New precision frontiers: aN3LO PDFs

Giacomo Magni,
Nikhef Theory Group and VU Amsterdam

The LHC precision program
Centro de Ciencias de Benasque Pedro Pascual
02 October 2023

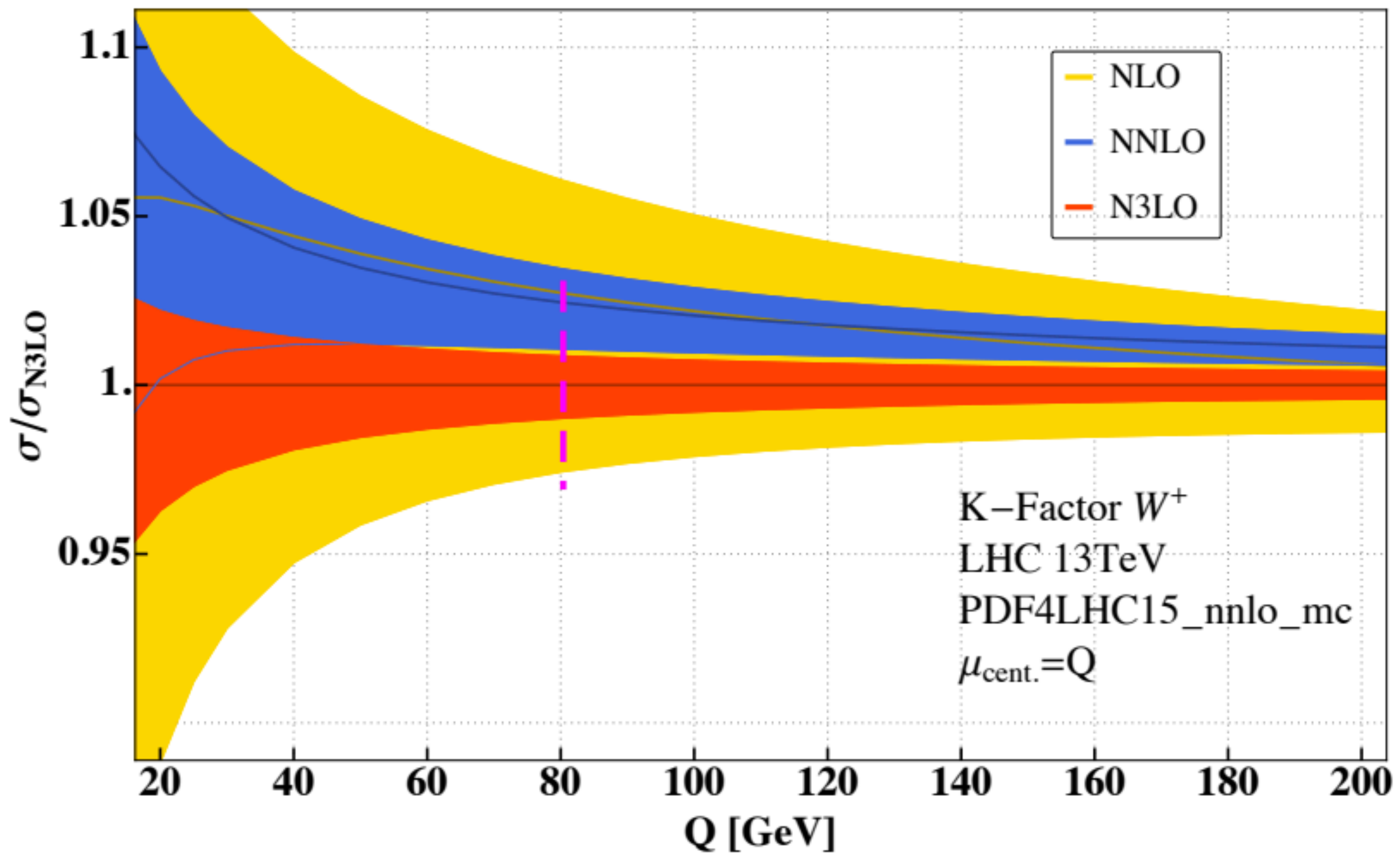
email: gmagni@nikhef.nl

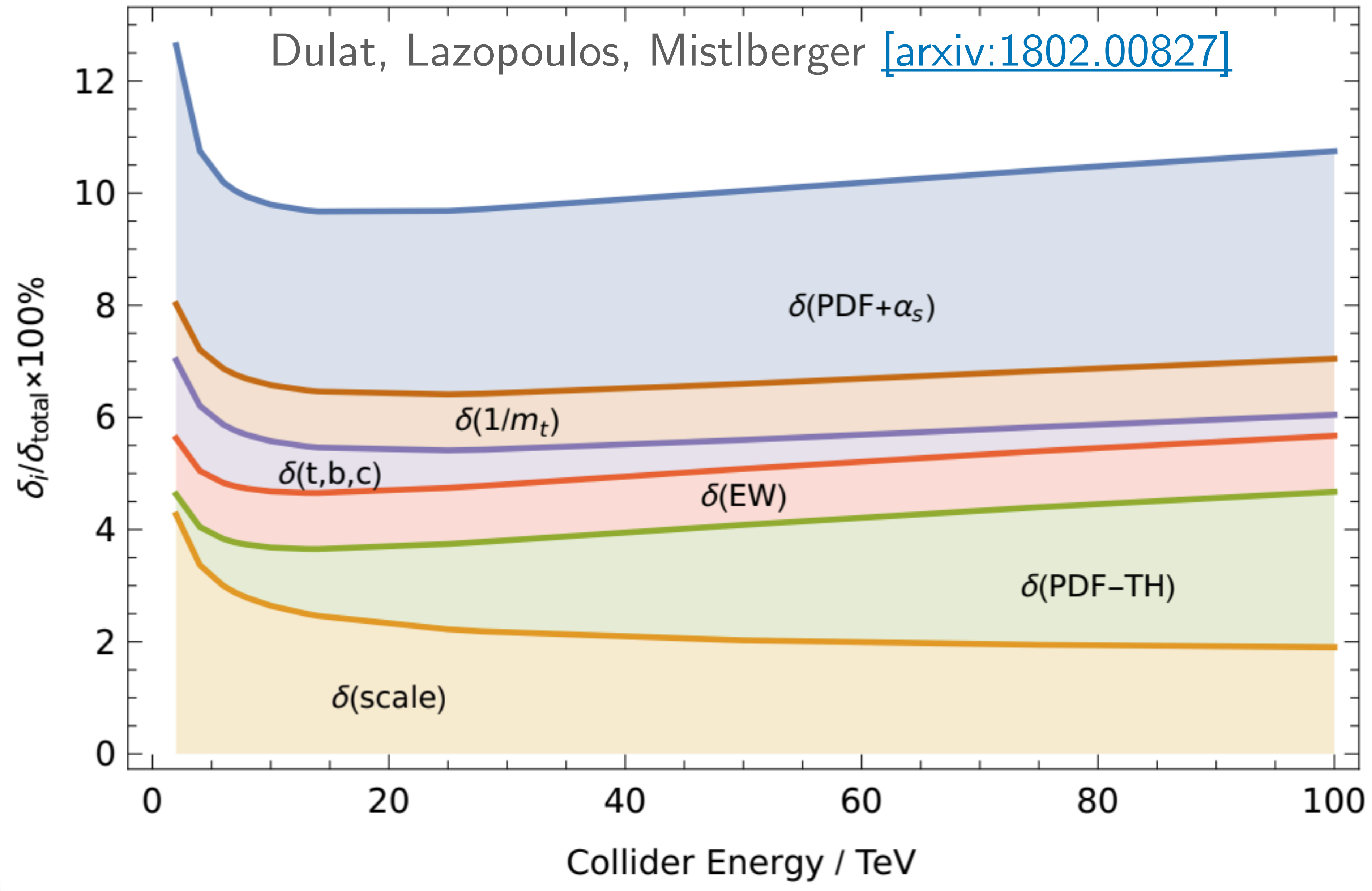
Introduction & Motivations

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

- Predictions for LHC observes 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**: $gg \to H$ [arxiv:1503.06056] $qq \to H\ (VBF)$ [arxiv:1606.00840]; Duhr, Dulat, Mistlberger [arxiv:1904.09990]; Duhr, Dulat, Hirschi, Mistlberger [arxiv:2004.04752] $pp \to W^{\pm}$ Duhr, Dulat, Mistleberger [arxiv:2007.13313]; Chen, Gehrmann, Glover, Huss, Yang, Xing Zhu [arxiv:2205.11426] $pp \to Z/\gamma$, $pp \to VH$ Baglio, Duhr, Mistlberger, Szafrond [arxiv:2209.06138]; Chen, Gehrmann, Glover, Huss, Yang, Xing Zhu [arxiv:2107.09085] Neumann, Campbell [arxiv: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.

Duhr, Dulat, Mistlberger [arxiv:2007.13313]





- **Theory inputs at N3LO.**
- Towards NNPDF4.0 aN3LO.
- MSHT20aN3LO.
-

PDFs determination @ aN3LO

Several theoretical inputs are needed in a PDF fit:

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

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

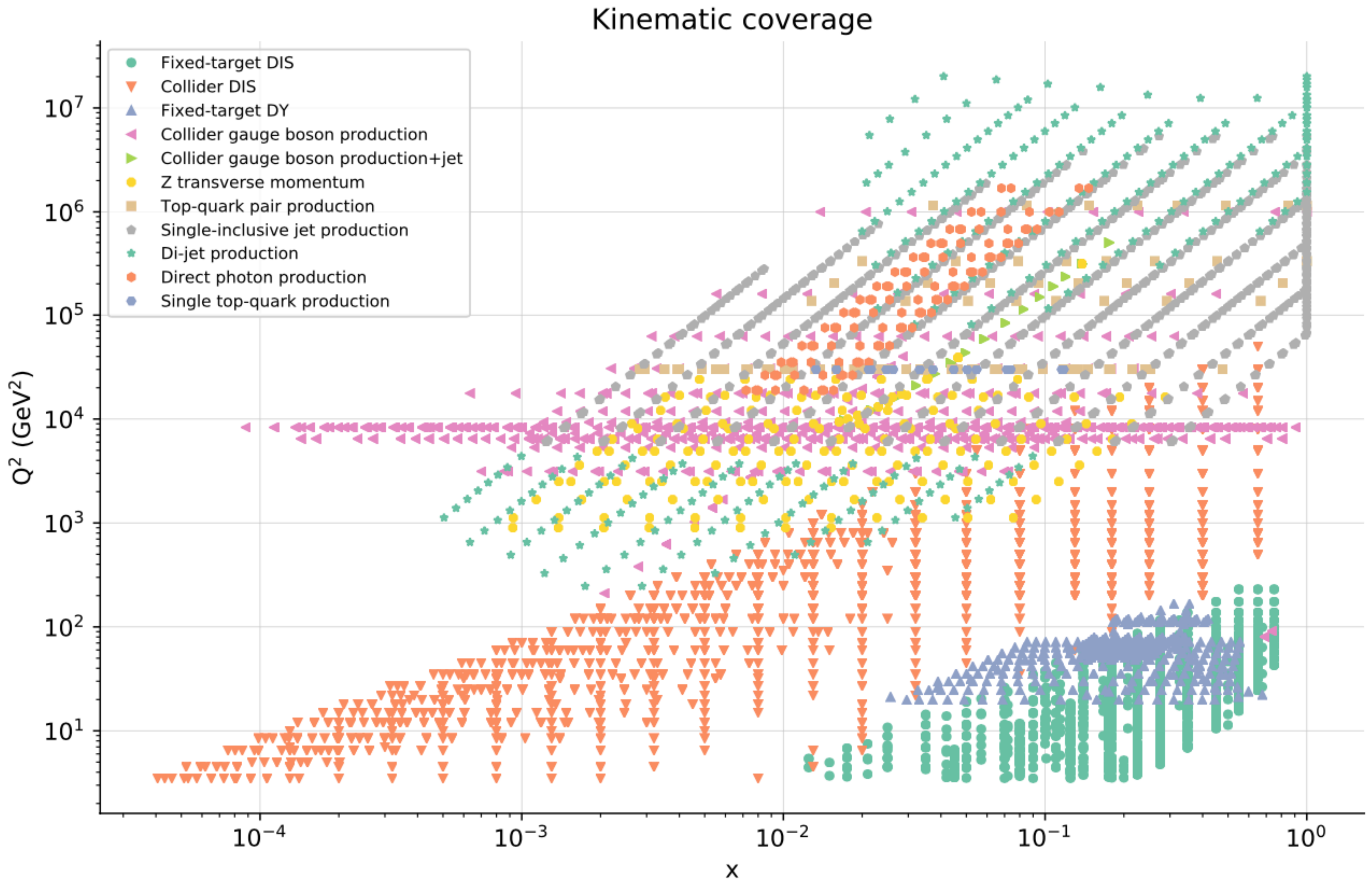
- **VFNS matching conditions** for each running component.

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

- **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

Analytical calculations of the complete N3LO spitting 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]; Gehrmann, Manteuffel, Sotnikov,Yan [arxiv:2308.07958] $\mathcal{O}(n_f^2), \mathcal{O}(n_f^3)$
- **Small-x limit:** Davies, Kom, Moch, Vogt. [arXiv:2202.10362] $P_{NS}^{(3)} \supset \sum_{k=0}^{6} \ln^k(x)$
- **Large-x limit:** Moch, Ruijl, Ueda, Vermaseren, Vogt [arXiv:1707.08315]

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

- 8 lowest **Mellin Moments:** [arXiv: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

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: $Q^2 \frac{dV}{dQ^2} = P_{NS,v} \otimes V$

$\longrightarrow$ 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 $P_{qq,PS}$
- **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:

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

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 **IHOU**

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

Mellin transformation:

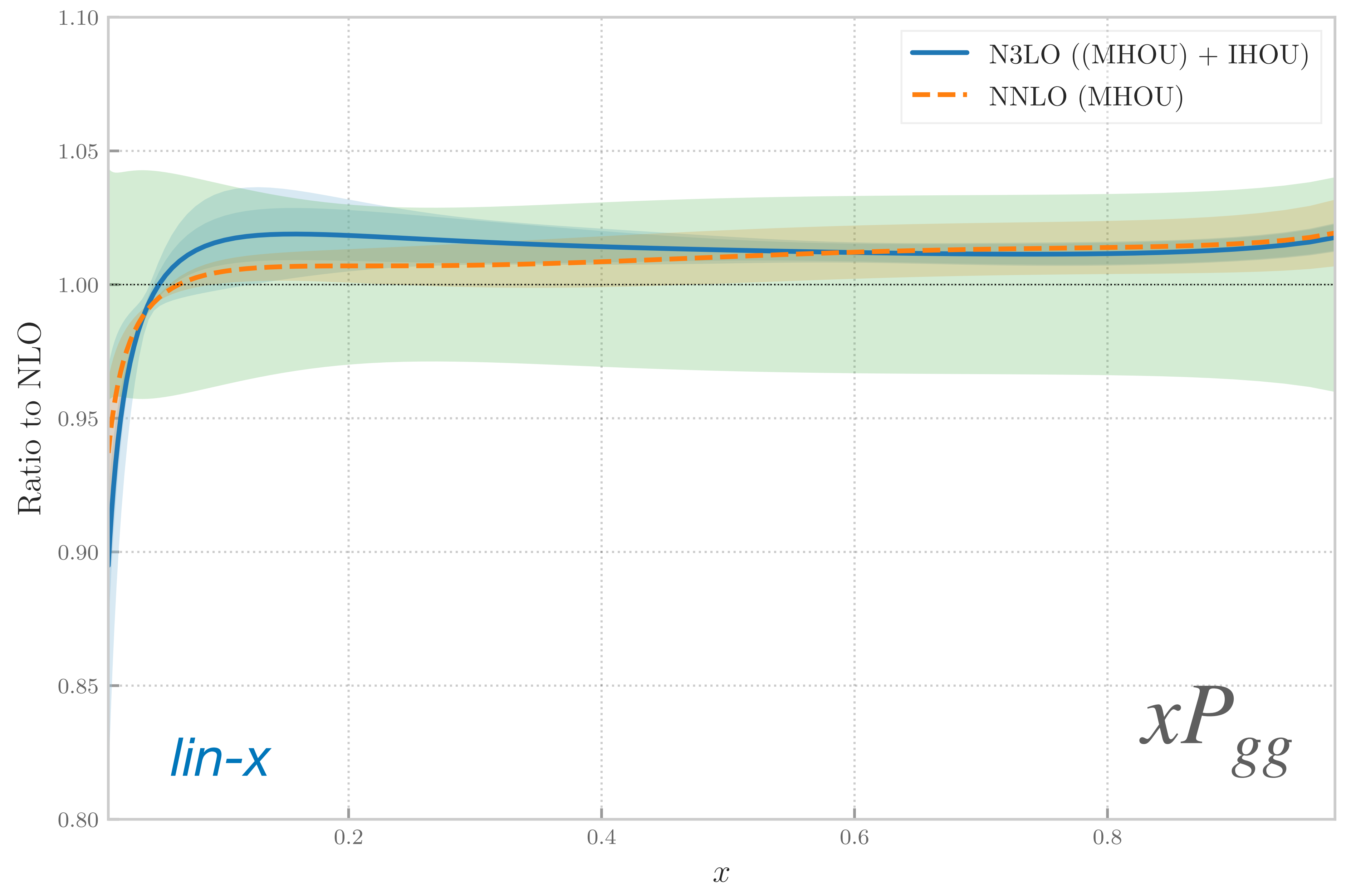
$$\tilde{\gamma}_{ij}(N) = \int_0^1 x^{N-1} P_{ij}(x) dx$$

