563], [arxiv:1008.3347], [arxiv:1402.0359], [arxiv:1409.1135], [arxiv:1406.4654], [arxiv:2211.0546], [arxiv:2311.00644] exception of $a^{(3)}_{H,g}$, computed in [arxiv:2403.00513]



DIS structure functions are computed in the **FONLL** scheme: [arxiv:1001.2312]

$$F_{FONLL} = F^{(n_f+1)}_{ZM} + F^{(n_f)}_{FFNS} - \lim_{m_h \to 0} F^{(n_f)}_{FFNS}$$

- Extended up to N^{3}LO for the Heavy structure functions F_{heavy}.
- Extended up to NNLO for light F_{light} + massless N^{3}LO contributions.

ZM = massless scheme.
FFNS = massive scheme.

The NNPDF4.0 aN^{3}LO PDF set

To produce our aN^{3}LO PDF fit:

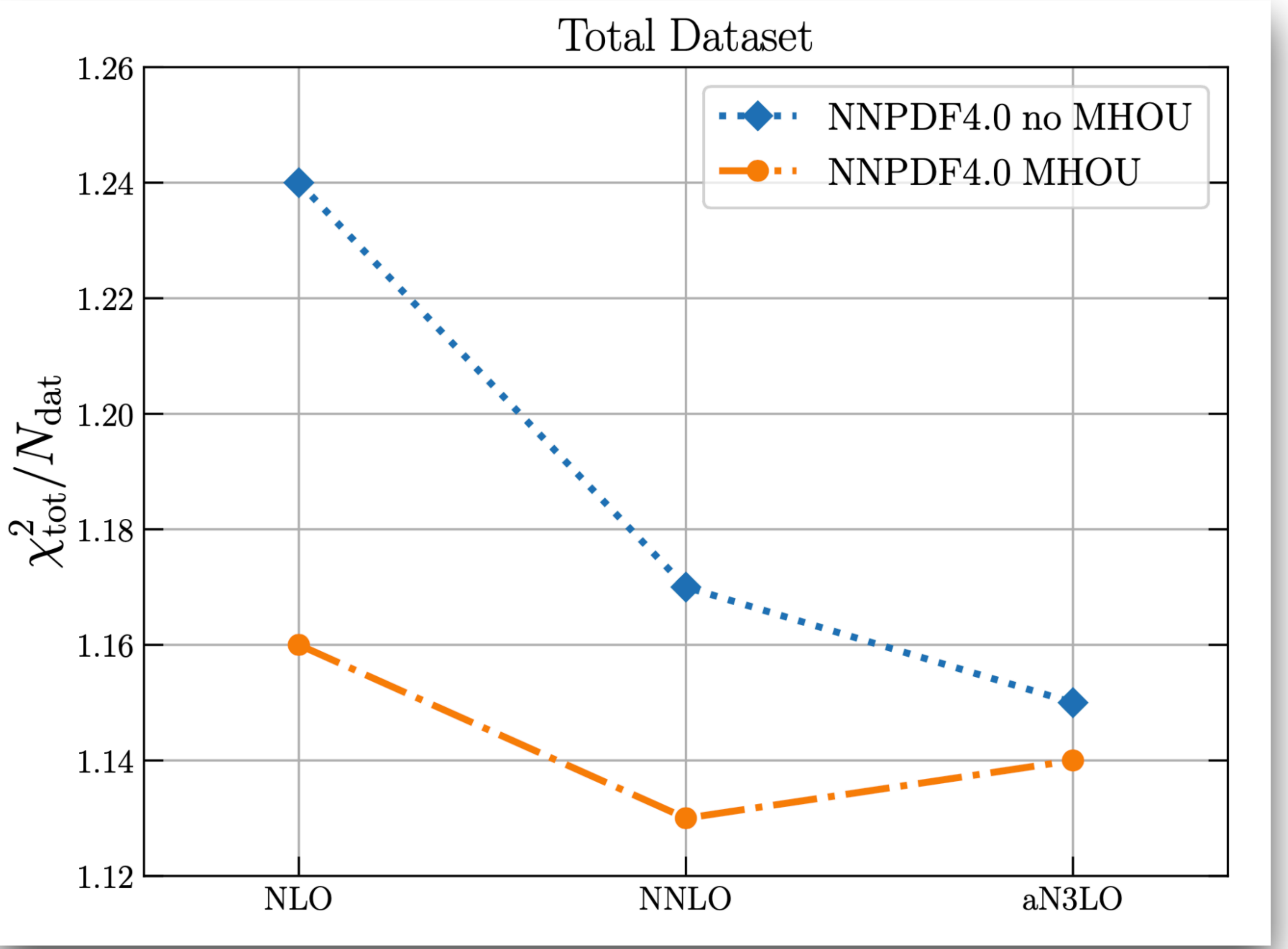
- We include **N^{3}LO corrections in DIS and DGLAP** with their respective IHOU.
- We adopt NNLO renormalisation scale variation to estimate *unknown* N^{3}LO effects in DY, Jets and Top data.
- **MHOU and IHOU** are propagated to PDF fit with the **covariance formalism**:

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

- Fit $\simeq 4000$ different experimental datapoints (DIS, Drell Yann, Jets, Top), with the **NNPDF4.0 methodology** parametrising PDFs at initial scale $Q_0 = 1.65$ GeV with a Neural Network.

$$f_i(x, Q_0) = x^{a_i}(1-x)^{b_i}\text{NN}(\theta, x,)_i,\ i = q_i, g$$

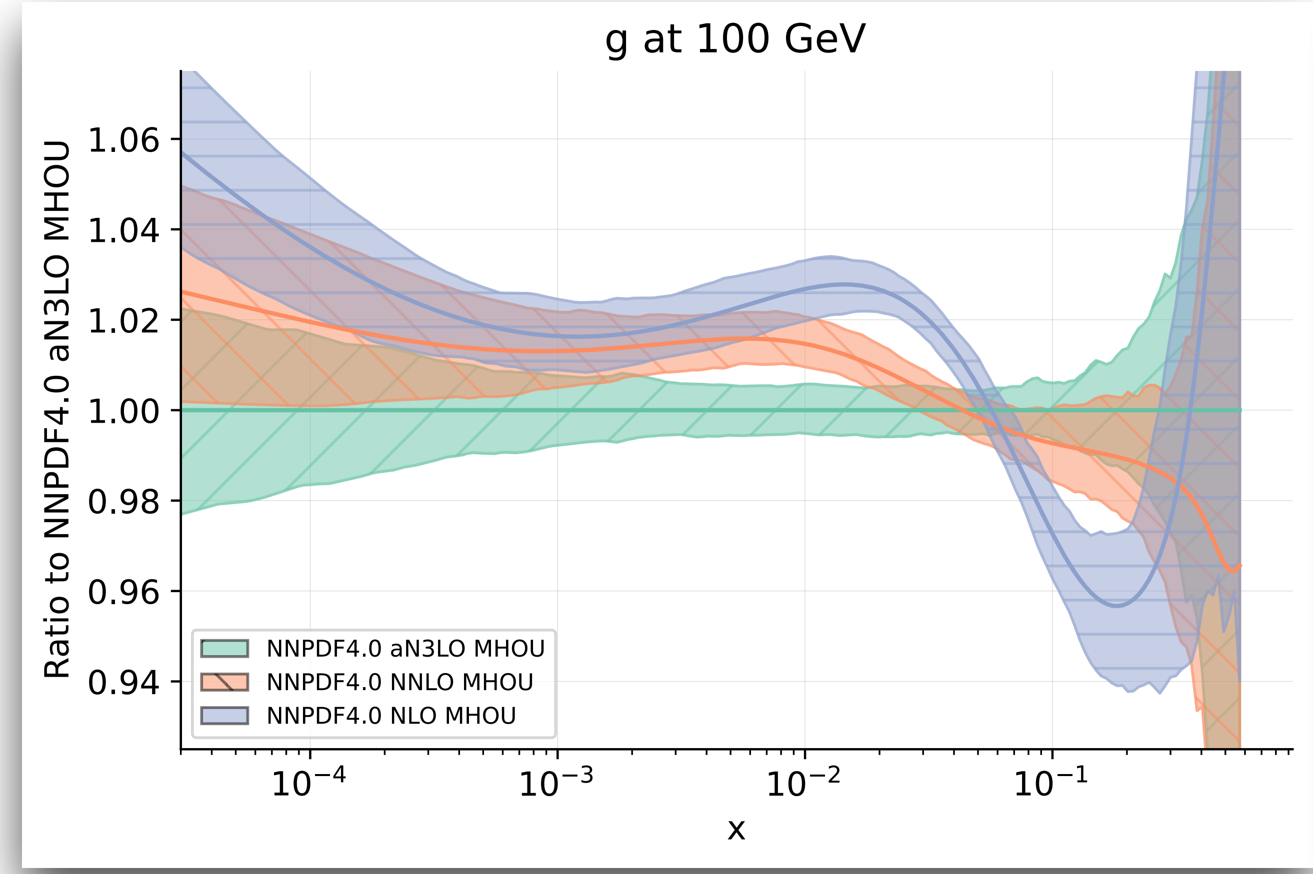
Total χ^2 at different pQCD orders

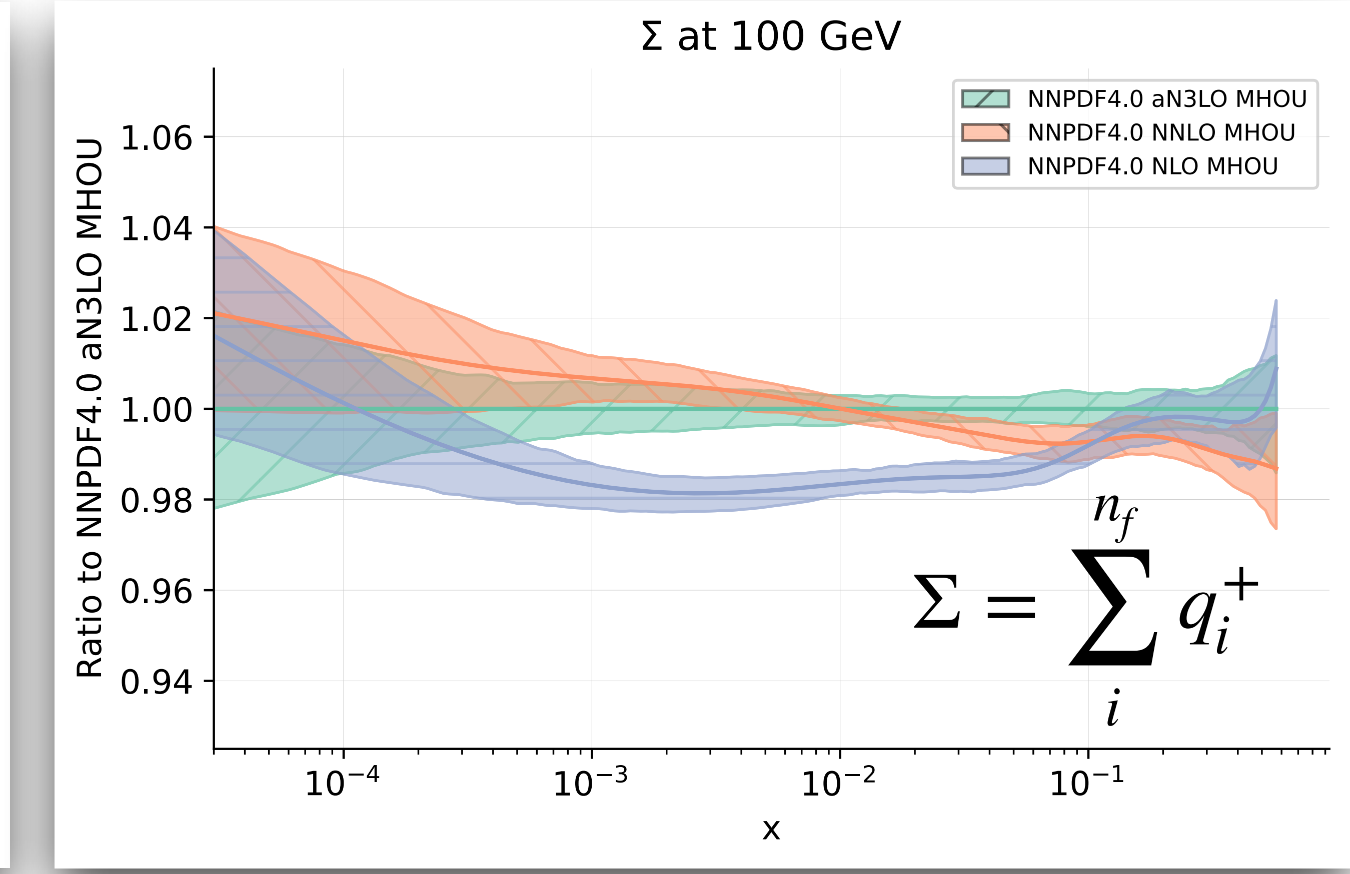


MHOU stabilise the fit: χ^2 is less dependent on QCD order.

