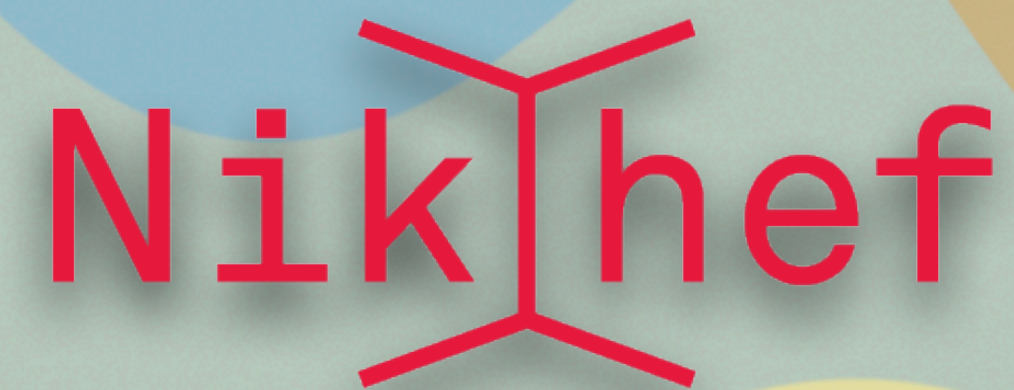


Approximate N3LO Parton Distributions with the NNPDF framework

Giacomo Magni,
Nikhef Theory Group and VU Amsterdam

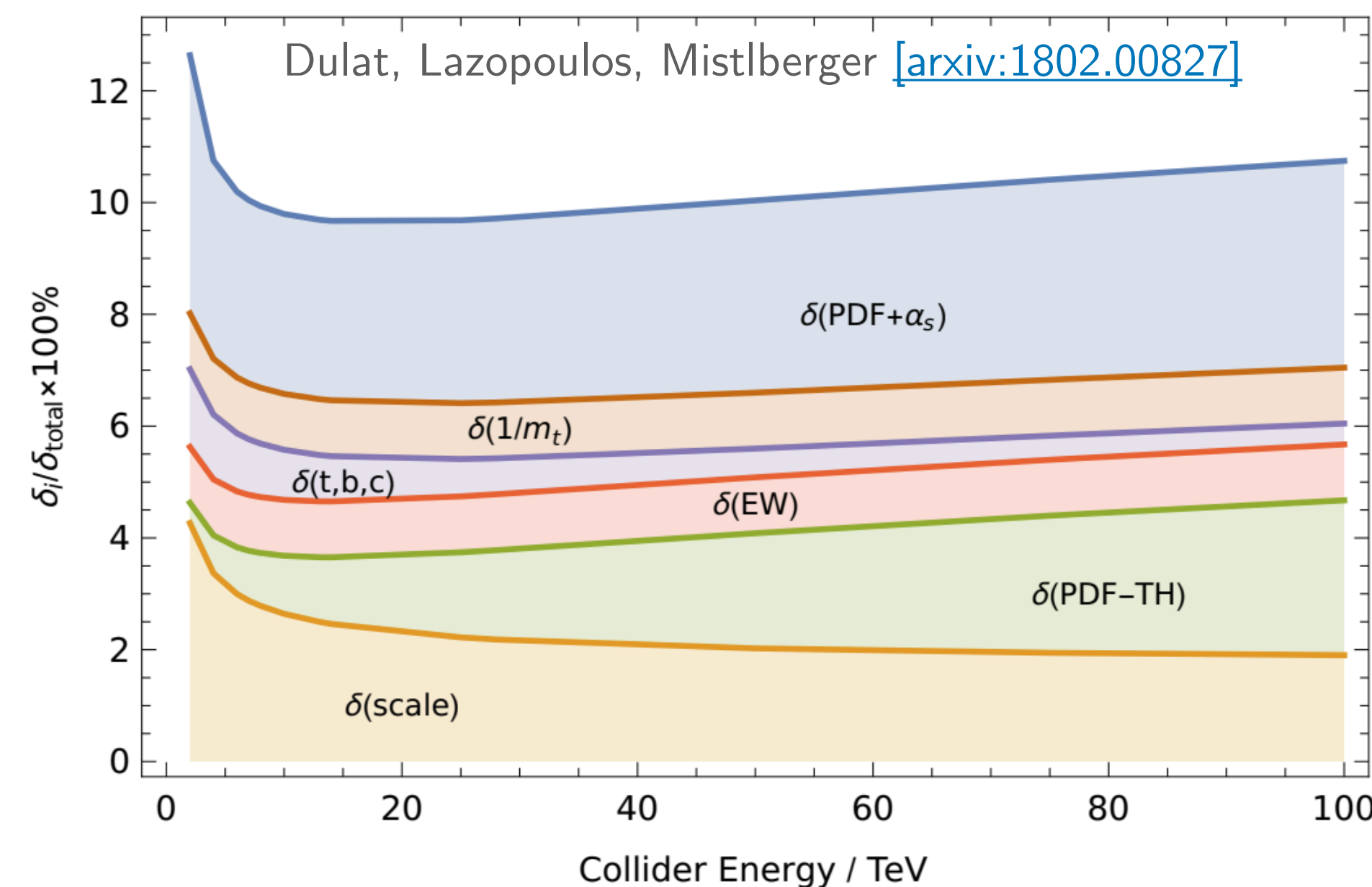
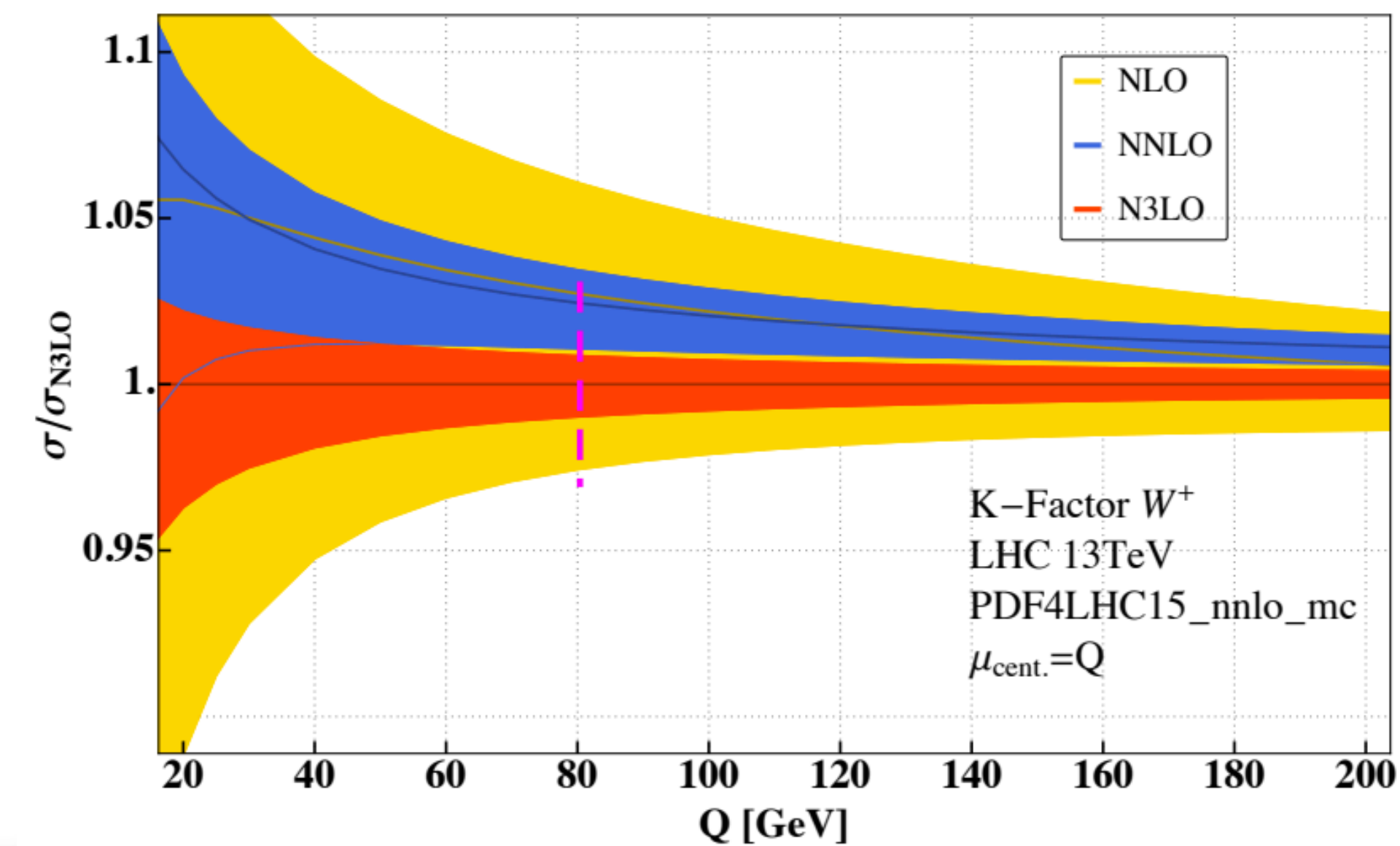
EFCA-NuPECC-APPEC workshop
DESY, Hamburg
14 December 2023



Introduction & Motivations

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

- ▶ Predictions for LHC observables relies on two main ingredients: **PDFs** and partonic **Matrix Elements**.
- ▶ In the last years many 2 to 1 processes have been calculated up to QCD at **N3LO**: $gg \rightarrow H$ [\[arxiv:1503.06056\]](https://arxiv.org/abs/1503.06056) $qq \rightarrow H$ (VBF) [\[arxiv:1606.00840\]](https://arxiv.org/abs/1606.00840); Duhr, Dulat, Mistlberger [\[arxiv:1904.09990\]](https://arxiv.org/abs/1904.09990); Duhr, Dulat, Hirschi, Mistlberger [\[arxiv:2004.04752\]](https://arxiv.org/abs/2004.04752) $pp \rightarrow W^\pm$ Duhr, Dulat, Mistlberger [\[arxiv:2007.13313\]](https://arxiv.org/abs/2007.13313); Chen, Gehrmann, Glover, Huss, Yang, Xing Zhu [\[arxiv:2205.11426\]](https://arxiv.org/abs/2205.11426) $pp \rightarrow Z/\gamma$, $pp \rightarrow VH$ Baglio, Duhr, Mistlberger, Szafrond [\[arxiv:2209.06138\]](https://arxiv.org/abs/2209.06138); Chen, Gehrmann, Glover, Huss, Yang, Xing Zhu [\[arxiv:2107.09085\]](https://arxiv.org/abs/2107.09085) Neumann, Campbell [\[arxiv:2207.07056\]](https://arxiv.org/abs/2207.07056)
- ▶ **PDFs uncertainties** are becoming a bottleneck for LHC precision calculations with the largest uncertainties along with the incomplete knowledge of α_s .
- ▶ Differences between PDF sets which are based on similar datasets have to be well motivated.



- 
- The background of the slide is a repeating pattern of various Feynman diagrams. These diagrams are rendered in several colors: black, blue, orange, and light green. They represent different types of particle interactions, including tree-level and loop-level processes, with various line styles such as straight lines for fermions and wavy lines for bosons. The diagrams are arranged in a grid-like fashion across the entire slide.
- ▶ **Theory inputs for aN3LO PDFs.**
 - ▶ Towards NNPDF4.0 aN3LO.
 - ▶ Impact on future observables.

PDFs determination at aN3LO

Several theoretical inputs are needed in a PDF fit:

- ▶ The main ingredient are the QCD **splitting functions** which controls the DGLAP evolution.

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

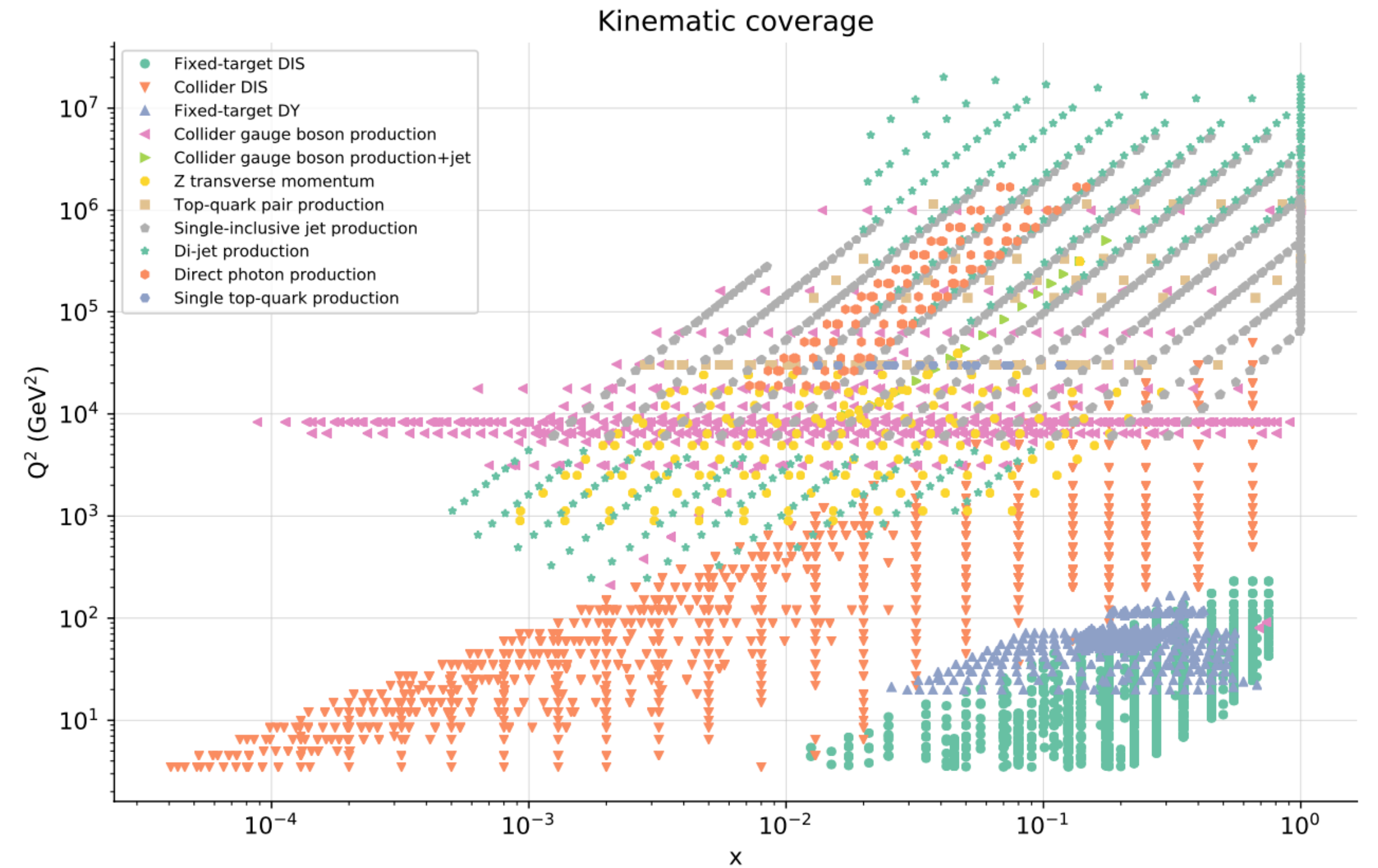
- ▶ **VFNS matching conditions** for each running component.

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

- ▶ **DIS partonic coefficients** functions, accounting for massive corrections when possible.

$$F_k = x \sum_{i=-n_f}^{n_f} C_{k,i}(x, \alpha_s) \otimes f_i(x, Q^2), \quad k = \{1,2,3\}$$

- ▶ **Hadronic coefficients.** At N3LO they can be included mainly through *k-factors*.



Not all of them are yet available at N3LO

- ◆ Construct reliable approximations from existing calculations.
- ◆ Determine theory uncertainties both from:

Incomplete Higher Order corrections (IHOU)

Missing Higher Order corrections (MHOU)

aN3LO splitting functions

See also G.Falcioni talk

Analytical calculations of the complete N3LO splitting functions are not available yet.
But many information are available.

In DGLAP evolution we can distinguish:

- ▶ 4 Singlet splitting functions: $Q^2 \frac{d}{dQ^2} \begin{pmatrix} g \\ \Sigma \end{pmatrix} = \begin{pmatrix} P_{gg} & P_{gq} \\ P_{qg} & P_{qq} \end{pmatrix} \otimes \begin{pmatrix} g \\ \Sigma \end{pmatrix}$
- ▶ **3 Non-Singlet** splitting functions: $Q^2 \frac{dV}{dQ^2} = P_{NS,v} \otimes V$



The **Non Singlet** splitting functions can be estimated with quite precise accuracy for phenomenological studies.

Non Singlet Know limits:

- ▶ **Large- n_f limit:** Davies, Vogt, Ruijl, Ueda, and Vermaseren. [[arXiv:1610.07477](https://arxiv.org/abs/1610.07477)]; Gehrmann, Manteuffel, Sotnikov, Yan [[arxiv:2308.07958](https://arxiv.org/abs/2308.07958)] $\mathcal{O}(n_f^2), \mathcal{O}(n_f^3)$
- ▶ **Small- x limit:** Davies, Kom, Moch, Vogt. [[arXiv:2202.10362](https://arxiv.org/abs/2202.10362)] $P_{NS}^{(3)} \supset \sum_{k=0}^6 \ln^k(x)$
- ▶ **Large- x limit:** Moch, Ruijl, Ueda, Vermaseren, Vogt [[arXiv:1707.08315](https://arxiv.org/abs/1707.08315)]

$$P_{NS}^{(3)} \approx A_4 \frac{1}{(1-x)_+} + B_4 \delta(1-x) + C_4 \ln(1-x) + D_4, \quad x \rightarrow 1$$

- ▶ 8 lowest **Mellin Moments:** [[arXiv:1707.08315](https://arxiv.org/abs/1707.08315)]


N3LO Non Singlet splitting functions dependency on active flavors

	n_f^0	n_f^1	n_f^2	n_f^3
$\gamma_{ns,-}^{(3)}$	✓	✓	✓	✓
$\gamma_{ns,+}^{(3)}$	✓	✓	✓	✓
$\gamma_{ns,s}^{(3)}$		✓	✓	

aN3LO splitting functions

See also G.Falcioni talk

In DGLAP evolution we can distinguish:

- ▶ **4 Singlet** splitting functions: $Q^2 \frac{d}{dQ^2} \begin{pmatrix} g \\ \Sigma \end{pmatrix} = \begin{pmatrix} P_{gg} & P_{gq} \\ P_{qg} & P_{qq} \end{pmatrix} \otimes \begin{pmatrix} g \\ \Sigma \end{pmatrix}$ 
- ▶ 3 Non-Singlet splitting functions: $Q^2 \frac{dV}{dQ^2} = P_{NS,v} \otimes V$

The **Singlet** splitting functions are way more challenging and can be determined only with a finite accuracy.