Rule of thumb:
small-N → small-x,
large-N → large-x

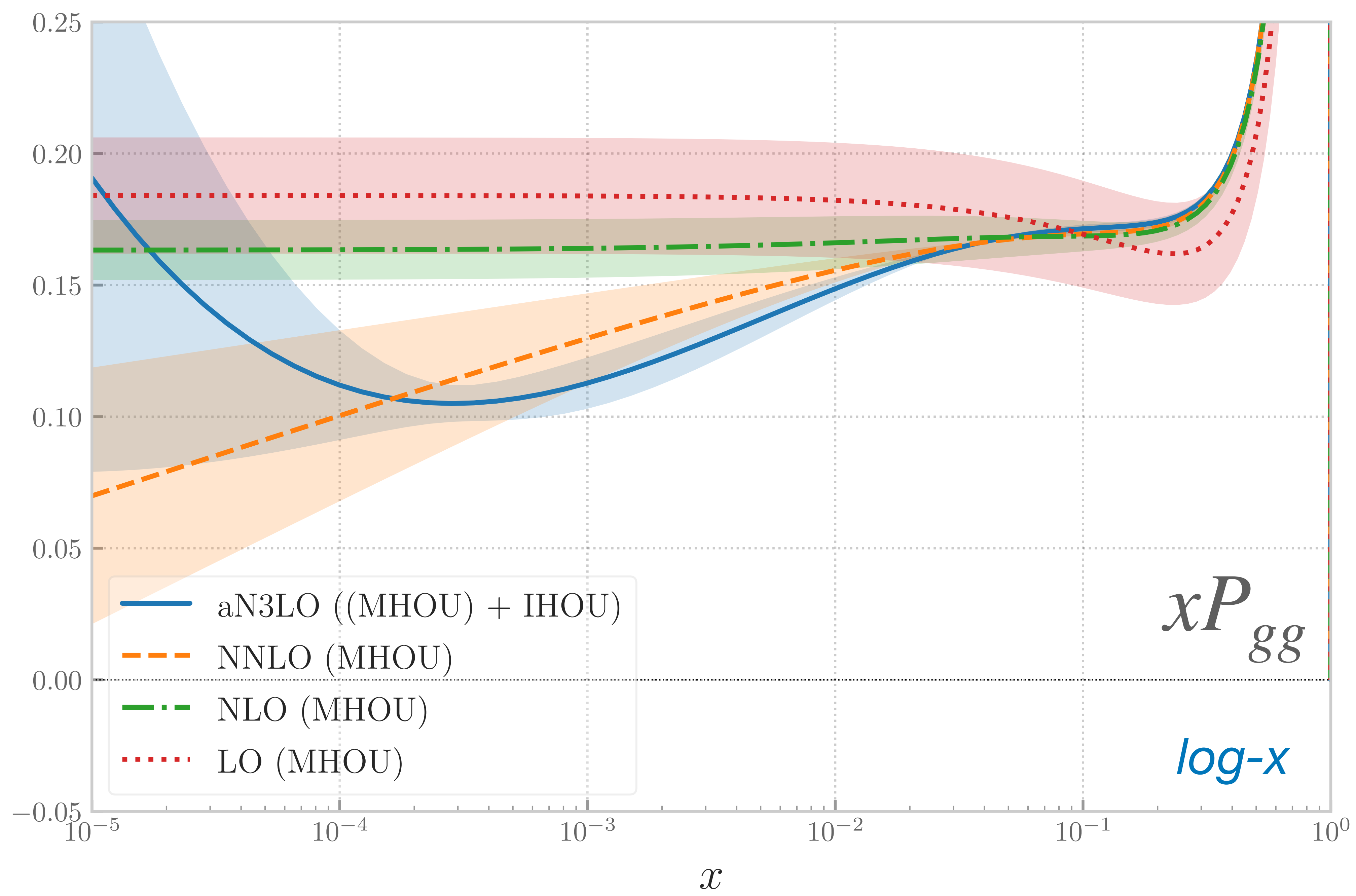
Adopted basis function for $\tilde{\gamma}_{qq}^{(3)}$

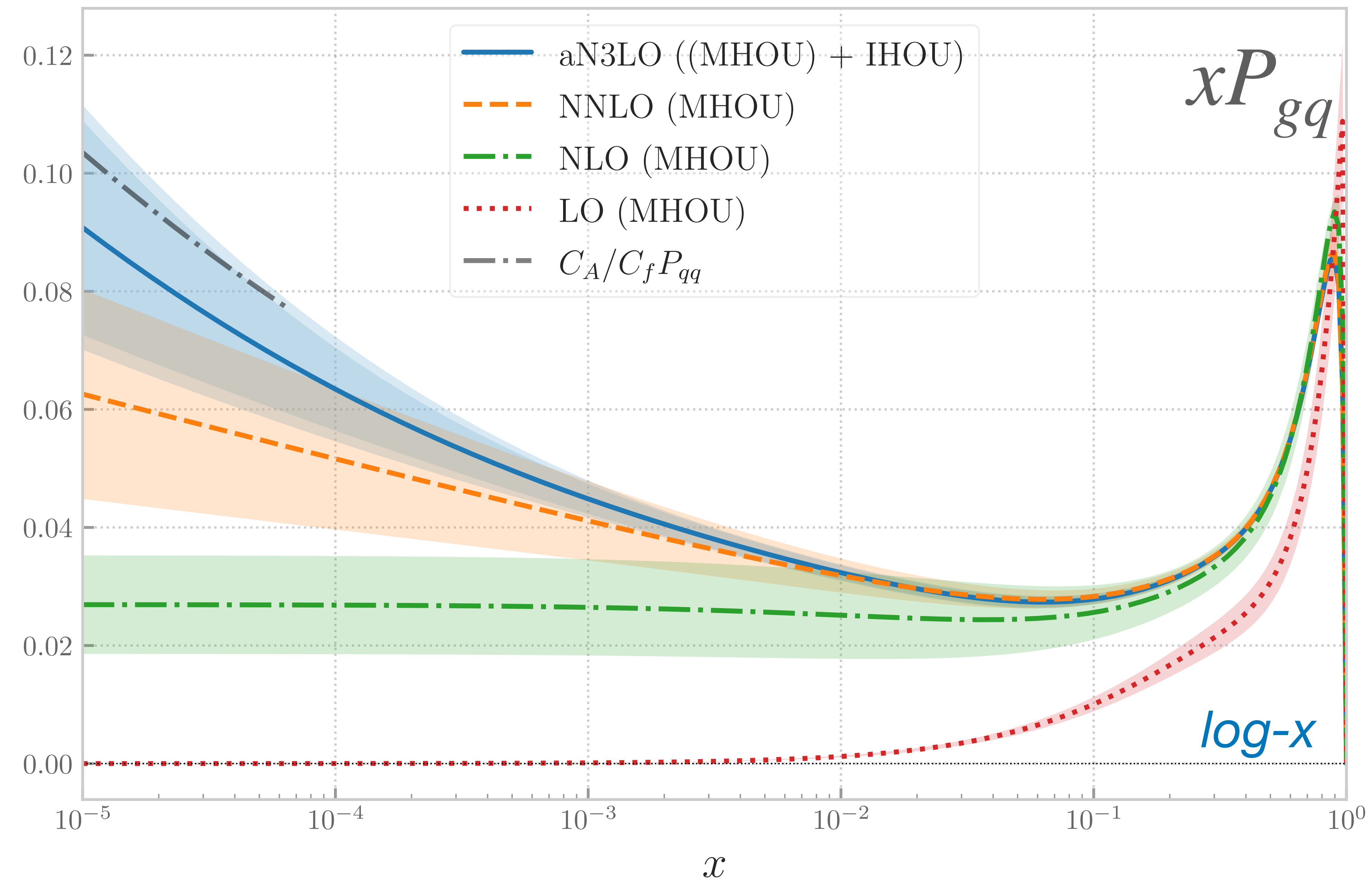
$G_1(N)$	$\mathcal{M}[(1-x)\ln^2(1-x)]$
$G_2(N)$	$-\frac{1}{(N-1)^2} + \frac{1}{N^2}$
$G_3(N)$	$\frac{1}{N^4}$, $\frac{1}{N^3}$, $\mathcal{M}[(1-x)\ln(1-x)]$ $\mathcal{M}[(1-x)^2\ln(1-x)^2]$, $\frac{1}{N-1} - \frac{1}{N}$, $\mathcal{M}[(1-x)\ln(x)]$
$G_4(N)$	$\mathcal{M}[(1-x)(1+2x)]$, $\mathcal{M}[(1-x)x^2]$,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

aN3LO splitting functions

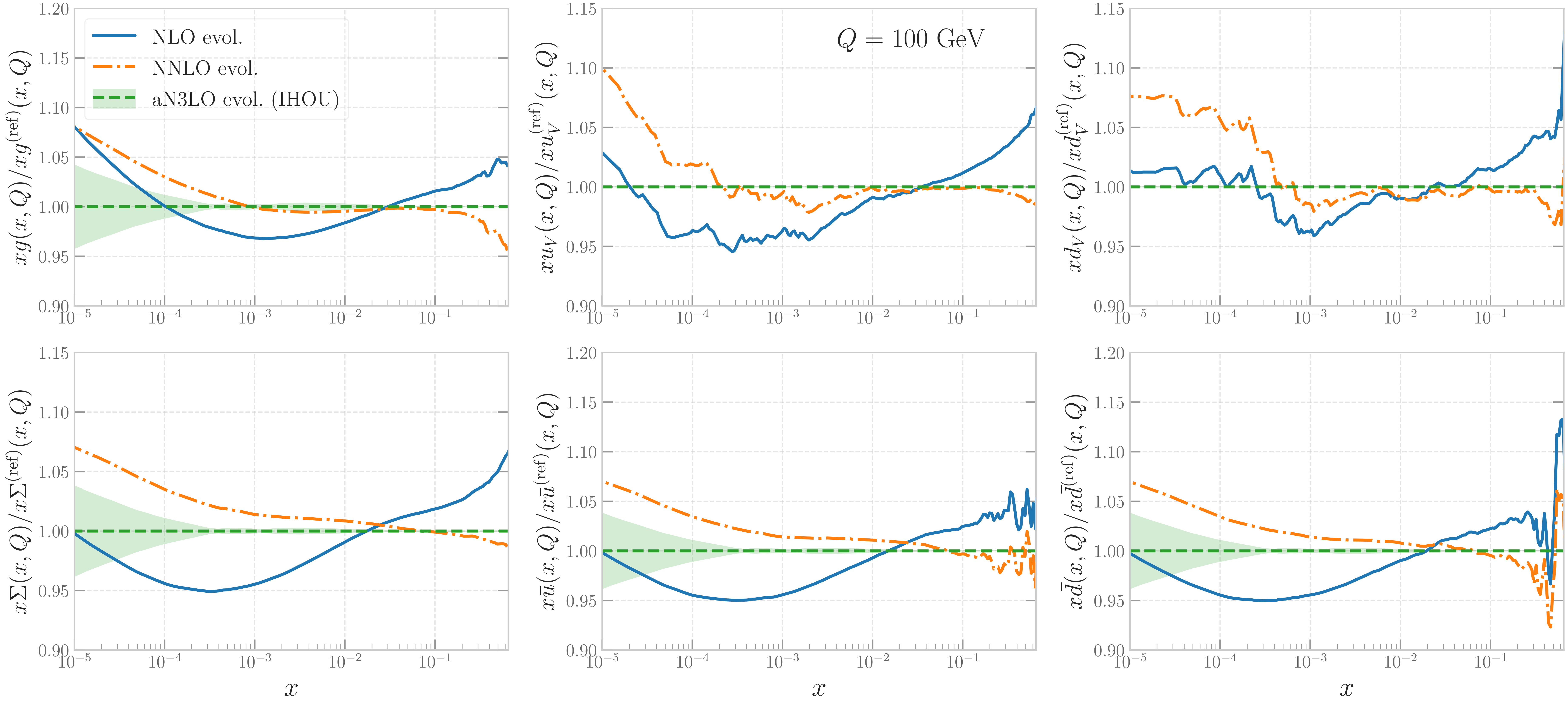


- Large logs $1/x \ln^3(x)$, $1/x \ln^2(x)$ arise at N3LO. MHOU (from scale variations) fails in small-x region.
- Good agreement between different perturbative orders at large-x.
- IHOU are not negligible. Having 10 moments available would be enough to reduce IHOU.
- Off diagonal terms P_{qg}, P_{gq}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





aN3LO DGLAP evolution



NNPDF4.0 NNLO evolution from, $Q = 1.65 \to 100$ GeV

- Valence-like PDFs display good perturbative convergence on all the x-range.
- Impact of the N3LO corrections is at percent level.

- Ongoing benchmark study with MSHT and FHMV to asses a region in which agreement between different aN3LO splitting functions approximations can be found.

DIS Structure Functions

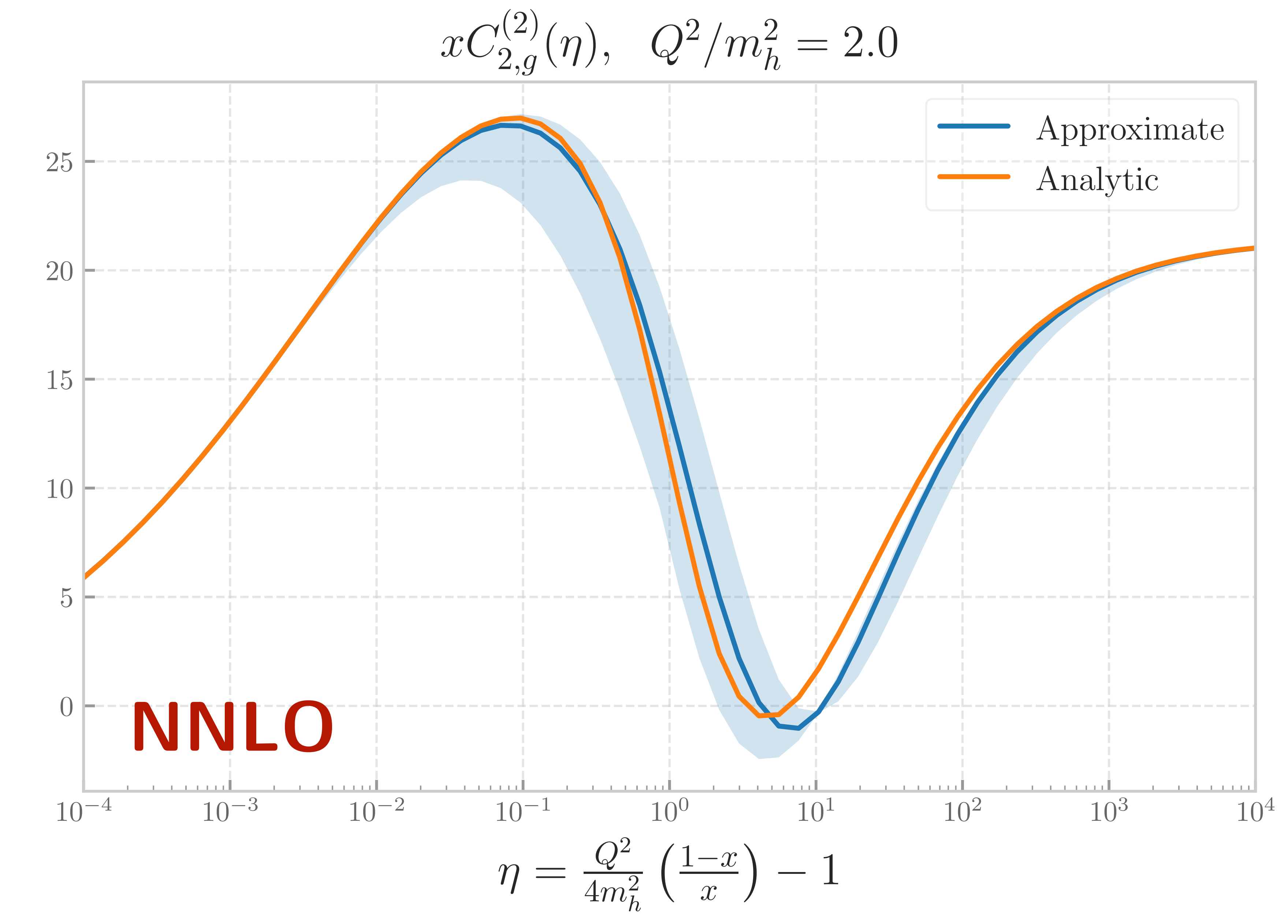
DIS structure functions are known at N3LO in the **massless limit (ZM-VFNS)** for F_2, F_L, F_3:

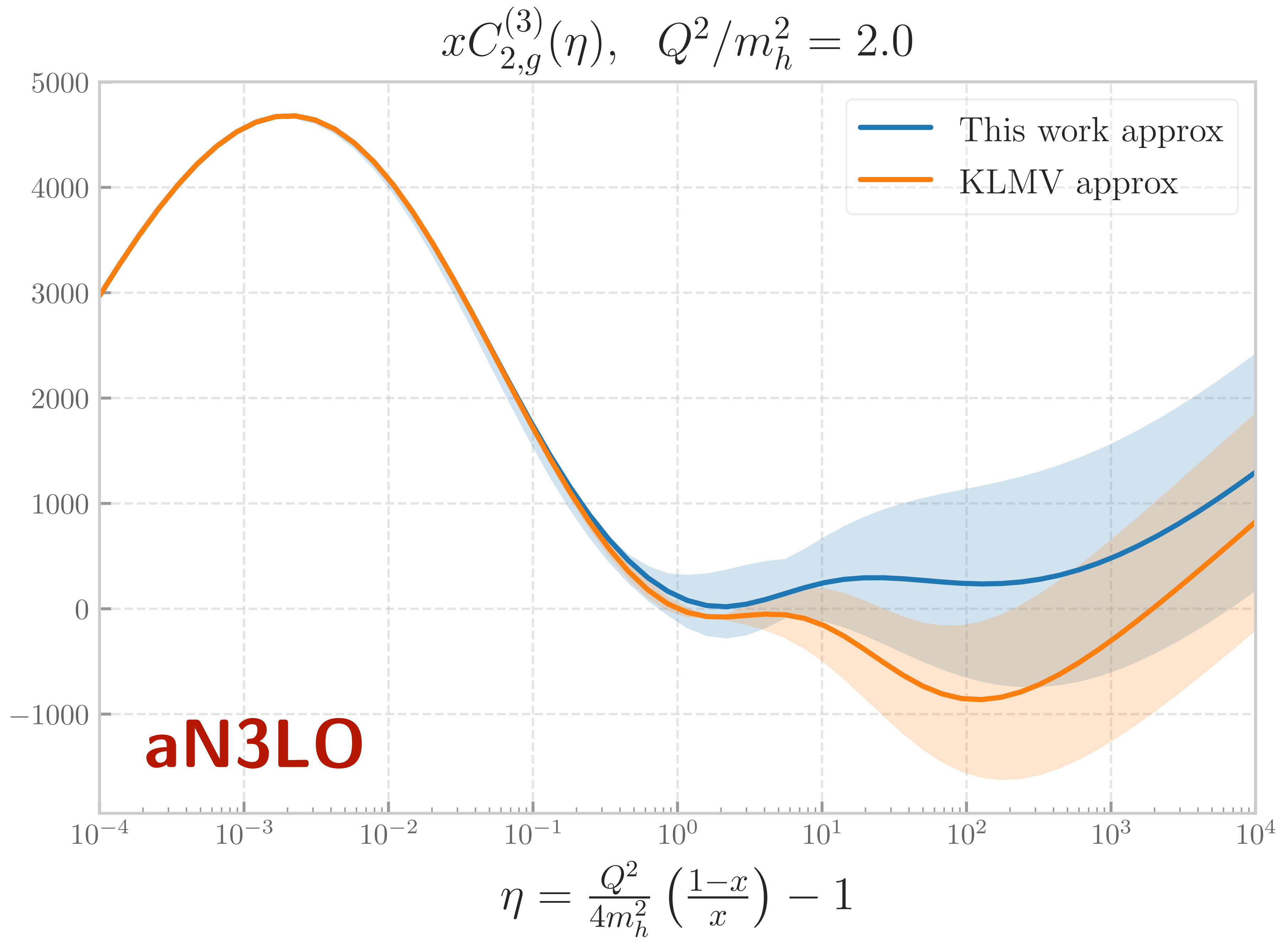
- DIS NC: Larin, Nogueira, Van Ritbergen, Vermaseren [arxiv:9605317] Moch, Vermaseren, Vogt [arxiv:0411112], [arxiv:0504242]
- DIS CC: Davies, Moch, Vermaseren, Vogt [arxiv:0812.4168] [arxiv:1606.08907]