The NNPDF4.0 aN^{3}LO PDF set

Perturbative convergence

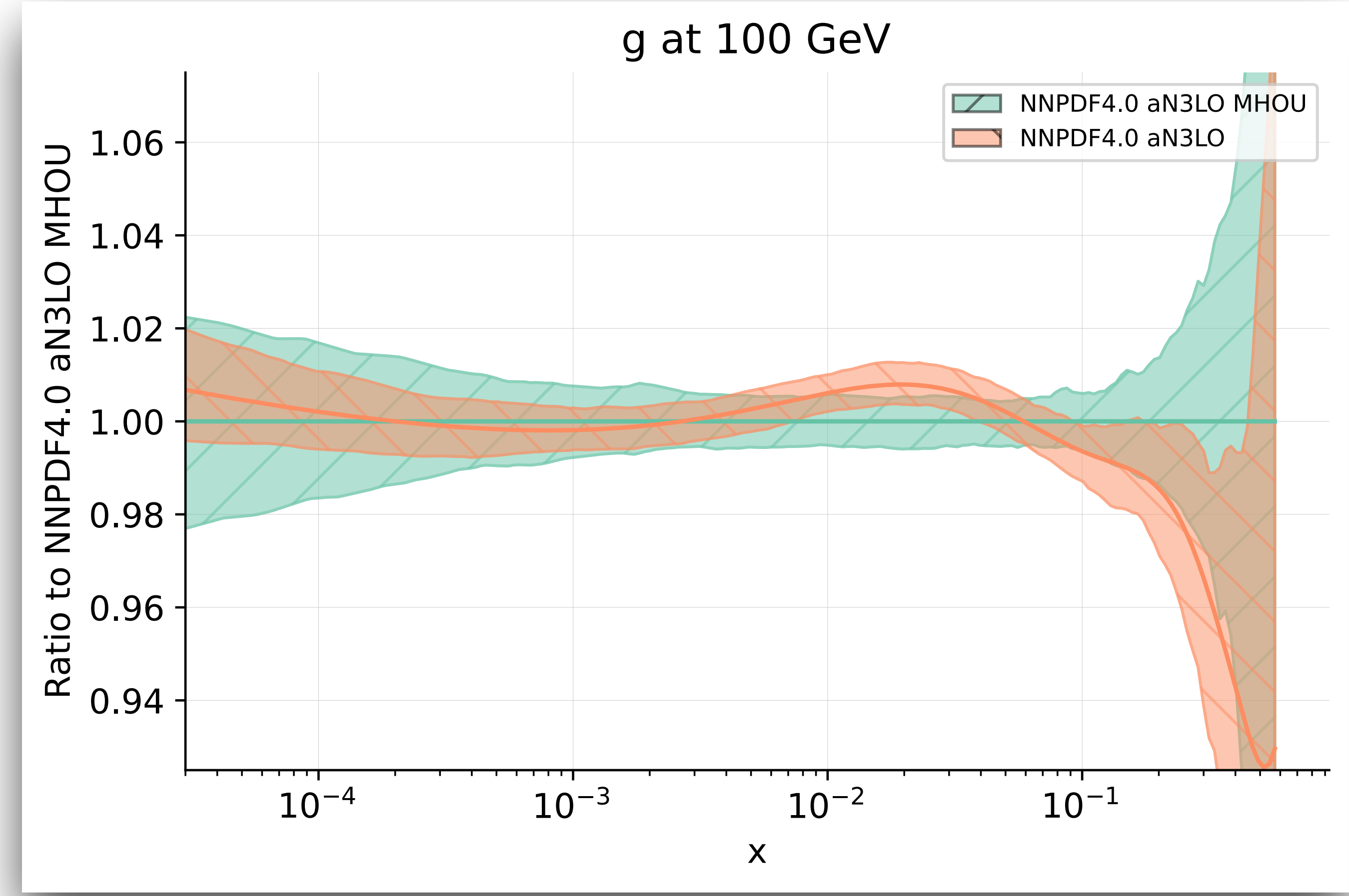


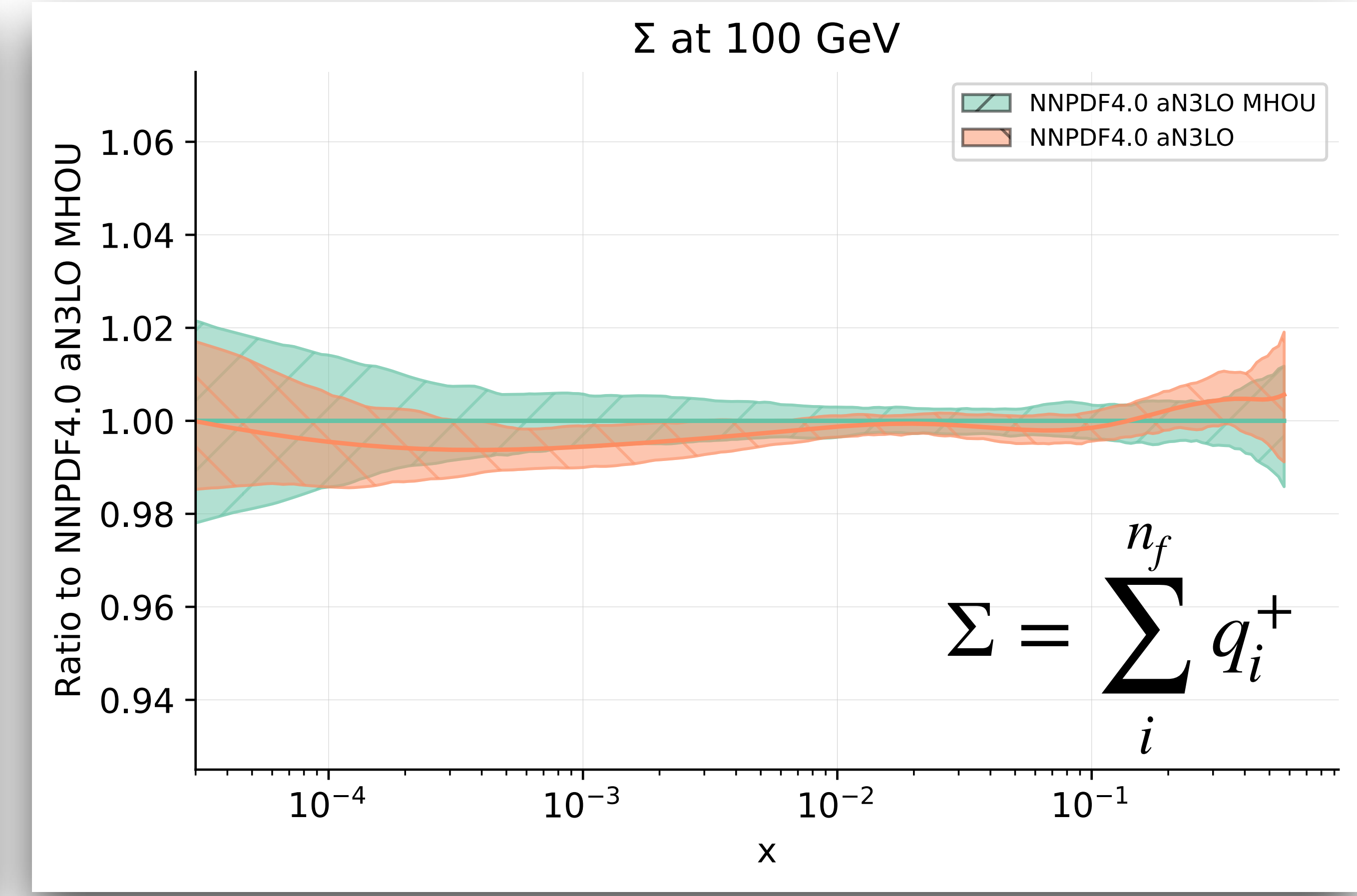


- Fairly good perturbative convergence in the data region $x \in [10^{-4}, 0.7]$.
- **Impact of aN^{3}LO** corrections is **mild on quarks PDFs.**
- $\sim 2\,\%$ depletion of the **gluon around $x \approx 10^{-2}$ w.r.t. NNLO.**

Impact of MHOU

- aN^{3}LO PDFs with/without MHOU are compatible.
- MHOU can shift central value, resolve tensions among datasets. Mainly de-weight jets datasets.
- aN^{3}LO corrections have a larger effect on the small-x, low-Q DIS data.





Comparison to MSHT20 aN3LO

McGowan, Cridge, Harland-Lang, Thorne [arxiv:2207.04739]

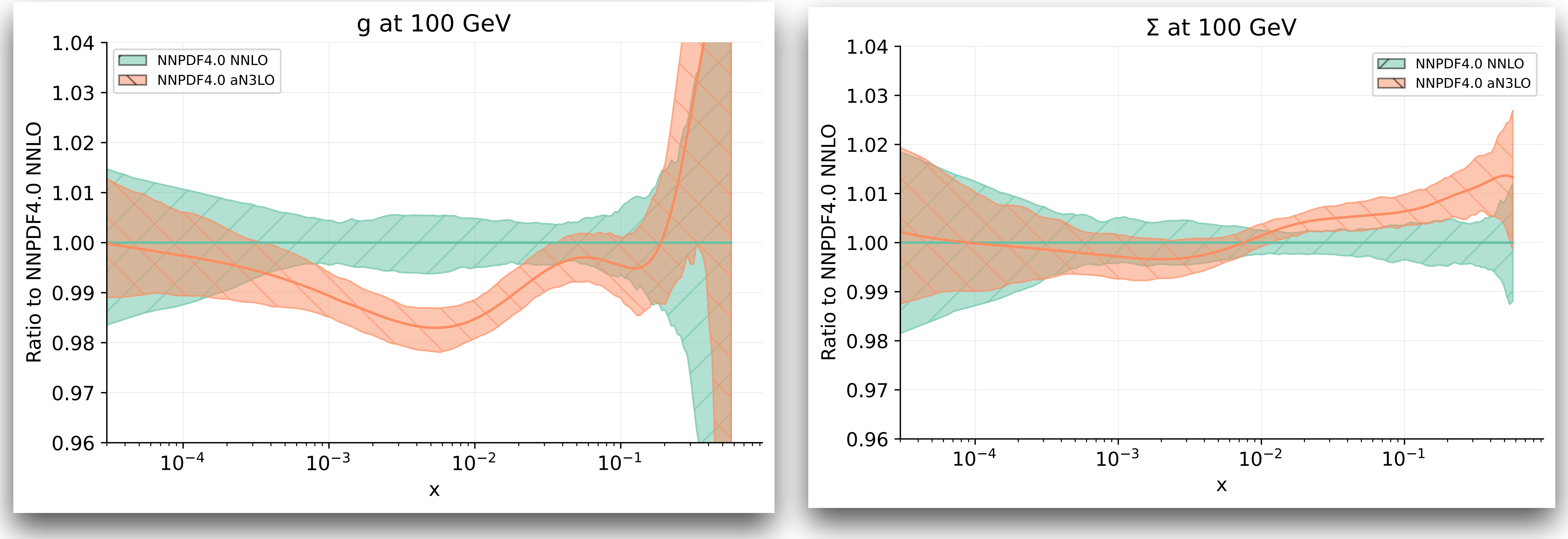
Main differences originates from:

- Splitting functions approximations: moments computed in the last 2 years.
- Inclusion of other approximate coefficients: hadronic k-factors, massive DIS ...
- Theory uncertainty methodology: nuisance parameters (MSHT) vs covariance matrix (NNDPF).
- Fitting methodology and experimental data.

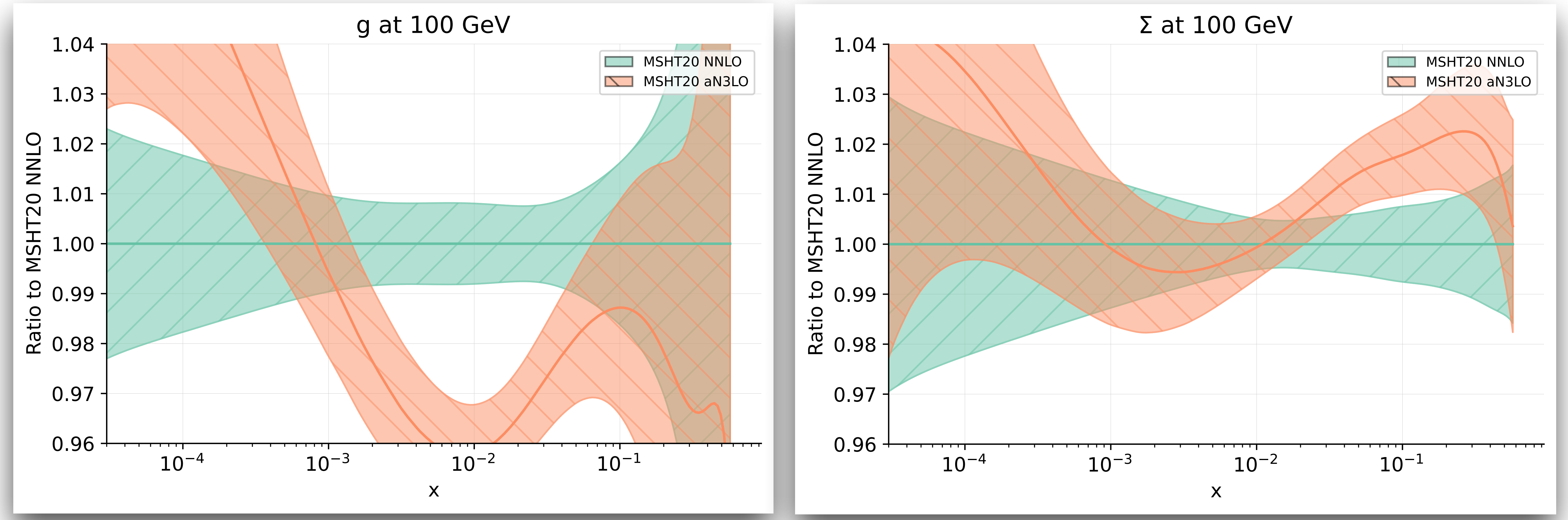
Qualitative aN^3LO / NNLO ratio is similar, with aN^3LO effects larger in MSHT.

A PDF combination for LHC phenomenology is technically feasible.