Singlet known limits:

- ▶ **Large- n_f limit:** Davies, Vogt, Ruijl, Ueda, Vermaseren. [\[arXiv:1610.07477\]](#); $\mathcal{O}(n_f^3)$
Gehrmann, Manteuffel, Sotnikov, Yan [\[arxiv:2308.07958\]](#) $\mathcal{O}(n_f^2)$ only for $P_{qq,PS}, P_{qg}$
- ▶ **Small- x limit:** Bonvini, Marzani [\[arXiv:1805.06460\]](#) $P_{ij}^{(3)} \supset \sum_{k=0}^3 \frac{\ln^k(x)}{x}$
- ▶ **Large- x limit:** Duhr, Mistlberger, Vita [\[arXiv:2205.04493\]](#); Henn, Korchemsky, Mistlberger [\[arXiv:1911.10174\]](#); Soar, Moch, Vermaseren, Vogt [\[arXiv:0912.0369\]](#).

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

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

- ▶ 5 (10) lowest **Mellin Moments:** Moch, Ruijl, Ueda, Vermaseren, Vogt [\[arXiv:2111.15561\]](#); Falcioni, Herzog, Loch, Moch, Vogt [\[arXiv:2302.07593\]](#), [\[arxiv:2307.04158\]](#)

N3LO Singlet splitting functions dependency on active flavors

	n_f^0	n_f^1	n_f^2	n_f^3
$\gamma_{gg}^{(3)}$	✓	✓	✓	✓
$\gamma_{gq}^{(3)}$	✓	✓	✓	✓
$\gamma_{qg}^{(3)}$		✓	✓	✓
$\gamma_{qq,ps}^{(3)}$		✓	✓	✓

aN3LO splitting functions

How can do we combine the different limits ?

The approximation procedure is performed in **Mellin** space for each n_f part independently:

$$\gamma_{ij}^{(3)} = \gamma_{ij,n_f}^{(3)} + \gamma_{ij,N \rightarrow \infty}^{(3)} + \gamma_{ij,N \rightarrow 0}^{(3)} + \tilde{\gamma}_{ij}^{(3)}$$

The parametrised part is constructed as:
$$\tilde{\gamma}_{ij} = \sum_l a_{ij}^{(l)} G_l(N)$$

1. A function G_1 for the leading unknown **large- N** contribution.
2. A function G_2 for the leading unknown **small- N** contribution.
3. 3 (8) functions G_l for the sub-leading small- N and large- N contributions.
4. Vary the functions G_l to generate a variety of approximations. This will estimate **IHO**

- ▶ **Only theoretical inputs** are considered.
- ▶ All the implemented approximations respect momentum sum rules.

Mellin transformation:

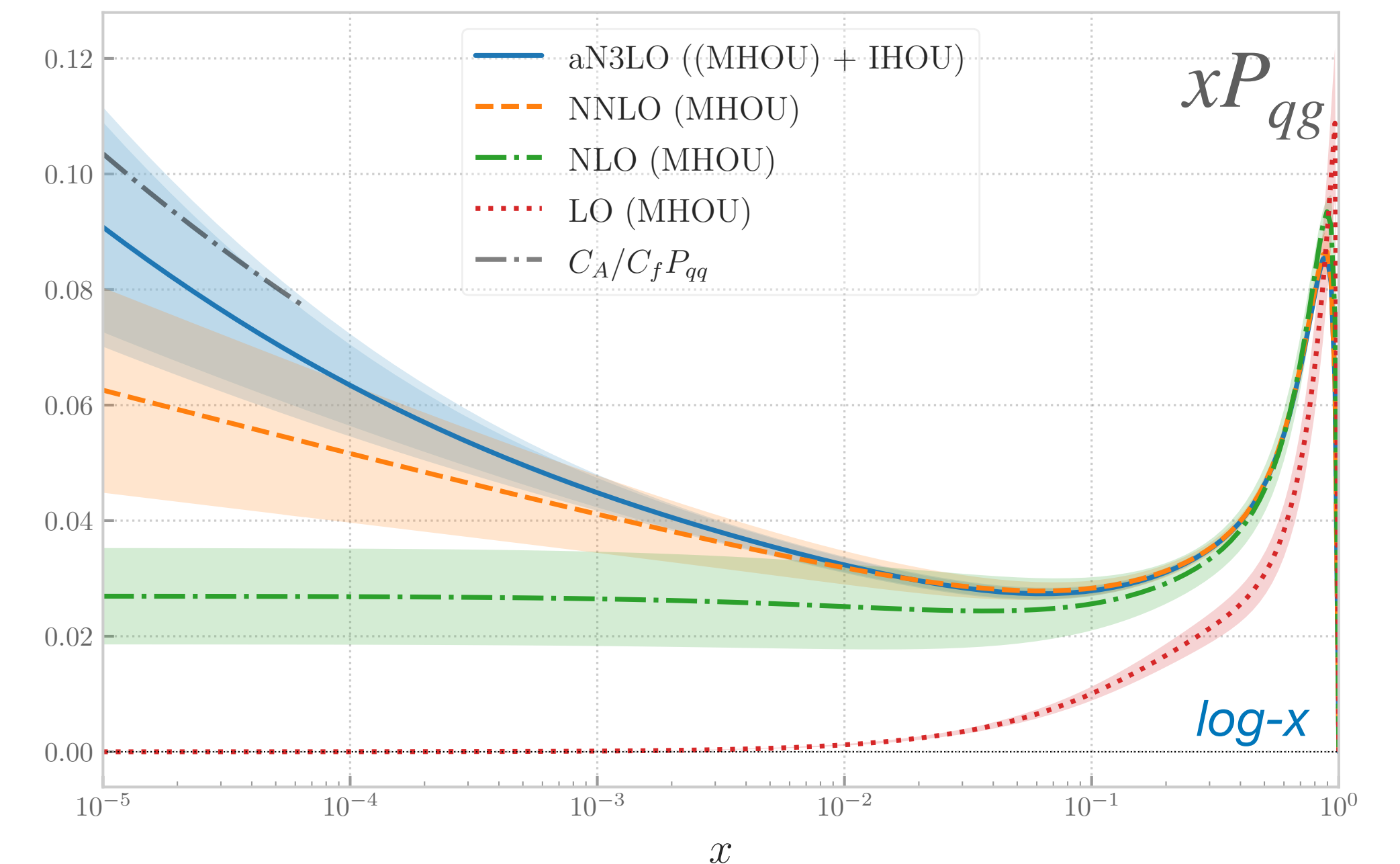
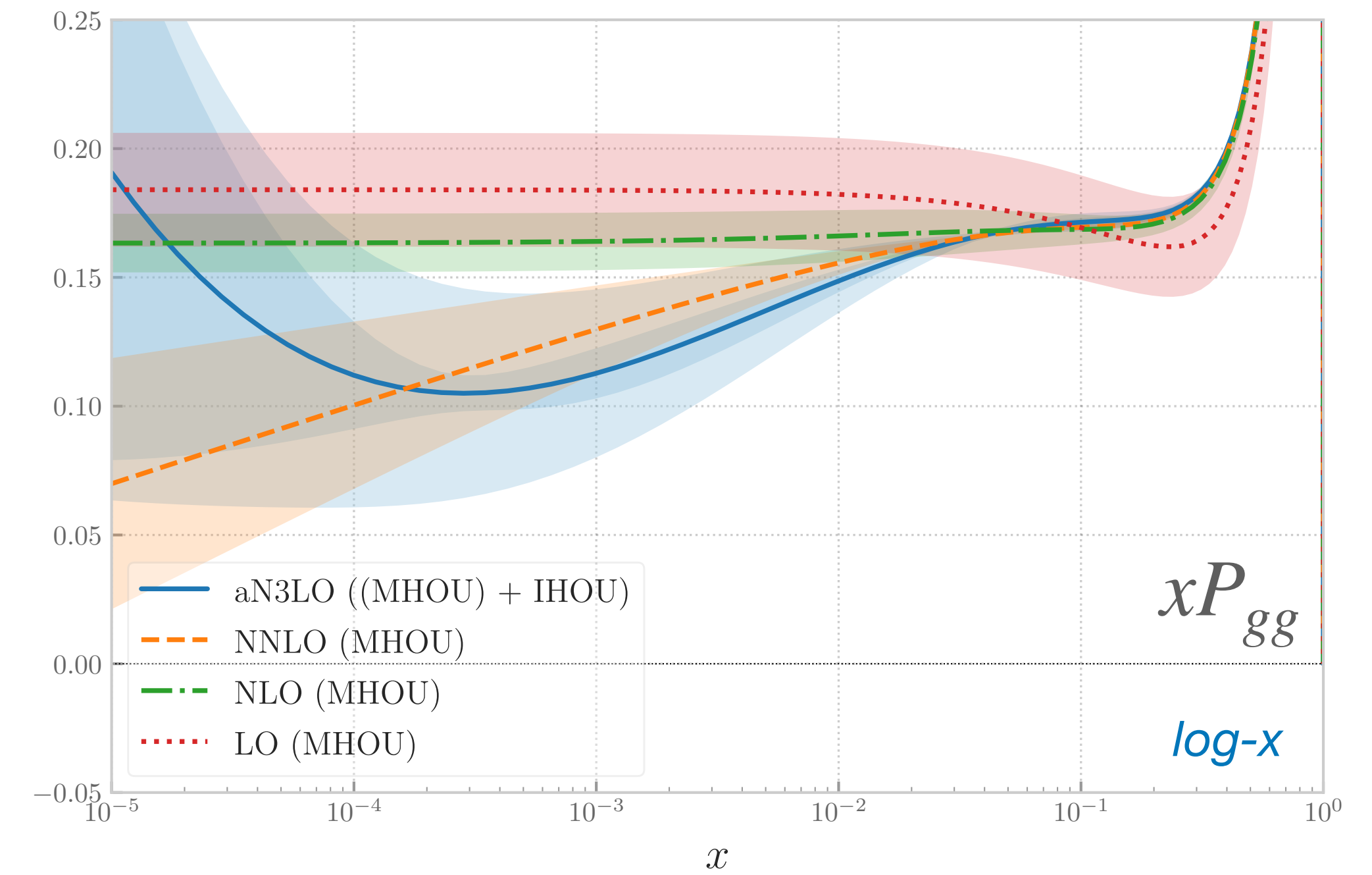
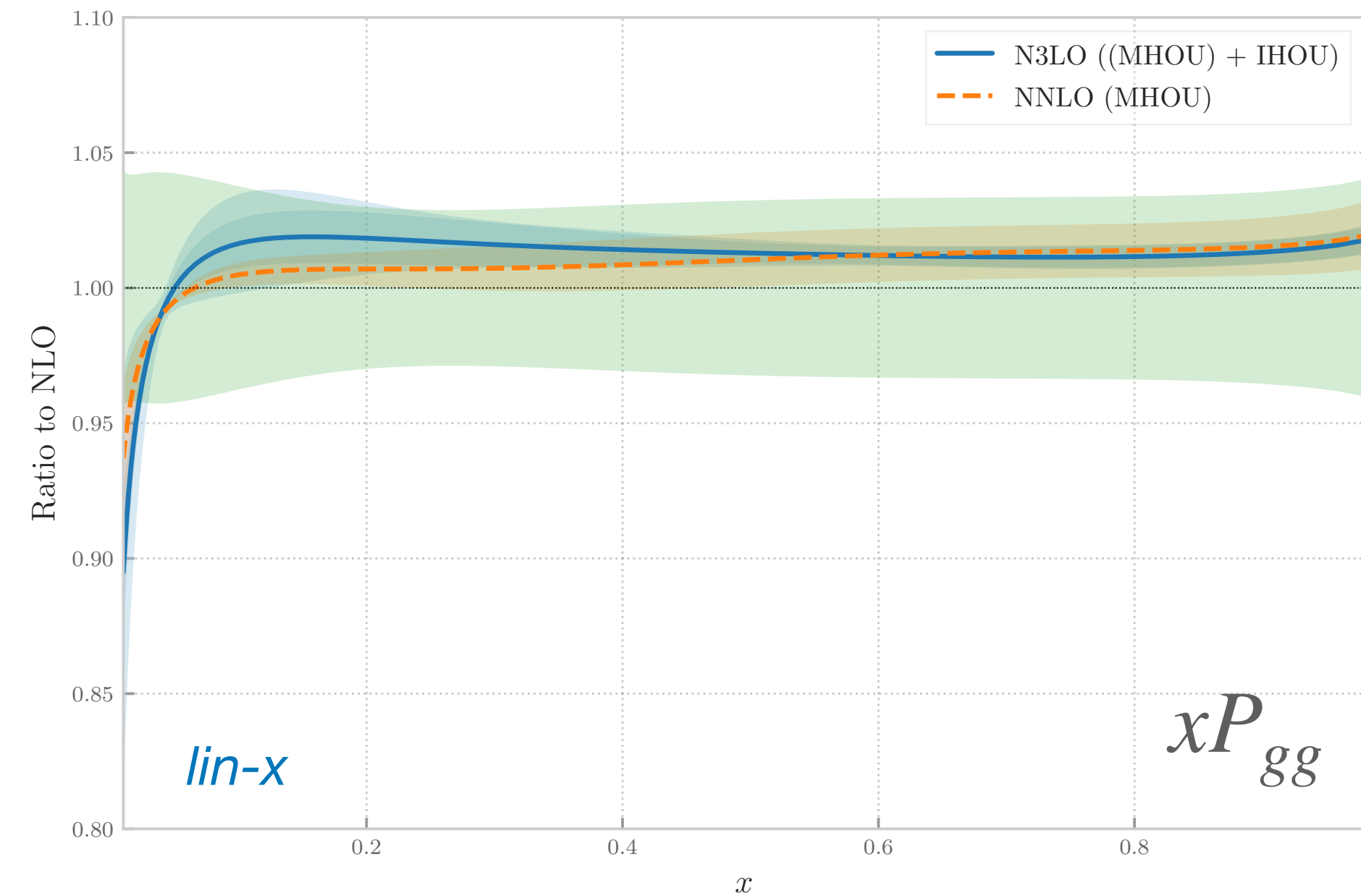
$$\tilde{\gamma}_{ij}(N) = \int_0^1 x^{N-1} P_{ij}(x) dx$$

*Rule of thumb:
small- $N \rightarrow$ small- x ,
large- $N \rightarrow$ large- x*

Adopted basis function for $\tilde{\gamma}_{qq}^{(3)}$

$G_1(N)$	$\mathcal{M}[(1-x) \ln^2(1-x)]$
$G_2(N)$	$-\frac{1}{(N-1)^2} + \frac{1}{N^2}$
$G_3(N)$	$\frac{1}{N^4}, \frac{1}{N^3}, \mathcal{M}[(1-x) \ln(1-x)]$
	$\mathcal{M}[(1-x)^2 \ln(1-x)^2], \frac{1}{N-1} - \frac{1}{N}, \mathcal{M}[(1-x) \ln(x)]$
$G_4(N)$	$\mathcal{M}[(1-x)(1+2x)], \mathcal{M}[(1-x)x^2],$ $\mathcal{M}[(1-x)x(1+x)], \mathcal{M}[(1-x)]$

aN3LO splitting functions

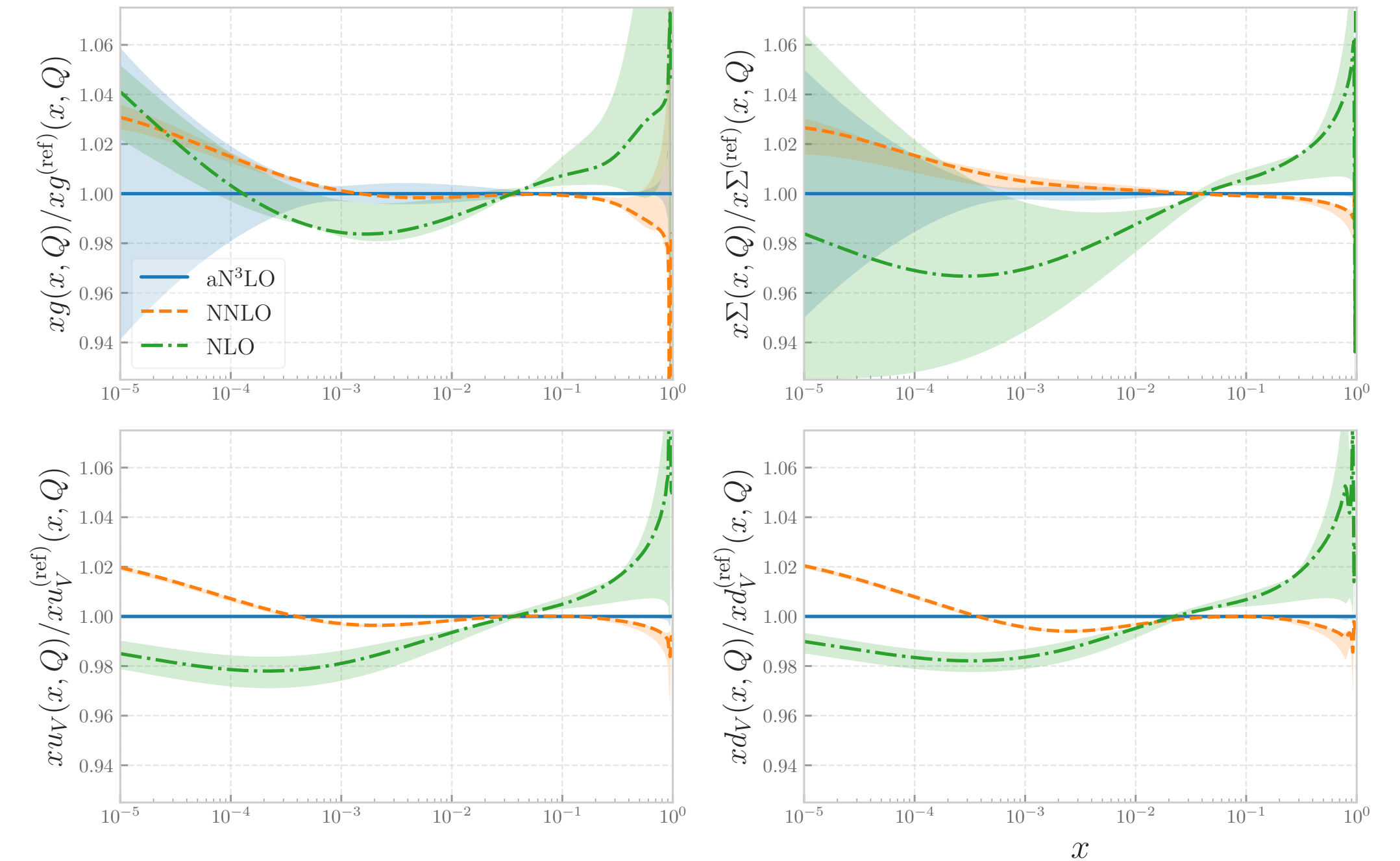


- ▶ Large logs $1/x \ln^3(x)$, $1/x \ln^2(x)$ arise at N3LO. MHO (from scale variations) fails in small- x region.
- ▶ Good agreement between different perturbative orders at large- x .
- ▶ IHOU are not negligible. Having 10 moments available would be enough to reduce IHOU.
- ▶ Off diagonal terms P_{qg} , P_{gq} are more difficult to estimate (large- $N \rightarrow 0$).