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

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

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





KLMV Kawamura, Lo Presti, Moch, Vogt [arxiv:1205.5727]

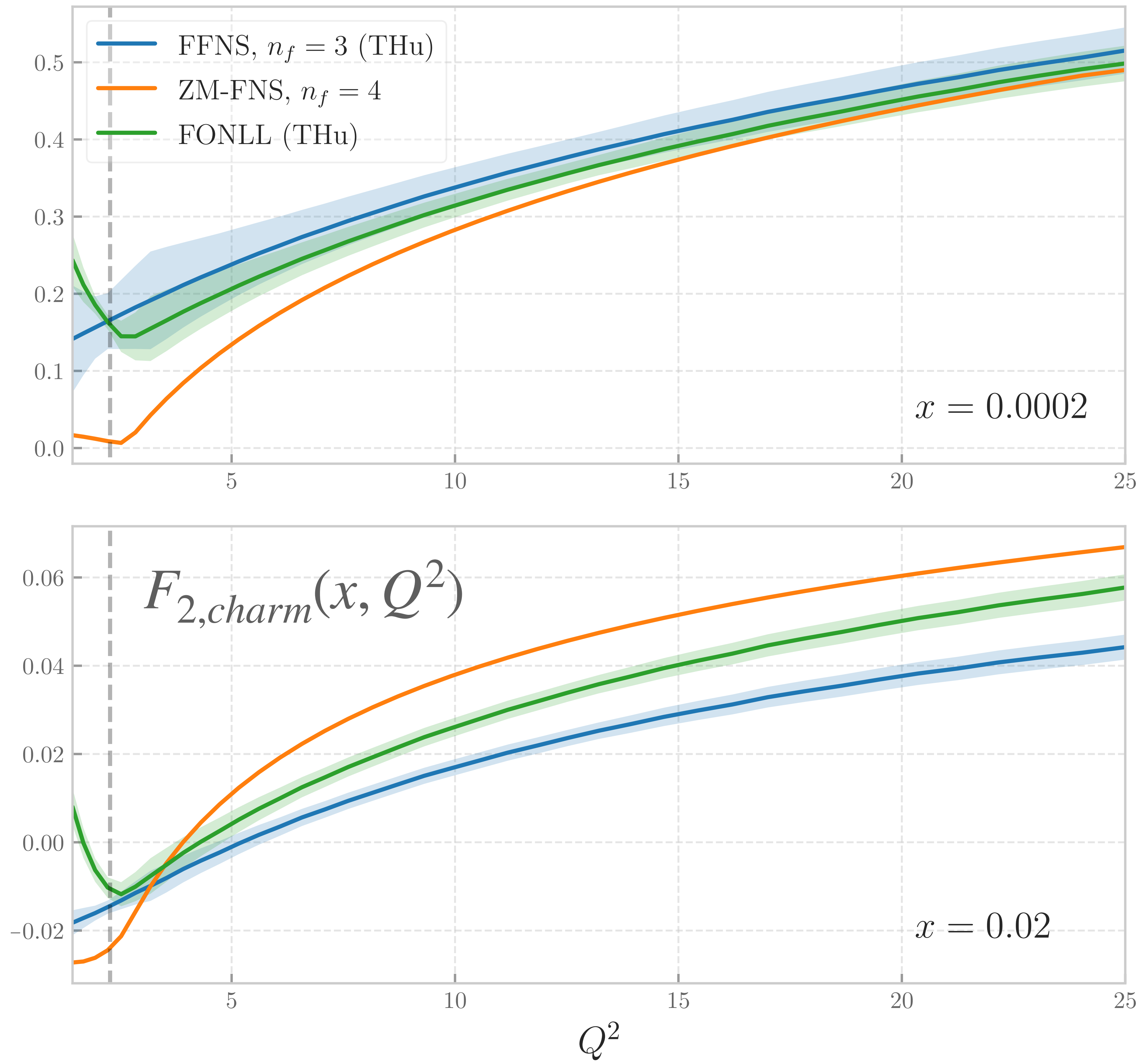
DIS VFNS@ aN3LO

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]. *(Other works see slide 24)*

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

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



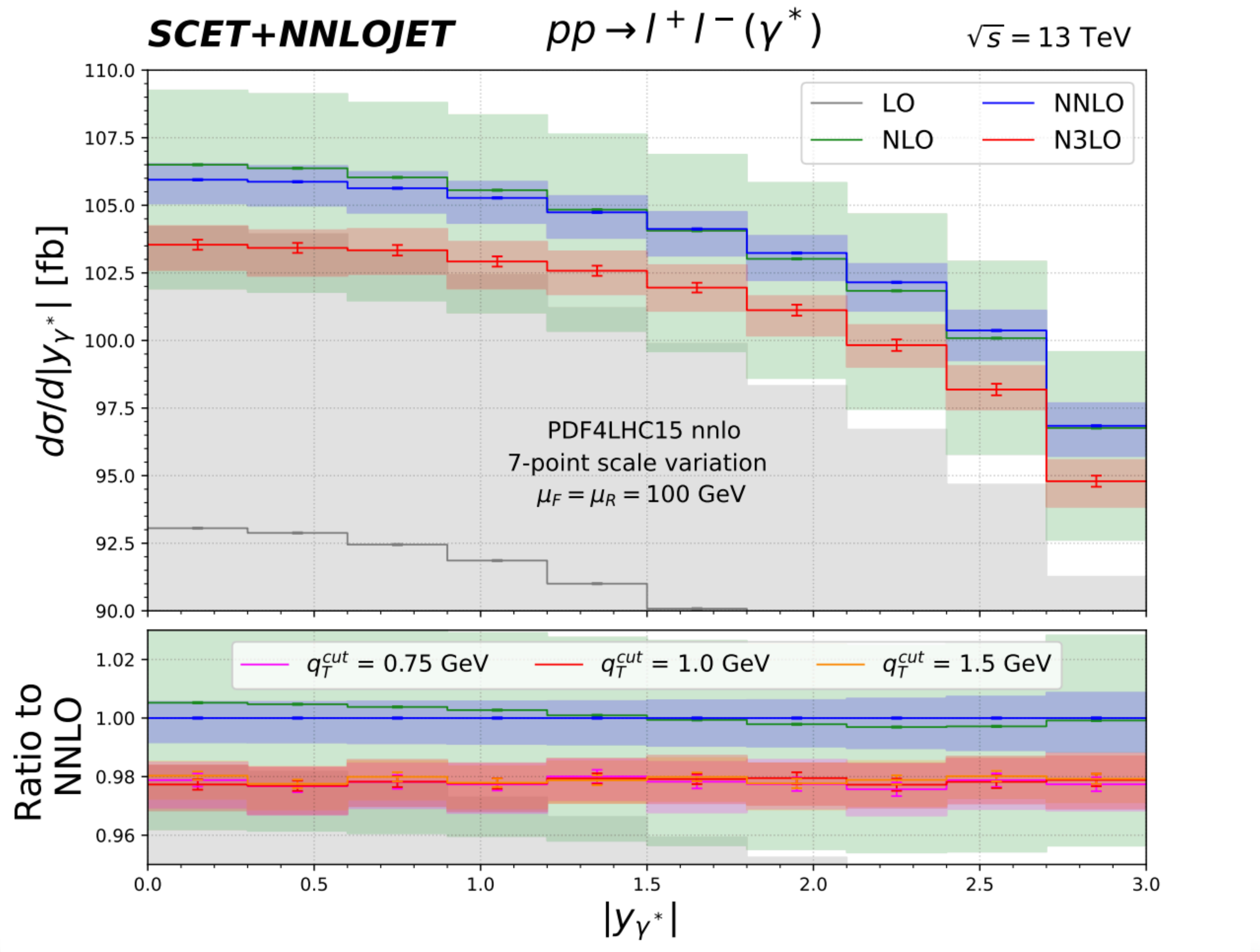
In NNPDF studies DIS structure functions are computed in the **FONLL** procedure [arxiv:1001.2312]:

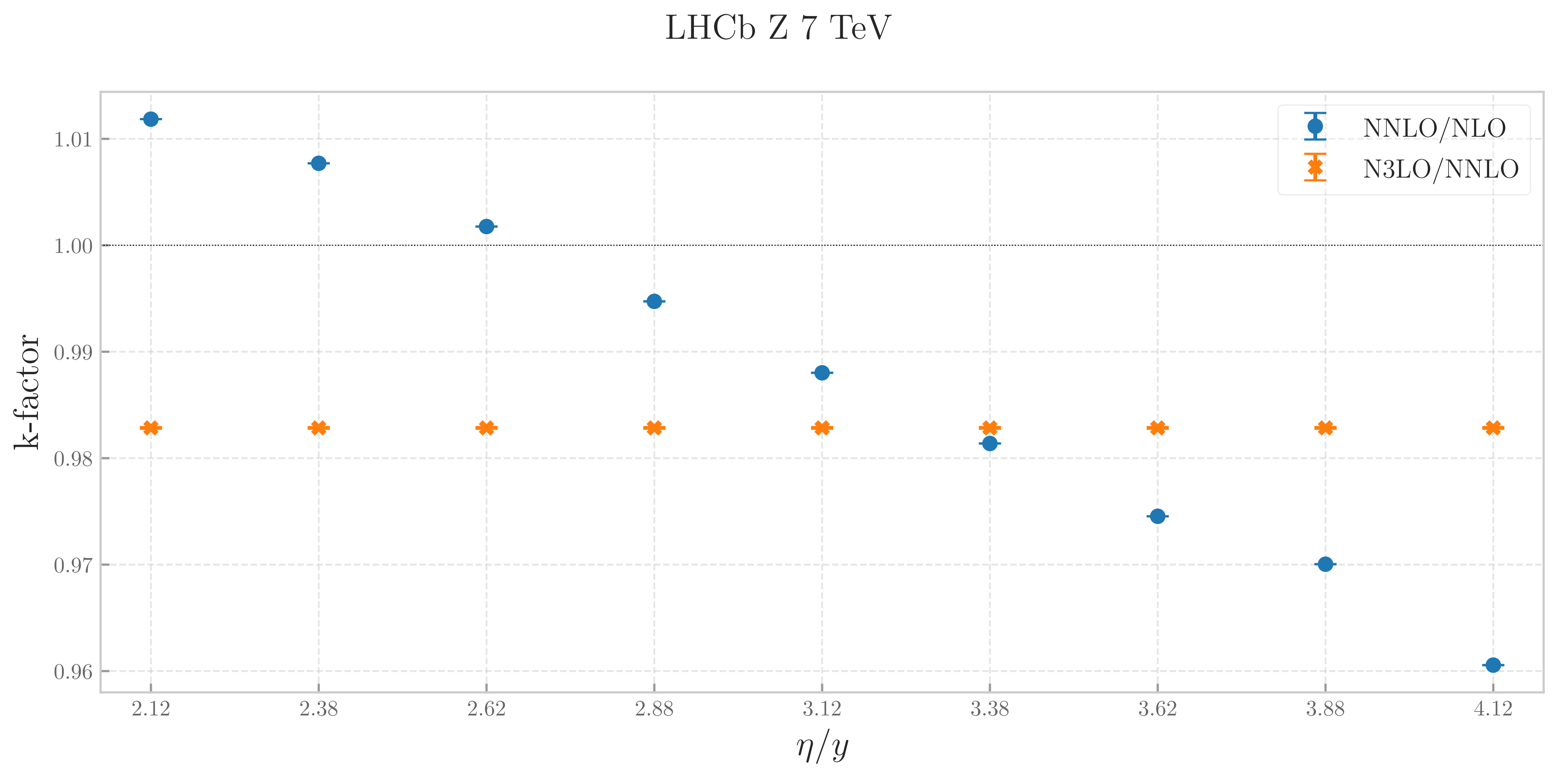
- Extended up to N3LO for the Heavy structure functions F_{heavy}
- Extended up to NNLO for light F_{light} + massless N3LO contributions.

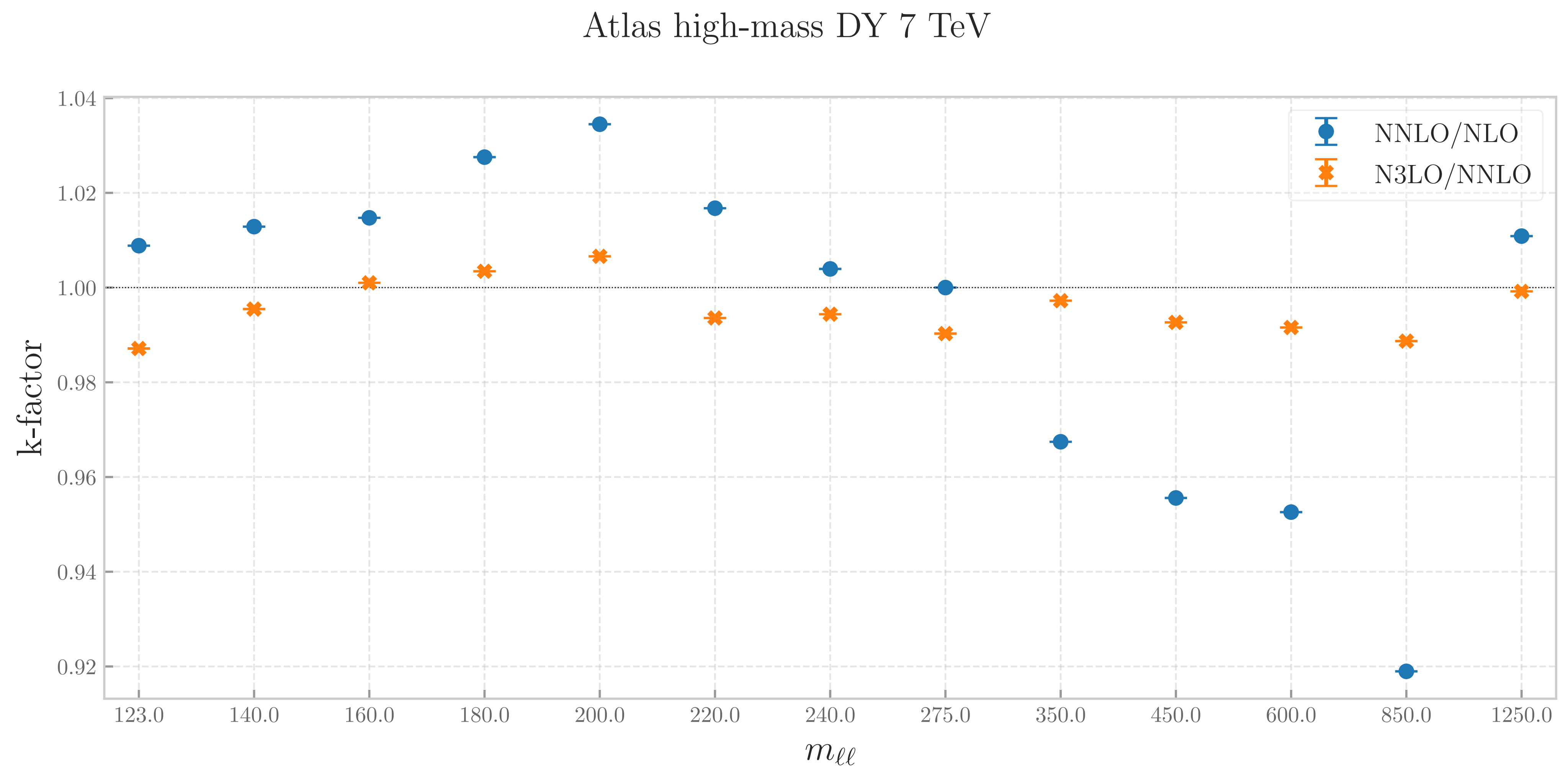
Collider DY @ aN3LO

- 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.

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







- Theory inputs at N3LO.
- **Towards NNPDF4.0 aN3LO.**
- MSHT20aN3LO.

PDF MHOU from scale variations

See also J.Rojo talk on Tuesday

NNPDF adopts Scale Variations to estimate **PDFs MHOU**.

For a given observable, MHOU are estimated by varying the unphysical scales. MSTH [arxiv:1811.08434], NNPDF [arxiv:1906.10698], [arxiv:2105.05114]

Scale variation advantages:

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

- Not a unique procedure. Differences are always higher orders.
- **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.

