Towards NNPDF aN3LO PDFs with theory uncertainties

Giacomo Magni,
Nikhef Theory Group and VU Amsterdam

Les Houches 2023,
16 June 2023

In collaboration with:

R.D.Ball, A.Barontini, A.Candido, S.Carrazza, J.Cruz-Martinez, L.D.Debbio, S.Forte,
T.Giani, F.Hekhorn, Z.Kassabov, N.Laurenti, E.R.Nocera, J.Rojo, T.Rabemananjara, C.Schwan, R.Stegeman, M.Ubiali.

email: gmagni@nikhef.nl

How can we improve theory accuracy of NNPDF4.0?

➡ NNPDF4.0 PDFs are still at NNLO accuracy in QCD, need to go **aN3LO**.

➡ Inclusion of **theory uncertainties** while determining PDFs is relevant at this level of accuracy.

How can we improve theory accuracy of NNPDF4.0?

➡ NNPDF4.0 PDFs are still at NNLO accuracy in QCD, need to go **aN3LO**.

➡ Inclusion of **theory uncertainties** while determining PDFs is relevant at this level of accuracy.

PRELIMINARY

Theory uncertainties from scale variations

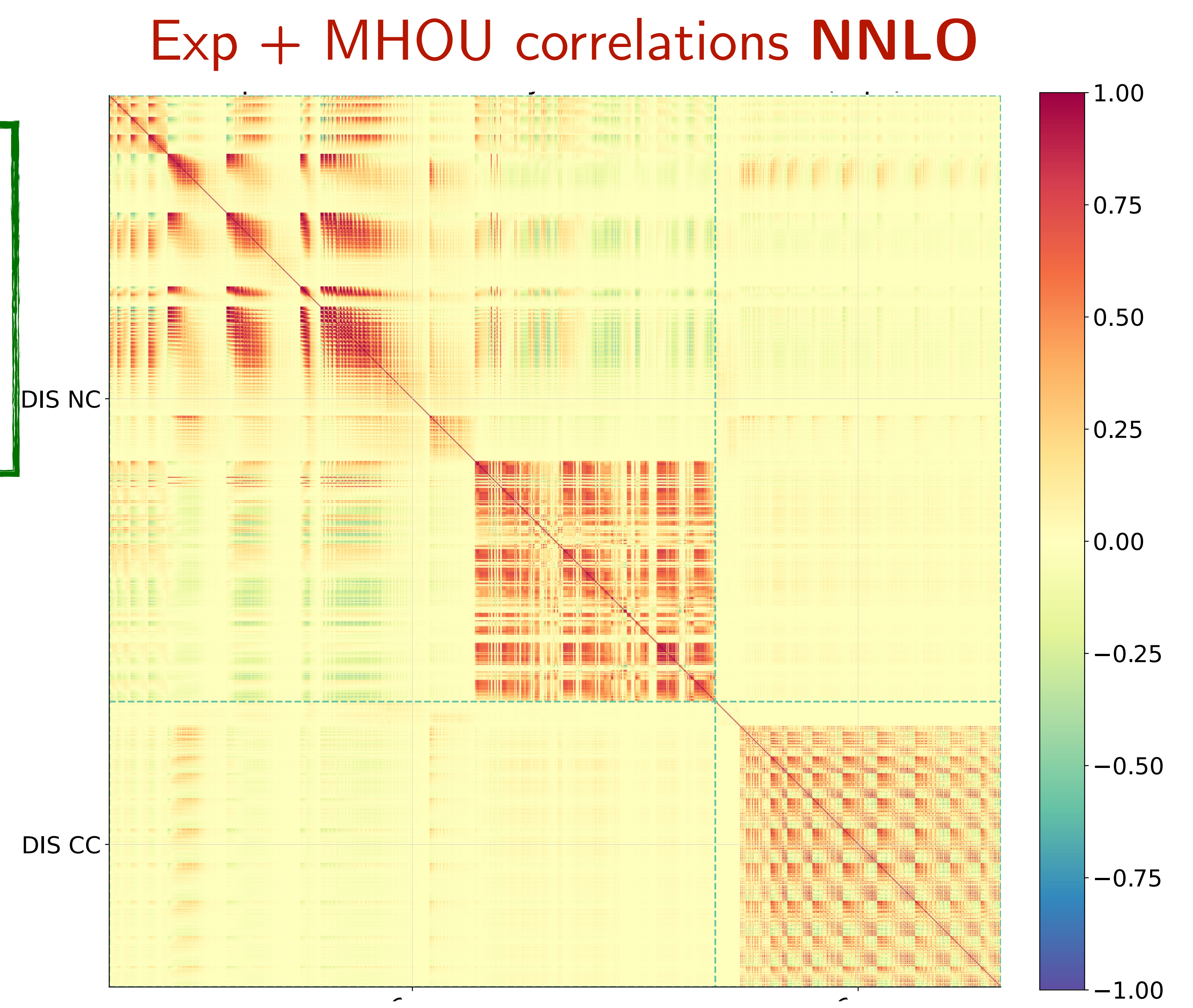
Scale variation advantages:

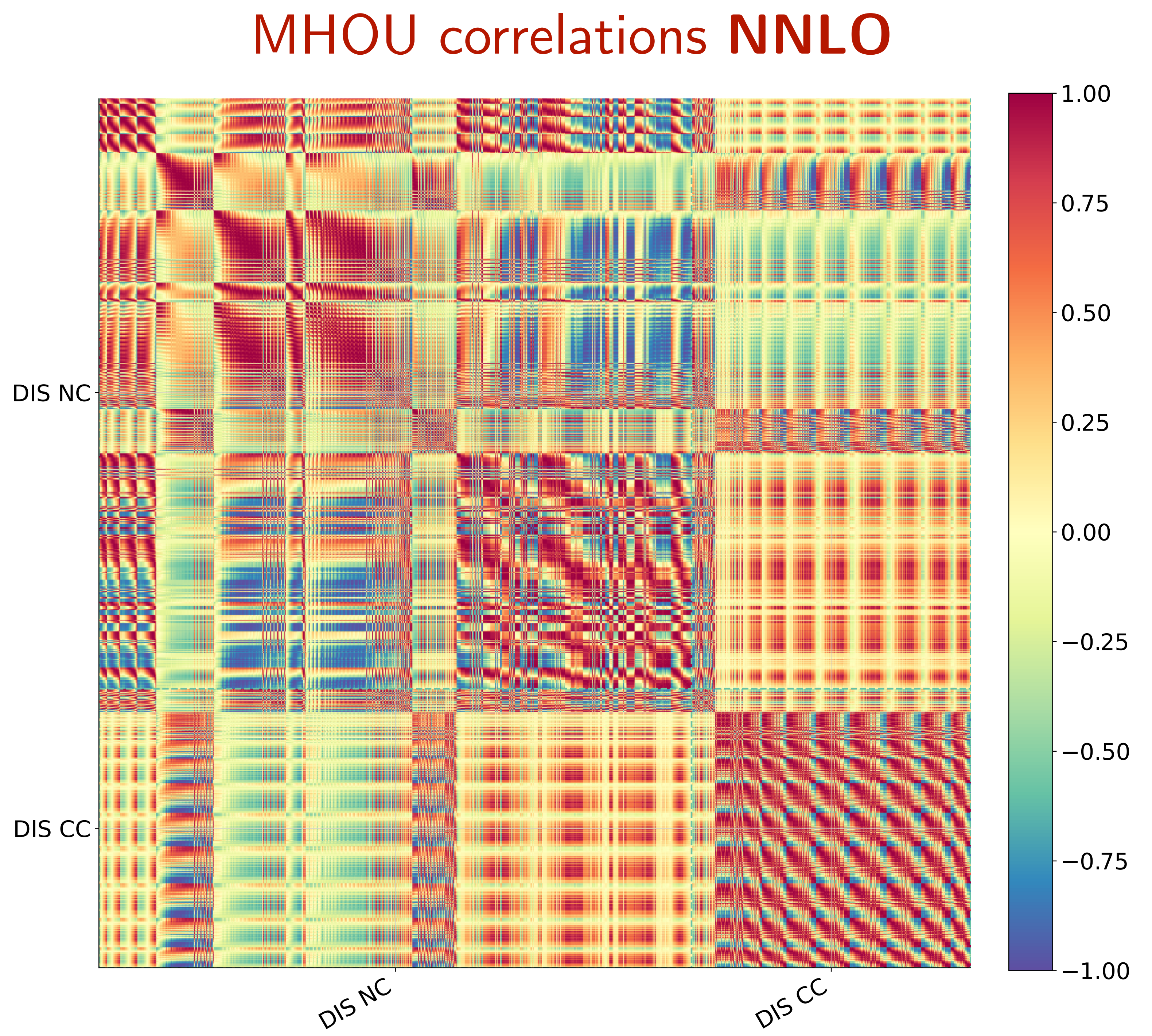
- Justified by RGE invariance.
- Valid for every process.