NNPDF4.0 aN^3LO / NNLO

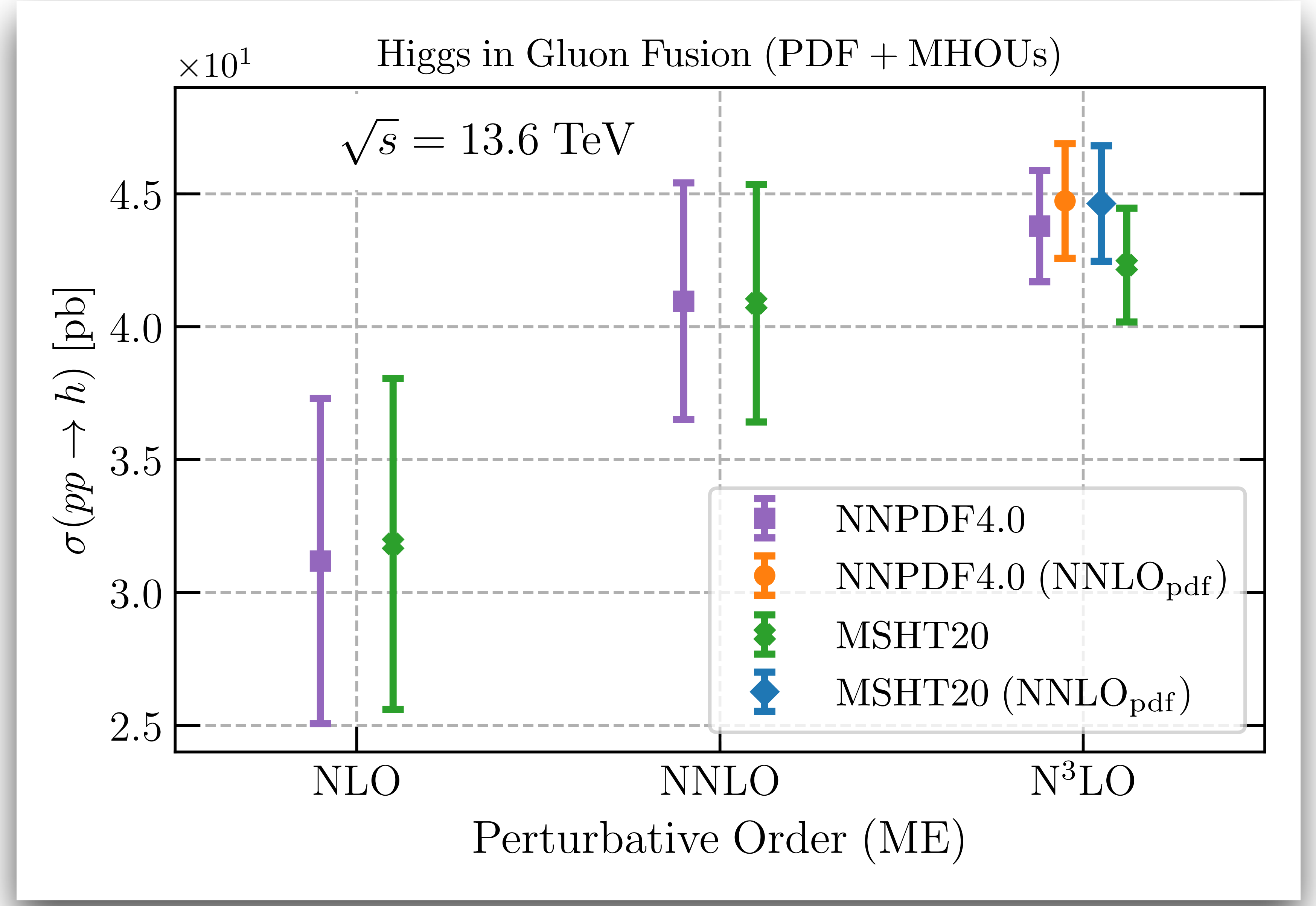


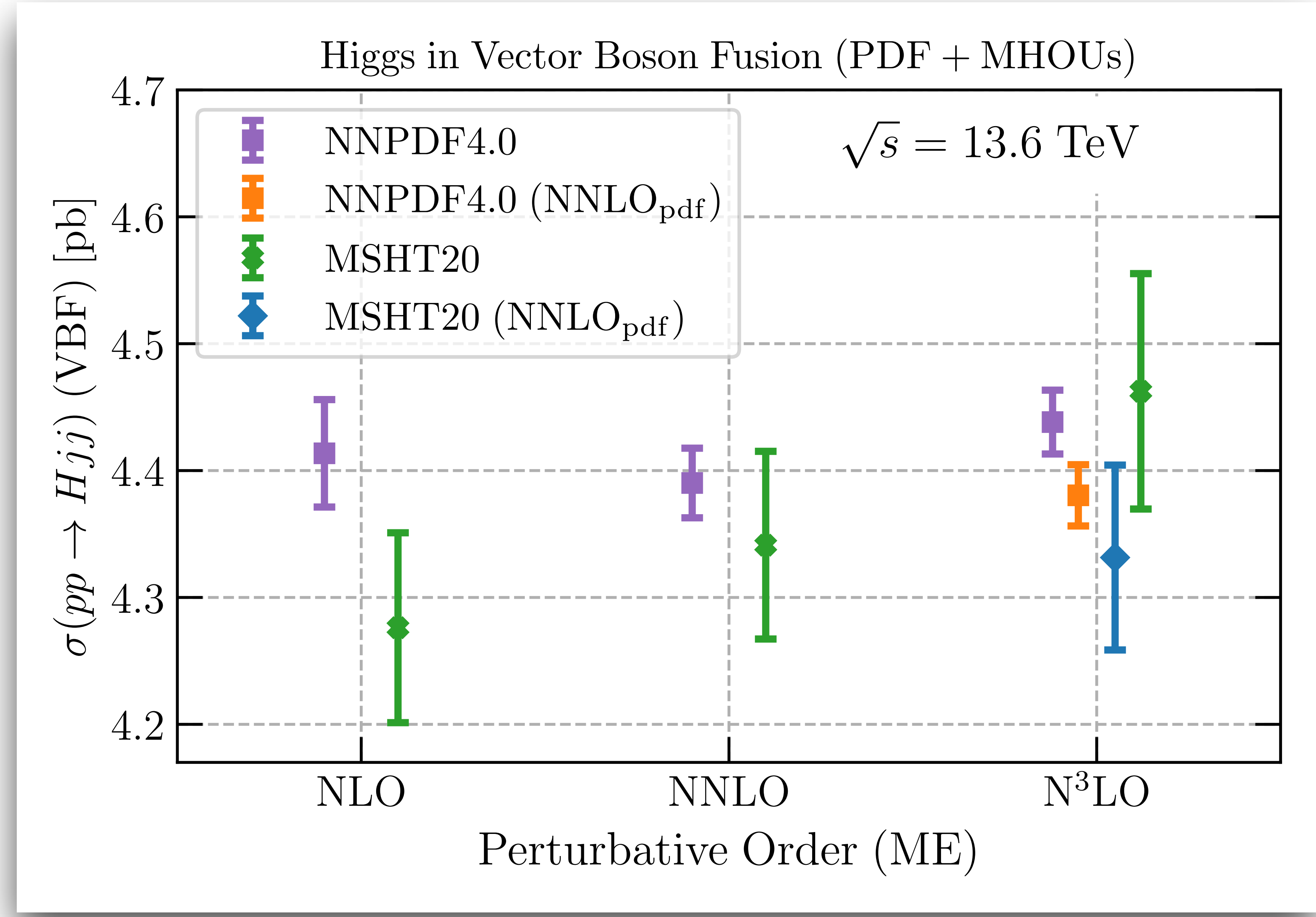
MSHT20 aN^3LO / NNLO



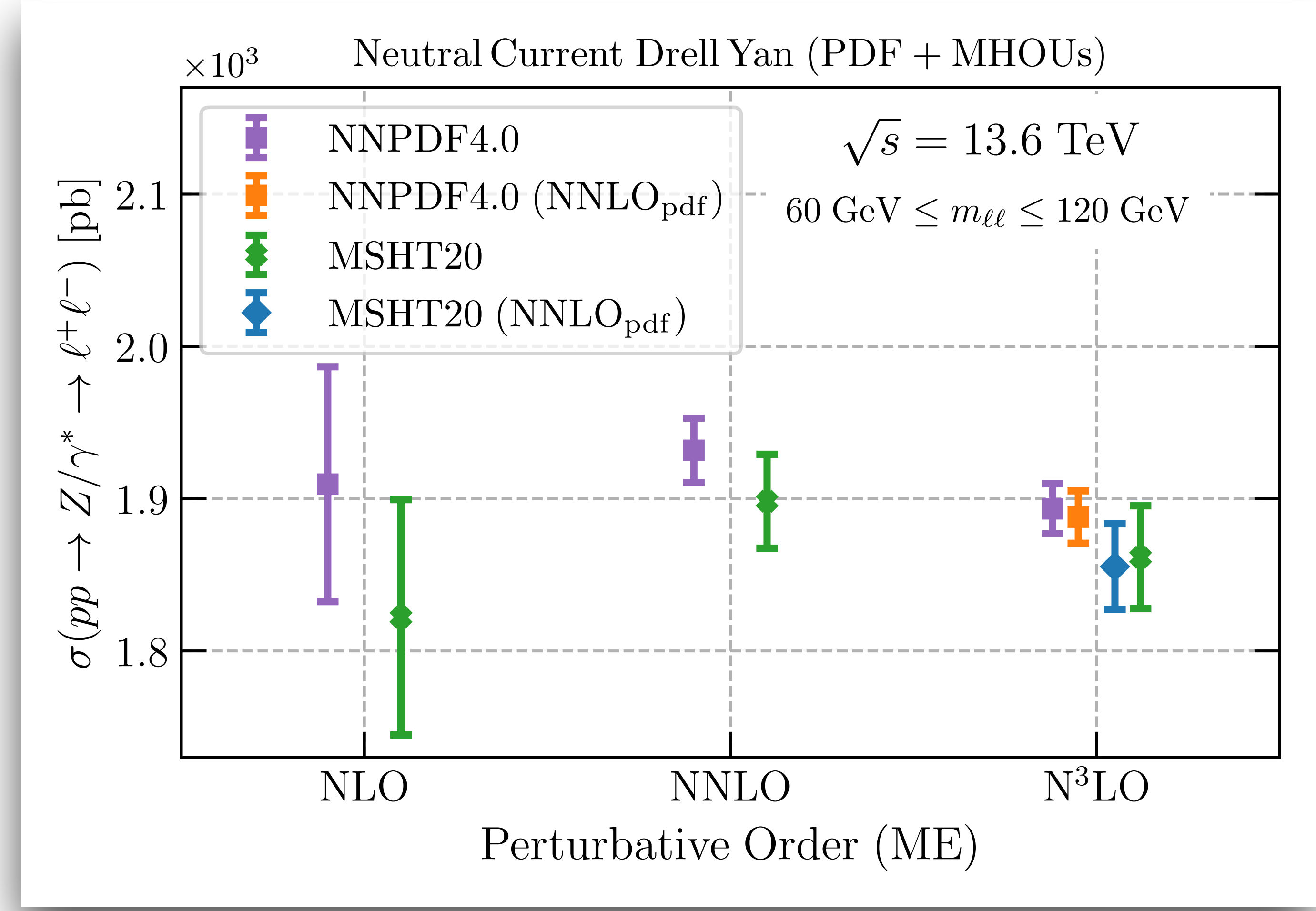
Impact on LHC phenomenology: Higgs production

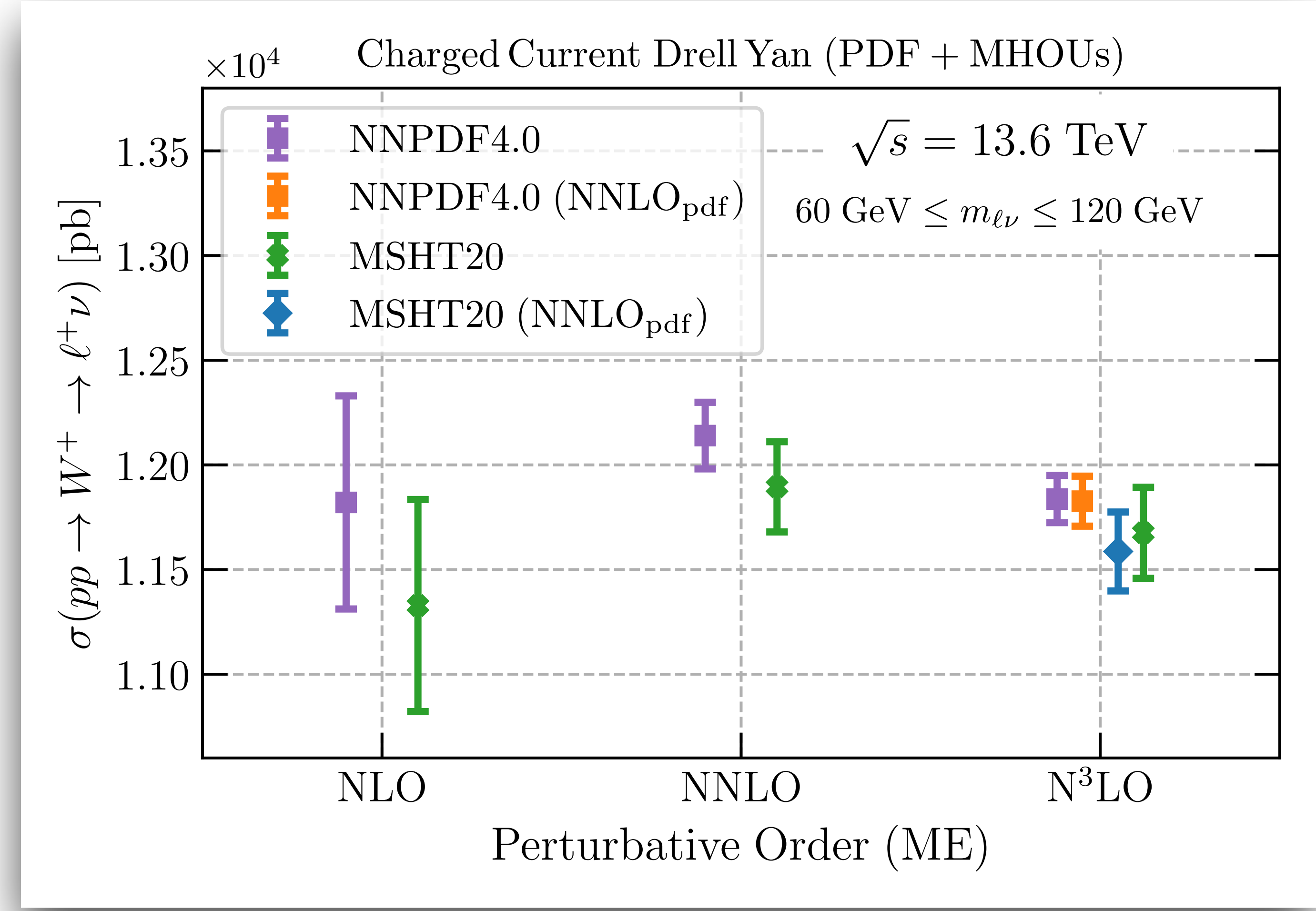
- **aN^{3}LO PDFs** effects are visible in **Higgs gluon fusion**, leading to a $2.1\,\%$ **suppression** w.r.t NNLO PDFs and N^{3}LO ME.
- Similar effect is visible in Higgs VBF. The cross-section is more stable at different perturbative orders. Improved compatibility with MHST20 aN^{3}LO PDF.

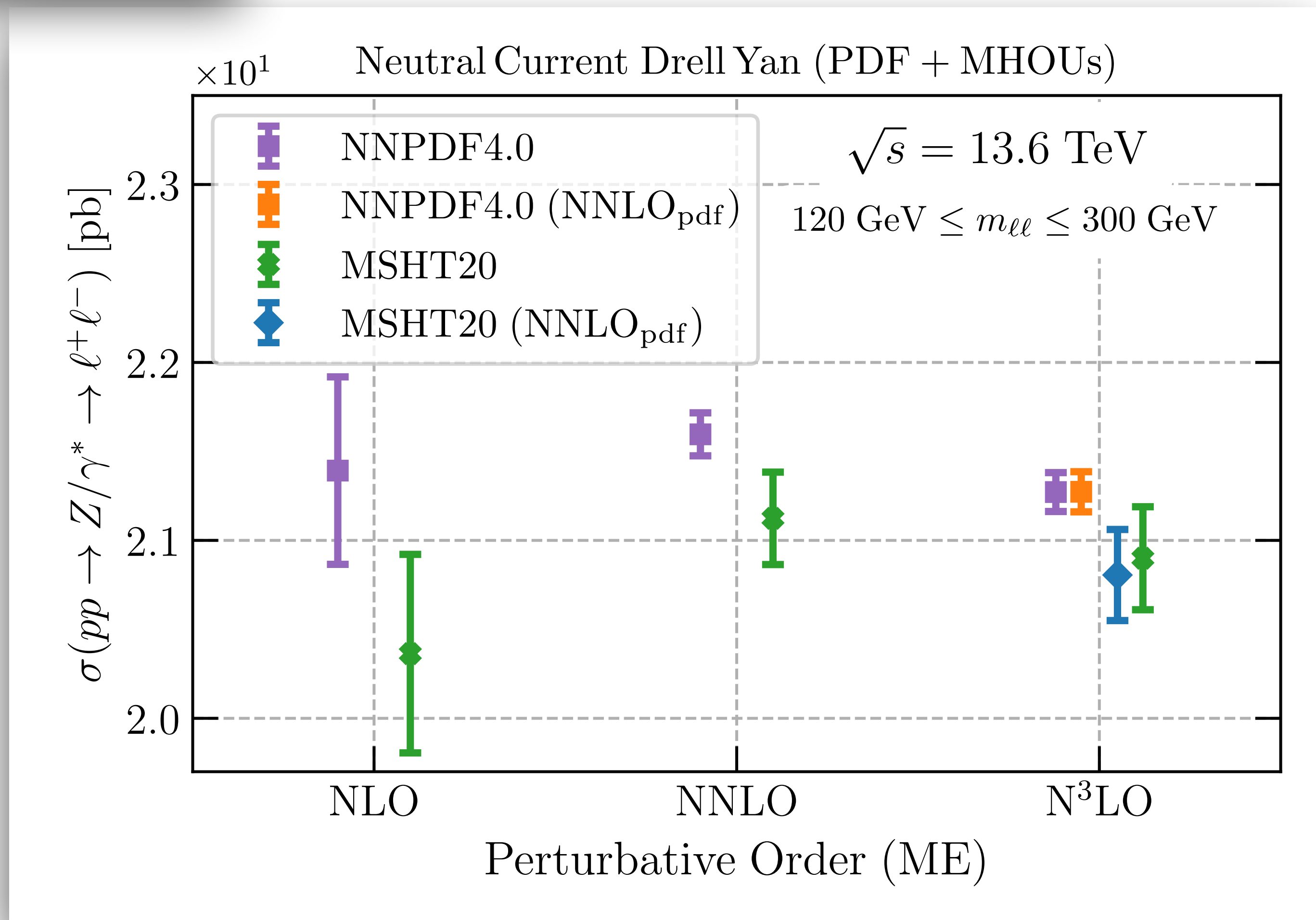


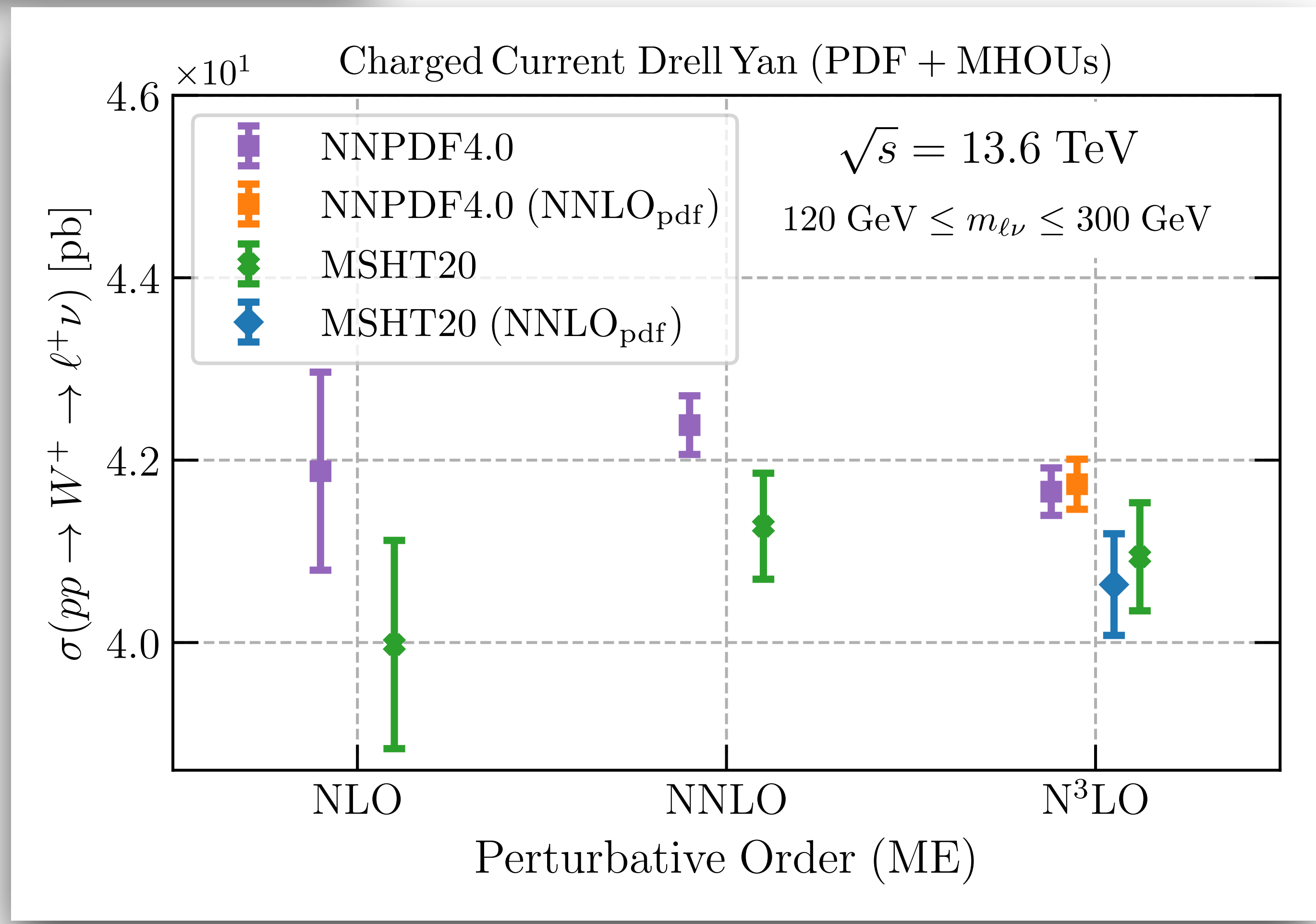


Impact on LHC phenomenology: Drell-Yan









Also for collider **gauge boson production**, usage of aN^{3}LO PDFs seems to **improve the perturbative convergence.**