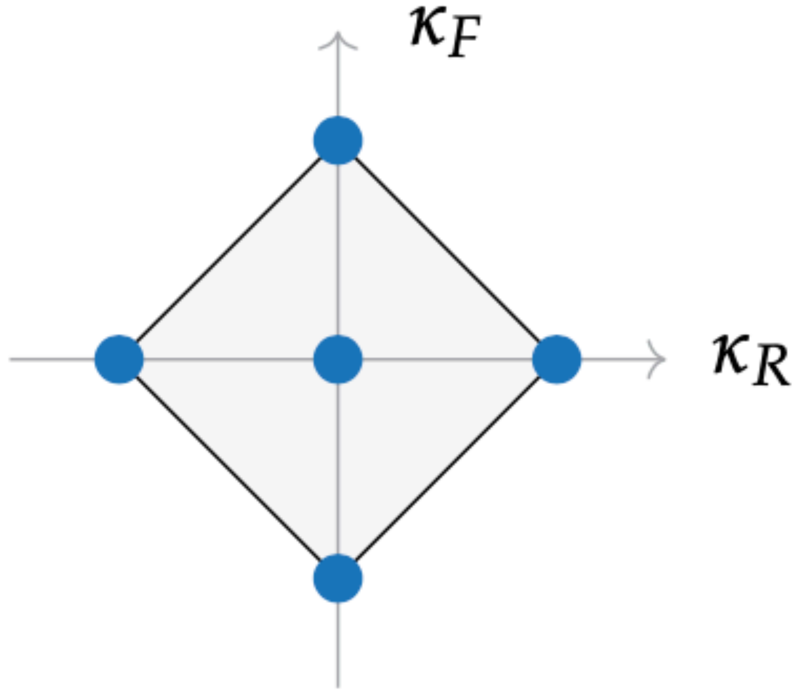
Observable **DGLAP Evolution**

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

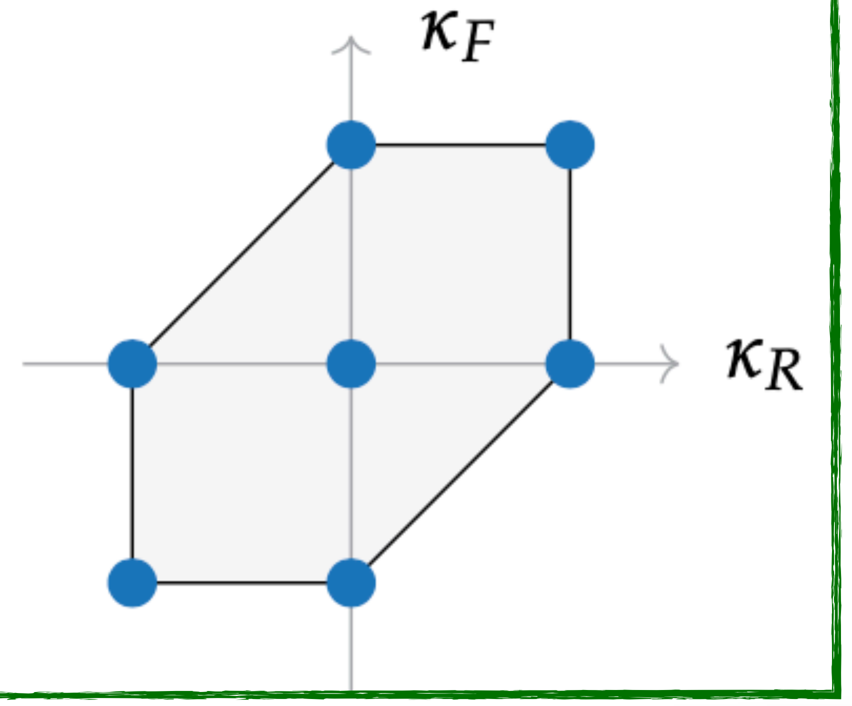
$$n = \{1 \ldots N_{dat}\}$$

Partonic coefficients

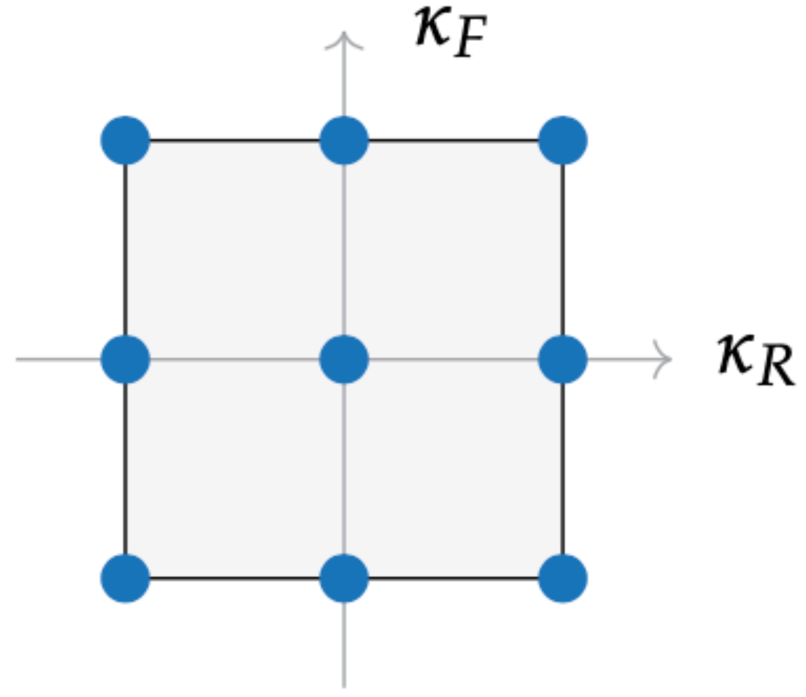
5 points



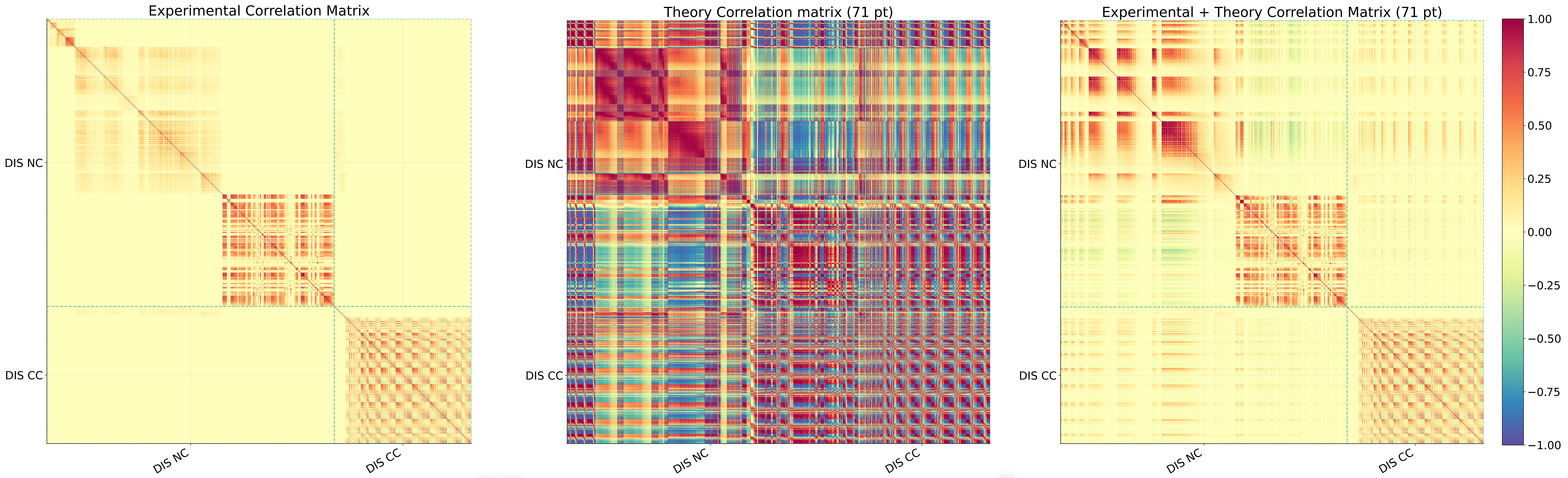
7 points



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:

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

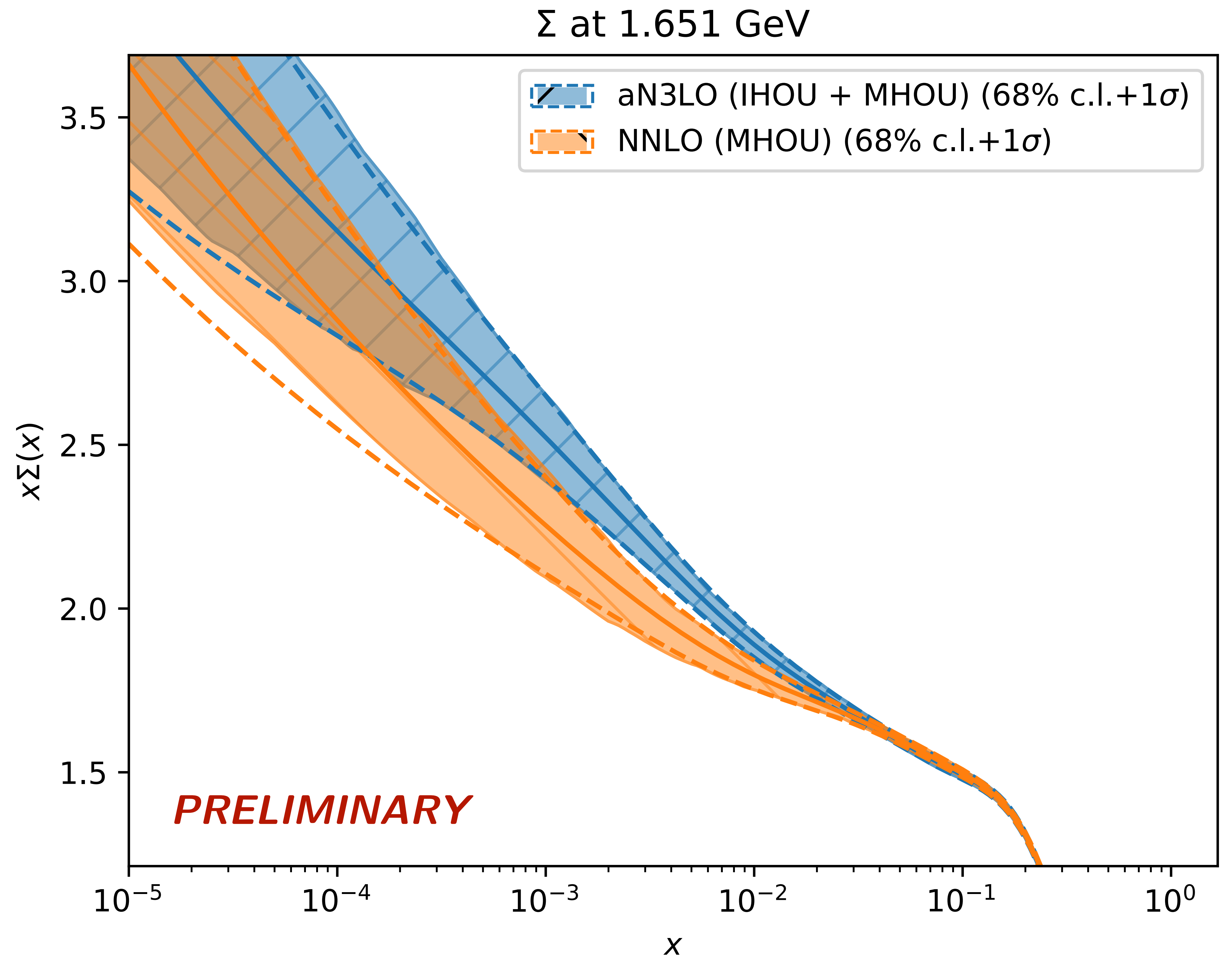
- **IHOU** are **independent** from **MHOU**, so they can be added in quadrature:

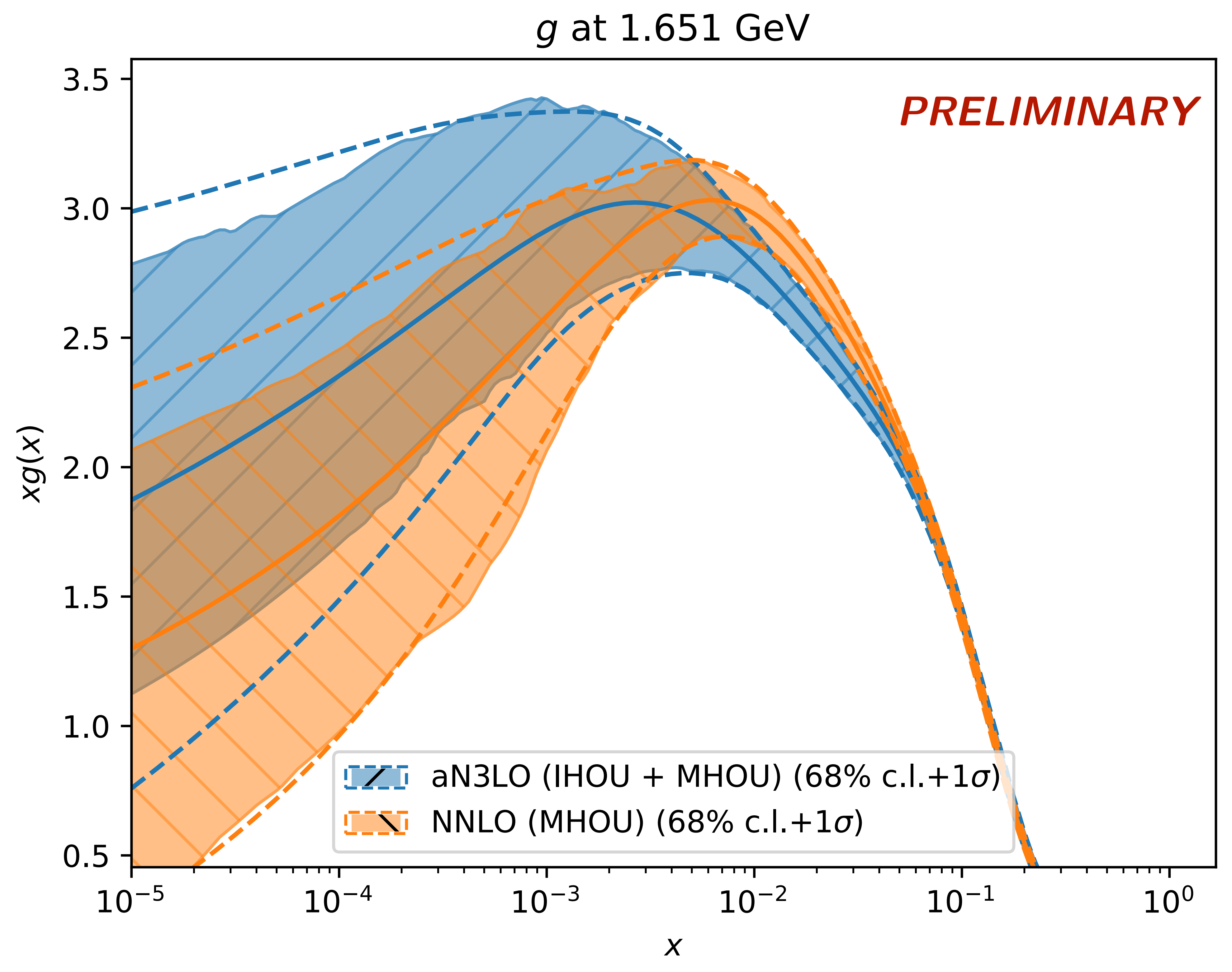
$$Cov_{ij} = Cov_{ij,EXP} + Cov_{ij,MHOU} + Cov_{ij,IHOU}$$

- Theory uncertainties correlate different processes and experiments.