General formalism how to introduce theory uncertainties in PDFs have been addressed in various studies:
MSTH [arxiv:1811.08434], NNPDF [arxiv:1906.10698], [arxiv:2105.05114]

$$Cov = Cov_{Exp} + Cov_{Th}$$

- Scale Variations are not a unique procedure. There are many different schemes that can be used to compute MHOU.
- **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.



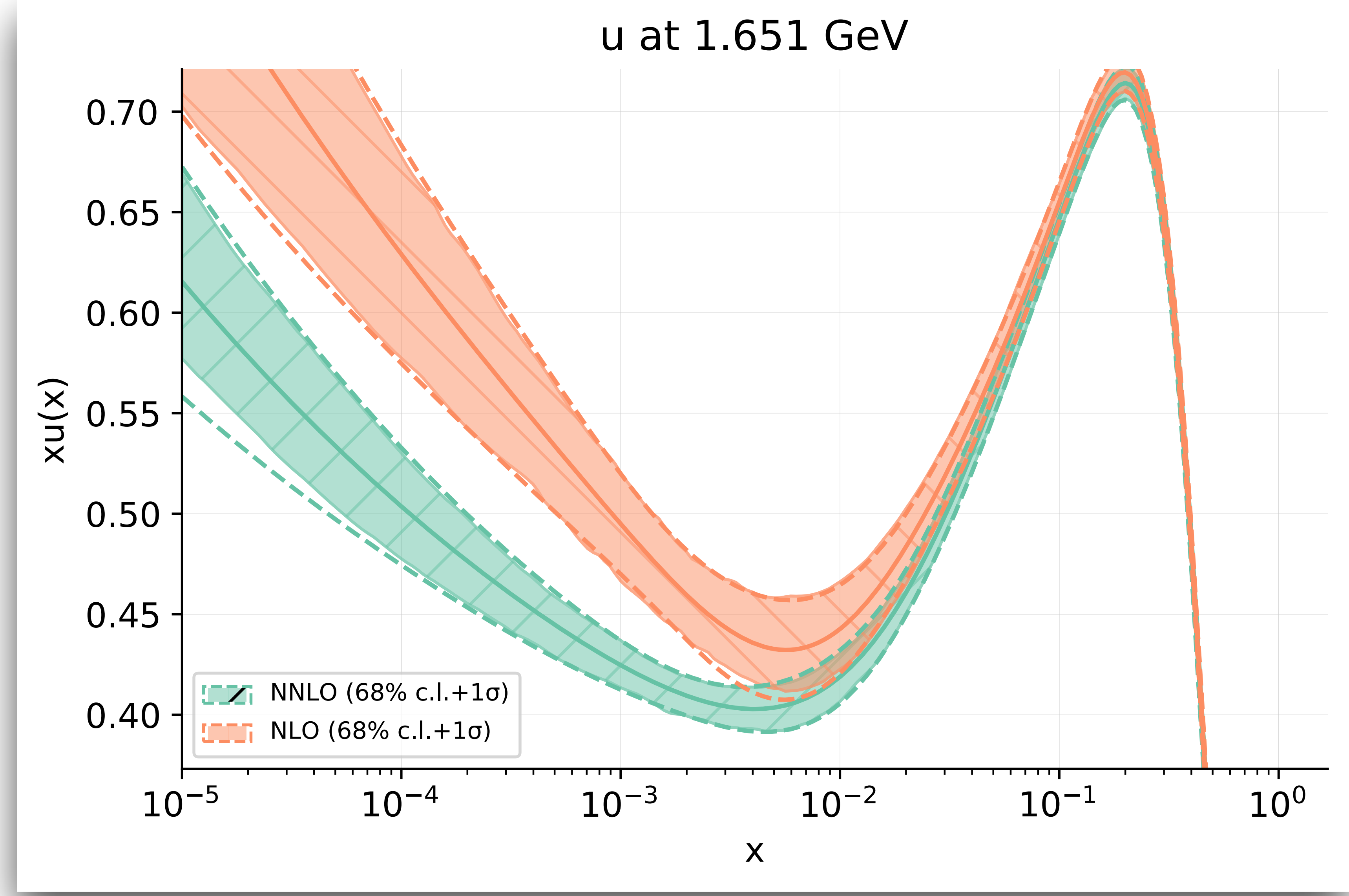