aN^3LO PDF with QED corrections

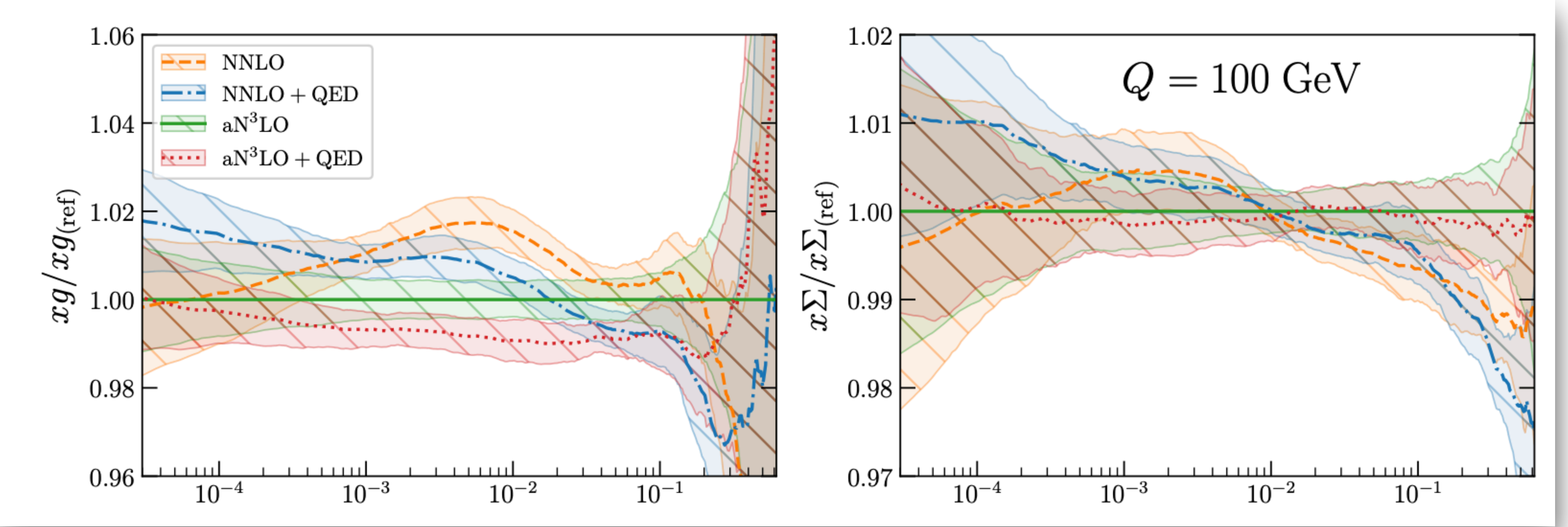
Barontini, Laurenti, Rojo [arxiv:2406.01779]

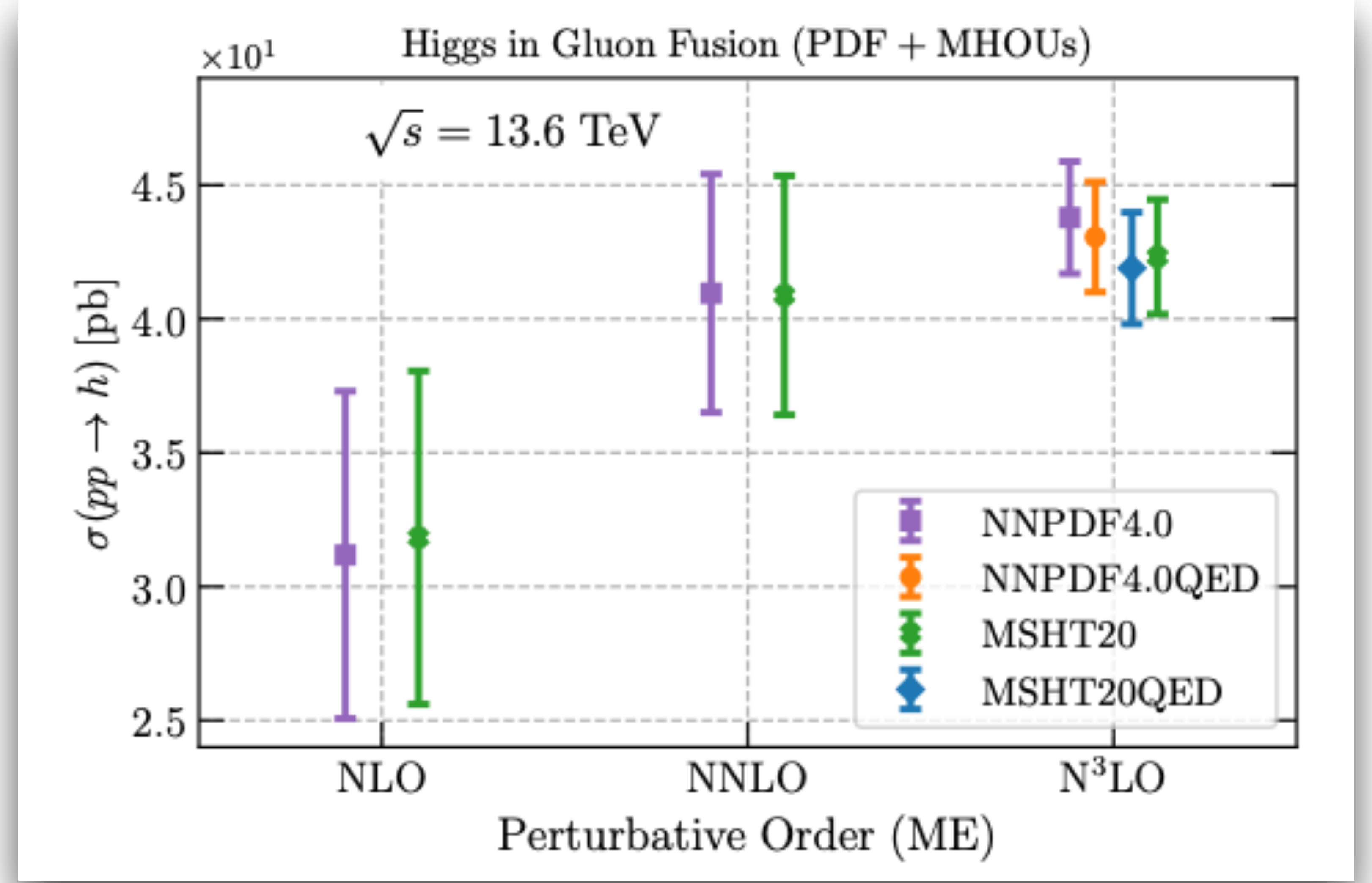
Recently we have also provided an additional global fits:

✓ **NNPDF40 QED aN3LO**

The photon **PDF is computed from DIS** structure functions at a given **high** Q^2 scale.
[`LuxQED` Manohar et al. [arxiv:1607.04266] [arxiv:1708.01256]]

DGLAP with mixed $QED \otimes QCD$: $\mathcal{O}(\alpha_s \alpha_{em}), \mathcal{O}(\alpha_{em}^2)$





- The photon PDF subtracts some momentum from other partons (especially gluon):

$$\int_0^1 xdx \left(g(x) + \sum_i q_i^+(x) + \gamma(x) \right) = 1$$

- **QED** effects on the PDFs **are comparable to QCD aN^3LO** corrections, **both must be taken into account** to achieve best accuracy.

- Recent $\gamma(x, Q^2)$ determination by MSHT collaboration is also available `MSTH20_aN3LO_QED` [arxiv:2312.07665]

an3lo4HXSWG PDF combination

Ball, Cridge, Forte, Harland-Lang, GM, Nocera, Rojo, Thorne, Ubiali **[In preparation]**

- NNPDF4.0 aN3LO and MSHT20an3lo have different uncertainties and different methodologies (kinematic coverage, fitting methodology ...).

- However, effects due to aN^{3}LO PDFs are mandatory for precise Higgs phenomenology.

- We can construct an unweighted combination of the PDFs w/wo QED effects:

  an3lo4HXSWG and **an3lo4HXSWG_qed**

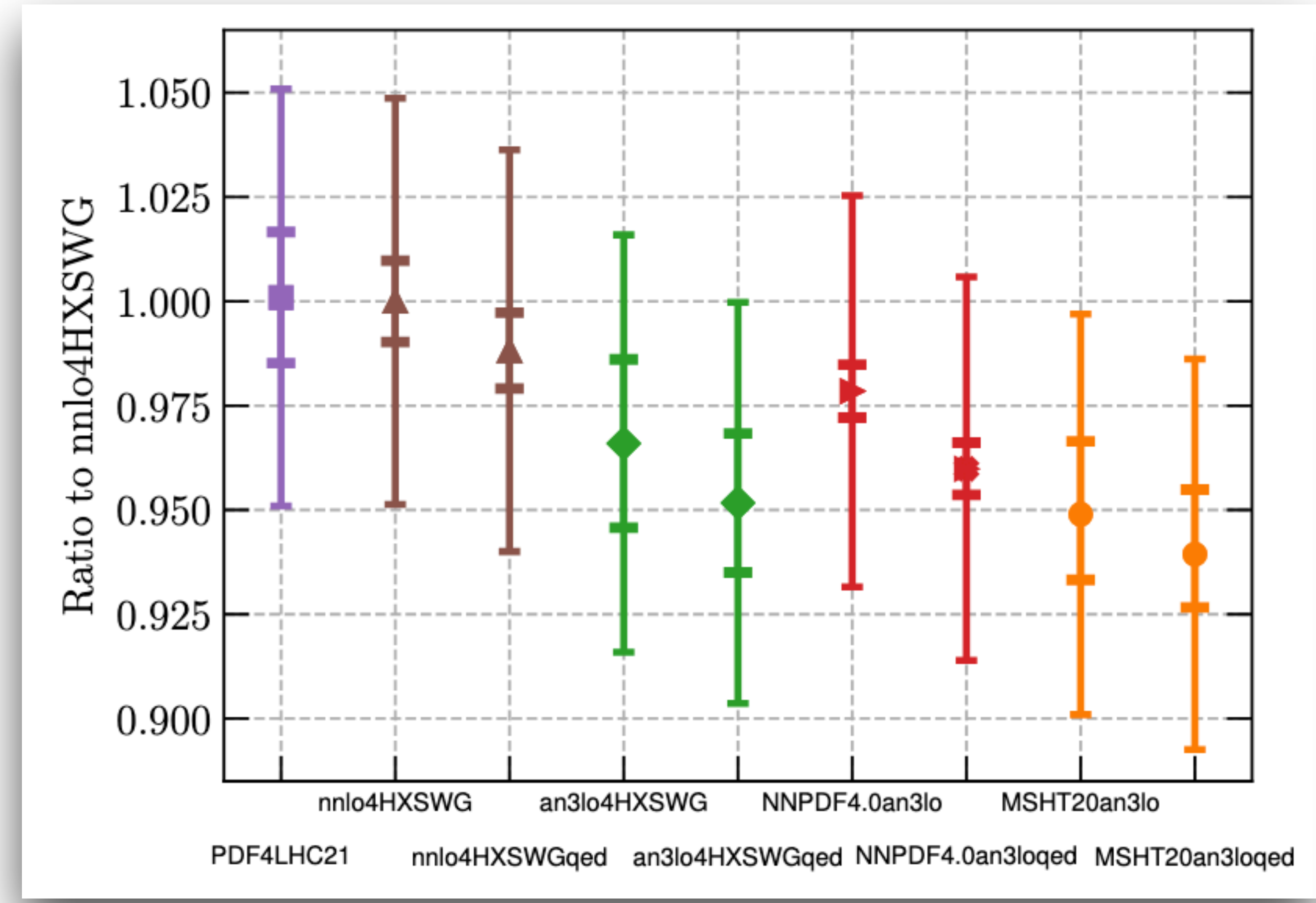
  it provides a conservative estimate of PDFu and gain in accuracy.

For Higgs ggF and VBF:

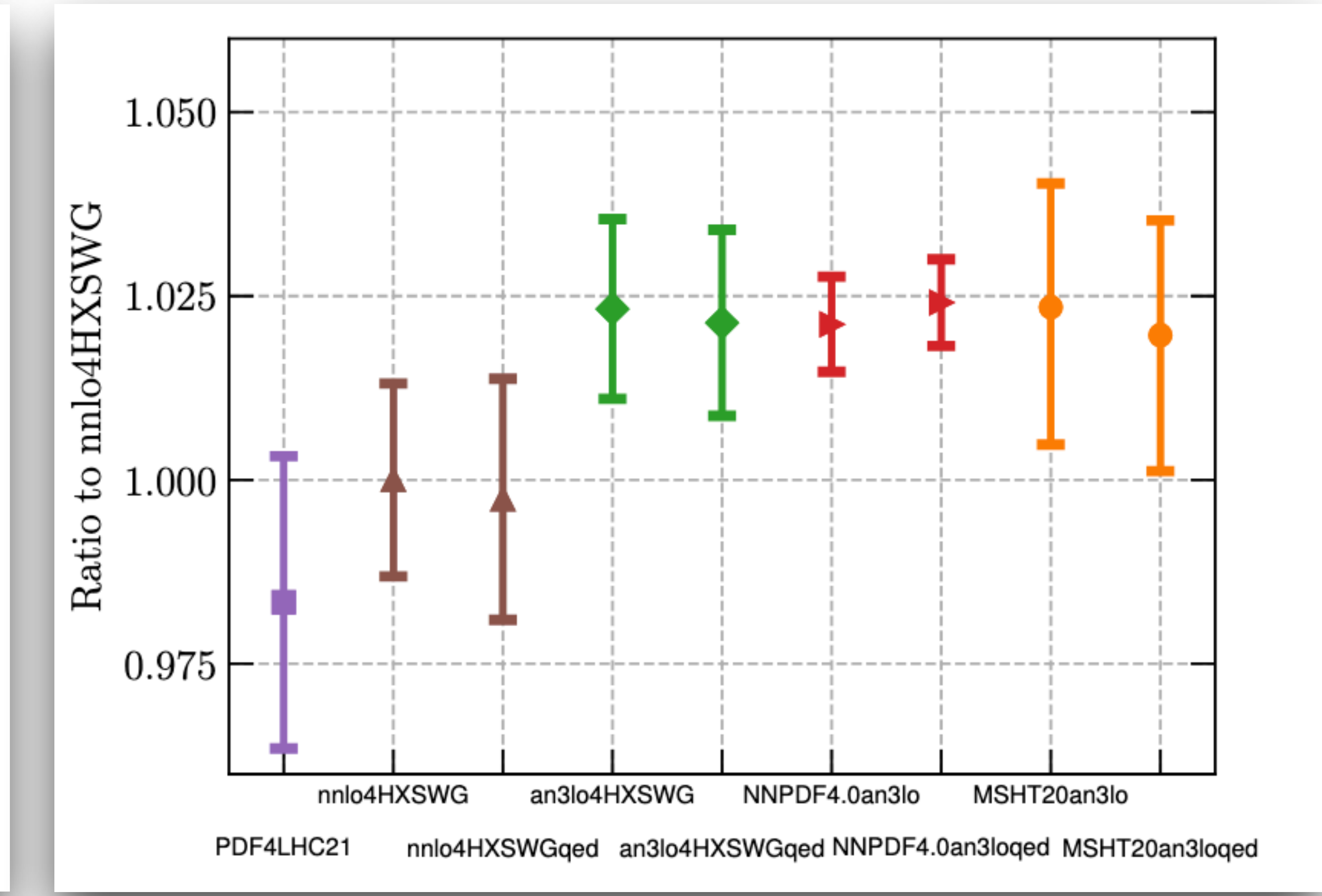
- The approximate estimate $\Delta^{\mathrm{app}}_{\mathrm{NNLO}}$ is very unreliable, and specifically it underestimates $\Delta^{\mathrm{exact}}_{\mathrm{NNLO}}$.
- Difference weighted and unweighted combination $\mathcal{O}(1\%)$ is smaller than the shift from NNLO to aN^{3}LO PDFs $\mathcal{O}(3\%)$.

$$\Delta^{\mathrm{exact}}_{\mathrm{NNLO}} \equiv \left| \frac{\sigma^{\mathrm{N^3LO}}_{\mathrm{N^3LO-PDF}} - \sigma^{\mathrm{N^3LO}}_{\mathrm{NNLO-PDF}}}{\sigma^{\mathrm{N^3LO}}_{\mathrm{N^3LO-PDF}}} \right| \qquad \Delta^{\mathrm{app}}_{\mathrm{NNLO}} \equiv \frac{1}{2} \left| \frac{\sigma^{\mathrm{NNLO}}_{\mathrm{NNLO-PDF}} - \sigma^{\mathrm{NNLO}}_{\mathrm{NLO-PDF}}}{\sigma^{\mathrm{NNLO}}_{\mathrm{NNLO-PDF}}} \right|$$

Higgs gluon fusion



Higgs VBF



PDF set	$\sigma(gg \to h)$	$\sigma(h\ \mathrm{VBF})$
$\Delta^{\mathrm{exact}}_{\mathrm{NNLO}}$ (NNPDF4.0)	2.2%	1.3%
$\Delta^{\mathrm{exact}}_{\mathrm{NNLO}}$ (MSHT20)	5.3%	2.3%
$\Delta^{\mathrm{exact}}_{\mathrm{NNLO}}$ (combination)	3.3%	2.3%
$\Delta^{\mathrm{app}}_{\mathrm{NNLO}}$ (NNPDF4.0)	0.2%	0.2%
$\Delta^{\mathrm{app}}_{\mathrm{NNLO}}$ (MSHT20)	1.4%	1.3%
$\Delta^{\mathrm{app}}_{\mathrm{NNLO}}$ (combination)	1.6%	0.5%

Summary & outlook

Newest NNPDF4.0 releases:

- ✓ aN^3LO QCD: state of the art **DGLAP** and **DIS**, along with theory uncertainties.
- ✓ NNLO theory uncertainties through scale variations, for NNLO fits and as proxy for unknown N^3LO ME.
- ✓ Determination of Photon PDF (NNLO and aN^3LO).