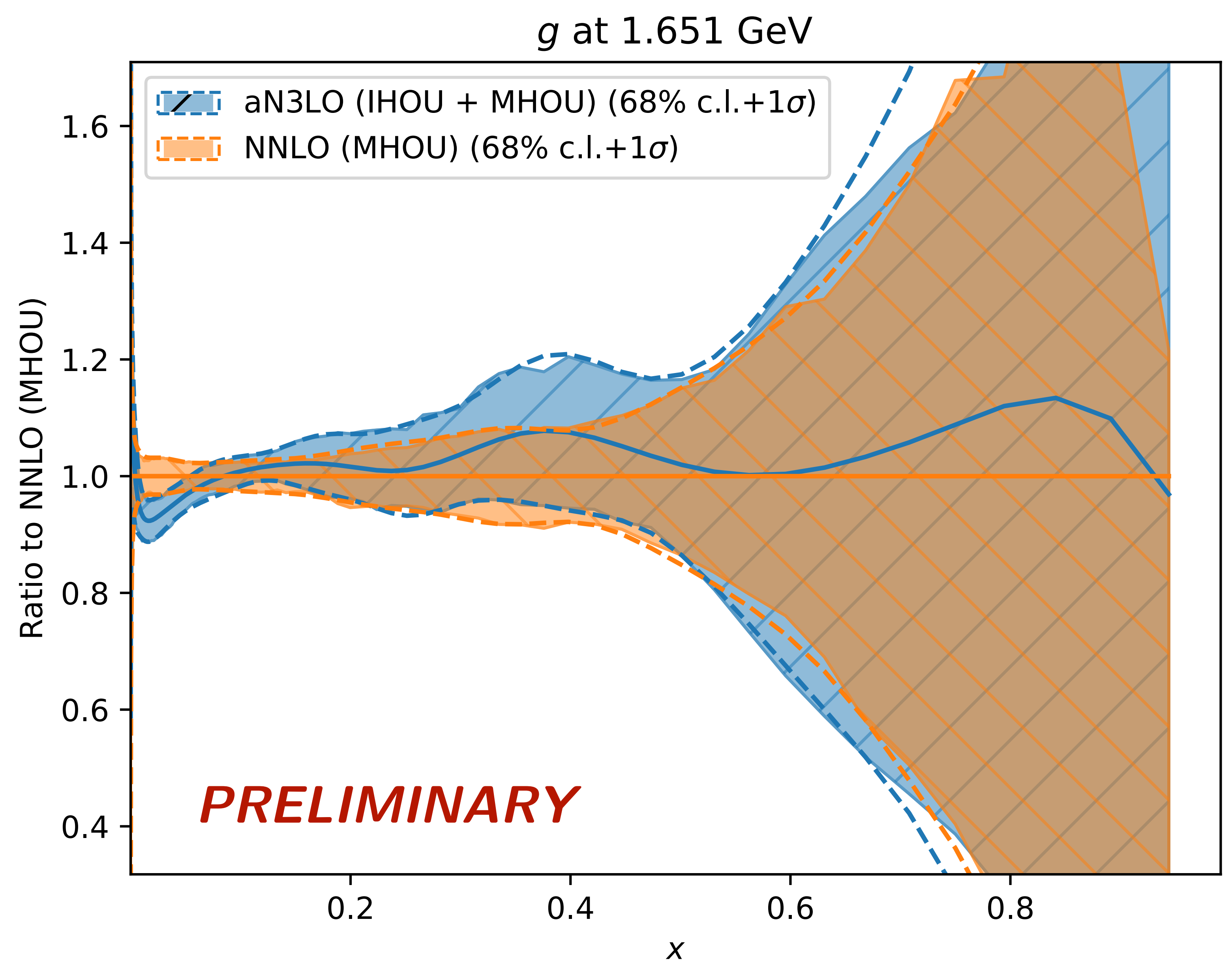
NNPDF4.0 aN3LO

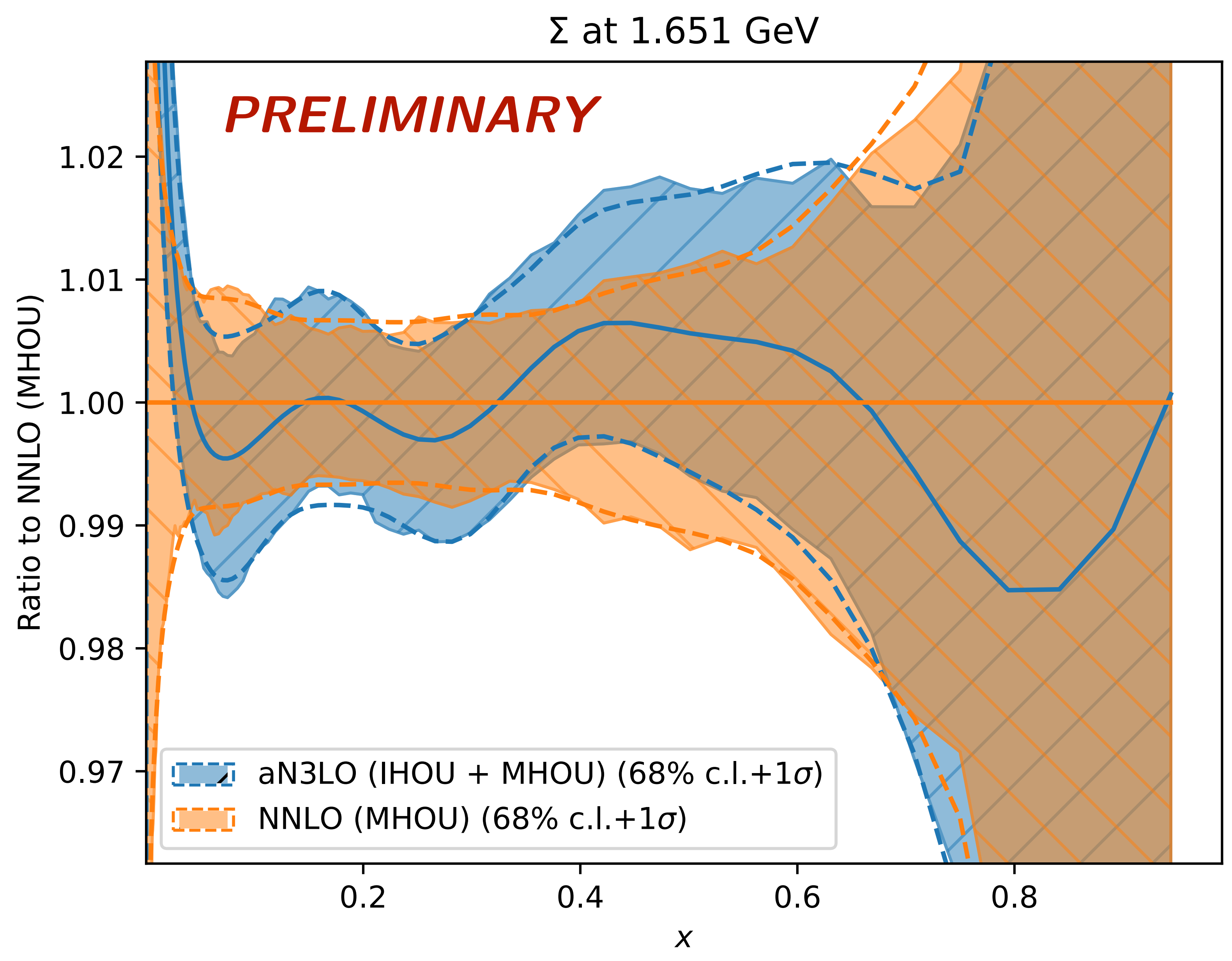
- Preliminary **aN3LO** fits show a quite visible impact of N3LO corrections in the **small-x** region for gluon g and Singlet Σ.
- MHOU have a non trivial effect and can induce **shifts** both in the **central value** and in **uncertainty** size.
- From lower orders we see that MHOUs improve perturbative convergence from NLO to NNLO.





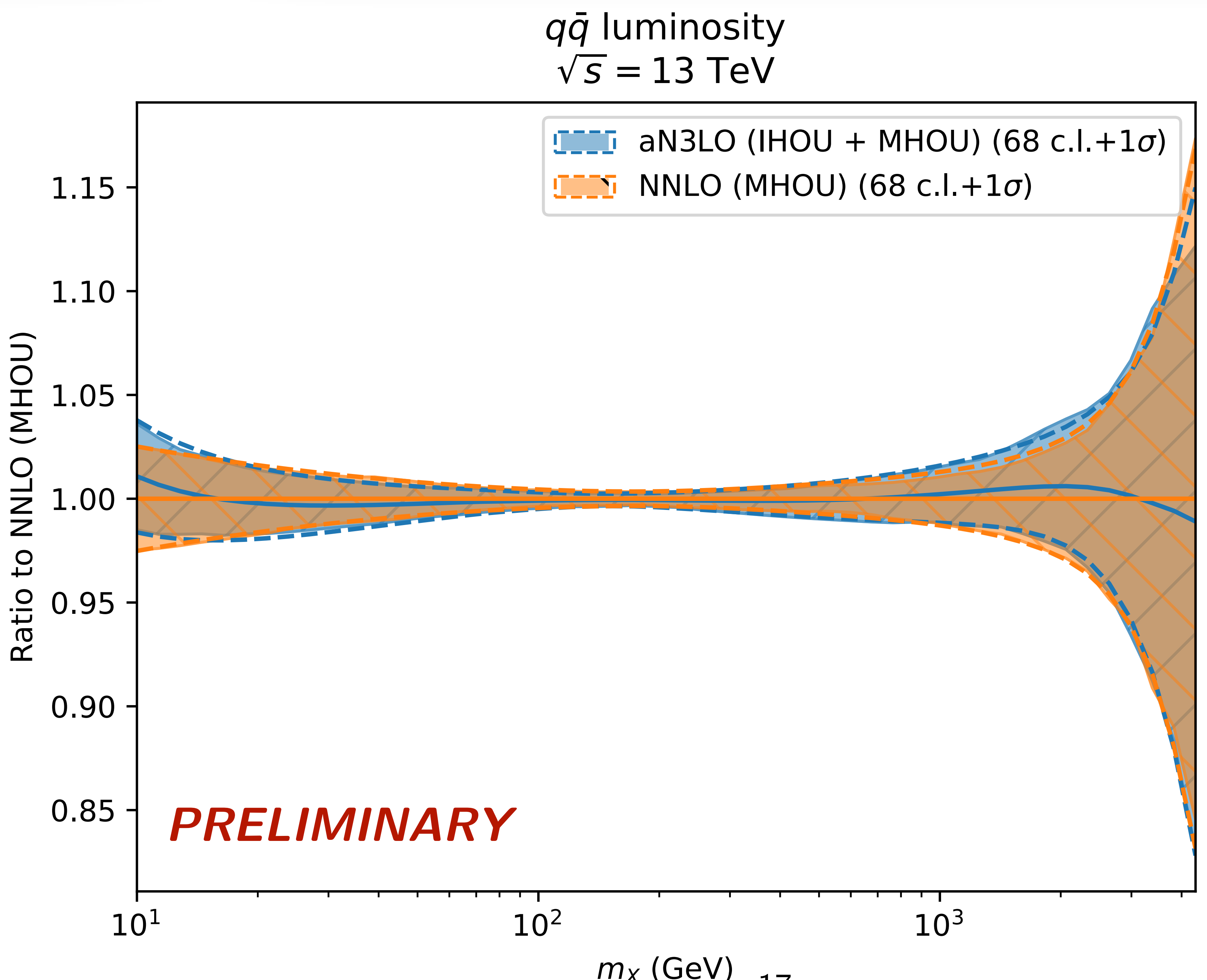
NNPDF4.0 aN3LO

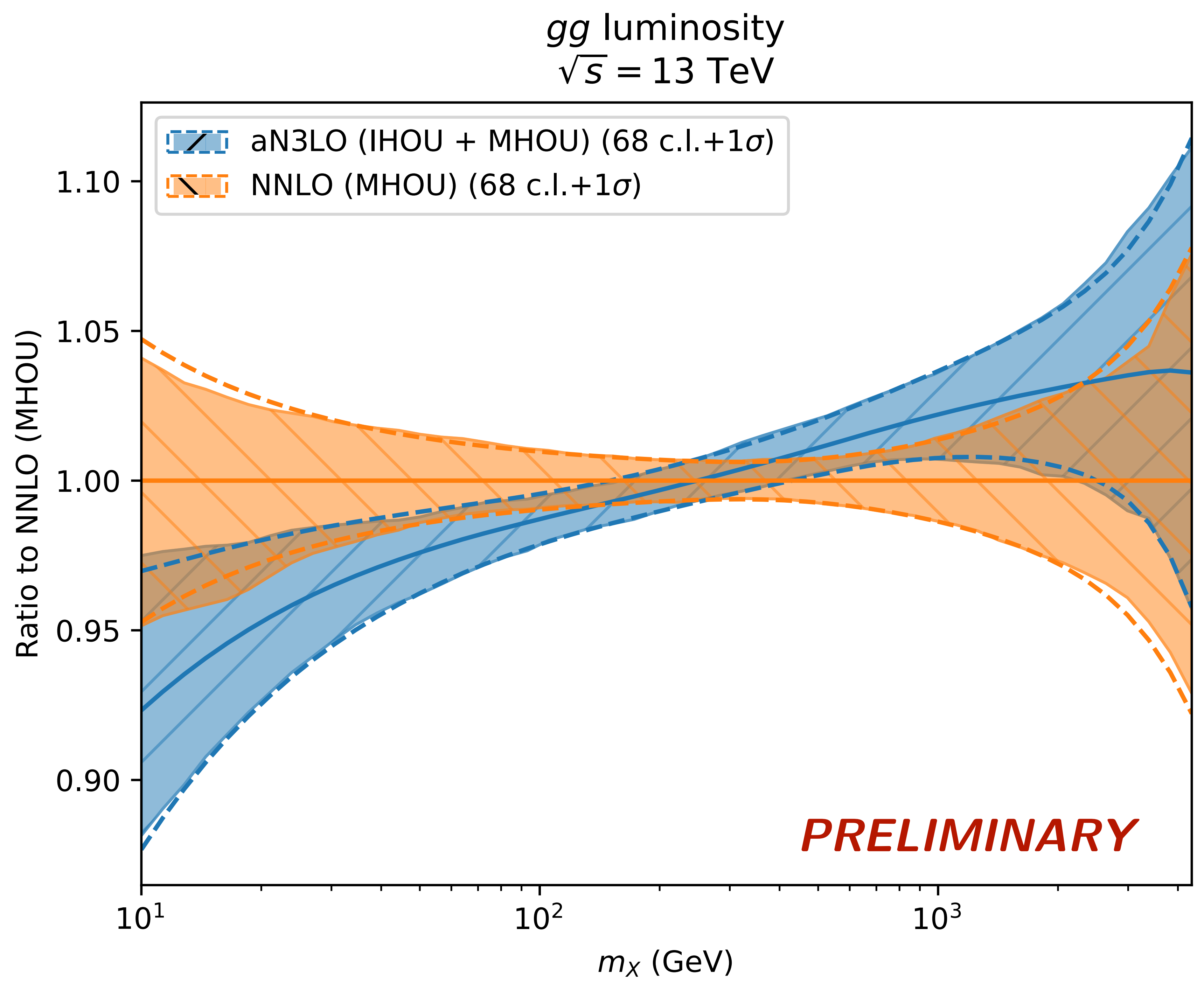




- At **large-x** PDFs are compatible within one sigma with NNLO and MHOU.

- Modification to partonic **luminosities** are visible especially for **gg,** which can be relevant for LHC.





- Theory inputs at N3LO.
- Towards NNPDF4.0 aN3LO.
- **MSHT20aN3LO**

MSTH20 aN3LO

[arxiv:2207.04739]

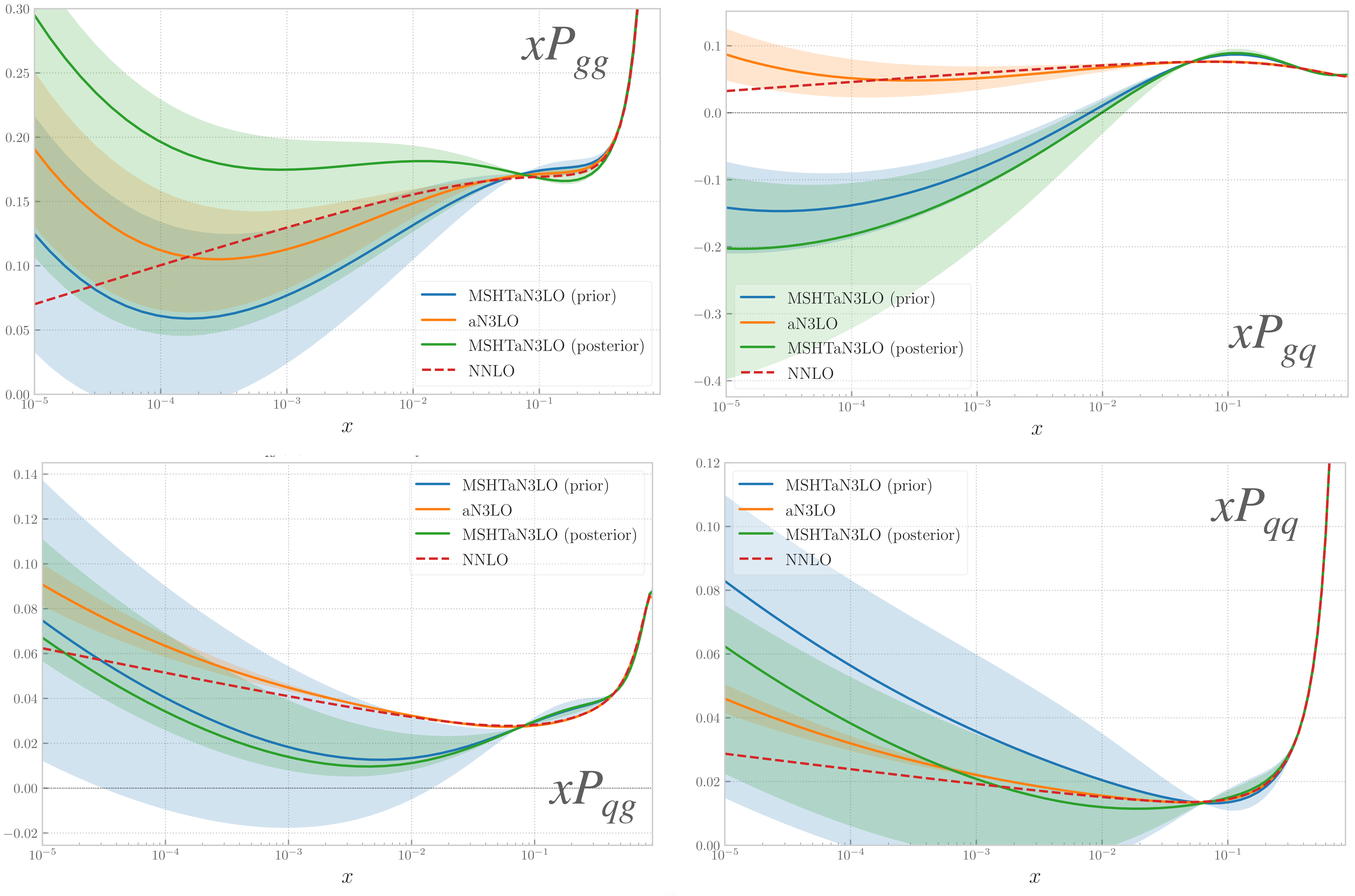
- The only public available aN3LO PDF determination is from the **MSHT** collaboration.

- **Similar** (but not identical) **theoretical inputs** are used: splitting functions limits, Mellin moments, ZM DIS coefficients, massive DIS limits.