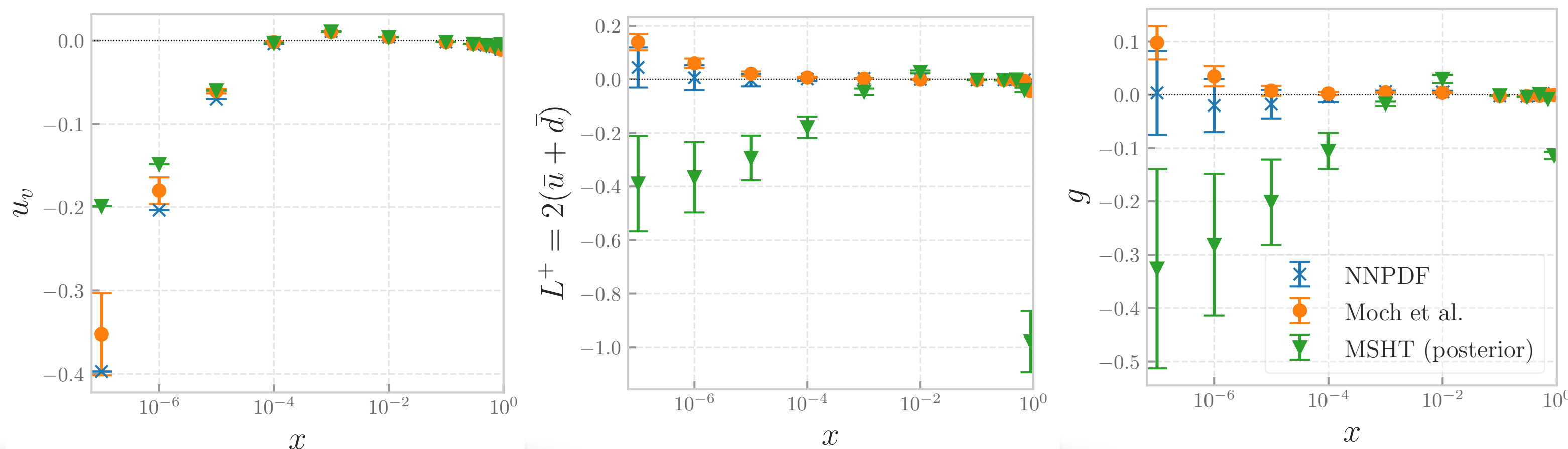
aN3LO DGLAP evolution

- ▶ Valence-like PDFs display good perturbative convergence on all the x-range.
- ▶ Impact of the N3LO corrections is **at most at percent level**.
- ▶ Ongoing **benchmark study** with MSHT and FHMV to assess a region in which agreement between different aN3LO splitting functions approximations can be found.

NNPDF4.0 NNLO evolution from, $Q = 1.65 \rightarrow 100 \text{ GeV}$



Relative difference to NNLO evolution from, $Q = 1.41 \rightarrow 100 \text{ GeV}$



See also T.Cridge talk

DIS Structure Functions

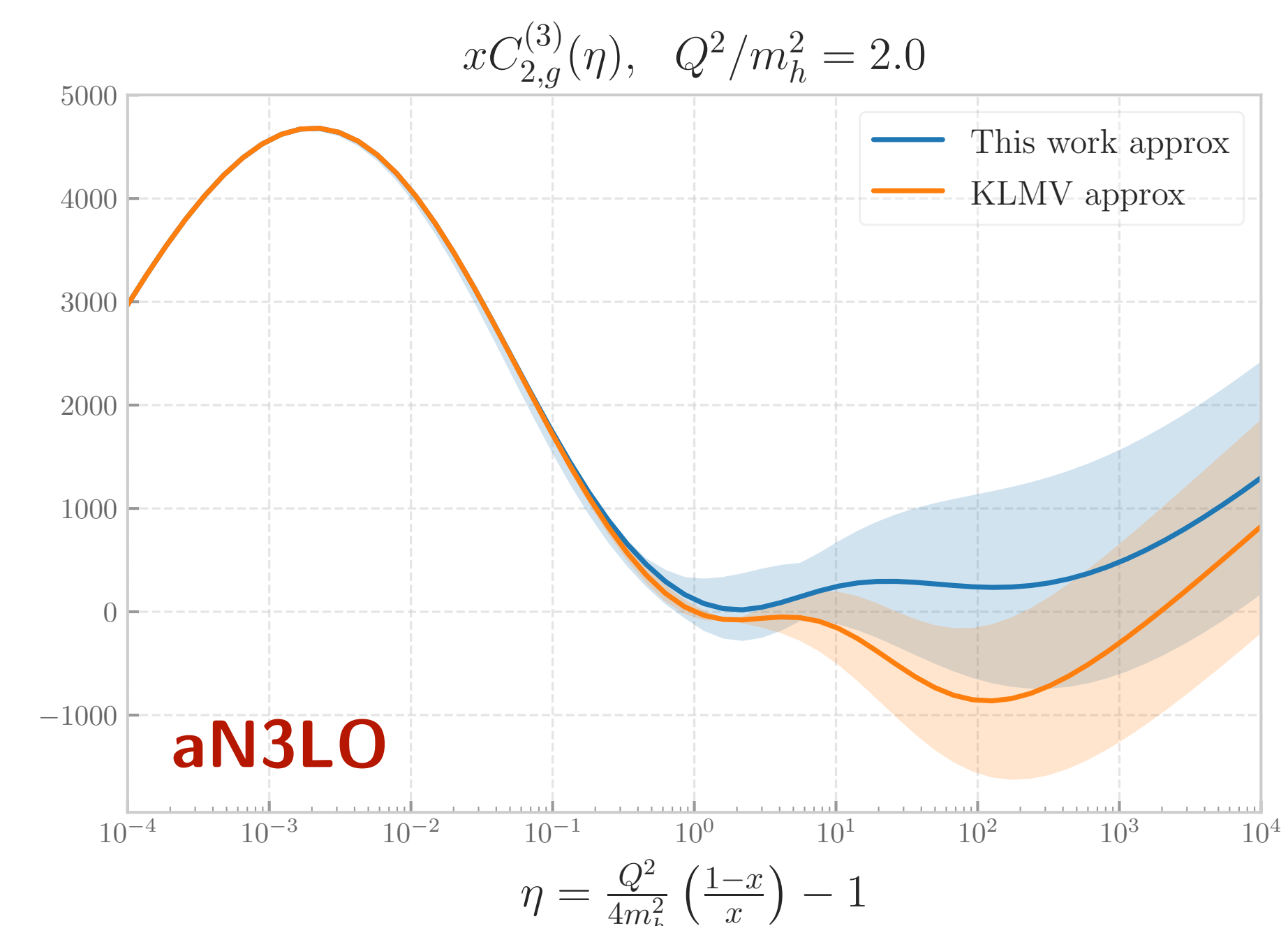
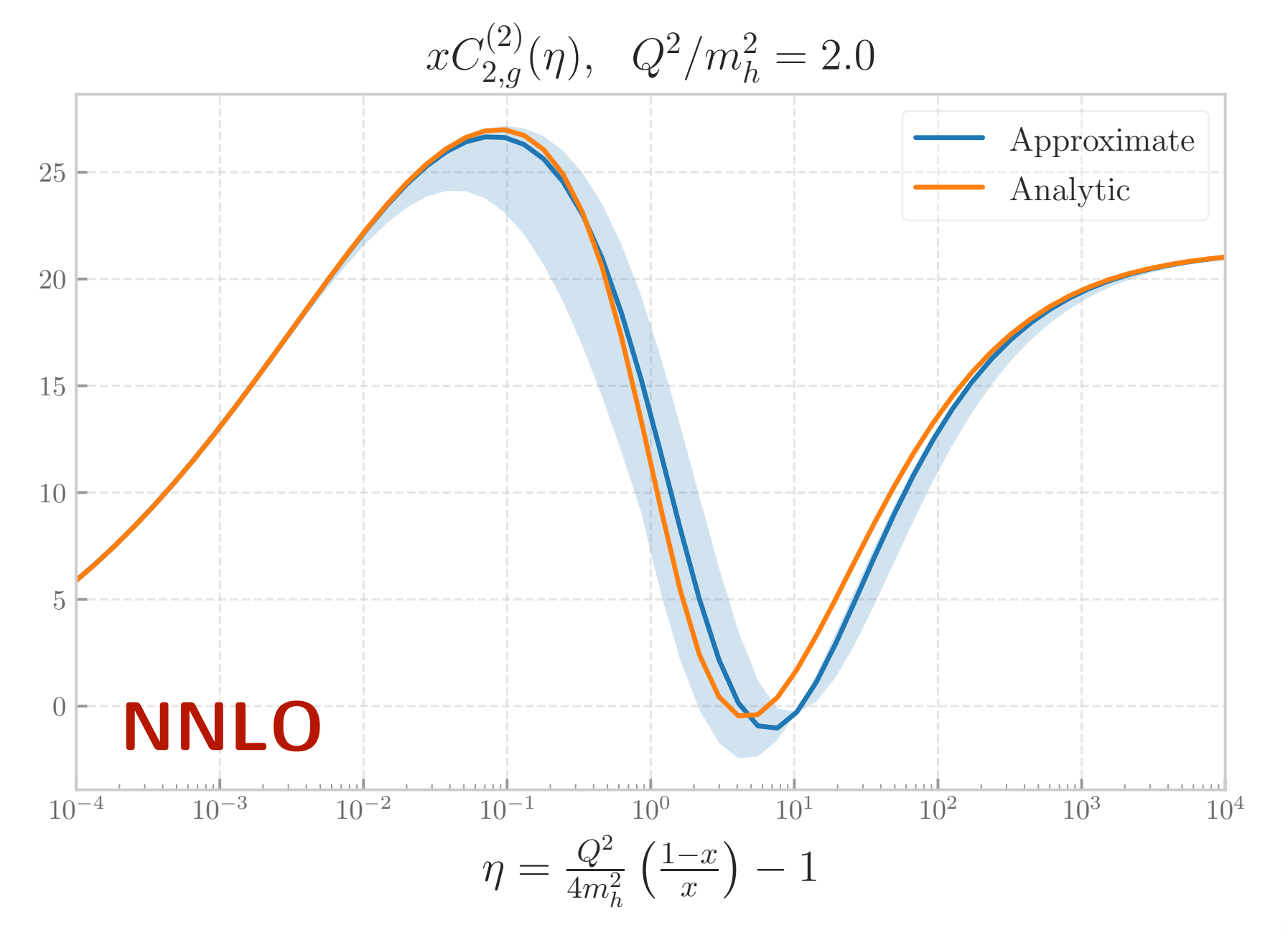
DIS structure functions are known at N3LO in the **massless limit (ZM-VFNS)** for F_2, F_L, F_3 :

- ▶ DIS NC: Larin, Nogueira, Van Ritbergen, Vermaseren [[arxiv:9605317](https://arxiv.org/abs/9605317)]
Moch, Vermaseren, Vogt [[arxiv:0411112](https://arxiv.org/abs/0411112)], [[arxiv:0504242](https://arxiv.org/abs/0504242)]
- ▶ DIS CC: Davies, Moch, Vermaseren, Vogt [[arxiv:0812.4168](https://arxiv.org/abs/0812.4168)]
[[arxiv:1606.08907](https://arxiv.org/abs/1606.08907)]

DIS **Heavy structure functions** can be parametrised joining the known limits ($Q \rightarrow m_h^2$ $Q \gg m_h^2$ and $x \rightarrow 0$) with proper damping functions f_1, f_2 .

$$C_{g,h}^3 = C_{g,h}^{(3,0)} + C_{g,h}^{(3,1)} \ln\left(\frac{\mu}{m_h}\right) + C_{g,h}^{(3,2)} \ln^2\left(\frac{\mu}{m_h}\right)$$

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



DIS VFNS at aN3LO

During a PDF fit different flavour schemes need to be joined together using a proper **Variable Flavor Number Scheme**

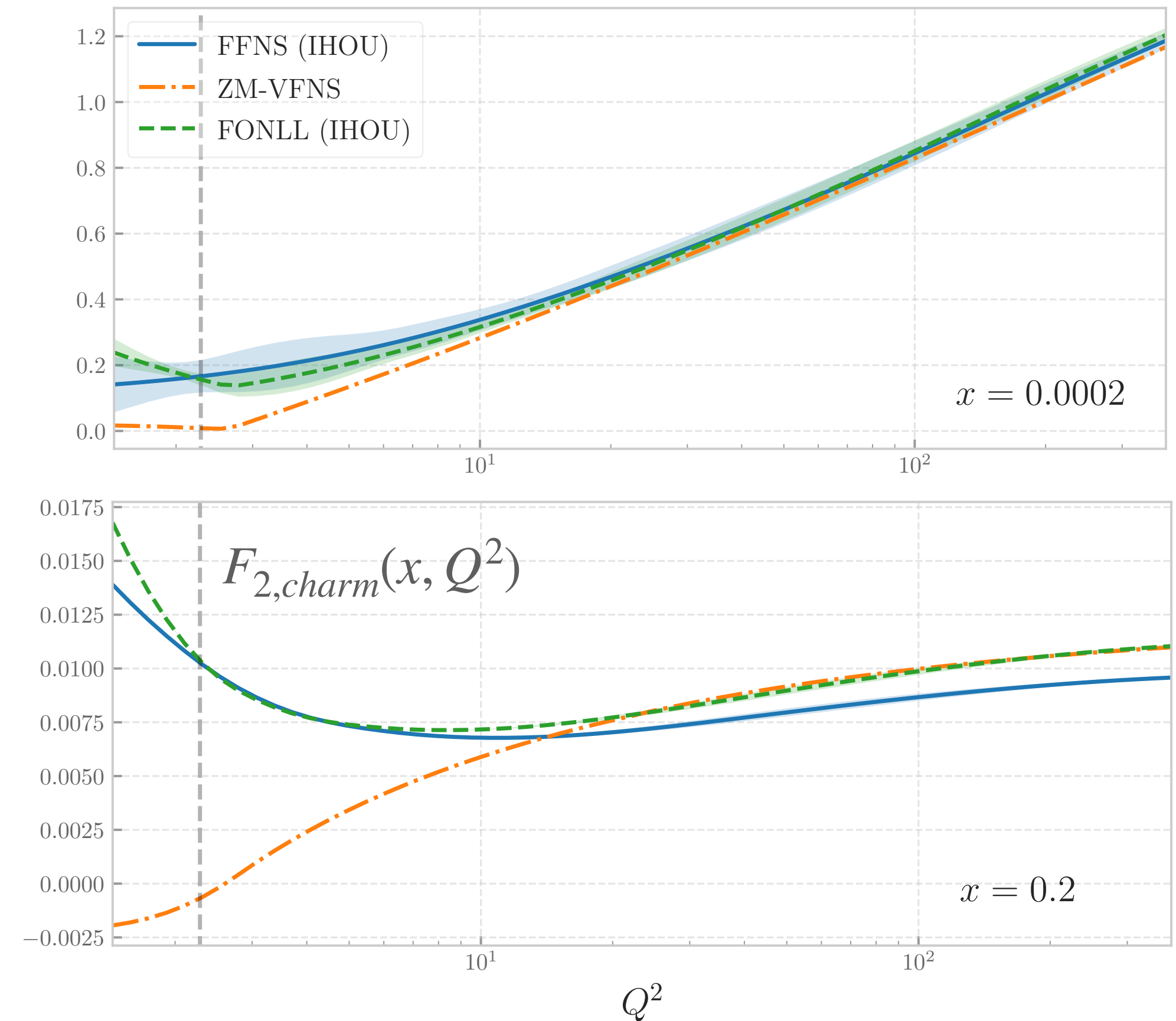
PDFs matching conditions are now available at

N3LO almost completely, with the exception of $a_{H,g}^{(3)}$: Bierenbaum,

Blümlein, Klein [arXiv:0904.3563] Ablinger, Behring, Blümlein, De Freitas, Hasselhuhn, von Manteuffel, Round, Schneider, Wißbrock. [arXiv:1406.4654]; Ablinger, Behring, Blümlein, De Freitas, Goedicke, von Manteuffel, Schneider Schonwald [arXiv:2211.0546].