NNPDF40 aN^3LO PDFs can be used:

- To **compute N^3LO cross sections** more precisely.
- To **evaluate missing higher order** effects on NNLO calculation more accurately.

Jan 2024:
NNPDF4.0 MHOU
NNPDF4.0 QED

Feb 2024:
NNPDF4.0 aN3LO

Jun 2024:
NNPDF4.0 QED aN3LO

...

WIP:
NNPDF4.1

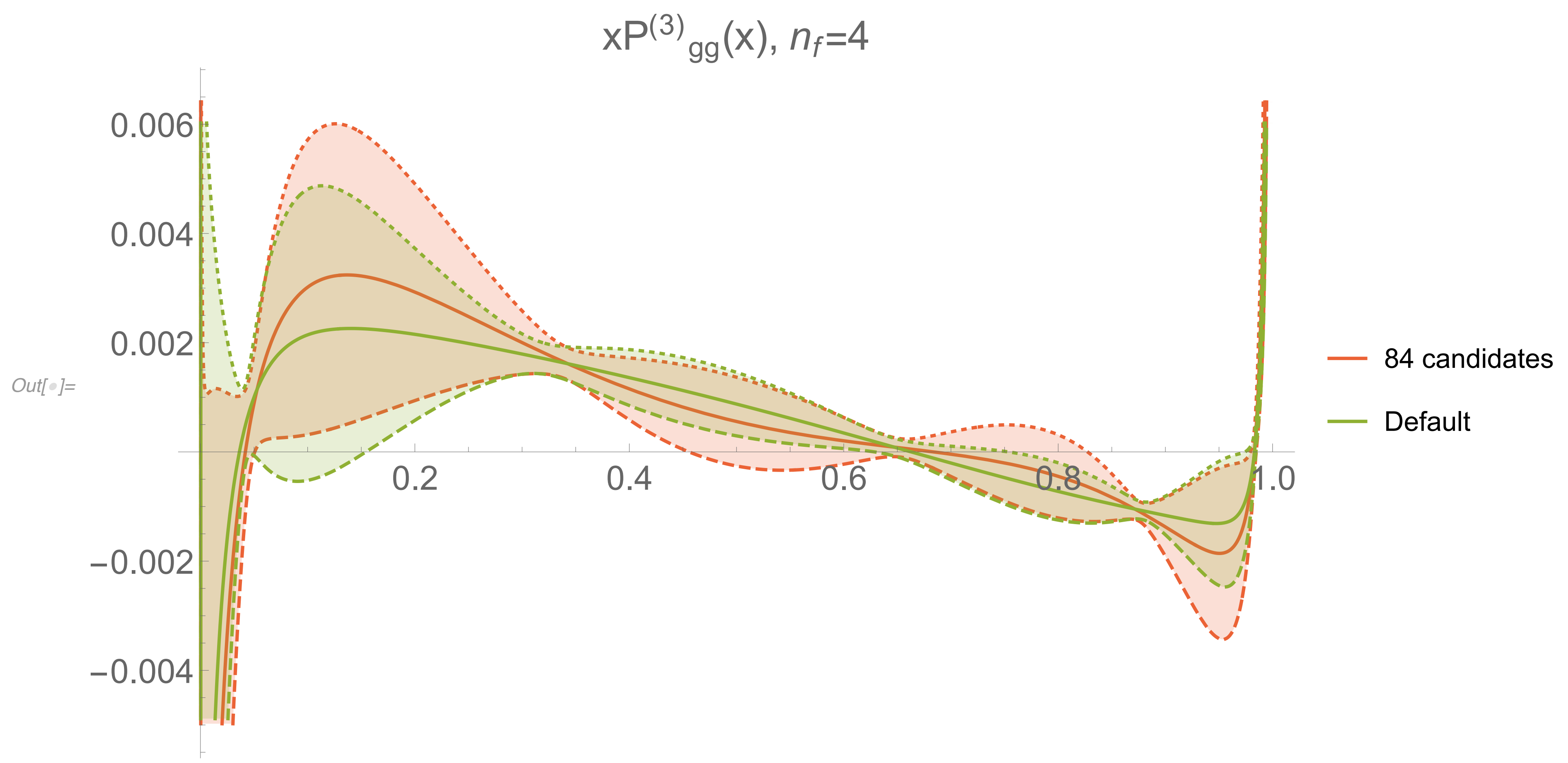
Future updates (NNPDF4.1):

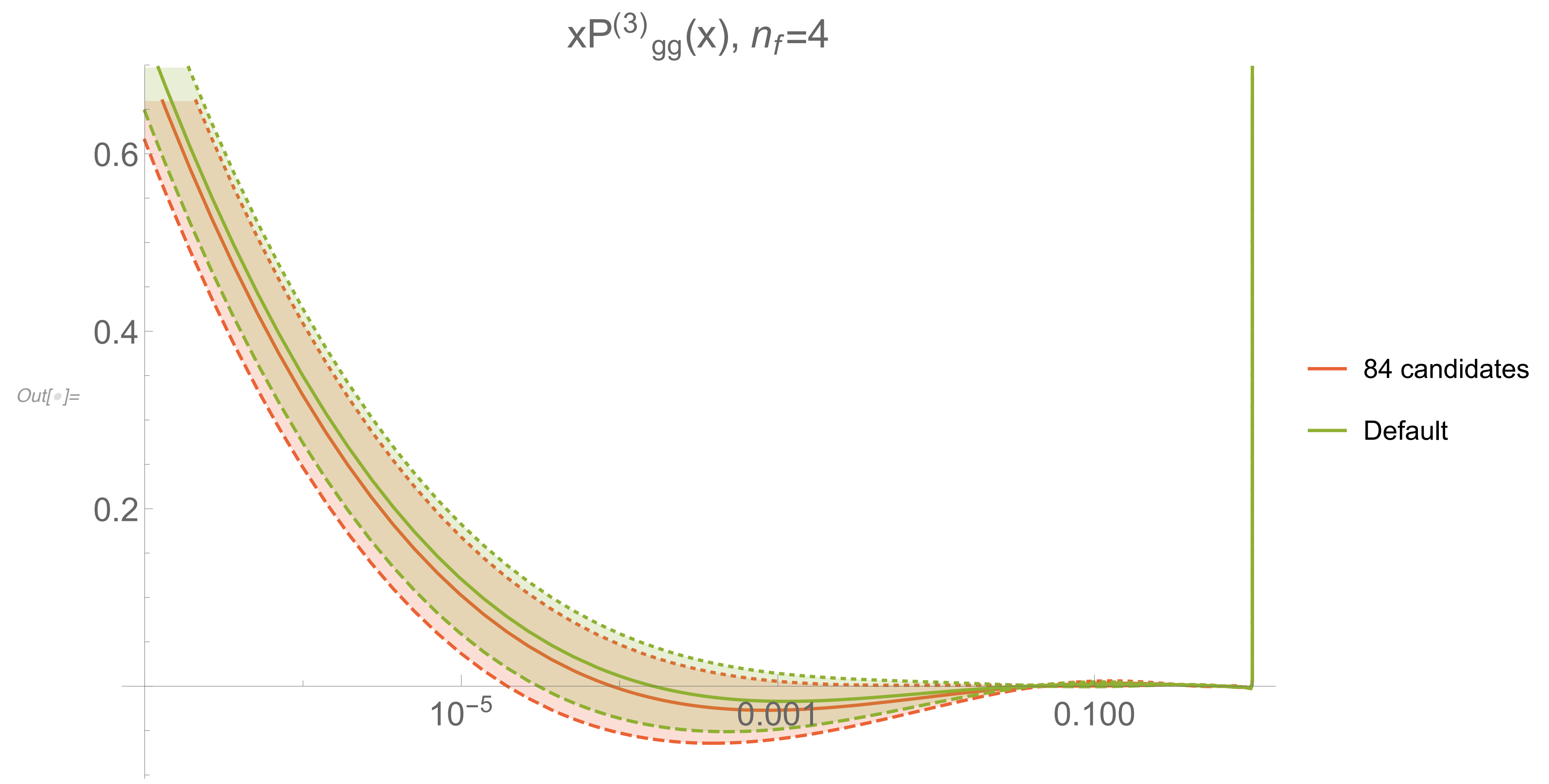
- Full NNLO: removal of NNLO k-factors.
- EWK corrections through k-factors
- Improved methodology: for ex. extended Hyperoptimization
- Extension of fitted data (LHC 13 TeV): DY, Top, Jets; DIS + Jet

Back up slides

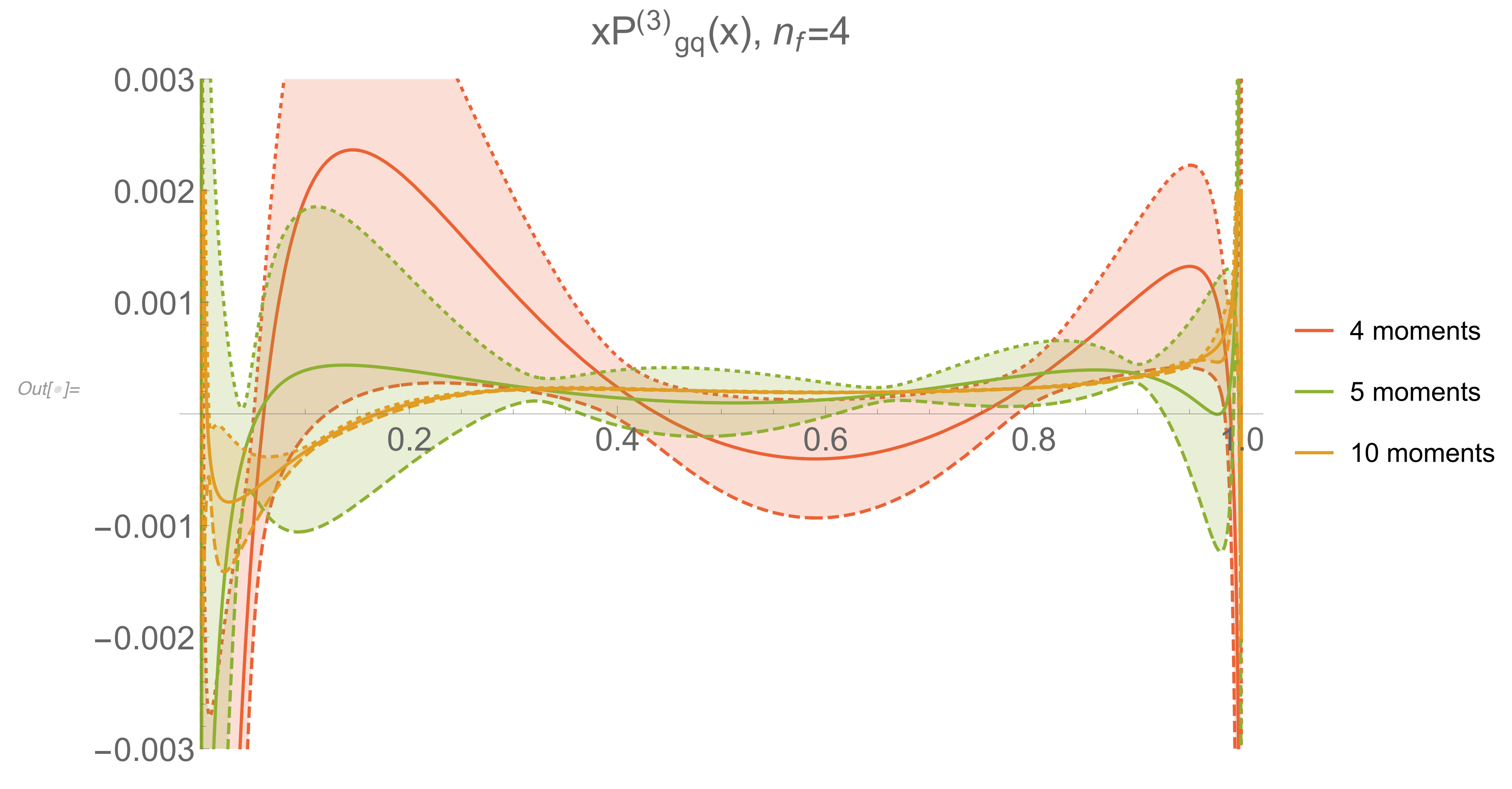
aN^{3}LO splitting functions approximation

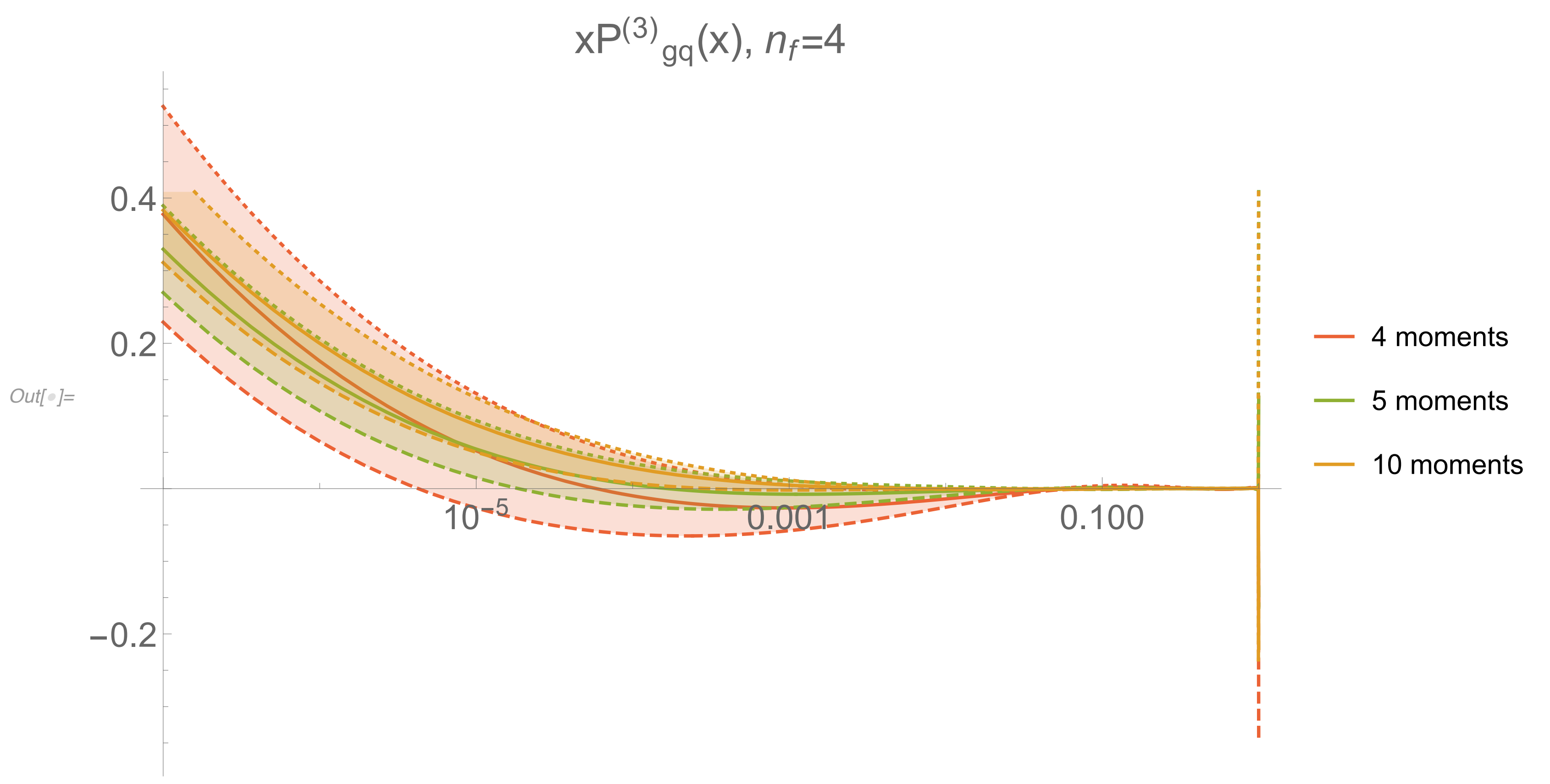
How does the approximation change if we add more test functions?