Differences:

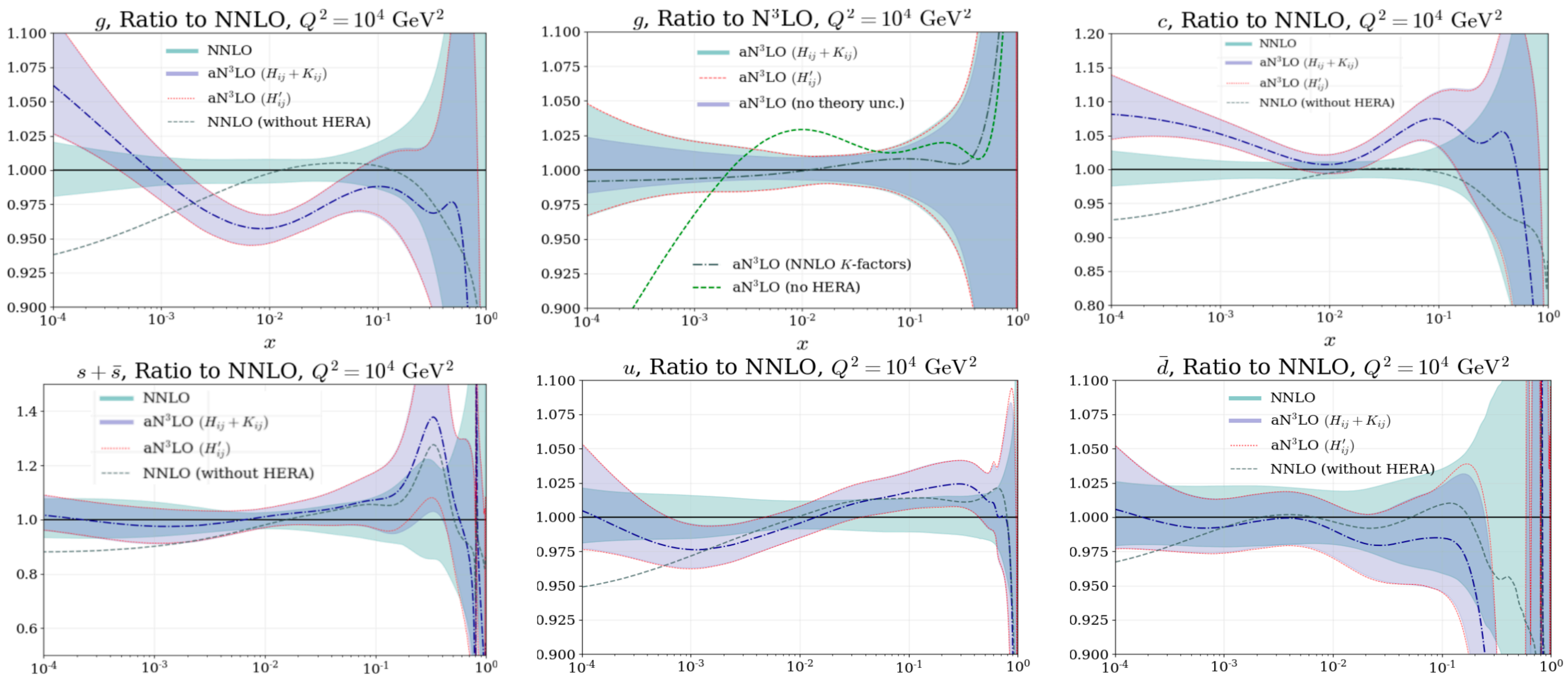
- Some N3LO contributions has been computed in the meantime.
- THu are estimated by means of **nuisance parameters**. No THu for NNLO fits.
- Hadronic k-Factors.
- Fitting methodology.
- Pertubative charm only.

Singlet aN3LO splitting functions comparison with MSHT aN3LO.



MSTH20 aN3LO PDFs set

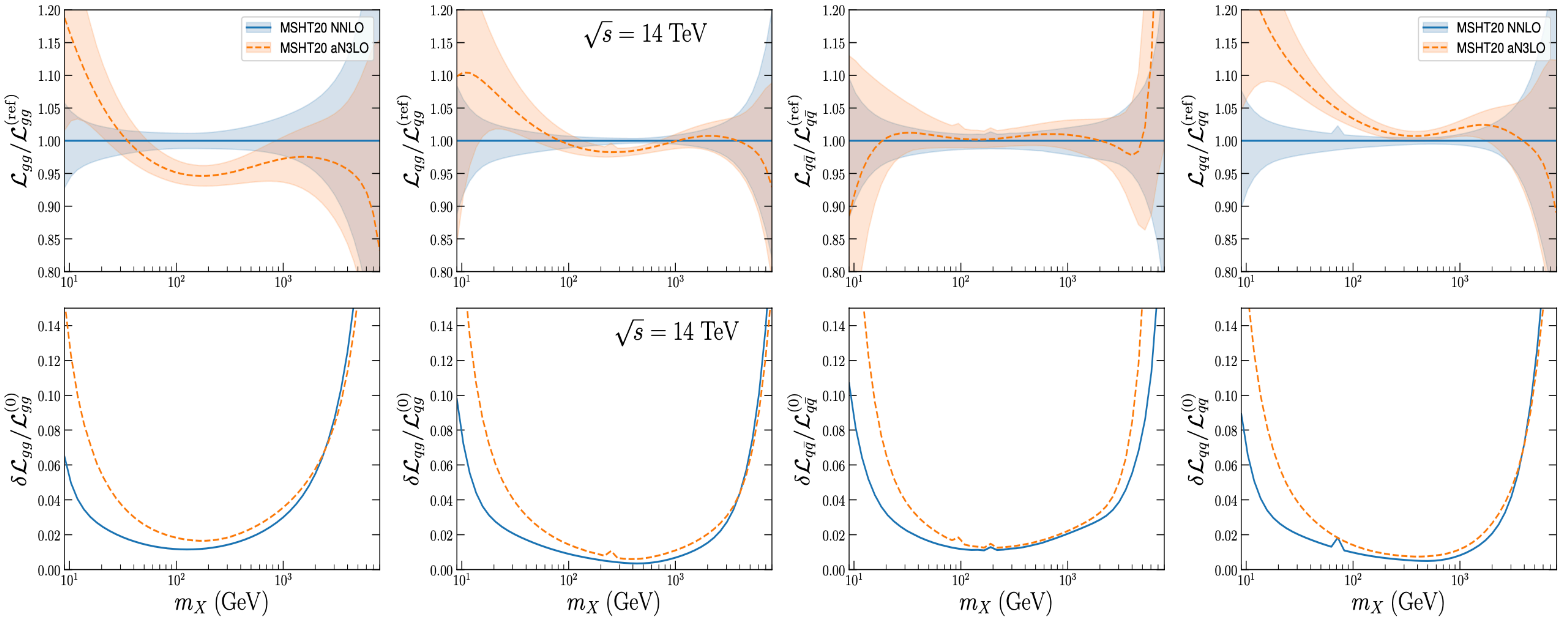
[arxiv:2207.04739]   From Thomas Cridge, Les Houches 2023



- N3LO corrections to gluon in mid-x are quite relevant (up to 4-5 %).
- Heavy quarks (perturbatively generated) raised.
- Uncertainties may be enlarged at low-x from THu.
- Improvement of the description of the HERA data and LHC jets (at the χ^2 level).

MSTH20 aN3LO luminosities

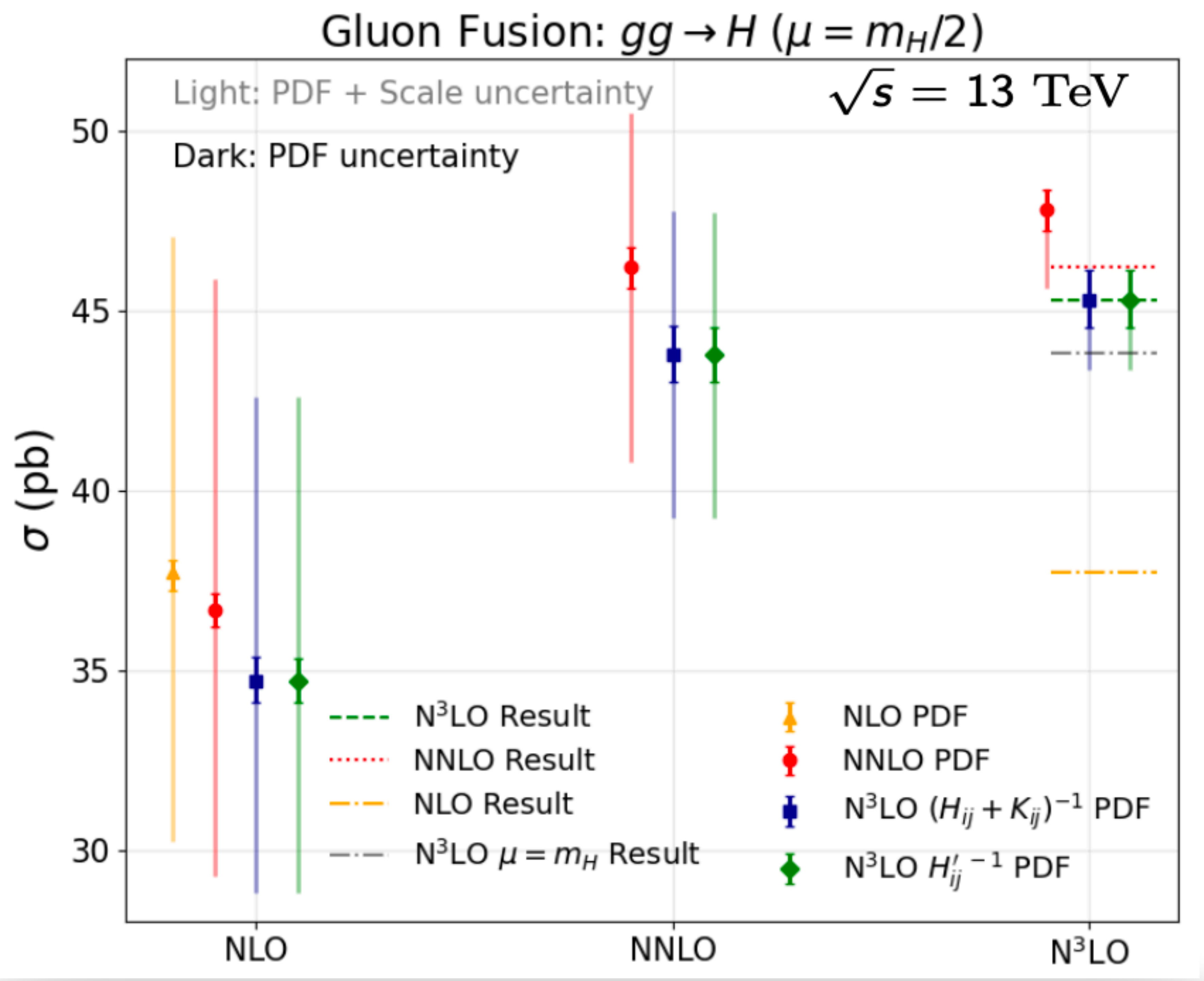
[arxiv:2207.04739]



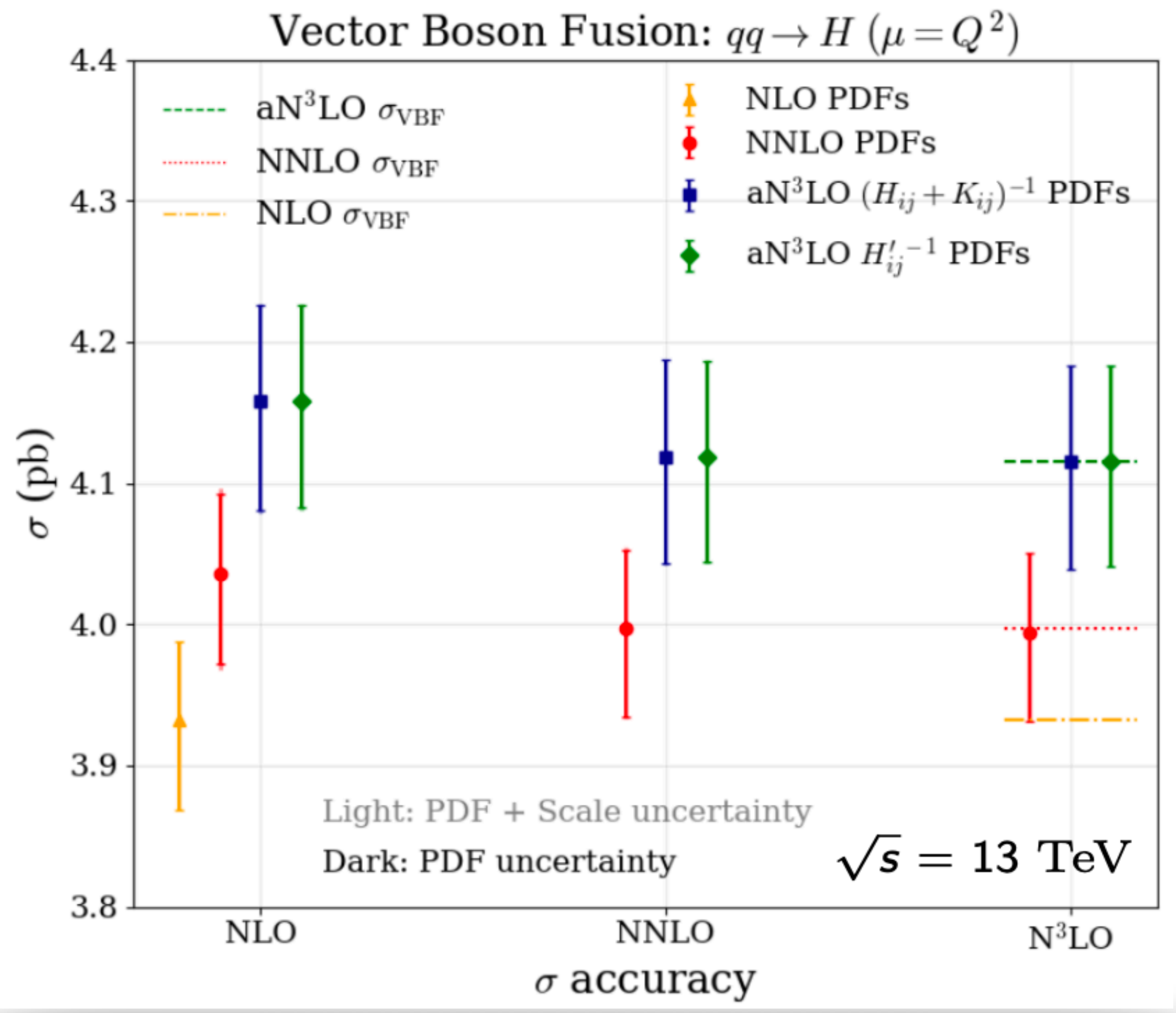
From Thomas Cridge, Les Houches 2023

Impact on H cross section

- A change in N3LO matrix elements can be compensated by reduction in PDFs at N3LO.
- MSHT20 aN3LO reports 5% ($gg \to H$) and 2.5% (VBF) effects for LHC Higgs cross sections.
- Changes in gluon and heavy quarks (large-x) are crucial for Higgs production at LHC.
- **N3LO predictions require N3LO PDFs.**



proVBF [arxiv:1606.00840]



ggHiggs [arxiv:1306.6633]

Summary & Conclusion

Summary & Conclusion

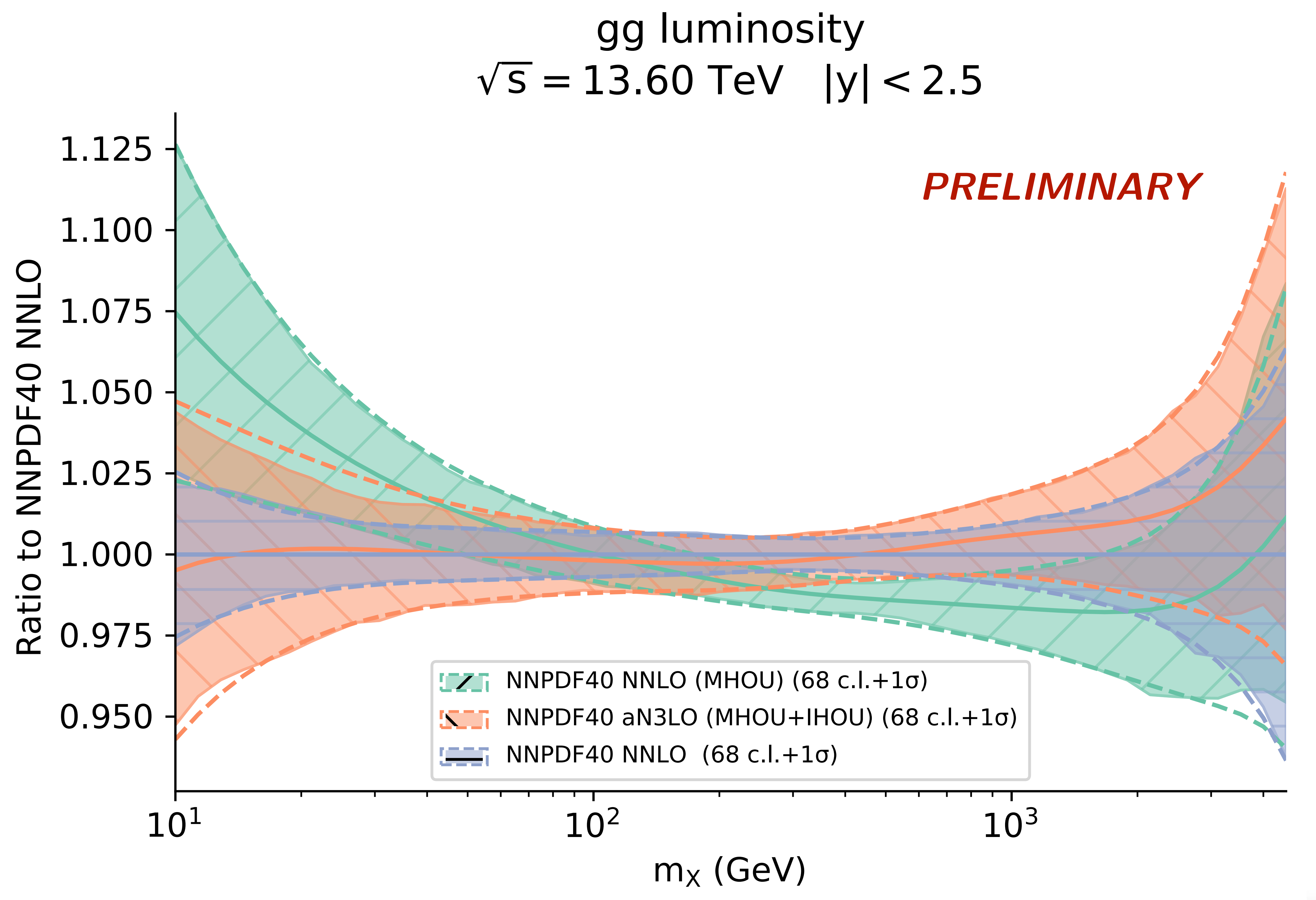
Latest NNPDF4.0 PDF fit doesn't contain theory uncertainties and is limited to NNLO QCD accuracy.