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

$$F_{h,FONLL} = F_{ZM}^{(n_f+1)} + F_{FFNS}^{(n_f)} - \lim_{m_h \rightarrow 0} F_{FFNS}^{(n_f)}$$



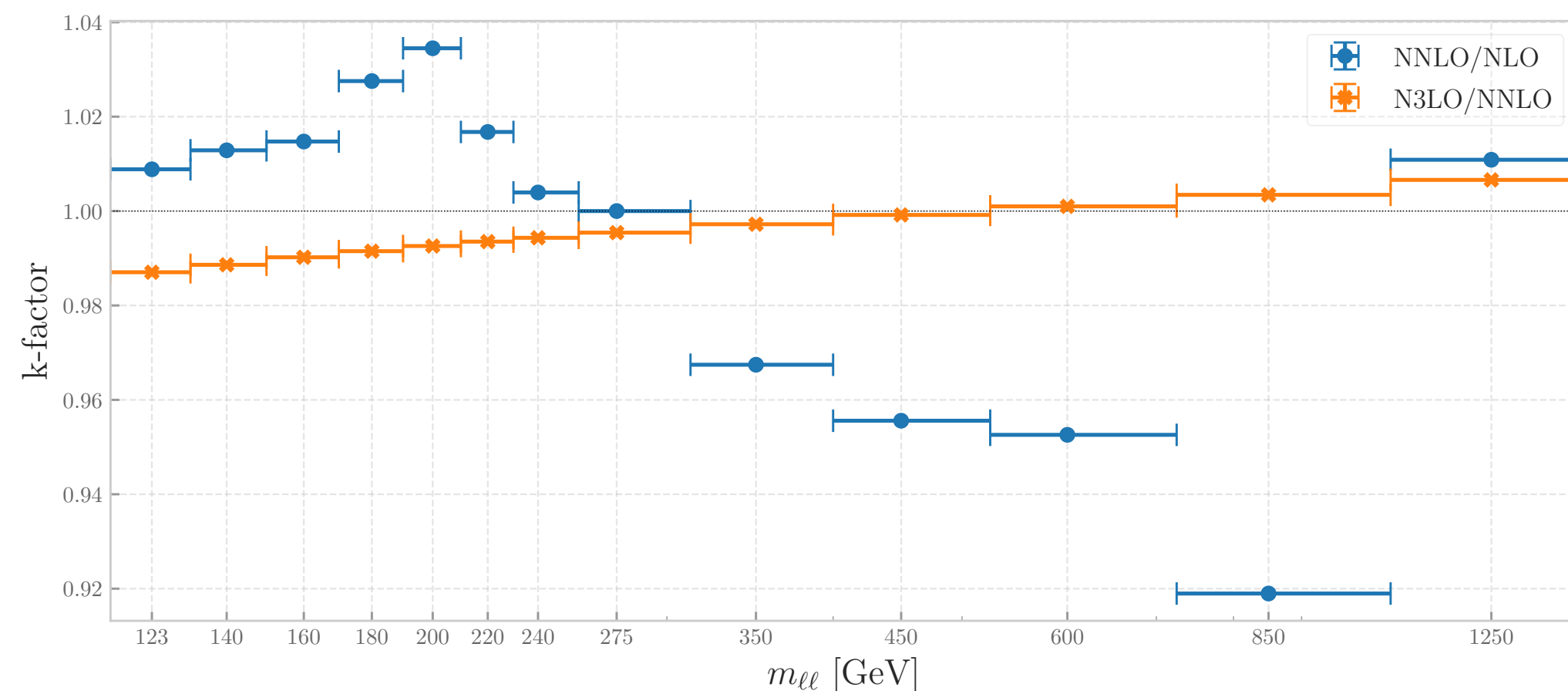
In NNPDF studies DIS structure functions are computed in the **FONLL** procedure [arxiv:1001.2312]:

- ▶ Extended up to N3LO for the Heavy structure functions F_{heavy}
- ▶ Extended up to NNLO for light F_{light} + massless N3LO contributions.

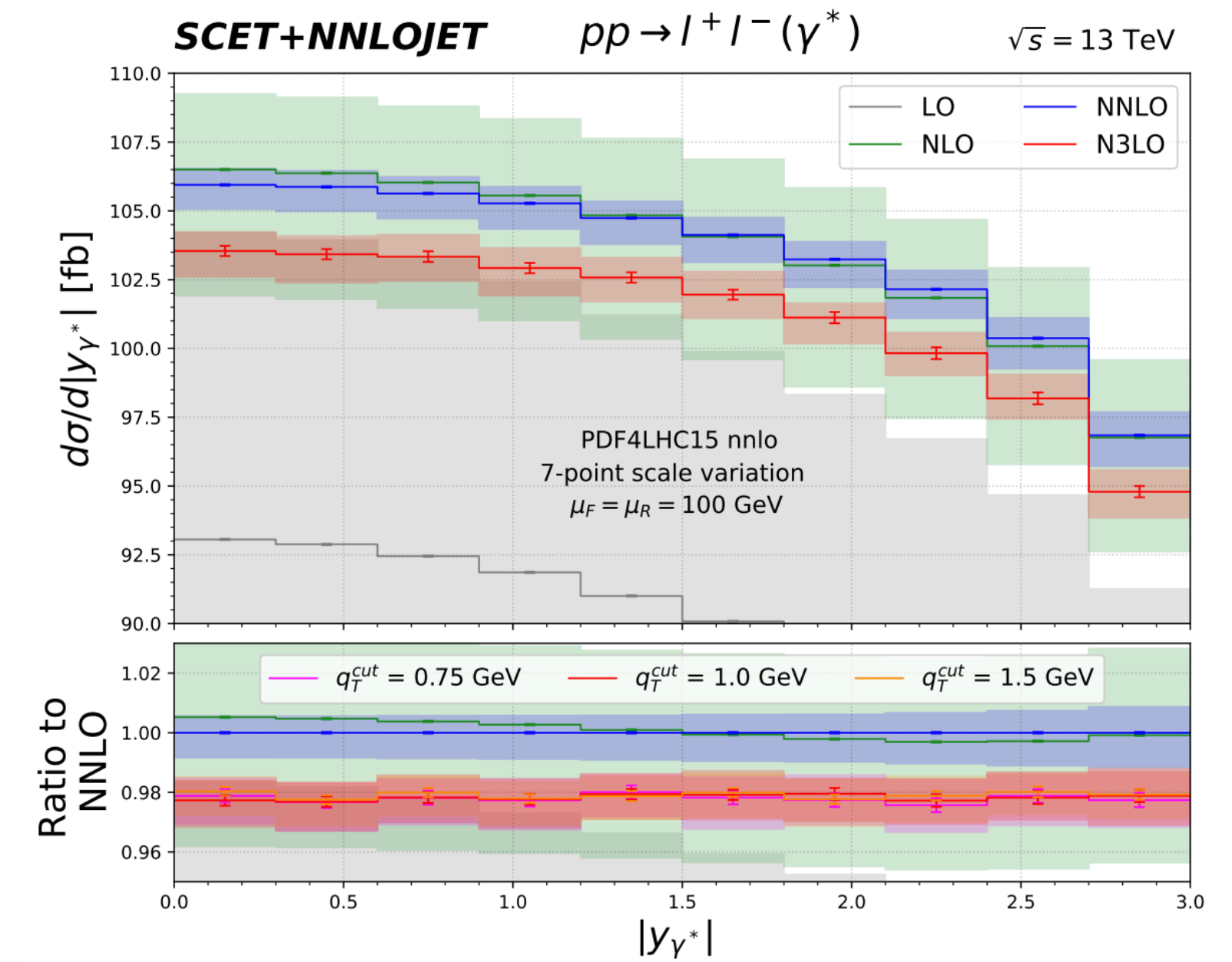
Collider DY @ aN3LO

- ▶ Corrections to **collider DY** and **W** productions (differential in $m_{\ell\ell}$ or y_Z) can be included through k-factors.
- ▶ N3LO effects are around 1-2% of the total cross sections for LHC experiments, and quite flat in the boson rapidity.
- ▶ Differential distributions in p_t are included only up to NNLO.
- ▶ N3LO corrections to other hadronic processes used in PDFs fits ($t, t\bar{t}, Jets, FTDY$) are not known or public available.
- ▶ Whenever N3LO ME are not available we introduce NNLO MHOU.

Atlas high-mass DY 7 TeV



Chen, Gehrmann, Glover, Huss, Yang, Zhu [[arxiv:2107.09085](https://arxiv.org/abs/2107.09085)]



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- The background of the slide is a repeating pattern of various Feynman diagrams. These diagrams are rendered in several colors: black, blue, orange, and light green. They represent different types of particle interactions, including tree-level and loop-level processes, with various line styles (solid, wavy, dashed) and arrow directions indicating the flow of particles and momentum.
- ▶ Theory inputs for aN3LO PDFs.
 - ▶ **Towards NNPDF4.0 aN3LO.**
 - ▶ Impact on future observables.

PDF MHOU from scale variations

For a given observable, MHOU are estimated by varying the unphysical scales. MSTH [[arxiv:1811.08434](https://arxiv.org/abs/1811.08434)], NNPDF [[arxiv:1906.10698](https://arxiv.org/abs/1906.10698)], [[arxiv:2105.05114](https://arxiv.org/abs/2105.05114)]

- ▶ Not a unique procedure. Scale variations are not the unique procedure.
- ▶ **Factorization scale variations** are introduced during the DGLAP evolution.
- ▶ **Renormalization scale variations** are retained inside the coefficient functions and varied differently for different kind of processes.
- ▶ The way in which μ_f, μ_r are varied simultaneously define a so called point prescription.

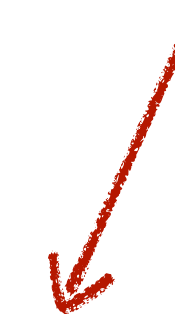
Scale variation advantages:

- ▶ Justified by RGE invariance.
- ▶ Valid for every process.

Observable



DGLAP Evolution



$$O_{i,n}(Q, \mu_f, \mu_r) = E_{ij,n}(Q, \alpha_s, \mu_f) \otimes C_{j,n}(Q/\mu_r, \alpha_s)$$

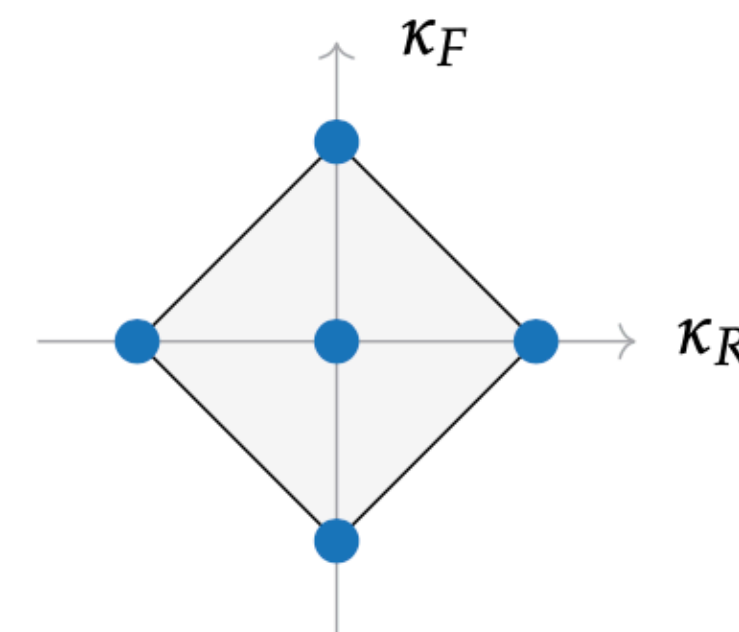
$$n = \{1 \dots N_{dat}\}$$



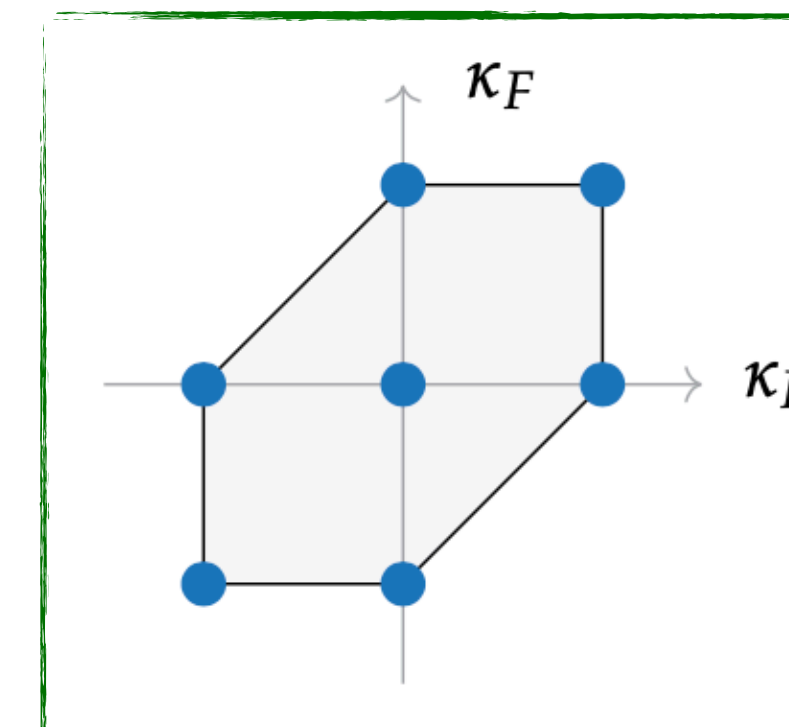
Partonic coefficients

- ◆ We use NNLO MHOU to estimate unknown N3LO effects.
- ◆ In addition we can add N3LO MHOU to account for further higher order corrections.

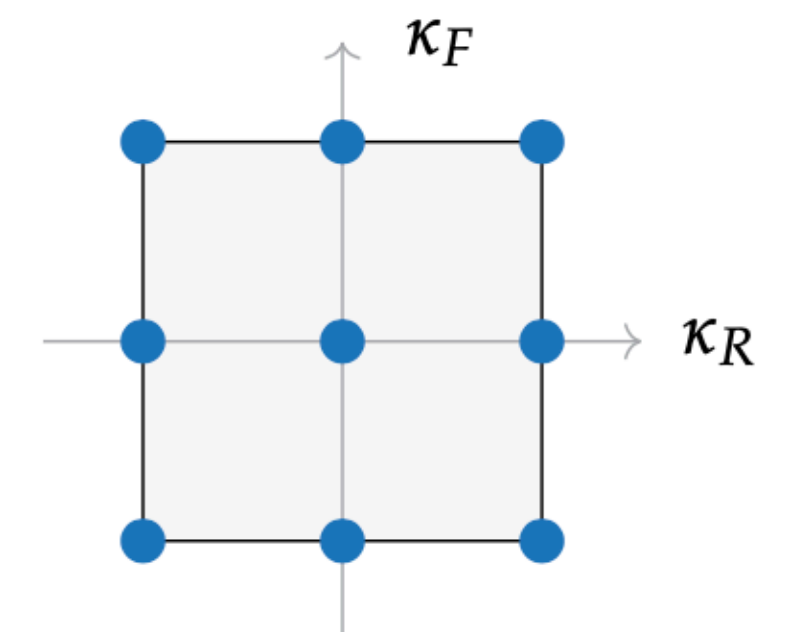
5 points



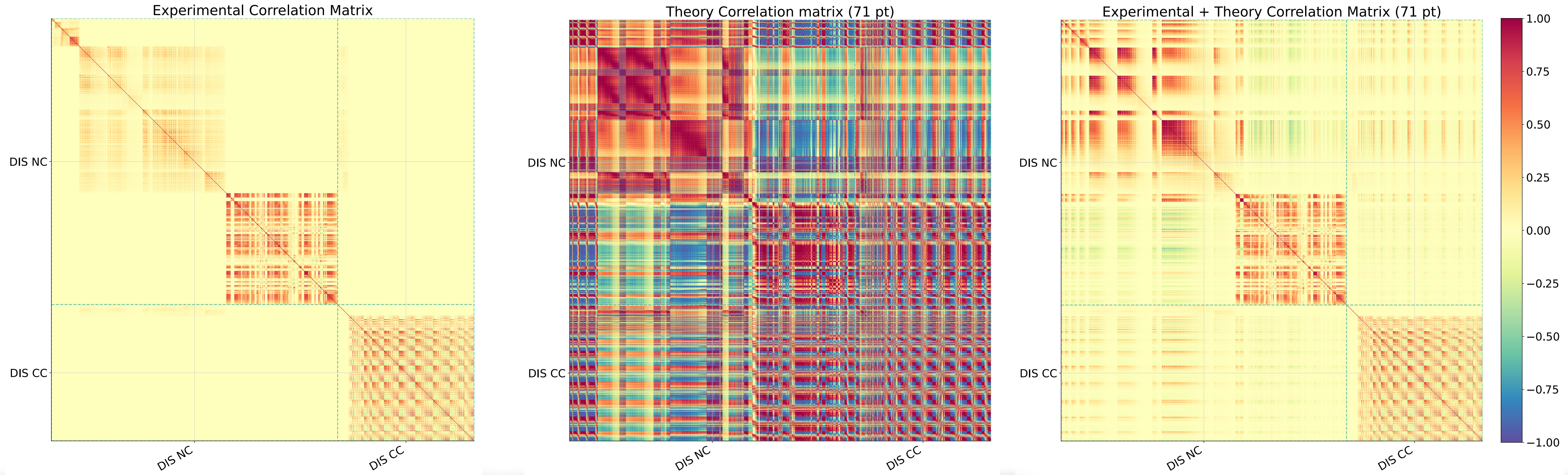
7 points



9 points



IHOU from aN3LO variations



- ▶ IHOU are propagated to the PDF fit by constructing a **covariance matrix** by varying a single splitting function (during the DGLAP evolution) or DIS coefficient at the time:

$$Cov_{ij,IHOU} = \sum_{l=1}^{N_{par}} \frac{1}{N_{var,l} - 1} \sum_{k=1}^{N_{var,l}} (T_{i,k} - \bar{T}_i)(T_{j,k} - \bar{T}_j) \quad i, j = 1, \dots, n_{data}$$

- ▶ **IHOU** are **independent** from **MHOU**, so they can be added in quadrature:

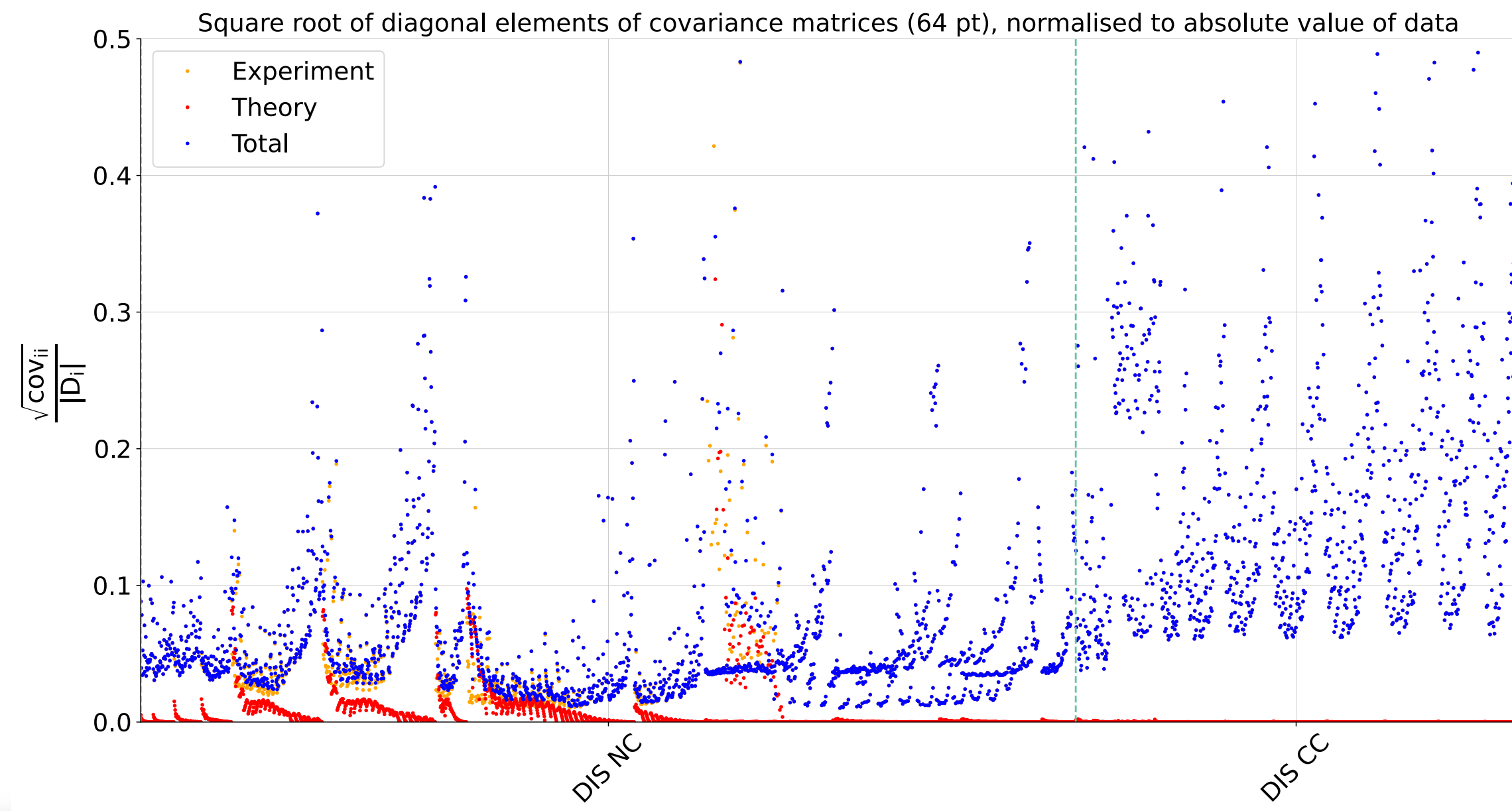
$$Cov_{ij} = Cov_{ij,EXP} + Cov_{ij,MHOU} + Cov_{ij,IHOU}$$

- ▶ Theory uncertainties correlate different processes and experiments.

See also E.R. Nocera talk

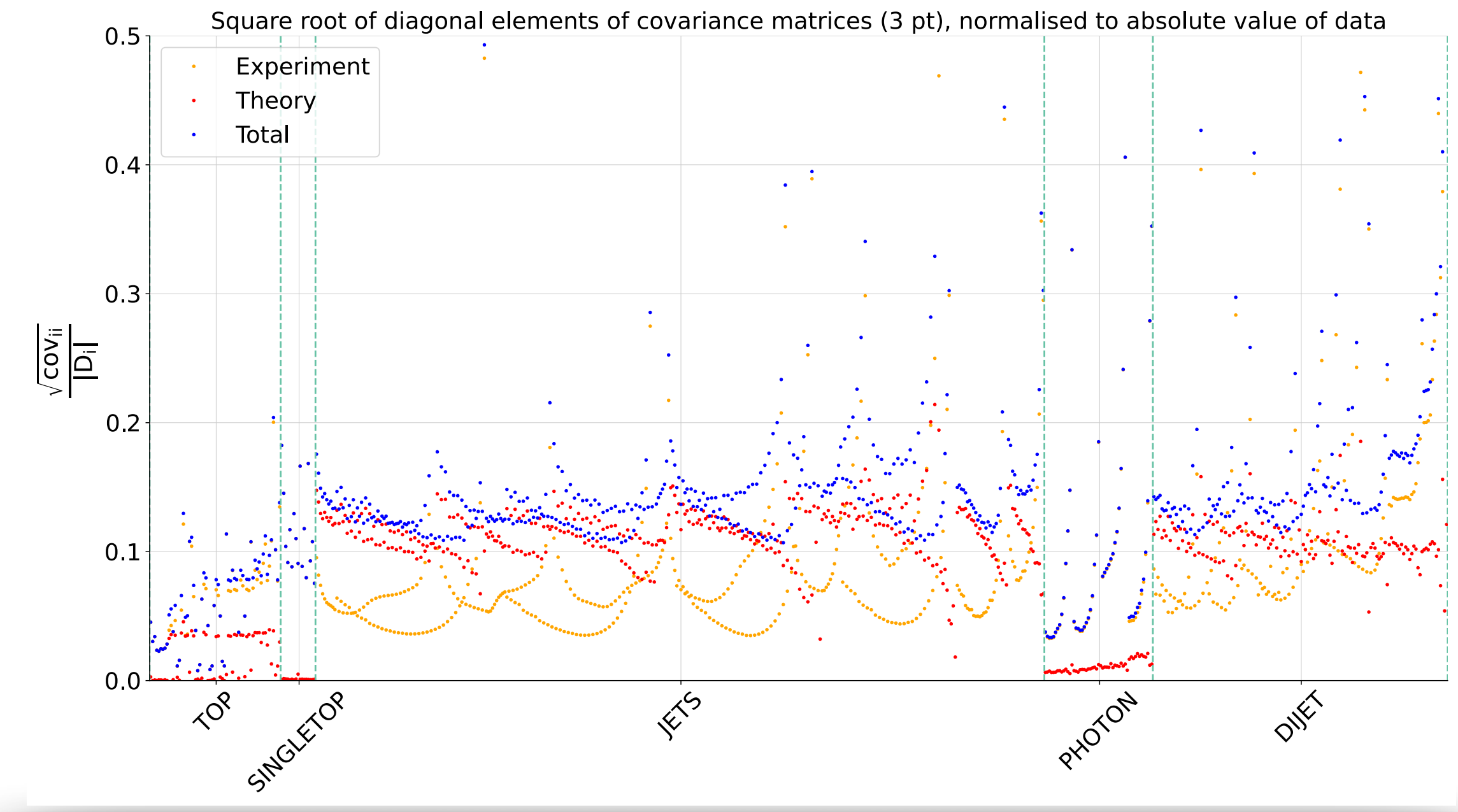
Impact of theory uncertainties

IHOU in DIS datasets



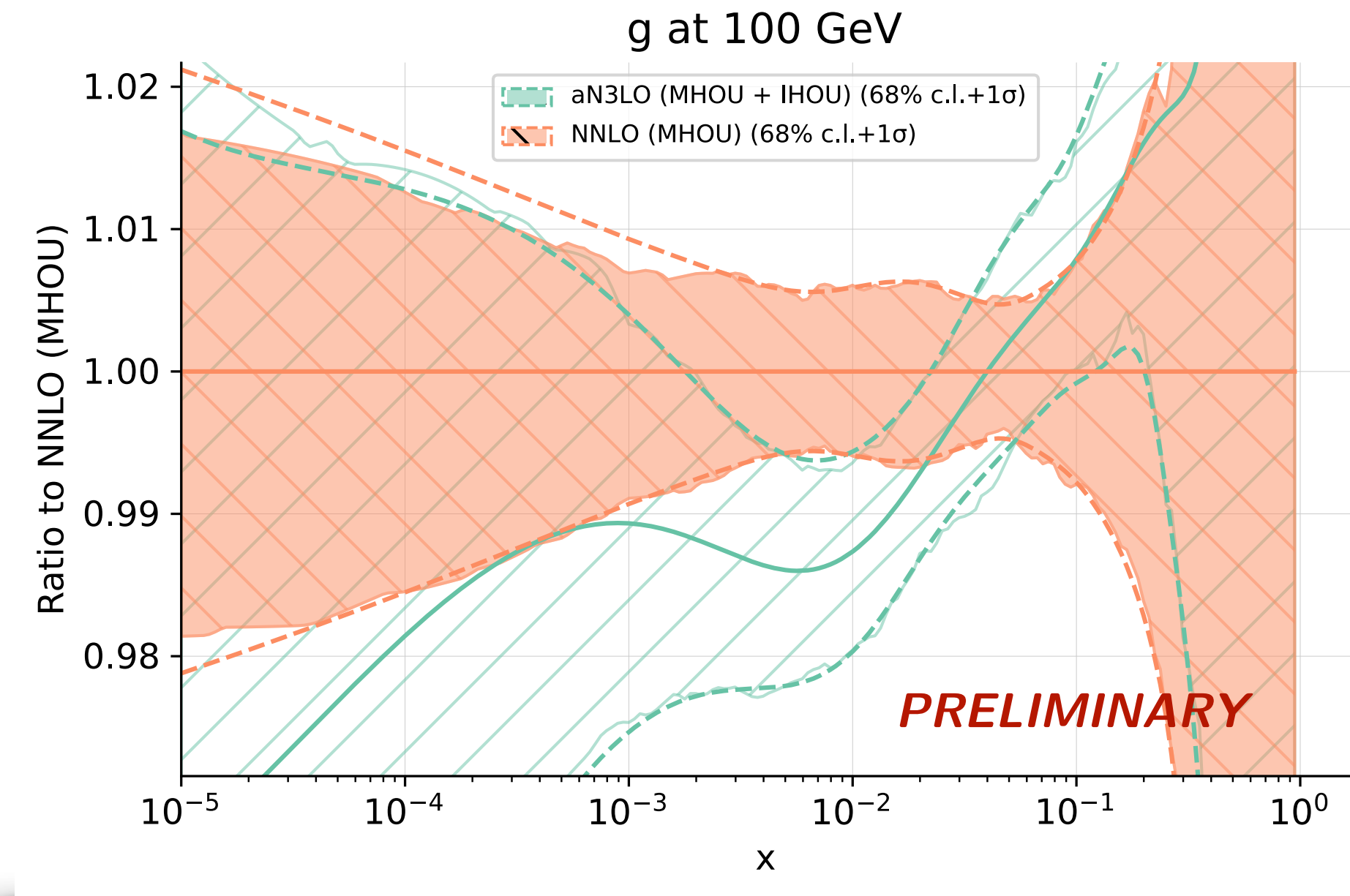
- ▶ **IHOU** have a larger effect on the **small-x, low-Q** DIS data.
- ▶ Approximations of DIS massive coefficient functions are included.

NNLO MHOU in LHC datasets



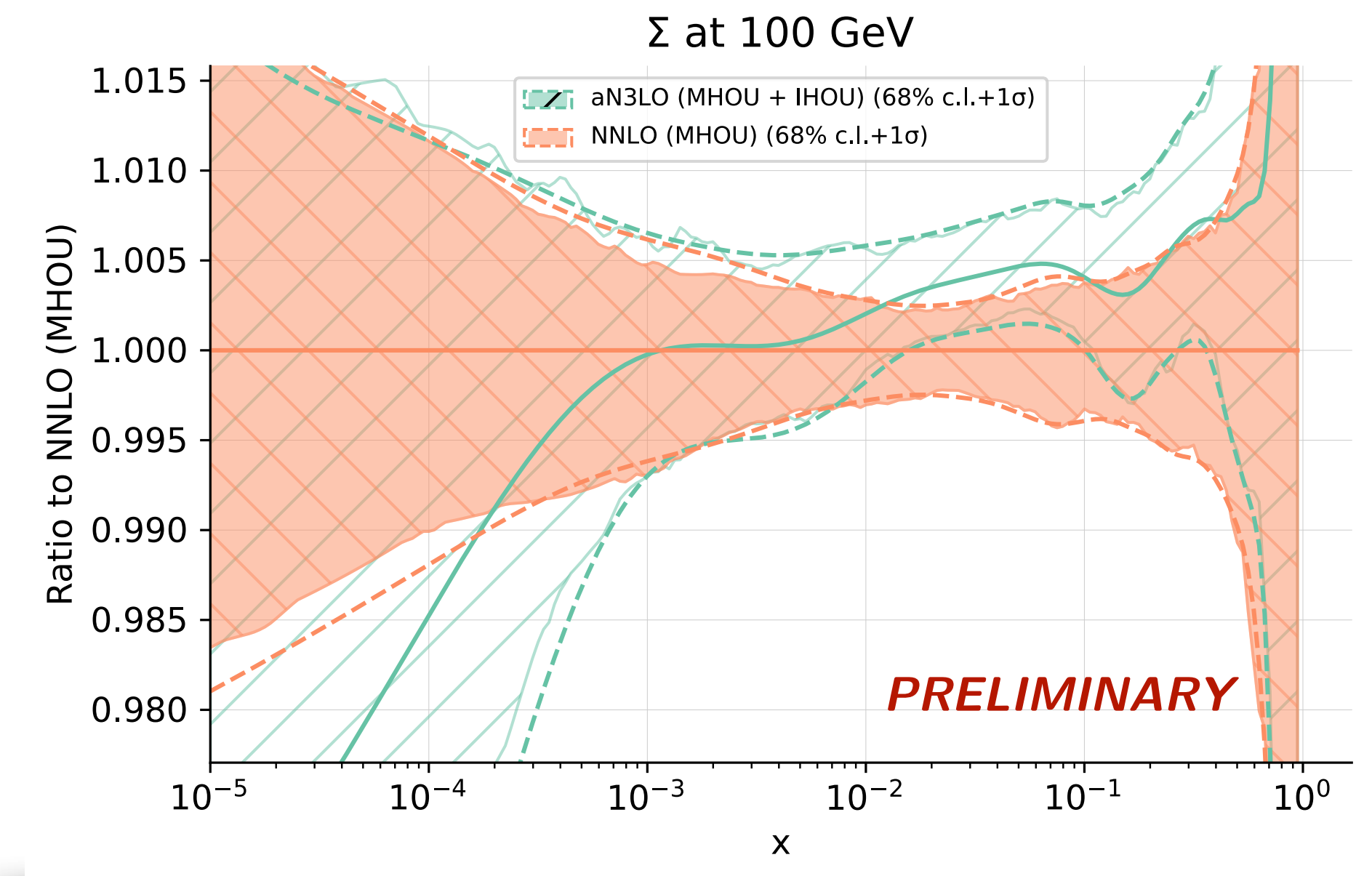
- ▶ **NNLO MHOU** from **renormalization scale variations** are included where N3LO ME are not available. Main effect is to deweight jets datasets.

NNPDF4.0 aN3LO



- ▶ Shift in N3LO - NNLO predictions is **within 1%** in most of the kinematic coverage.
- ▶ Exceptions are visible in **small- x DIS** data some collider **DY** data.

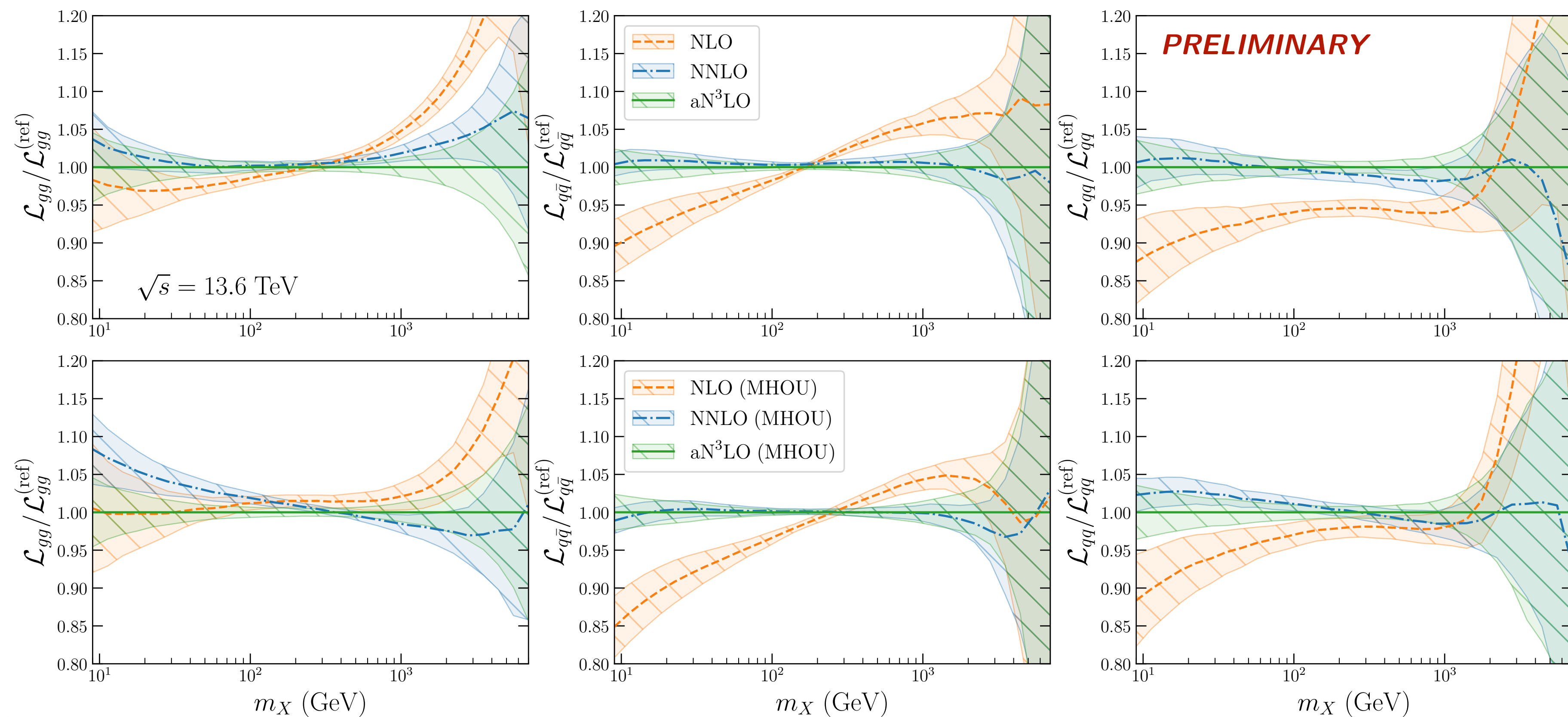
- ▶ Preliminary **aN3LO** fits show an effect of N3LO corrections specially for gluon g and Singlet Σ .
- ▶ At **large- x** PDFs are compatible within one sigma with NNLO determinations.