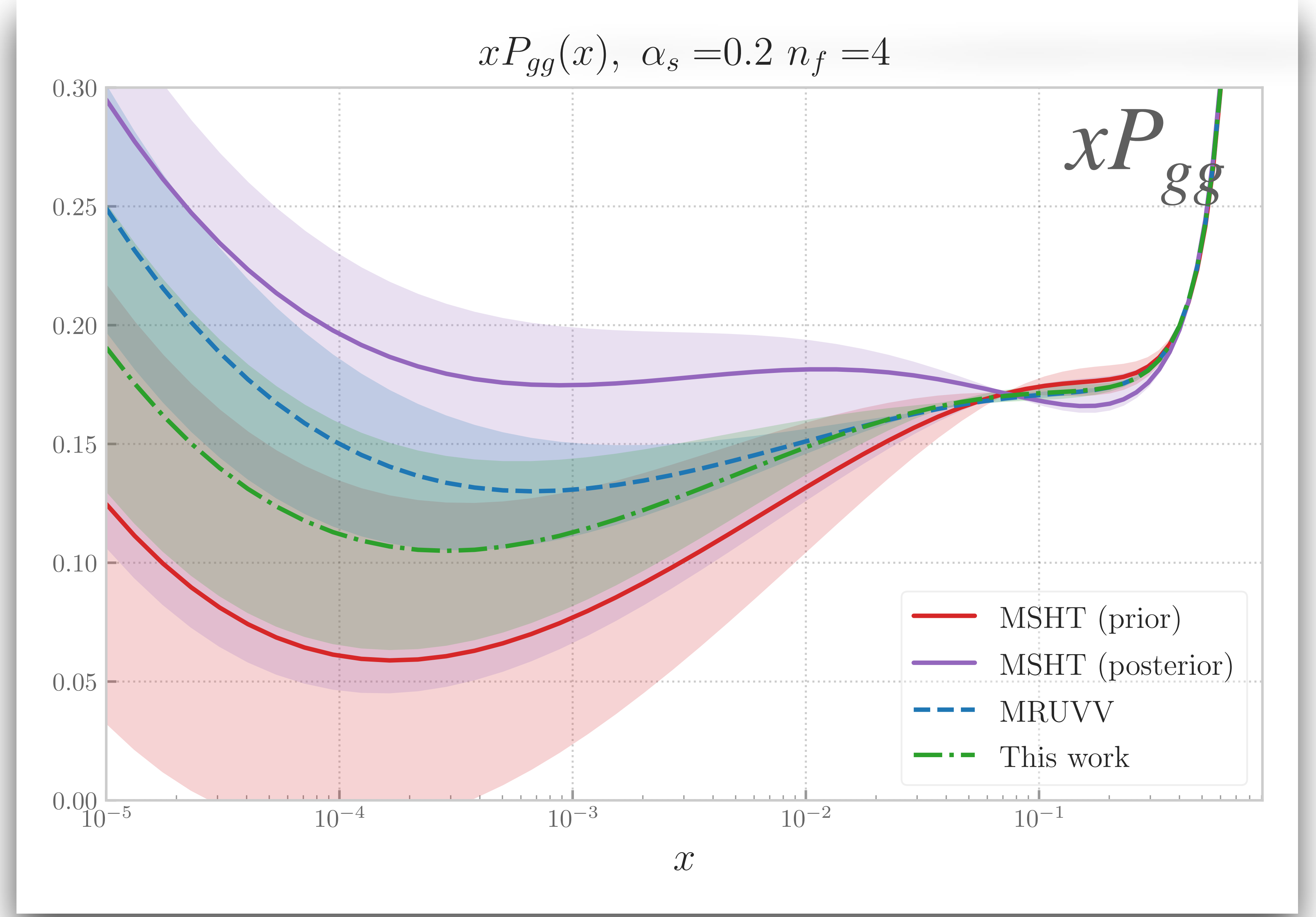


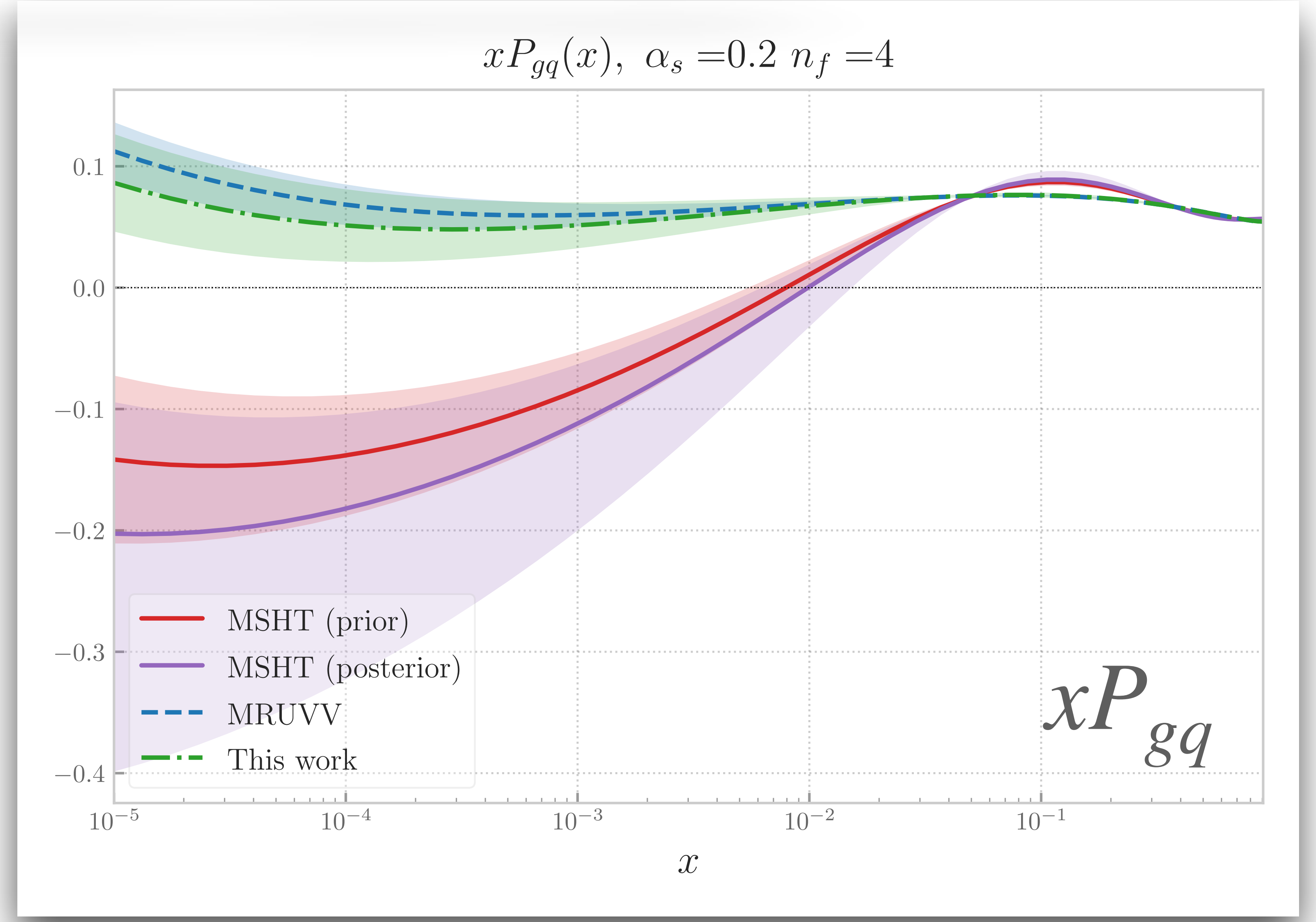
How does the approximation change if we add more Mellin moments?