We are about to release 3 updates:

✓ NNLO PDF determination with QED → **NNPDF4.0 QED**

✓ NNLO PDF with MHOU → **NNPDF4.0 MHOU**

✓ Approximate N3LO PDF → **NNPDF4.0 aN3LO**

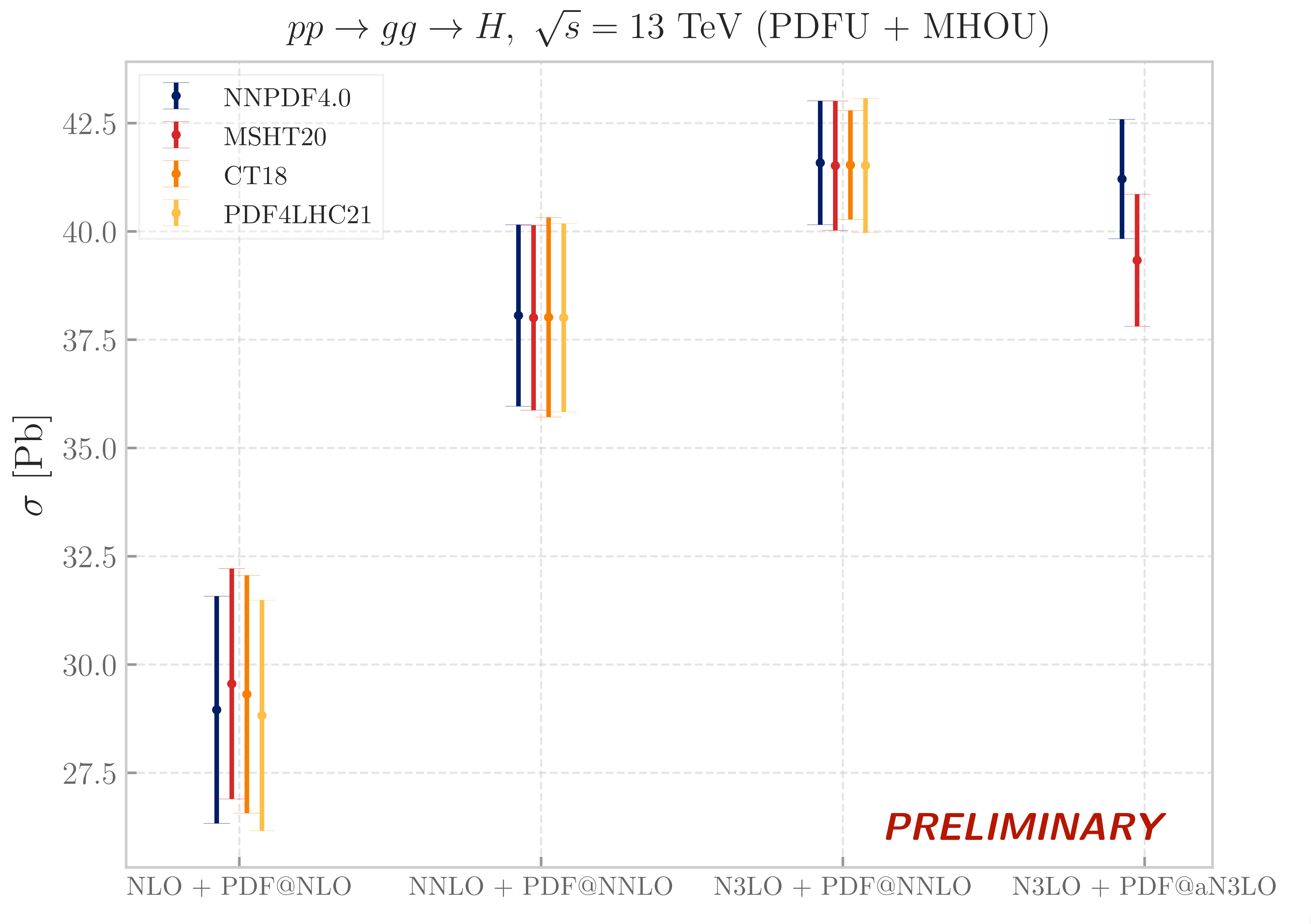


Further developments will be devoted to include EW corrections, validate fitting methodology and extend dataset included.

See also J.Rojo talk on Tuesday

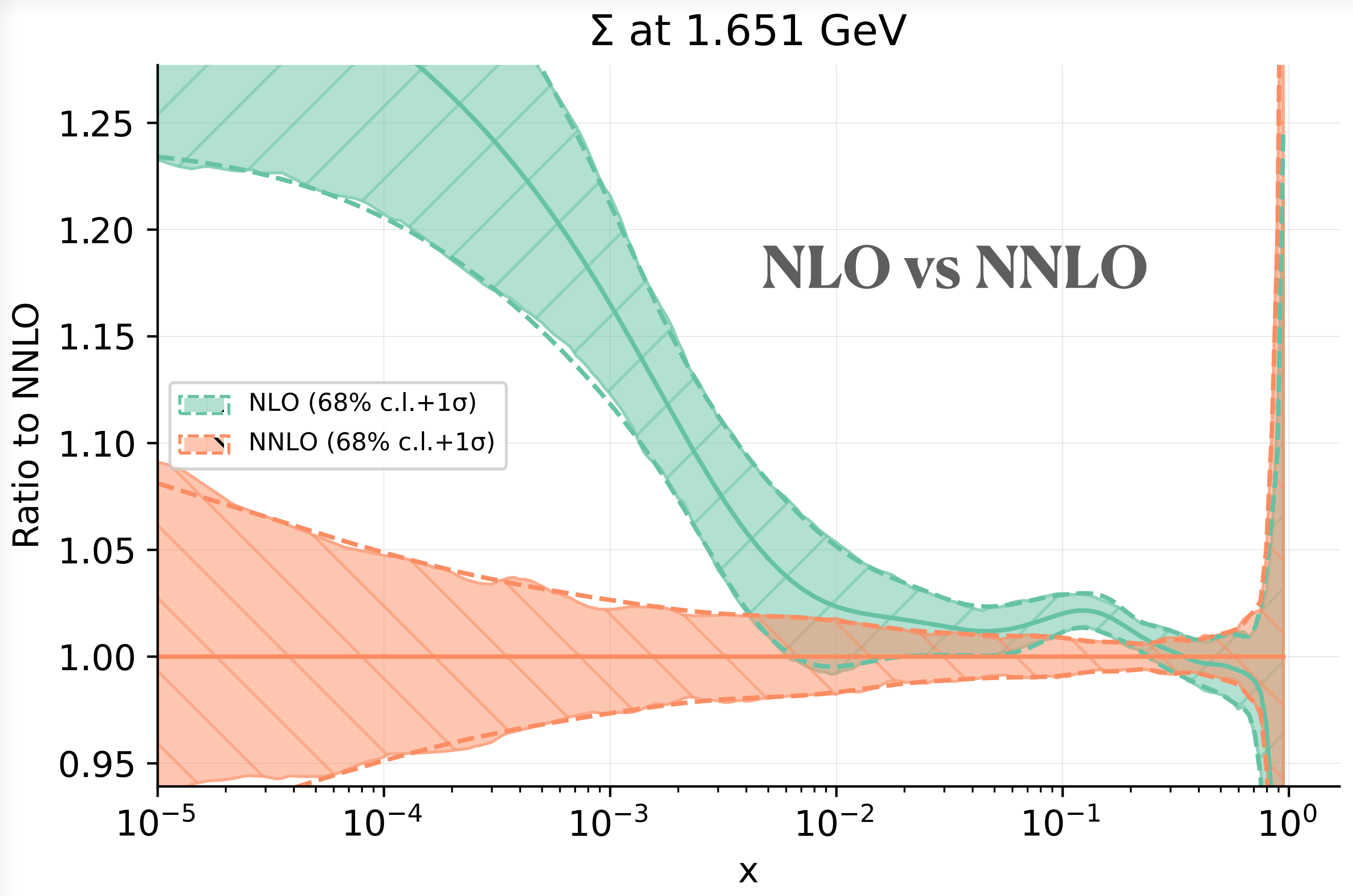
Summary & Conclusion

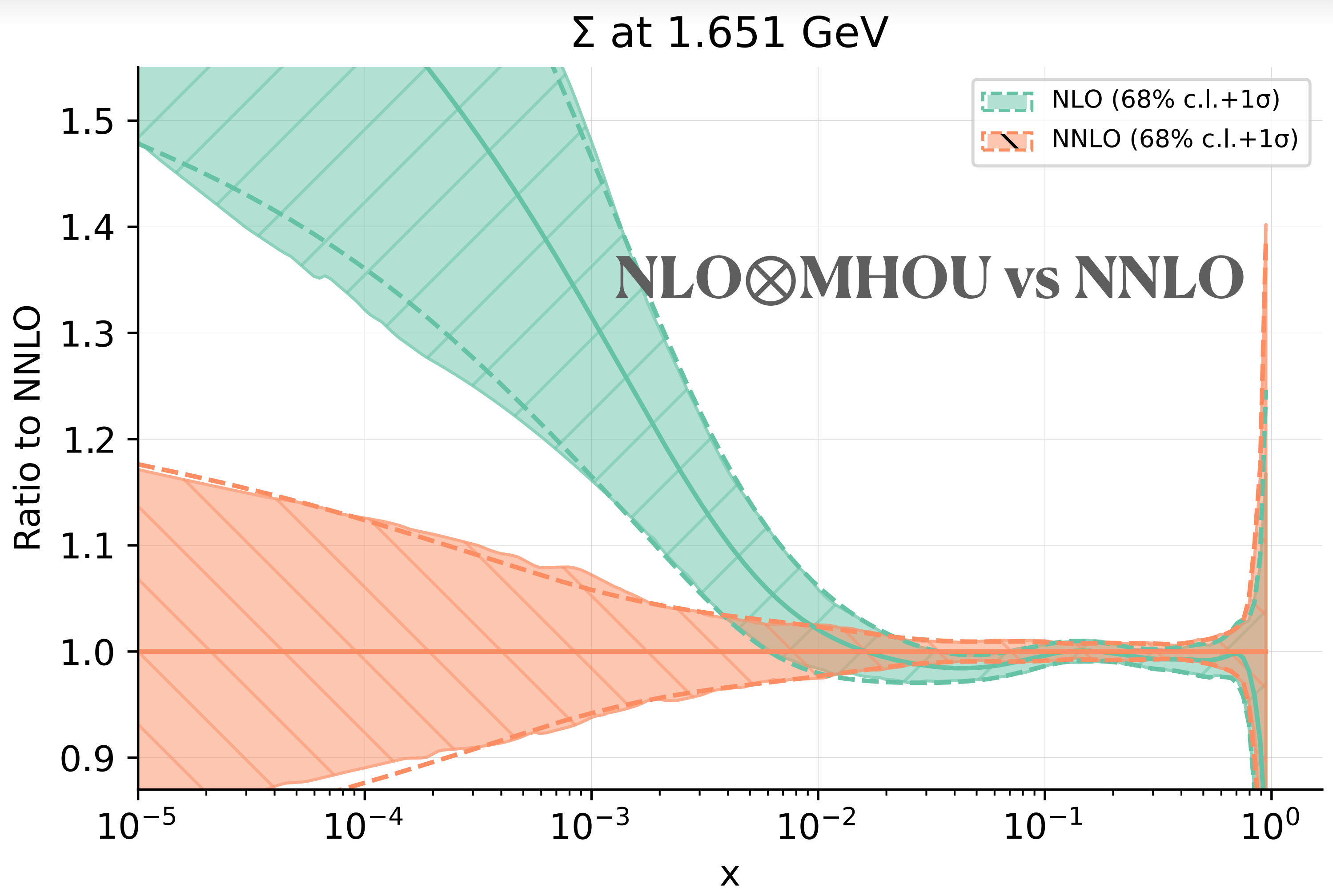
- Computing precise and accurate LHC observables require including theory uncertainties in PDFs.
- First aN3LO PDFs from the major fitting groups are (will be soon) available.
- Ongoing effort to benchmark inputs and validate these results.
- aN3LO PDFs mainly include aN3LO corrections to **DGLAP** and **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**.

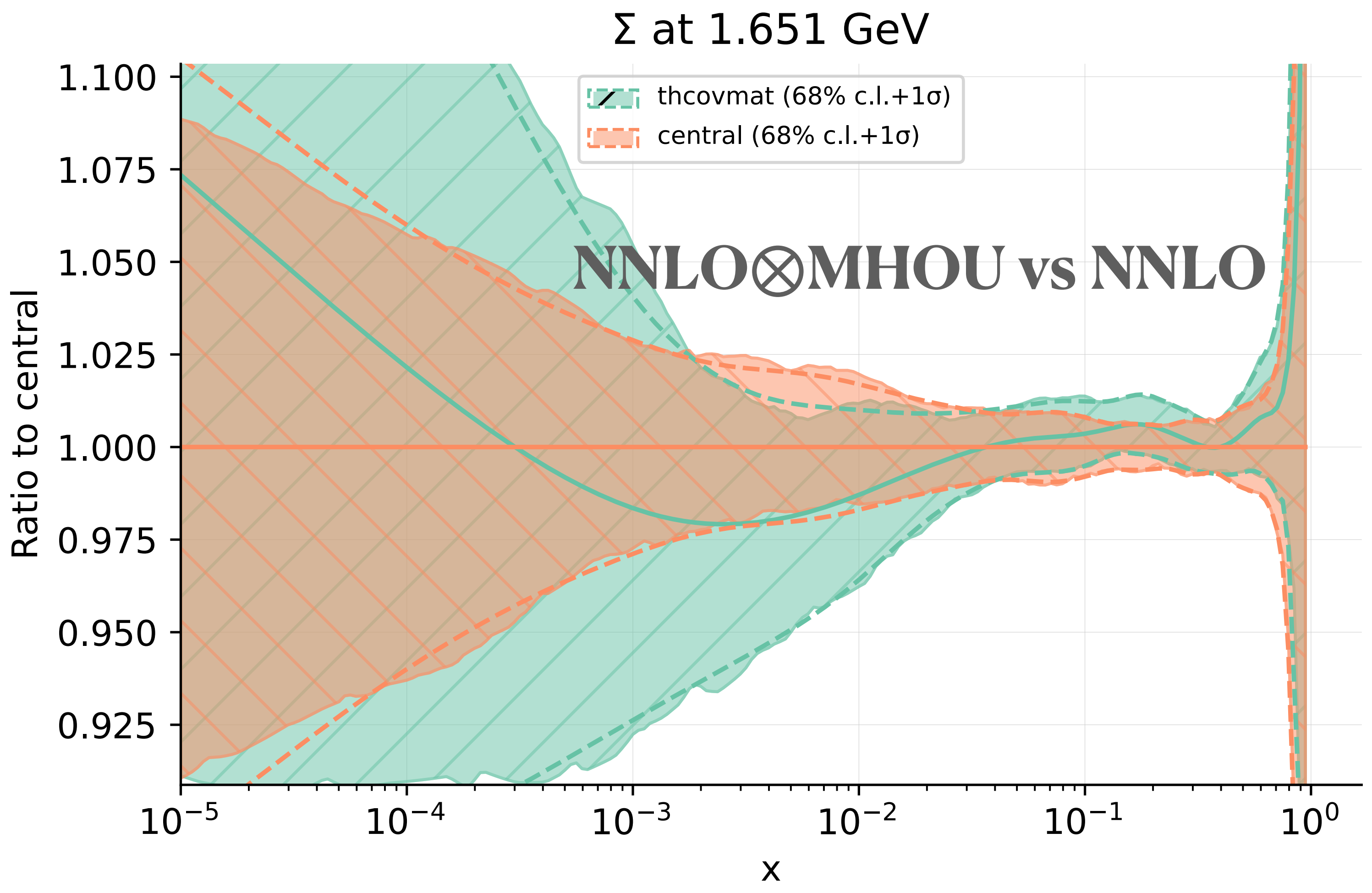


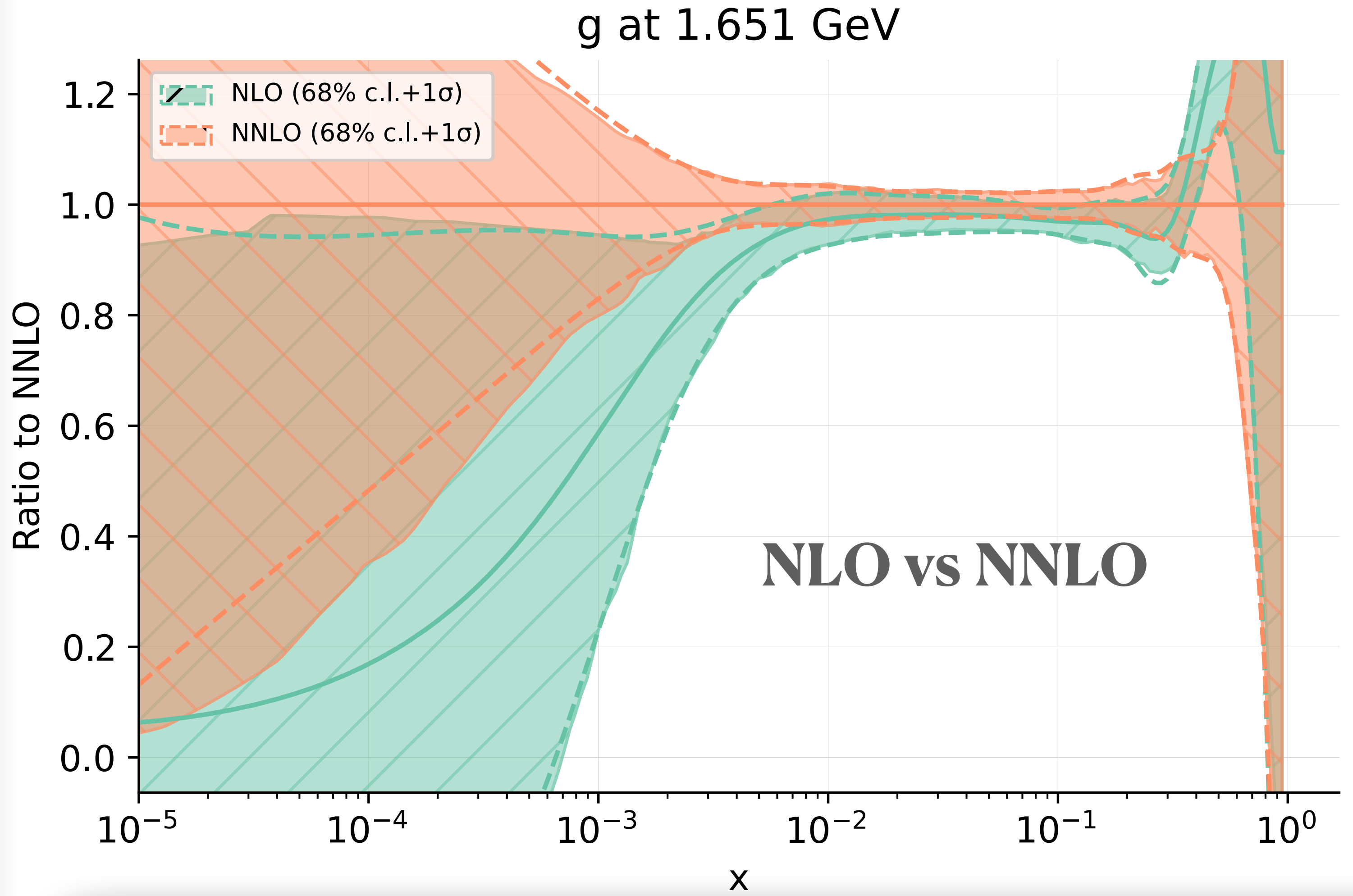
ggHiggs Bonvini et al. [arxiv:1306.6633]