NNPDF4.0 aN3LO

- MHOUs have a non trivial effect and can induce **shifts** both in the **central value** and in **uncertainty** size.
- MHOUs improve perturbative convergence, specially at NLO
- aN3LO MHOUs are generally smaller.

LHC RunIII partonic luminosities

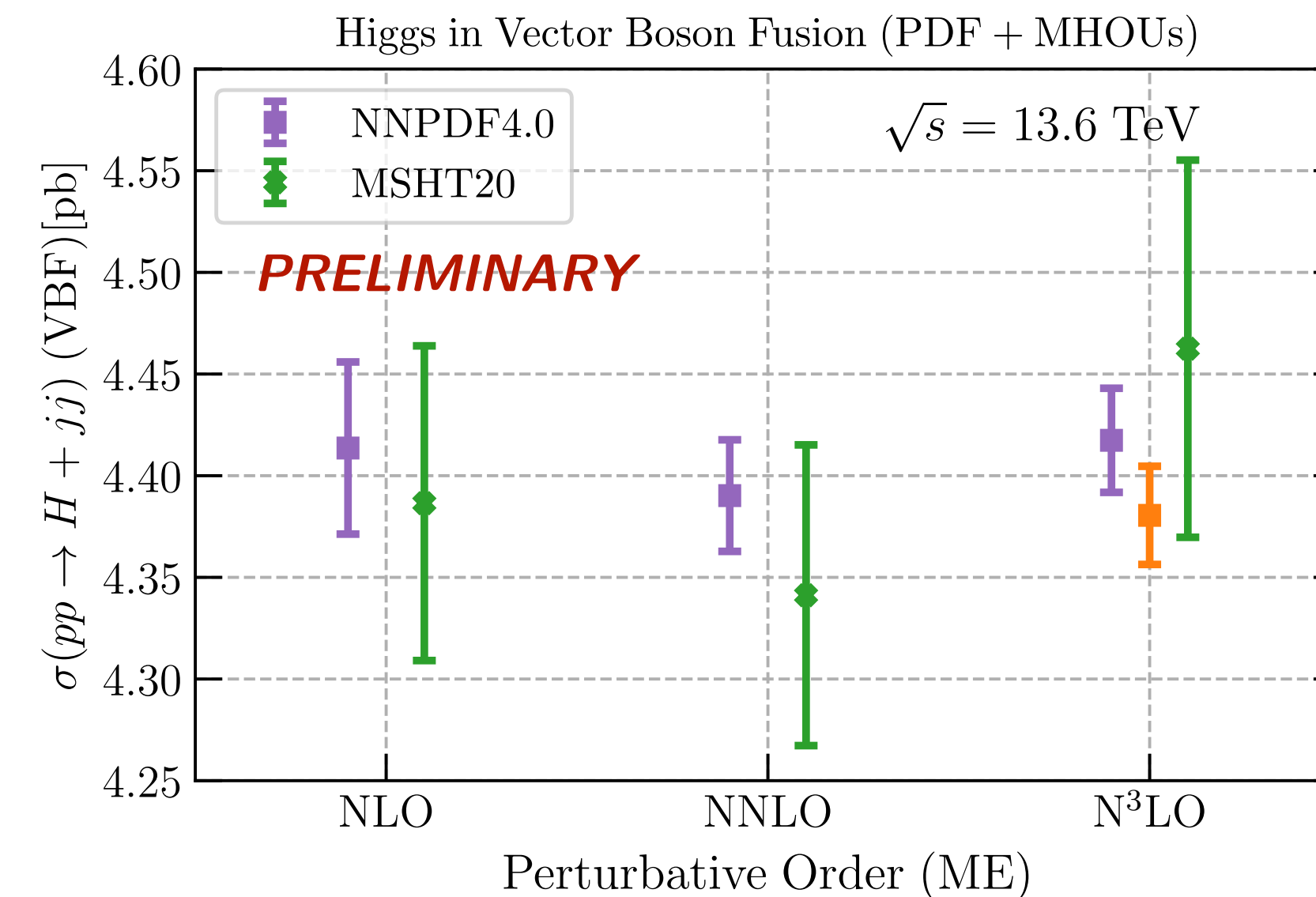
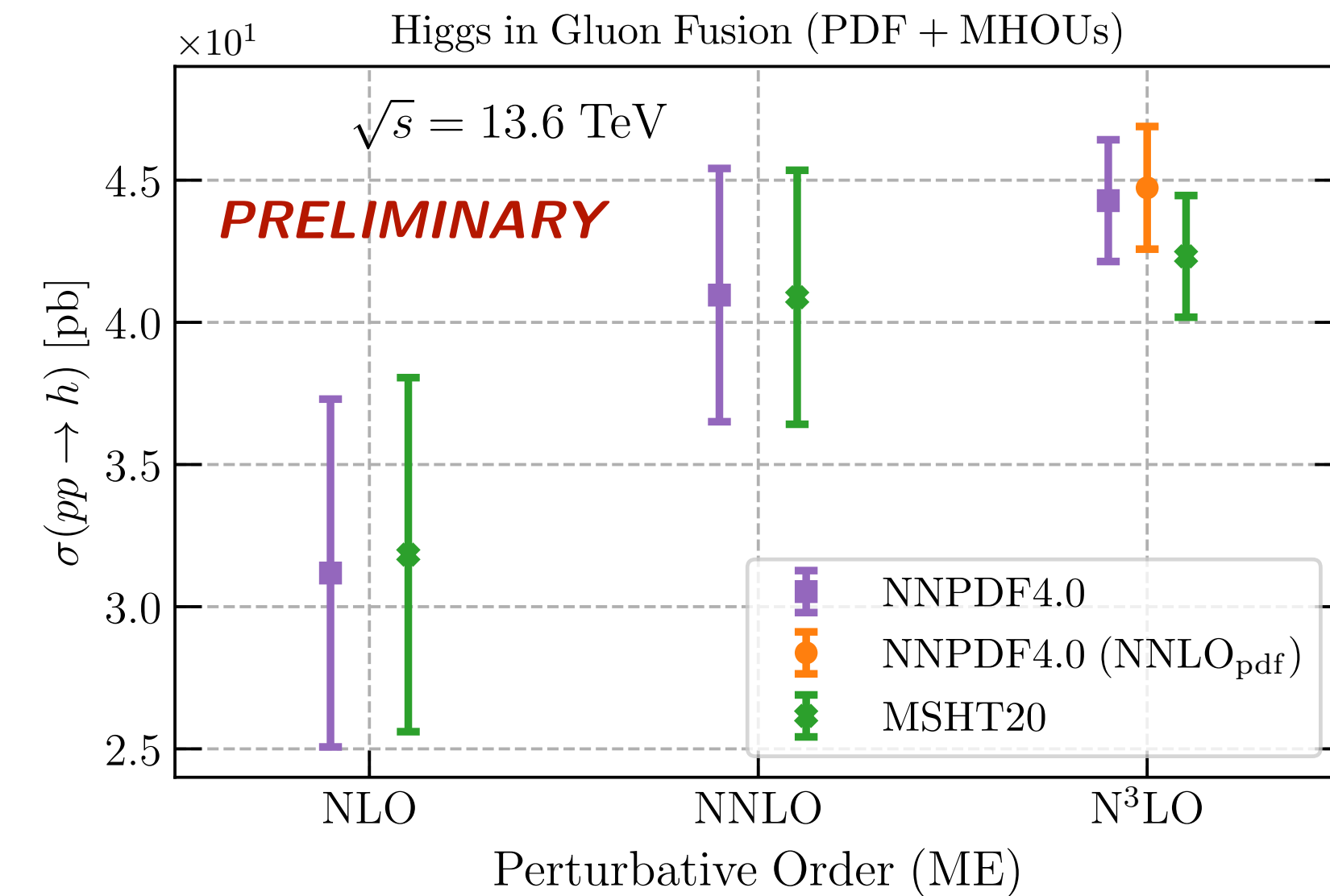


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- The background of the slide is a repeating pattern of Feynman diagrams. These diagrams are drawn with various colored lines (black, blue, orange, green) and arrows, representing different particle interactions and topologies. The diagrams are arranged in a grid-like fashion, creating a complex, textured background.
- ▶ Theory inputs for aN3LO PDFs.
 - ▶ Towards NNPDF4.0 aN3LO.
 - ▶ **Impact on future observables.**

Higgs Production at LHC

- ME for both **VBF** and **gluon fusion Higgs** production are available at N3LO: $gg \rightarrow H$ [[arxiv:1503.06056](https://arxiv.org/abs/1503.06056)] $qq \rightarrow H$ (VBF) [[arxiv:1606.00840](https://arxiv.org/abs/1606.00840)]

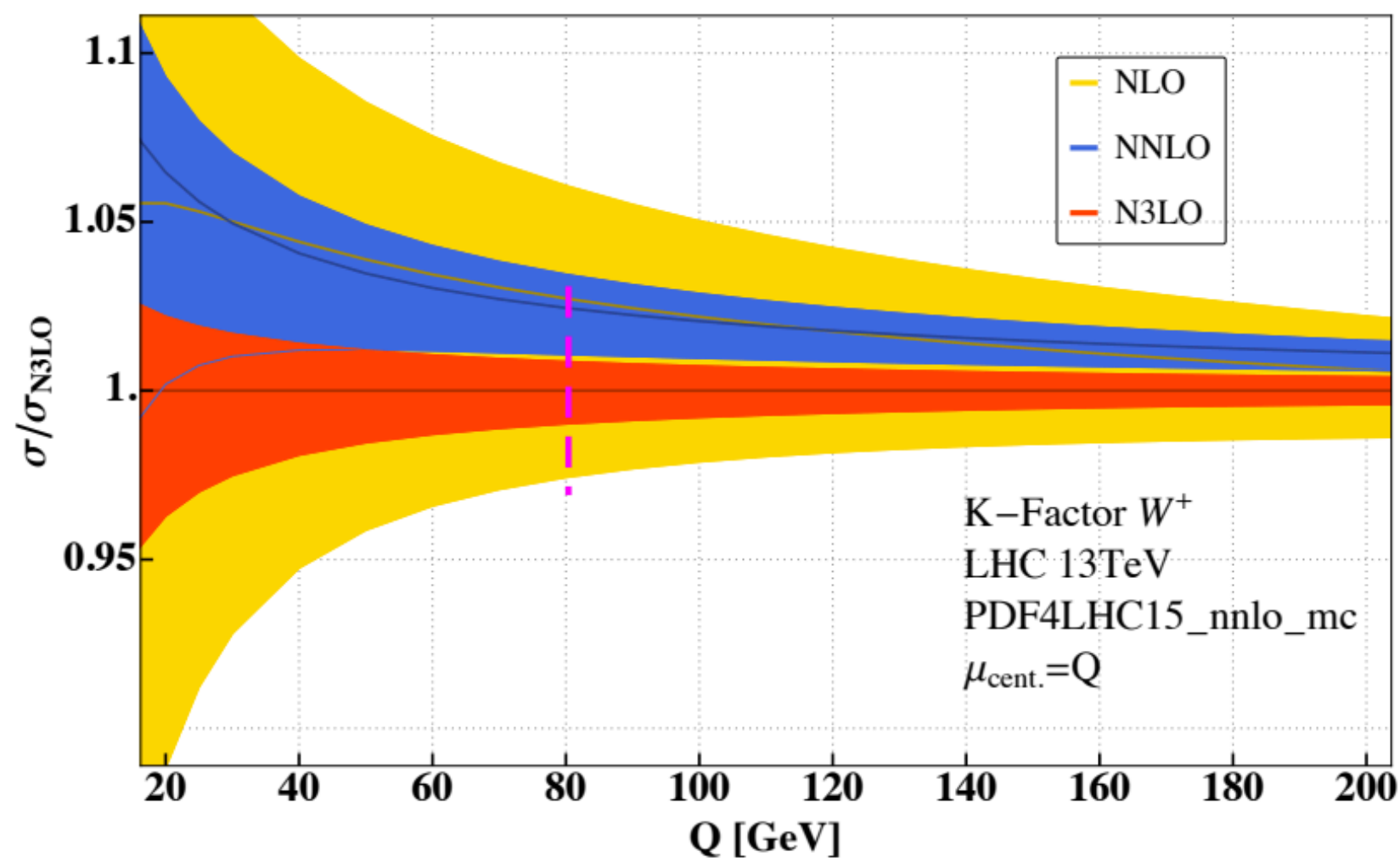
- Larger effects are visible in gluon fusion, leading to a small suppression w.r.t NNLO PDFs.
- Higgs VBF is more stable at different perturbative orders.