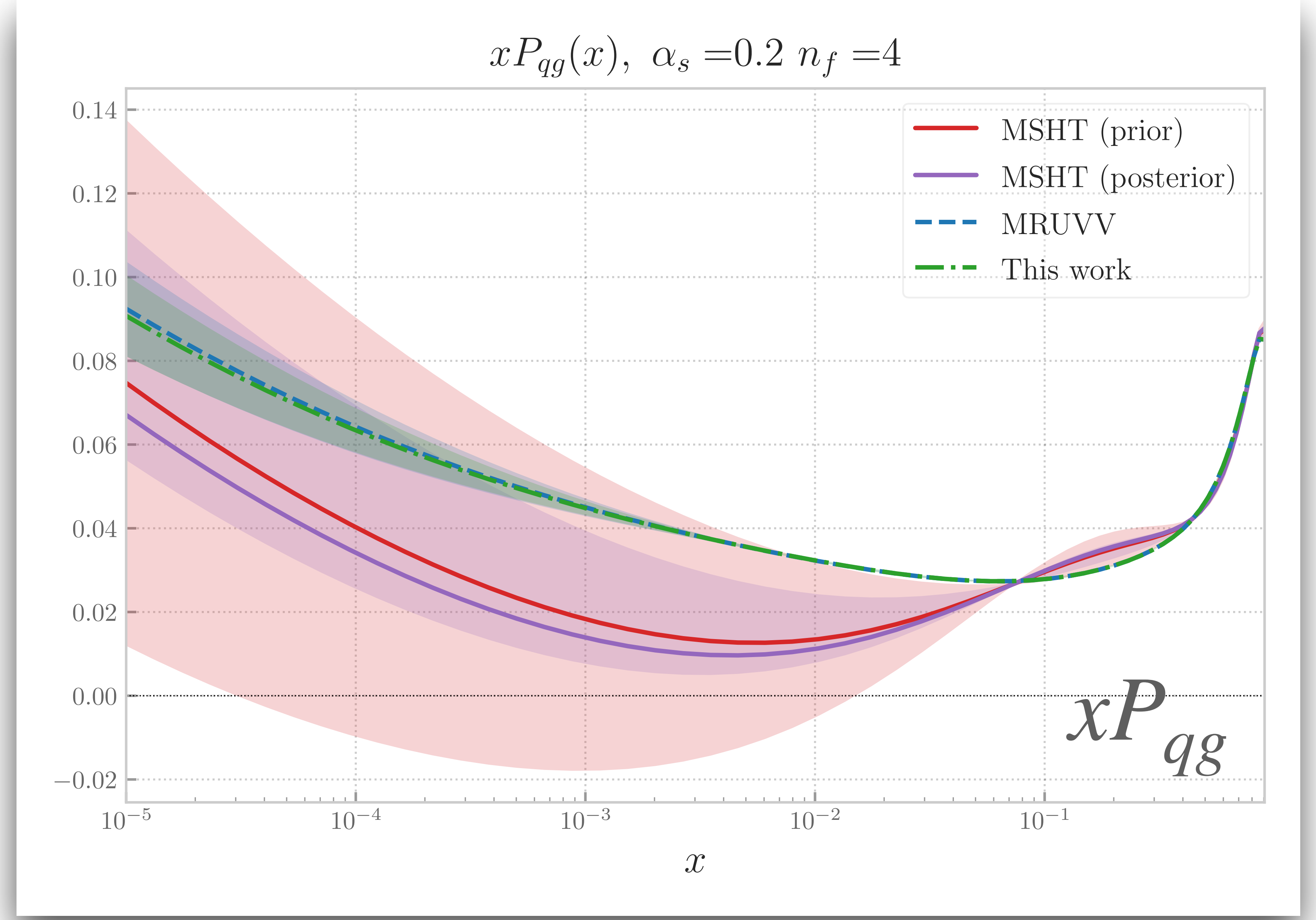


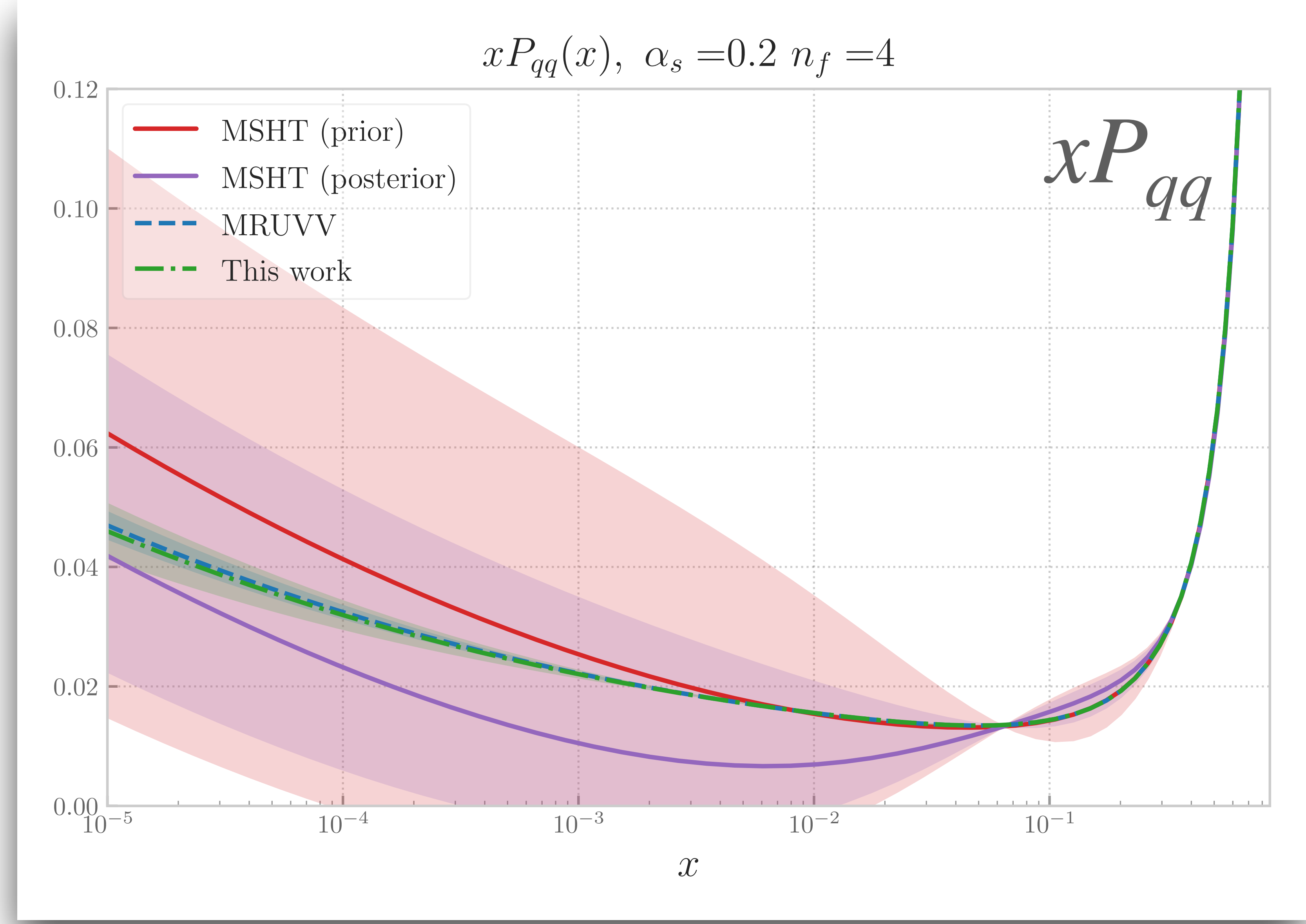


aN^{3}LO splitting functions benchmark



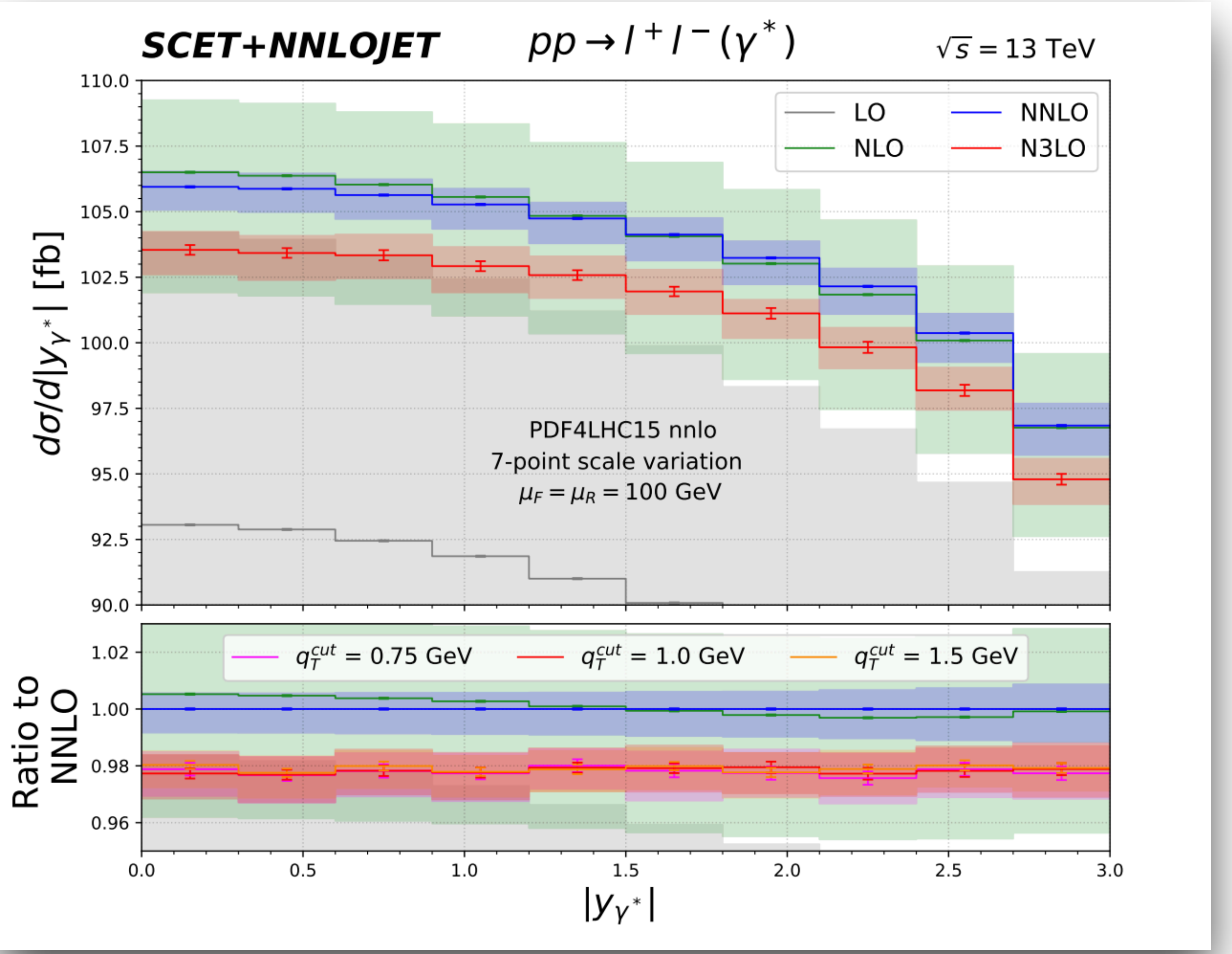






Hadronic processes: DY, Jets, Top

Chen, Gehrmann, Glover, Huss, Yang, Zhu [arxiv:2107.09085]



Single boson production (DY):

- N^3LO corrections to Z and $W^{\pm}$ differential in $m_{\ell\ell}$ or y_Z, can be included through k-factors. Effects are around 1-2% of the total cross sections, and quite flat in the boson rapidity.

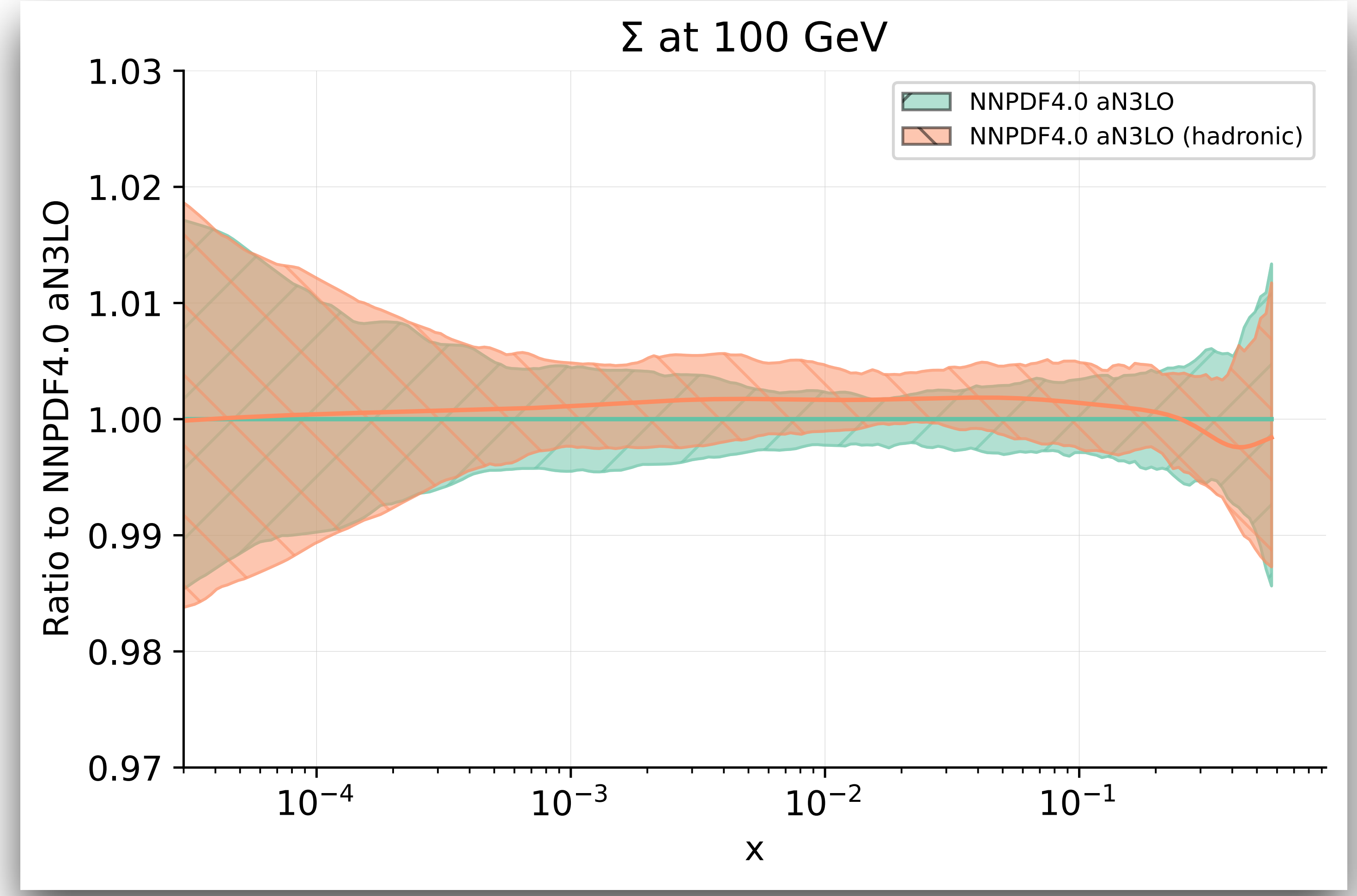
- Effect at PDF level is negligible (limited number of data). **N^3LO DY k-factors not included in the default fit**.

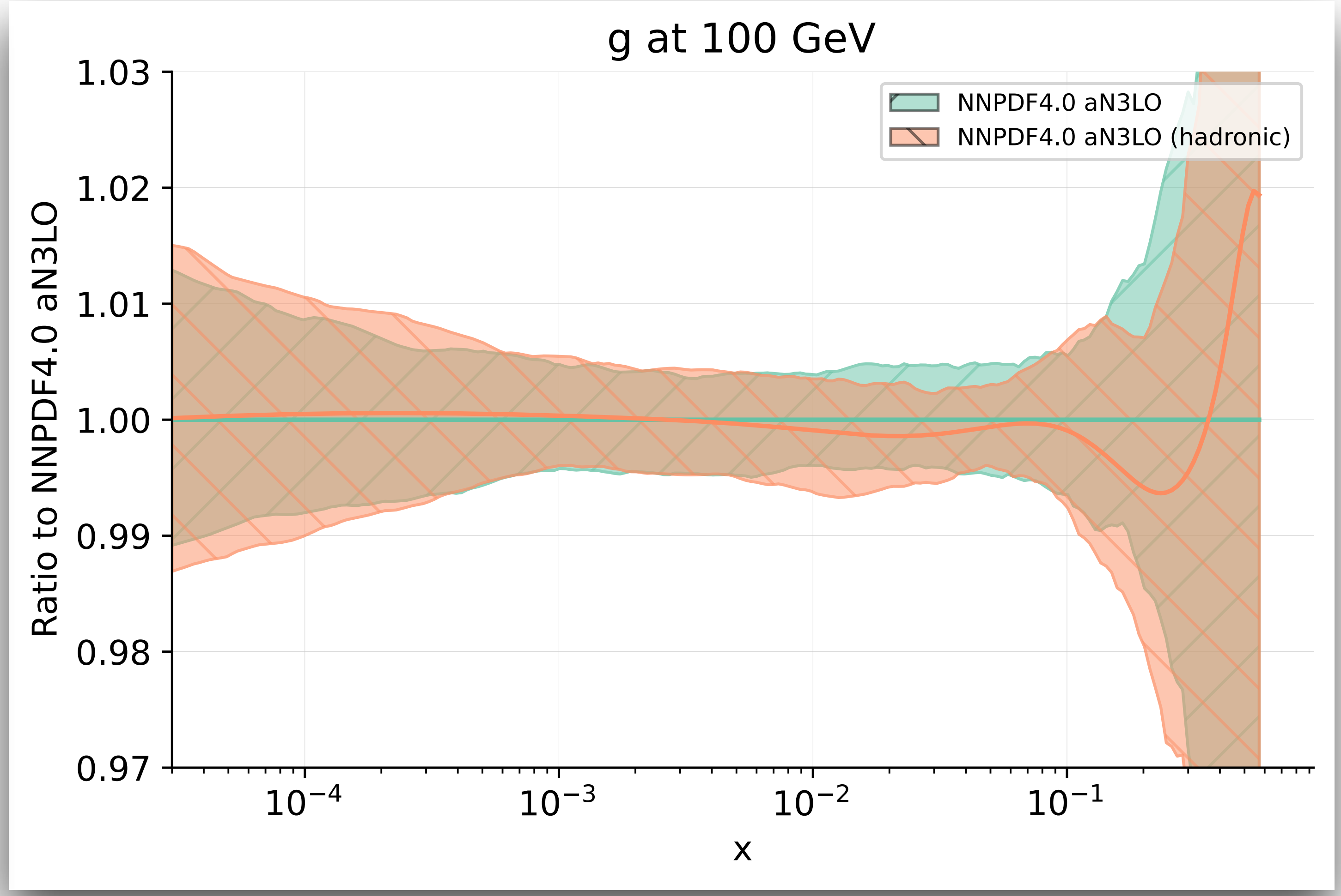
- Differential distributions in p_t are available only up to NNLO.

Jets, Dijets, Top:

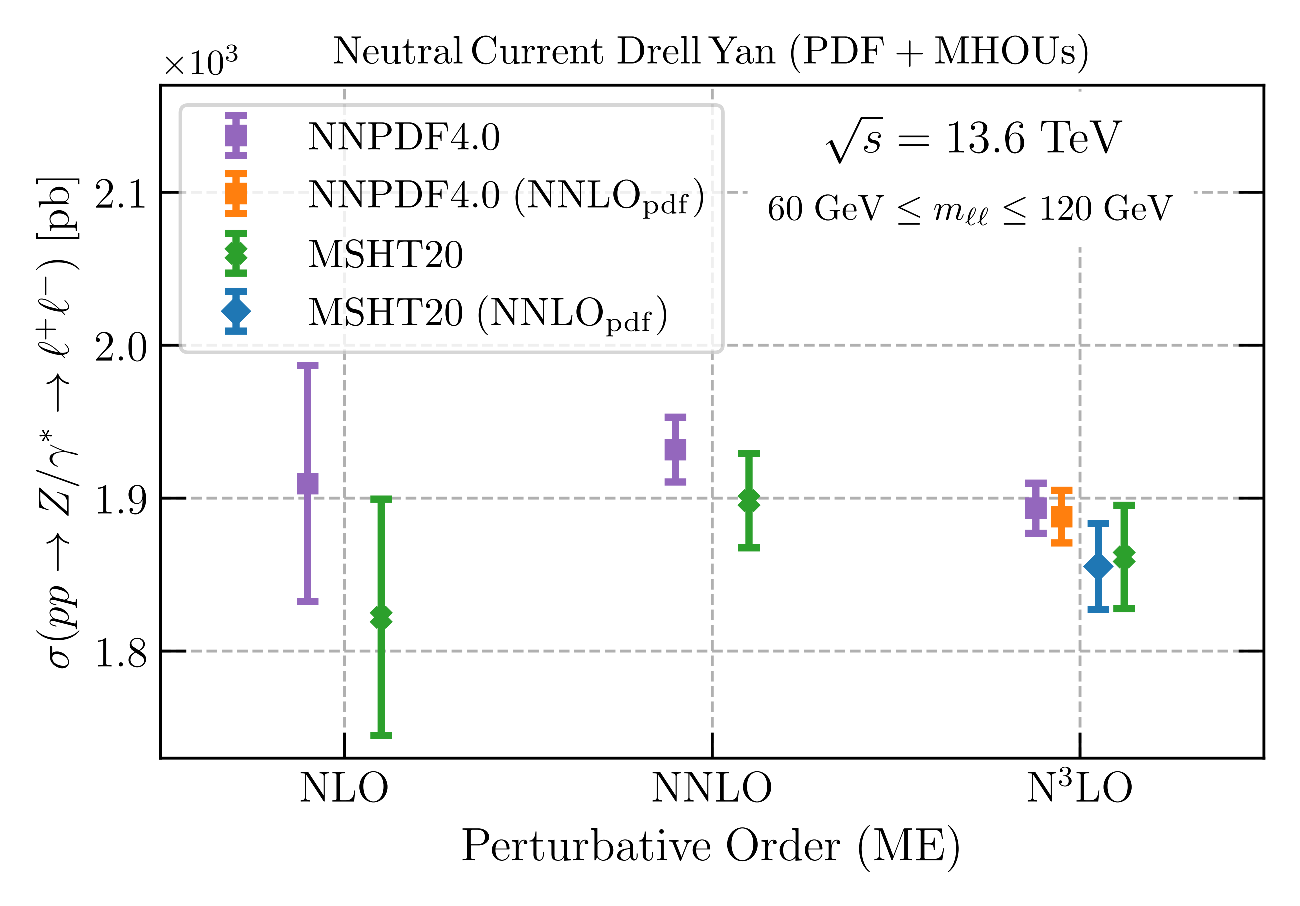
- N^3LO corrections are not known or public available.