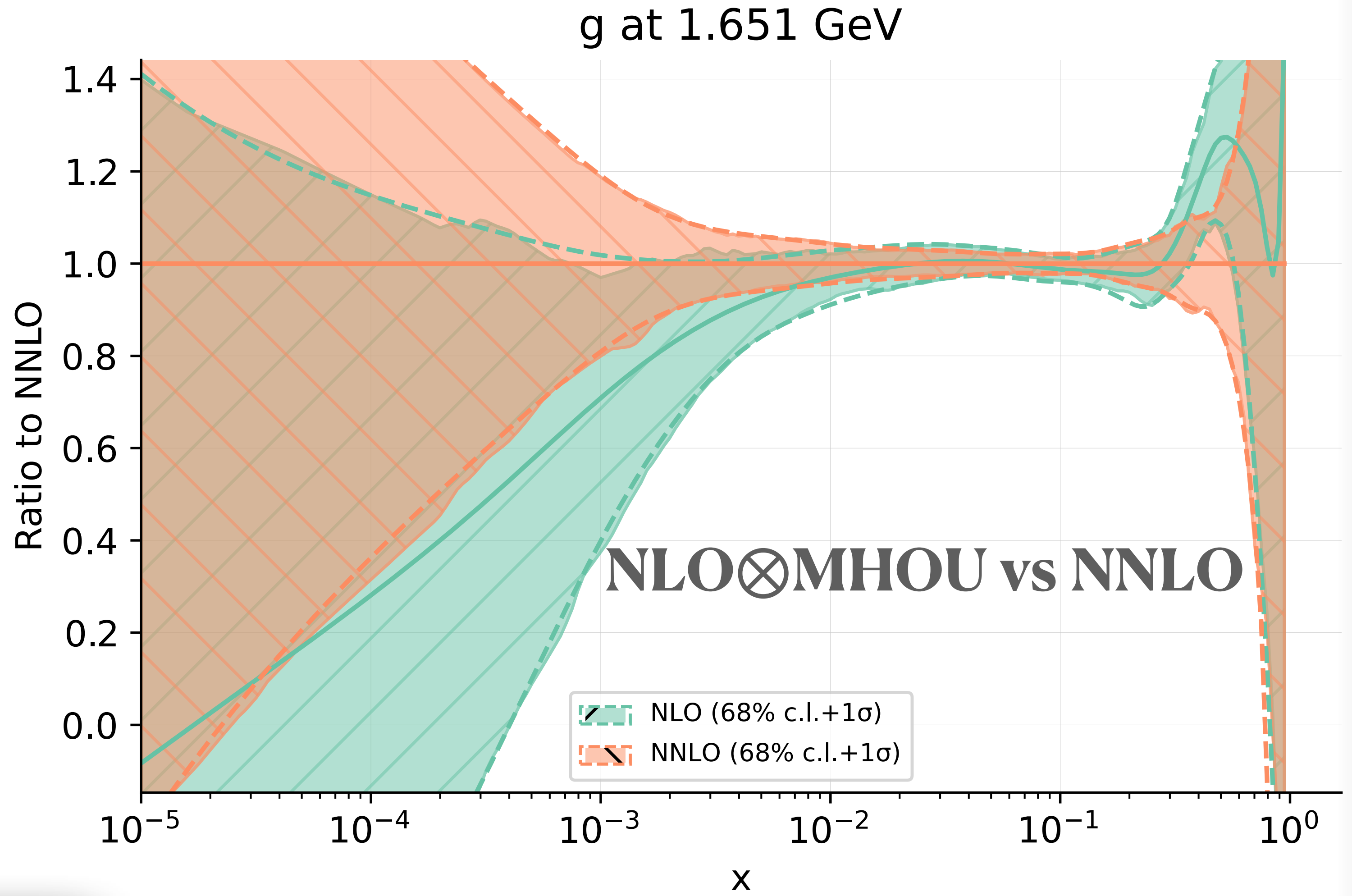
Impacts of MHOUs on PDFs

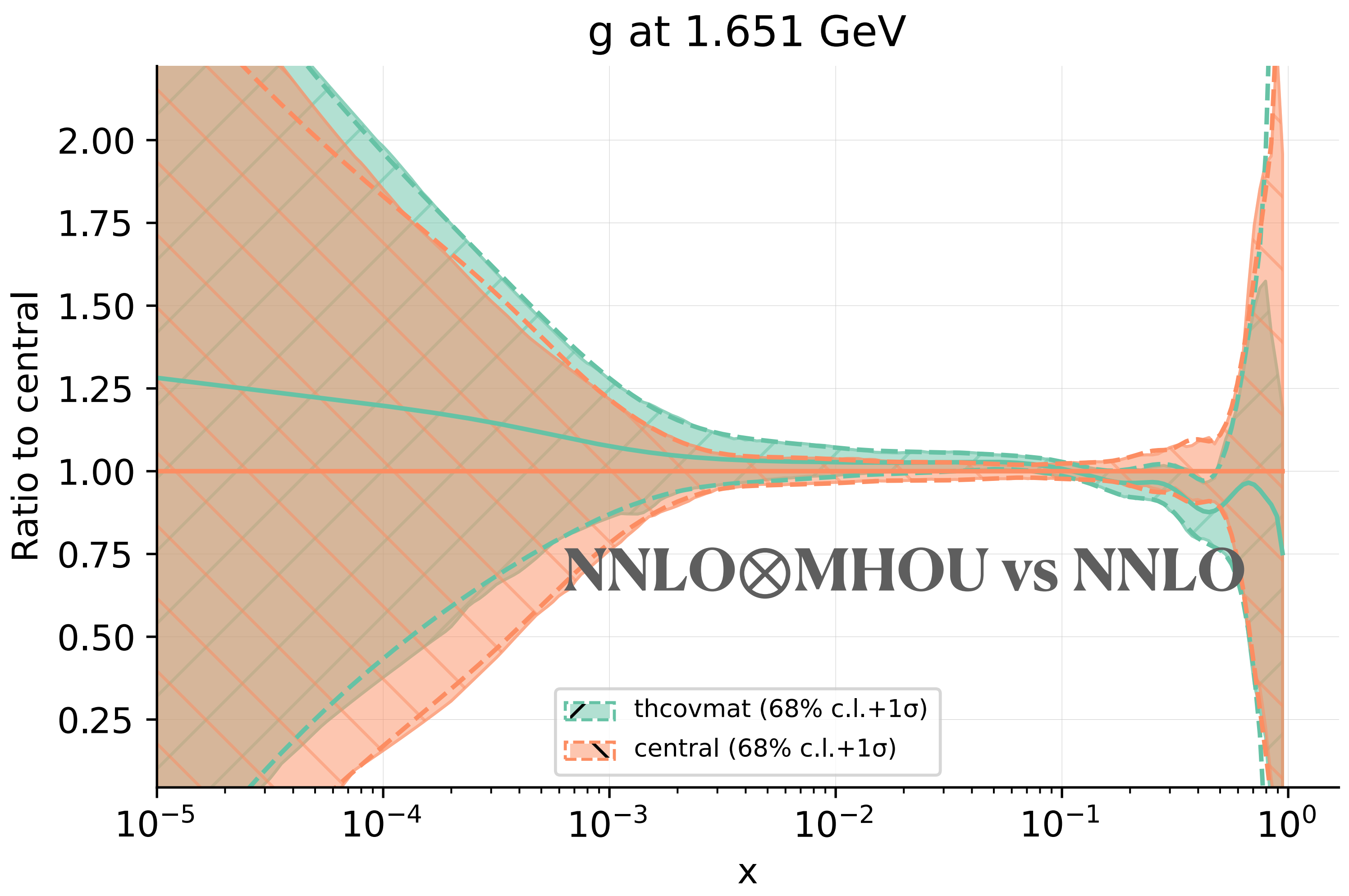








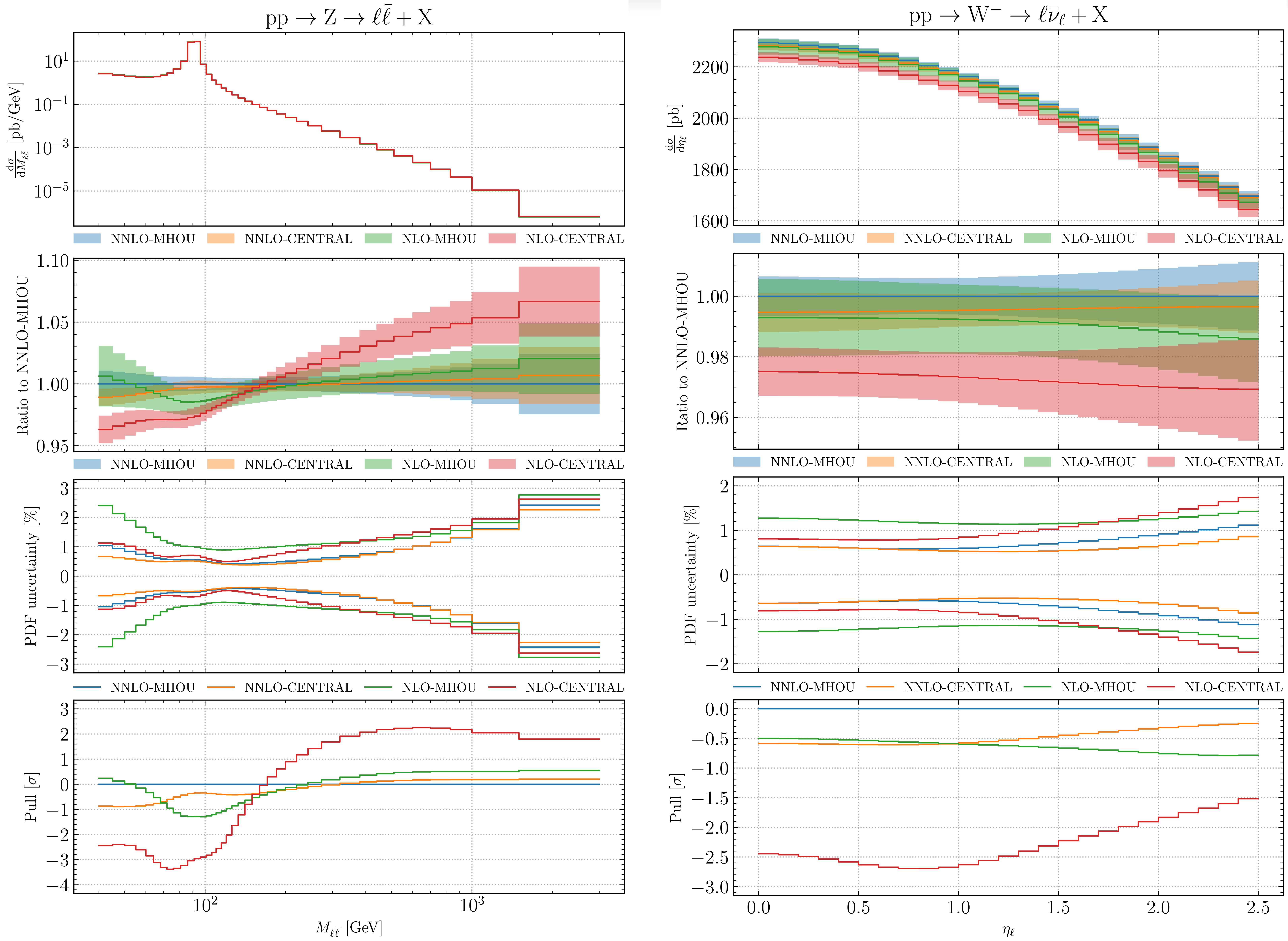




Compare Perturbative Convergence

From T. R. Rabemananjara

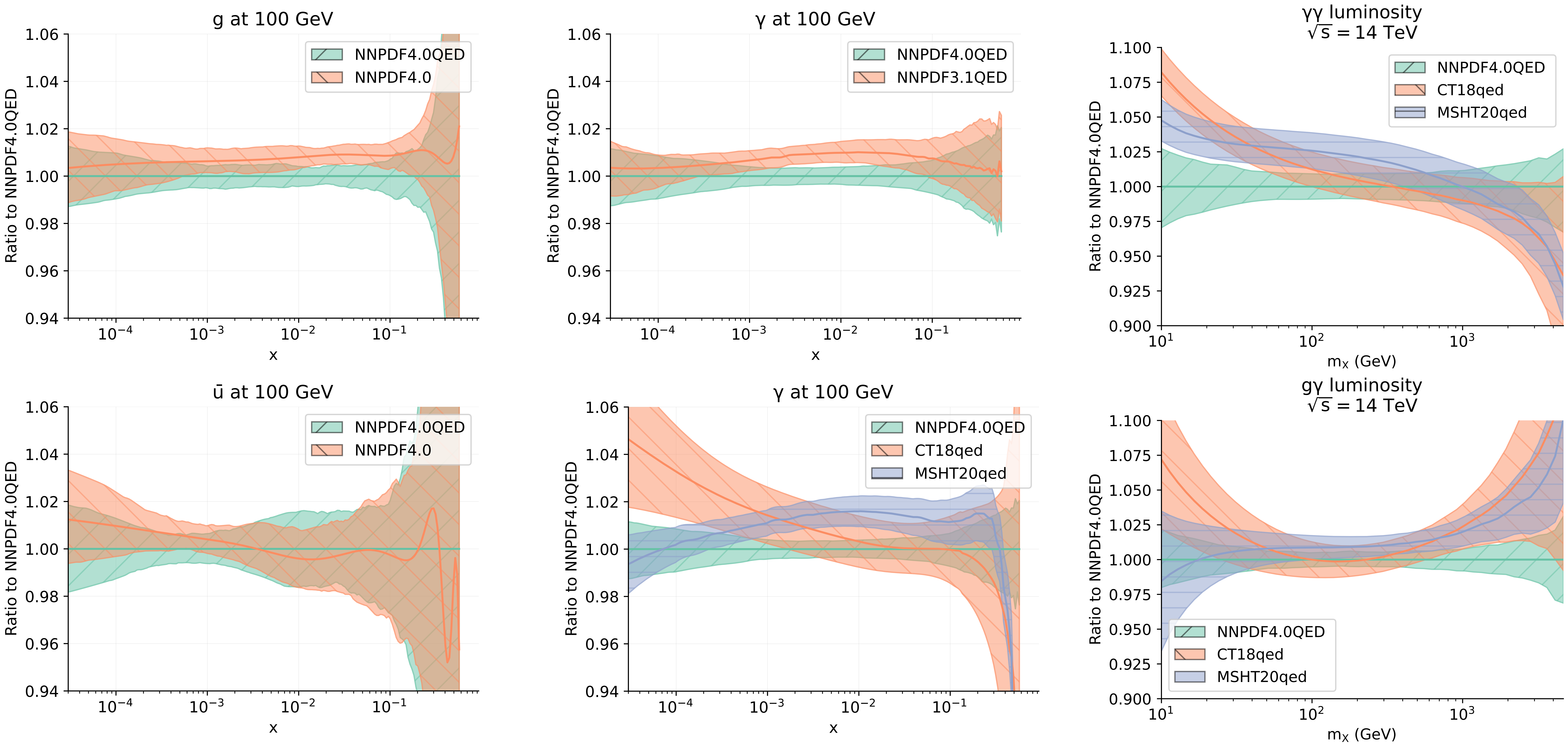
Phenomenological Impacts of MHOUs



- **NLO-MHOU** predictions are closer to **NNLO** than pure **NLO**.
- Very good agreement between **NNLO** and **NNLO-MHOU**.
- MHOUs **improve perturbative convergence** from **NLO** to **NNLO**.
- **NLO** vs. **NNLO** exhibit the **largest Uncertainty Pull**.

From T. R. Rabemananjara

NNLO QCD ⊗ QED PDFs



From T. R. Rabemananjara