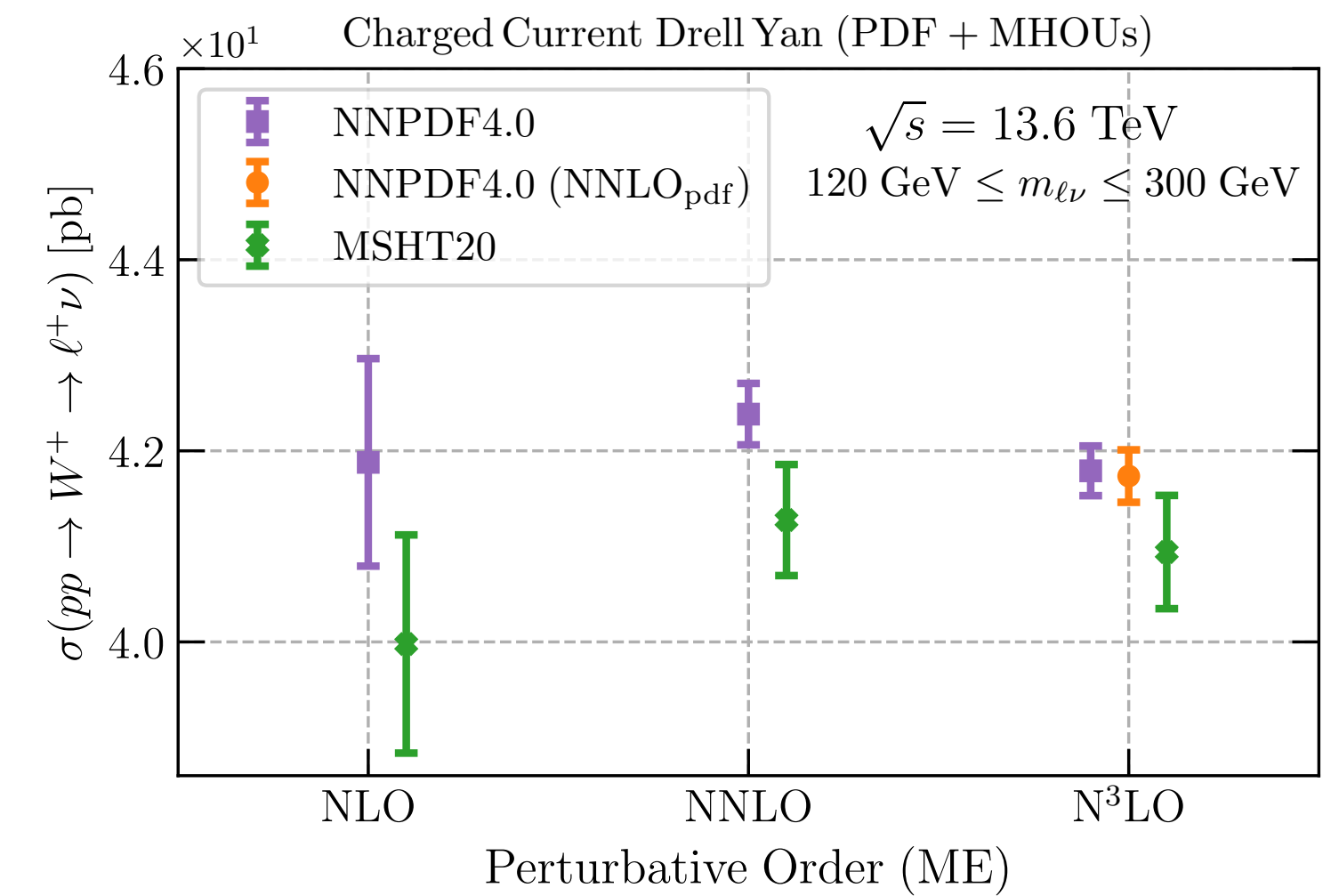
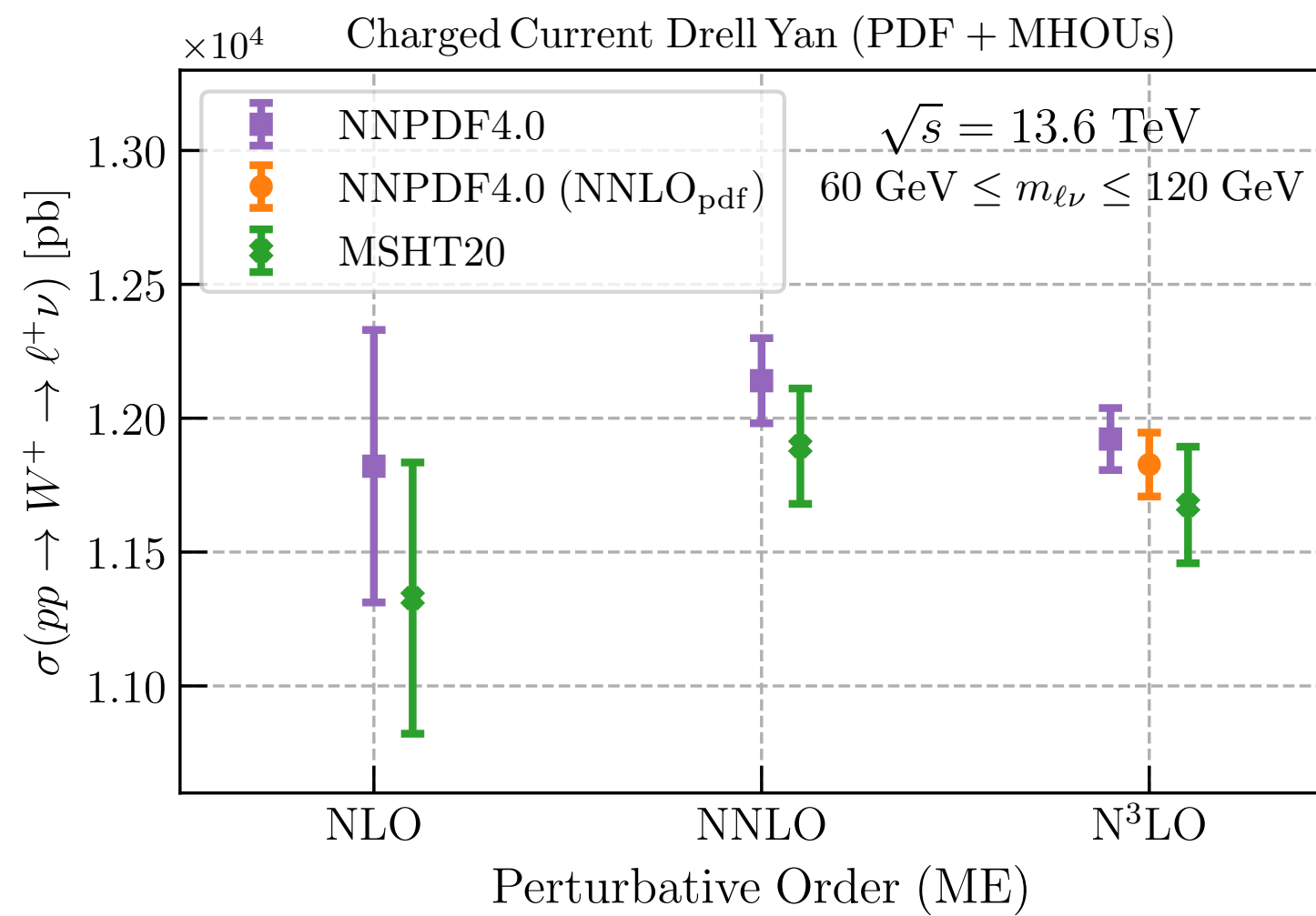
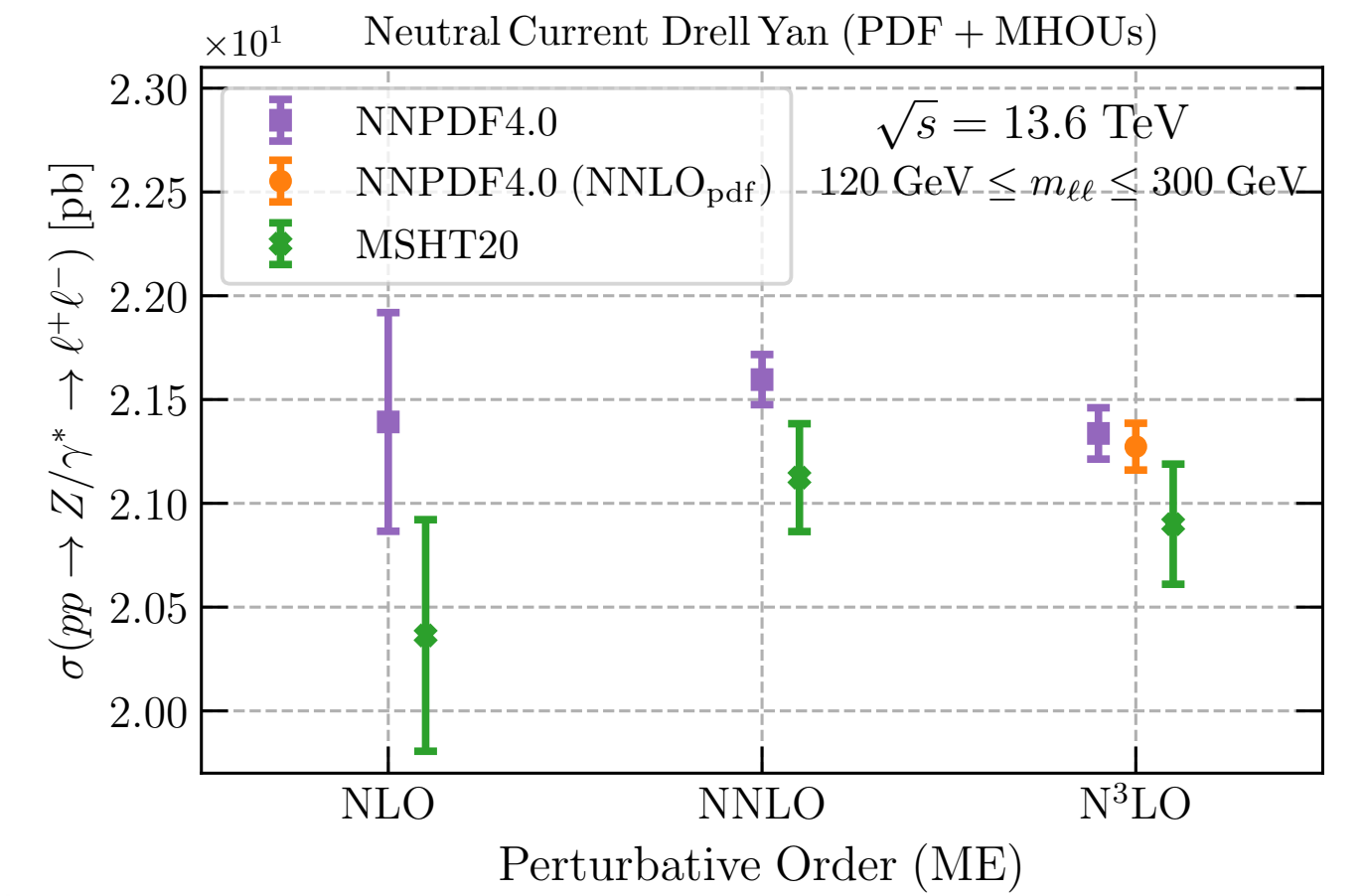
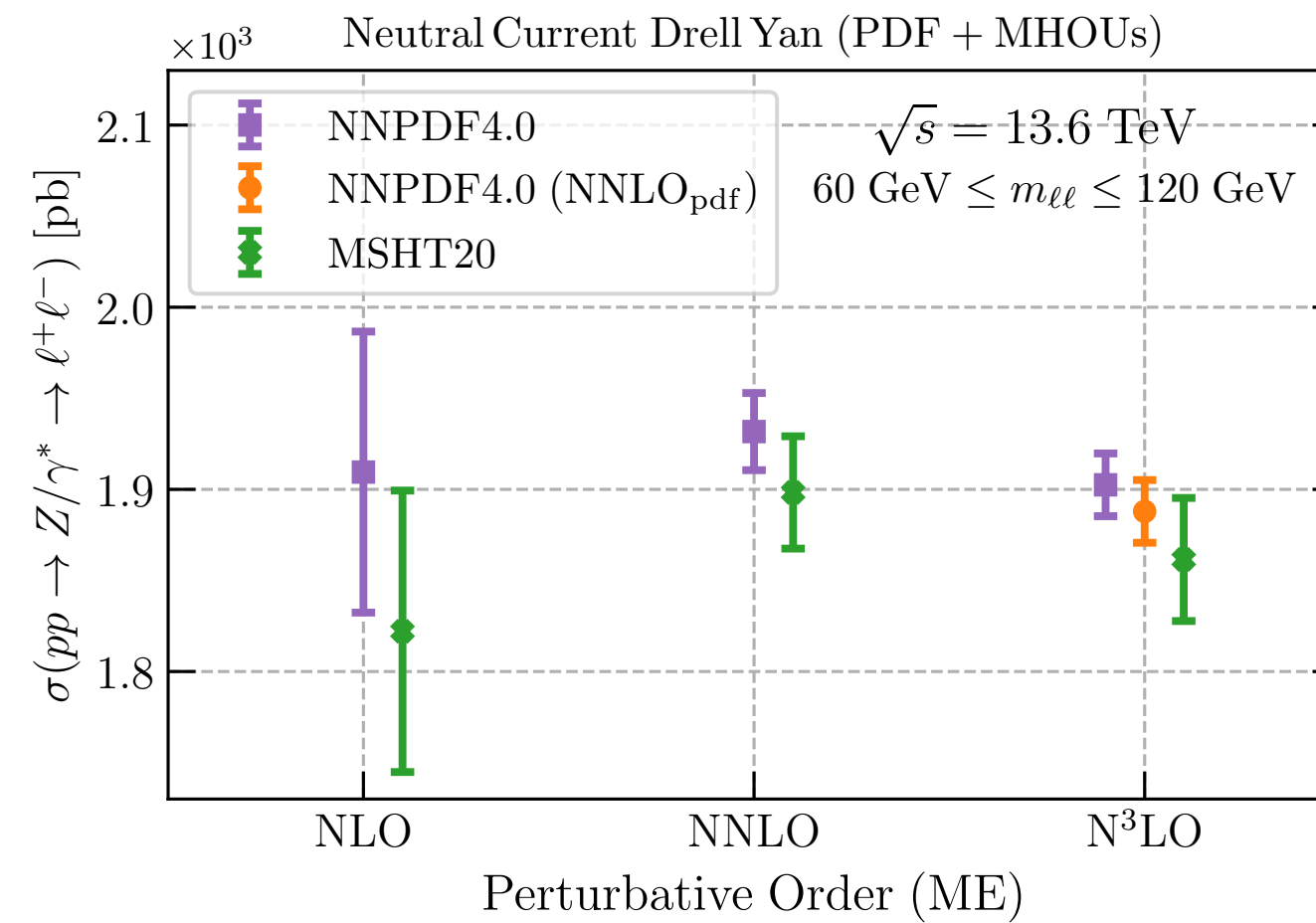
Drell-Yan at LHC

- ▶ Also for collider gauge boson production, usage of aN3LO PDFs seems to **improve the perturbative convergence**.
- ▶ Similar N3LO/NNLO ratio as in MSHT20 aN3LO.

Duhr, Dulat, Mistleberger [[arxiv:2007.13313](https://arxiv.org/abs/2007.13313)]



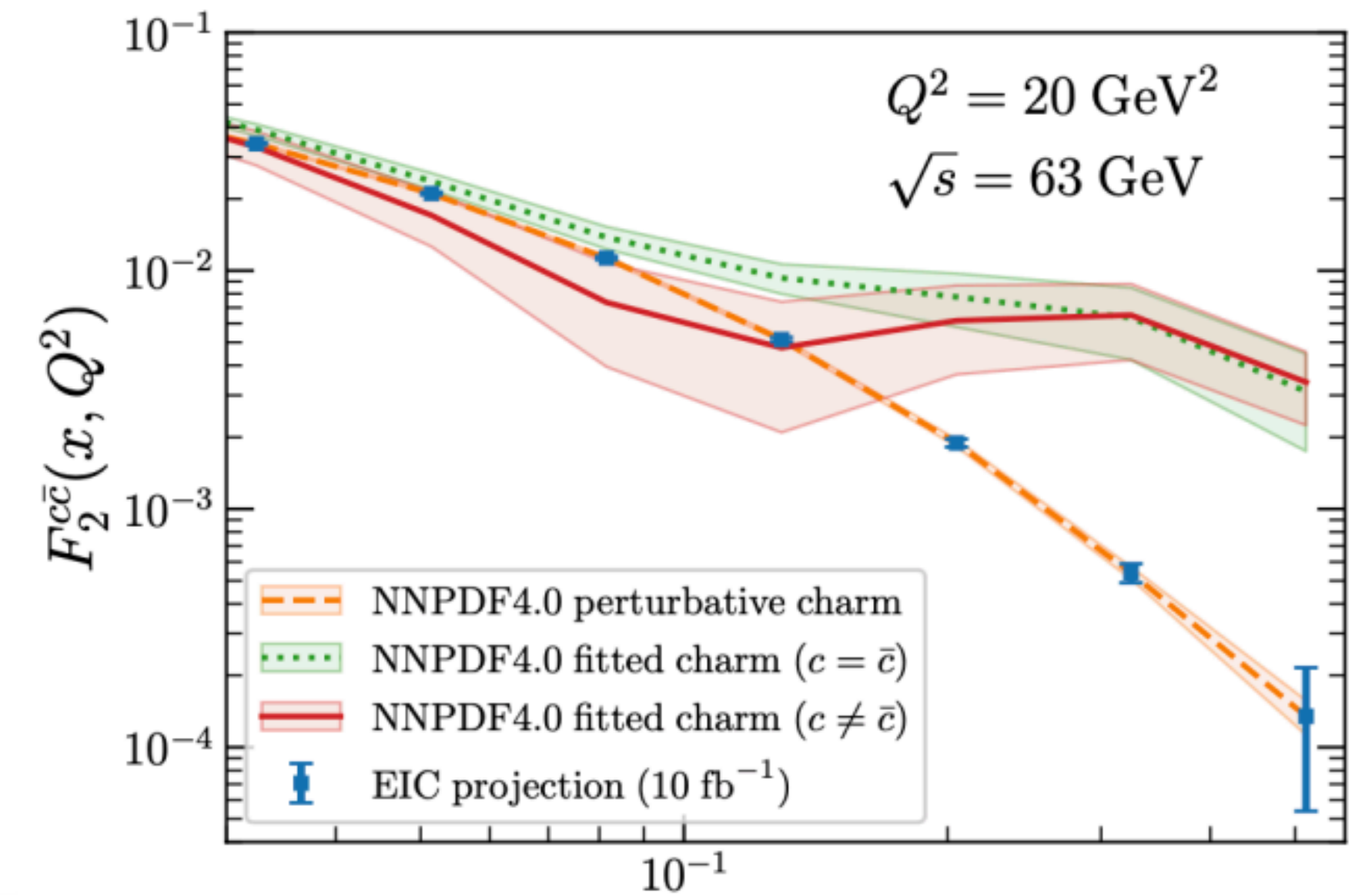
PRELIMINARY



DIS structure functions at EIC

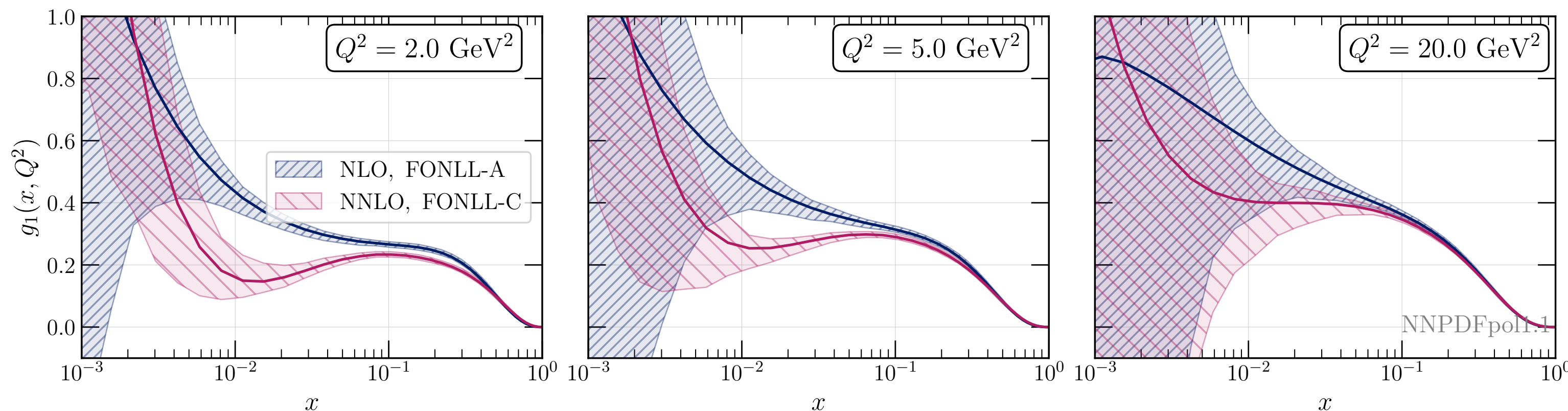
- ▶ At **EIC** we will be able to measure **many DIS observables**, with high precision, specially for **heavy quarks**.
- ▶ EIC will cover **large- x** kinematic regions, with higher accuracy than what we know so far.
- ▶ N3LO QCD corrections are just **one of the many required ingredients**.