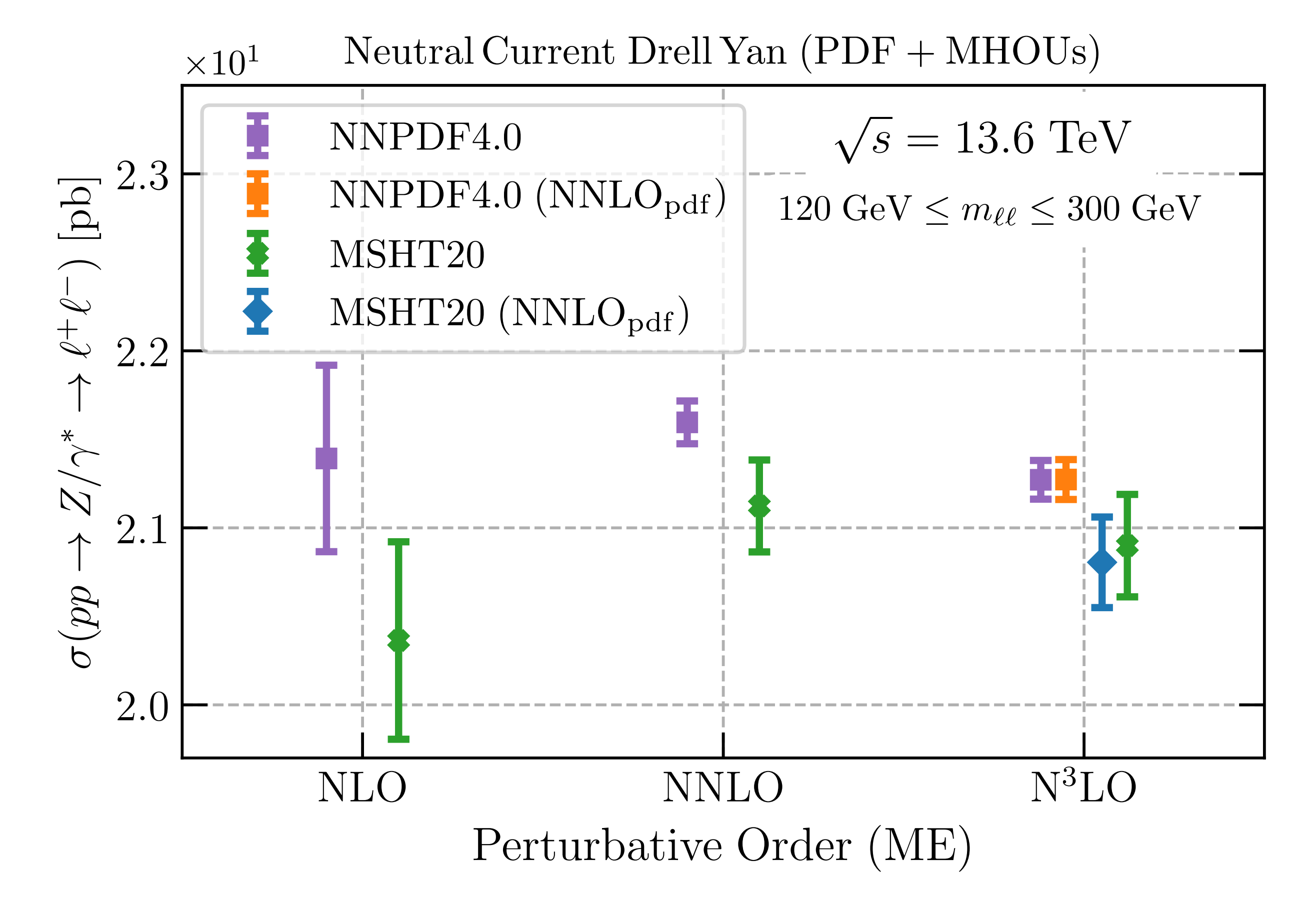
We use NNLO MHOU from 3 point renormalisation scale variation to estimate unknown N^3LO effects.

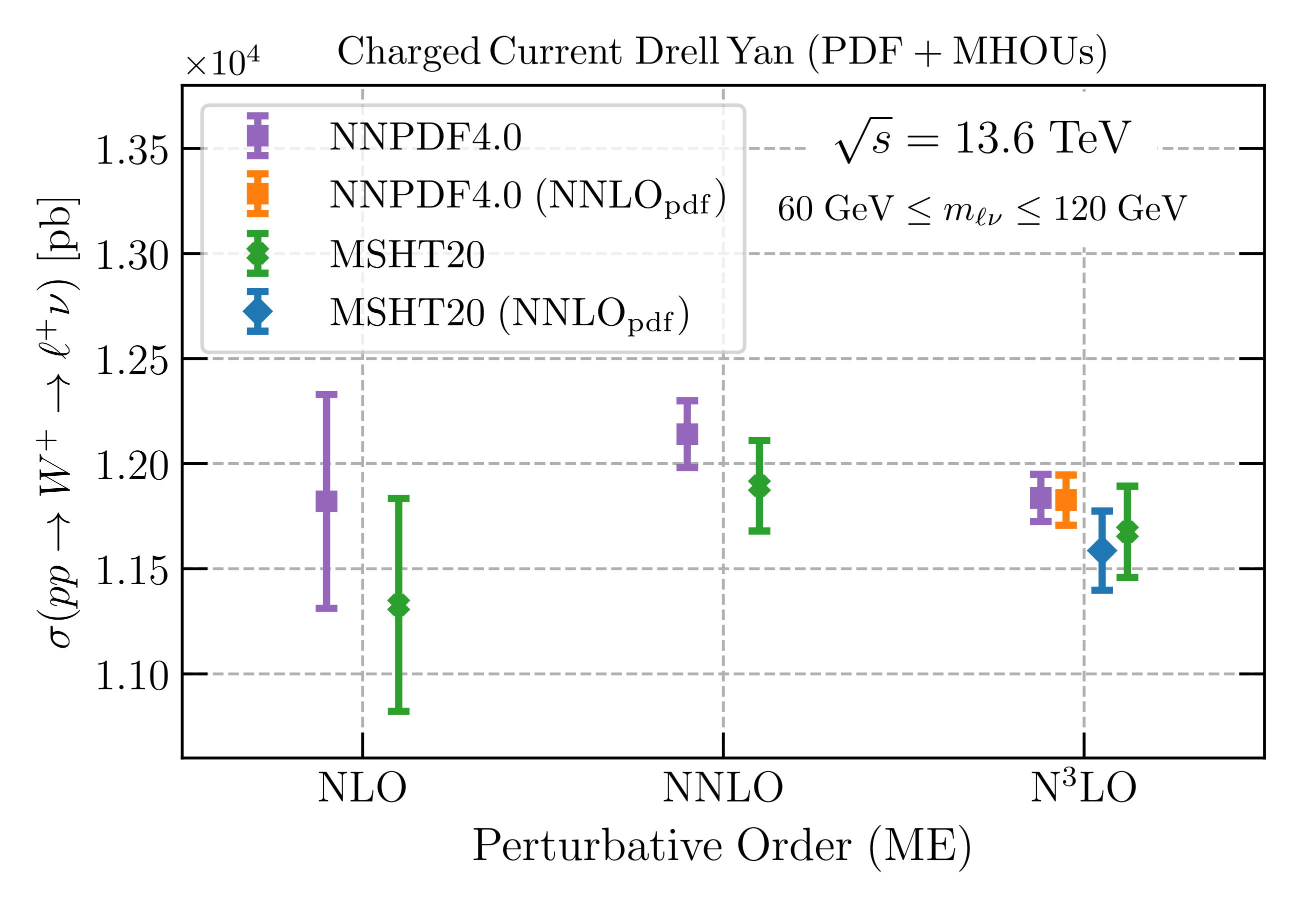


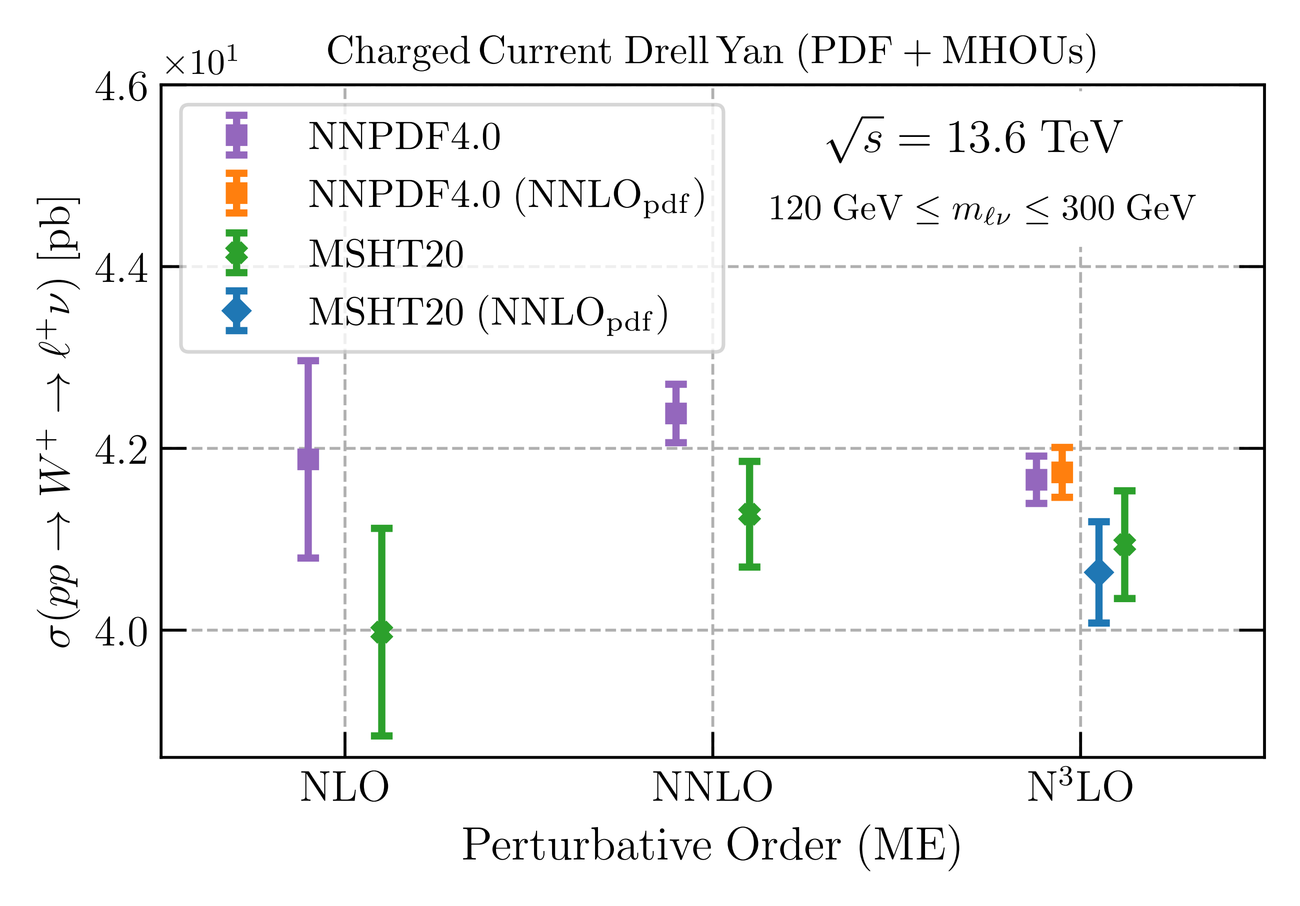


LHC phenomenology: Drell-Yan









Process	NNPDF4.0					
	σ (pb)	$\delta_{\rm th}$	$\delta_{\rm PDF}^{\rm noMHOU}$	$\delta_{\rm PDF}^{\rm MHOU}$	$\Delta_{\rm NNLO}^{\rm app}$	$\Delta_{\rm NNLO}^{\rm exact}$
W^+ (p)	1.2×10^4	1.0	0.5	0.5	1.1	0.1
W^- (p)	8.8×10^3	1.0	0.5	0.5	1.1	0.1
Z (p)	1.9×10^3	0.9	0.4	0.5	1.1	0.3
W^+ (hm)	4.7×10^{-4}	2.8	2.8	3.3	3.2	1.1
W^- (hm)	1.4×10^{-4}	2.9	2.9	3.3	3.3	0.1
Z (hm)	2.1×10^{-4}	2.3	2.3	2.5	3.4	0.3

aN^3LO PDF with QED corrections

Barontini, Laurenti, Rojo [arxiv:2406.01779]

The photon **PDF is computed from DIS** structure functions [arxiv:1607.04266] [arxiv:1708.01256]:

$$x\gamma(x,Q^2) = \frac{2}{\alpha_{em}} \int_x^1 \frac{dz}{z} \int_{\frac{M_p x^2}{1-z}}^{\frac{Q^2}{1-z}} \frac{d\mu^2}{\mu^2} \alpha_{em}(\mu^2) \left[(z P_{\gamma q} + \frac{2 x M_p}{Q^2}) F_2 - z^2 F_L \right] - \alpha_{em}(Q^2) z^2 F_2$$

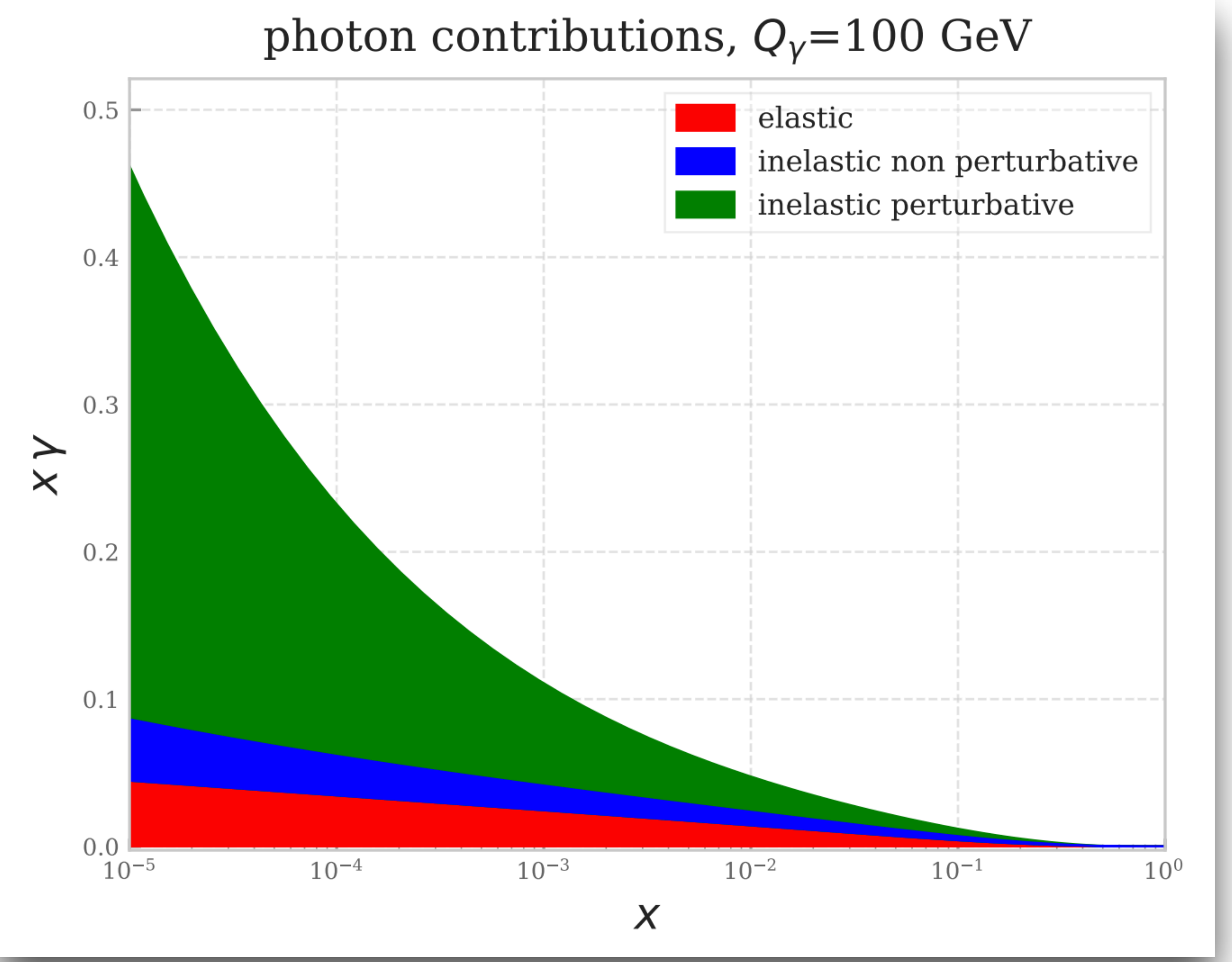
- Depending on the kinematic region the structure functions F_2, F_L are computed form: **pQCD DIS**, **Inelastic DIS**, **Elastic DIS**.

  ➡At **high** Q^2 scale the pQCD component is dominant.

- DGLAP evolution with mixed $QED \otimes QCD$: $\mathcal{O}(\alpha_s \alpha_{em}), \mathcal{O}(\alpha_{em}^2)$ corrections.

- Update the other partons with an iterative procedure from a QCD fit and modifying the momentum sum rule:

$$\int_0^1 xdx\ g(x) + \sum_i q_i^+(x) + \gamma(x) = 1$$



From NNPDF4.0 NNLO QED [arxiv:2401.08749]