Projection of $F_{2,charm}(x)$ at the EIC



See also [\[arxiv:2311.00743\]](https://arxiv.org/abs/2311.00743)

Polarised structure function $g_1(x)$ at the EIC



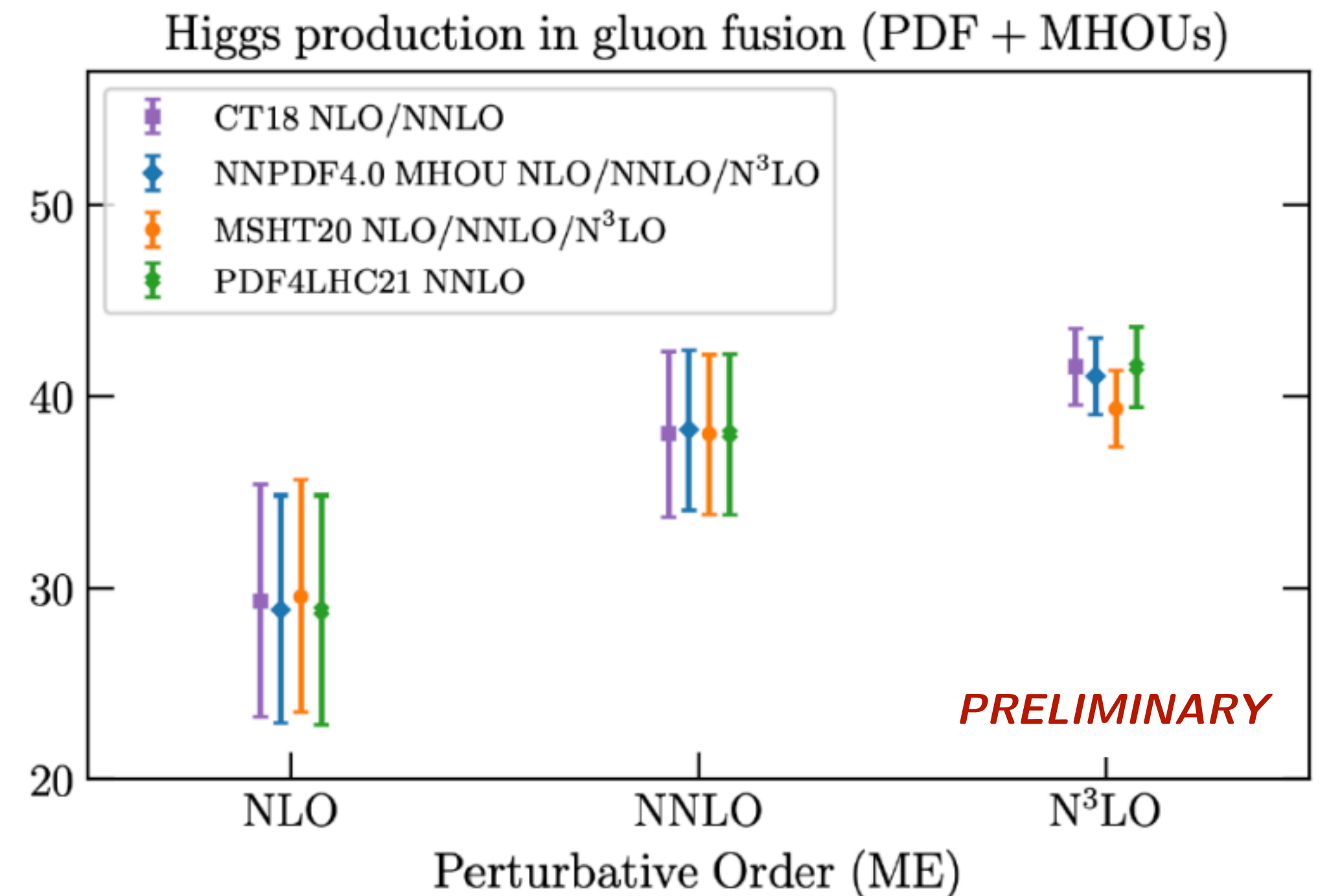
Heavy Quarks in Polarised Deep-Inelastic Scattering
 at the Electron-Ion Collider
 [in preparation]



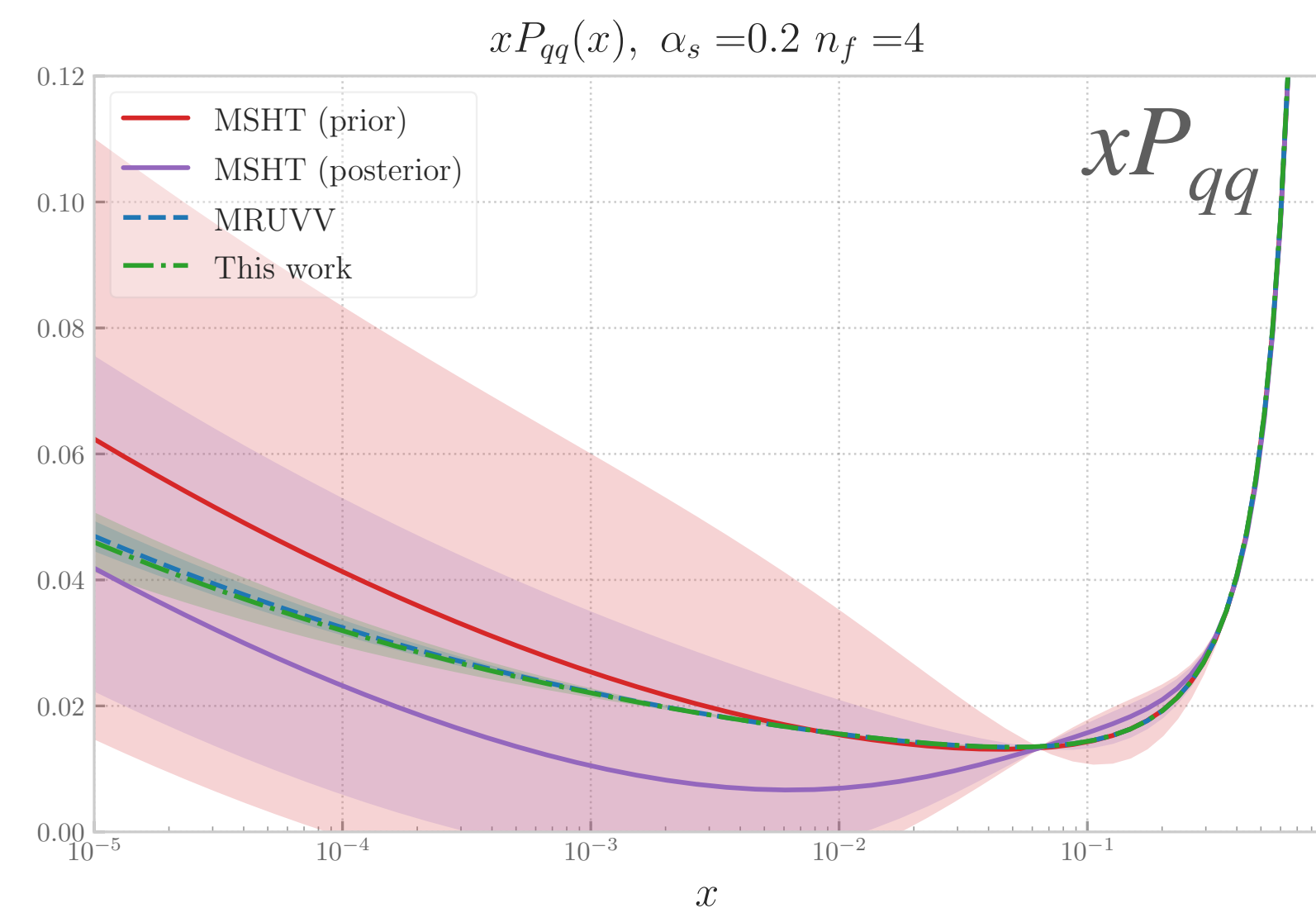
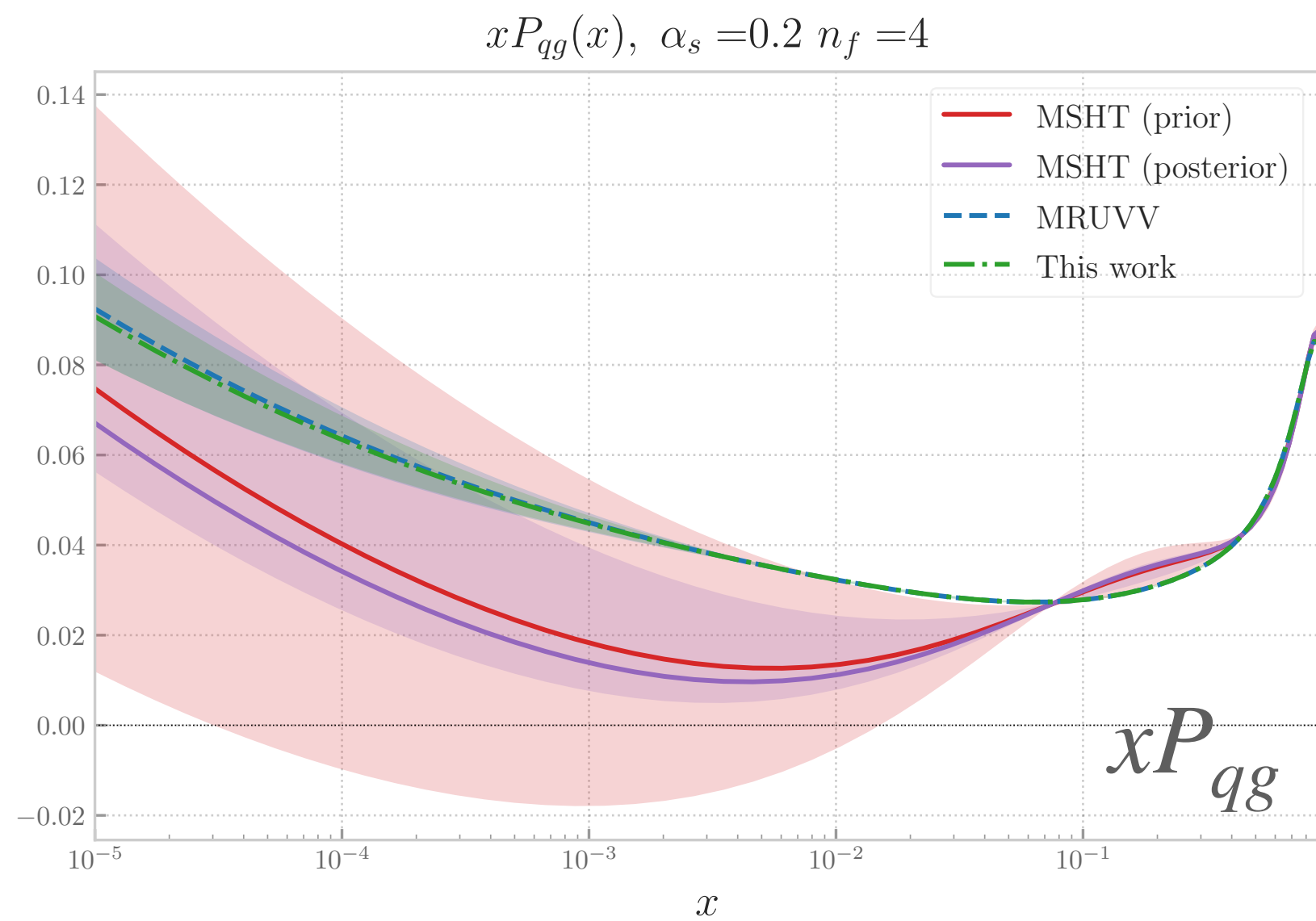
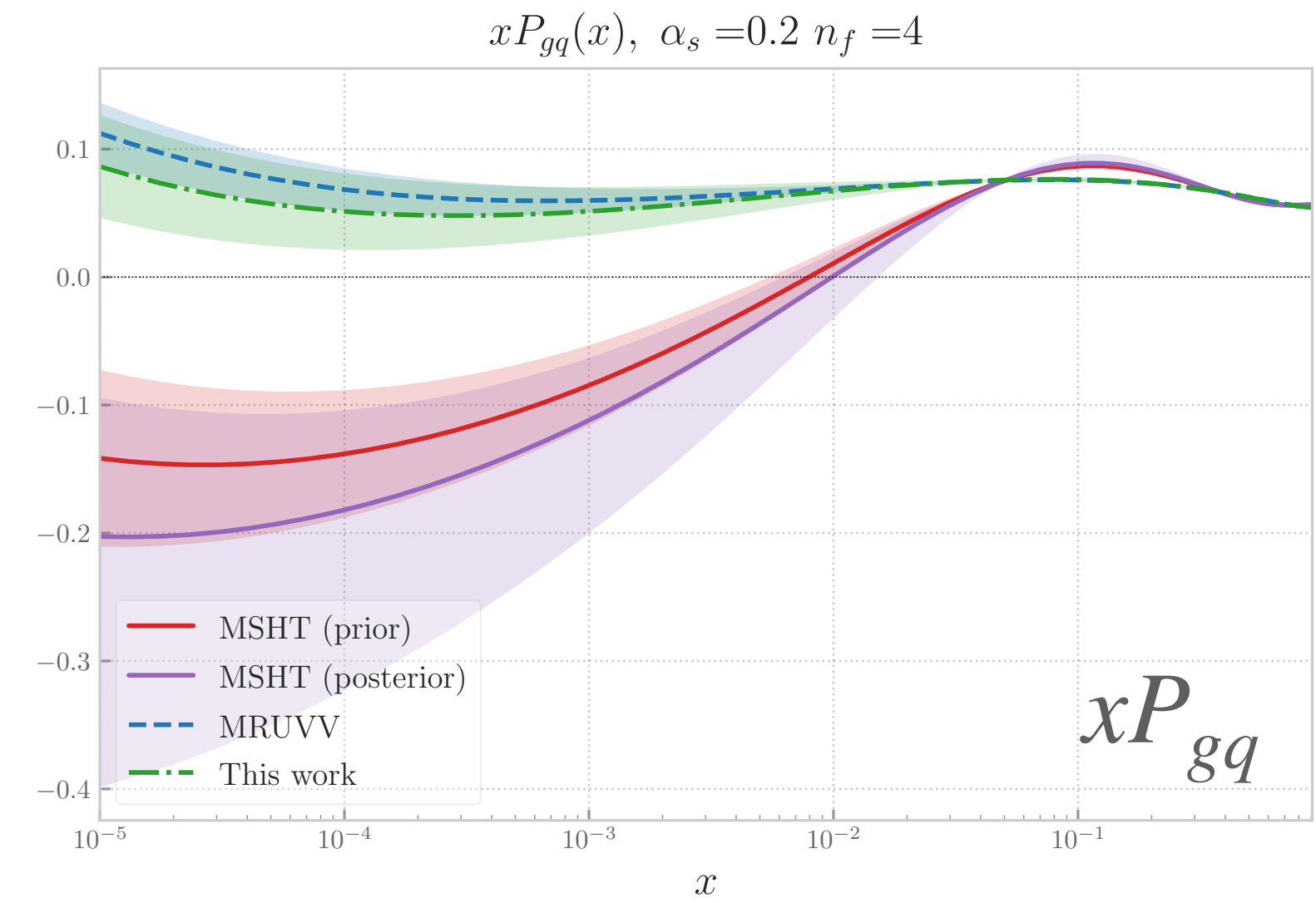
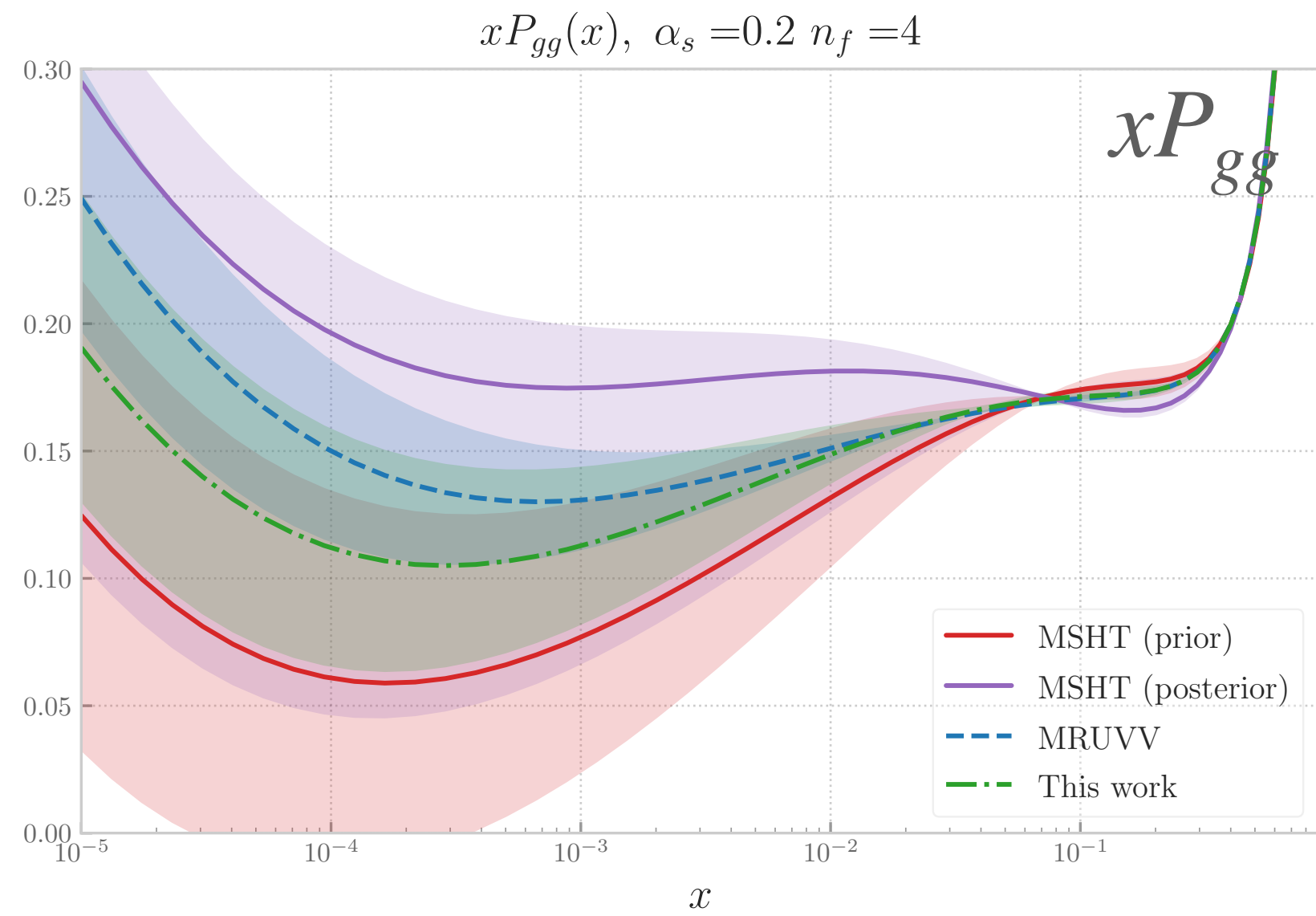
Summary & Conclusion

Summary & Conclusion

- ▶ Computing precise and accurate LHC observables require including theory uncertainties in PDFs.
- ▶ First aN3LO PDFs from the major fitting groups are (will be soon) available.
- ▶ Ongoing effort to benchmark inputs and validate these results.
- ▶ aN3LO PDFs mainly include aN3LO corrections to **DGLAP** and **DIS**.
- ▶ They can be used both with N3LO partonic cross section, but also to evaluate missing higher order effects as they are **provided with theory uncertainties**.



N3LO Splitting functions benchmarks



PDF comparison with MSHT20