Impact of MHOU theory uncertainties

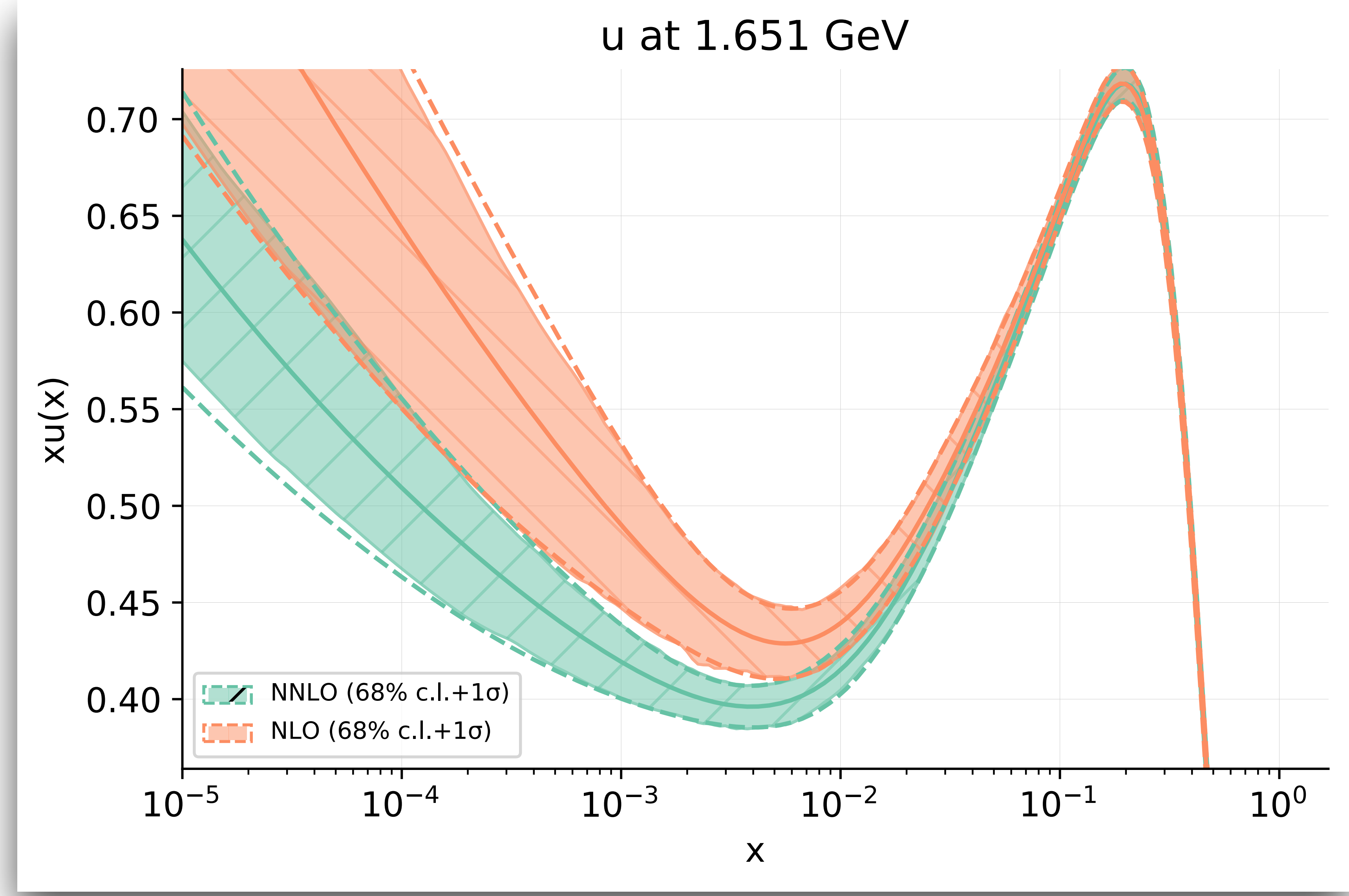
- μ_f/Q, μ_r/Q are varied in the range $[0.5,\ 1,\ 2]$
- 9 point prescription used.
- Effects on the PDF fit are non-trivial.

- Theory uncertainties add correlations between datasets, which are not taken into account in the experimental covariance mat.
- Reduction of χ^2/N_{dat} : $1.21 \rightarrow 1.19$
- Improvement in the perturbative convergence.

w/o Theory Uncertainties



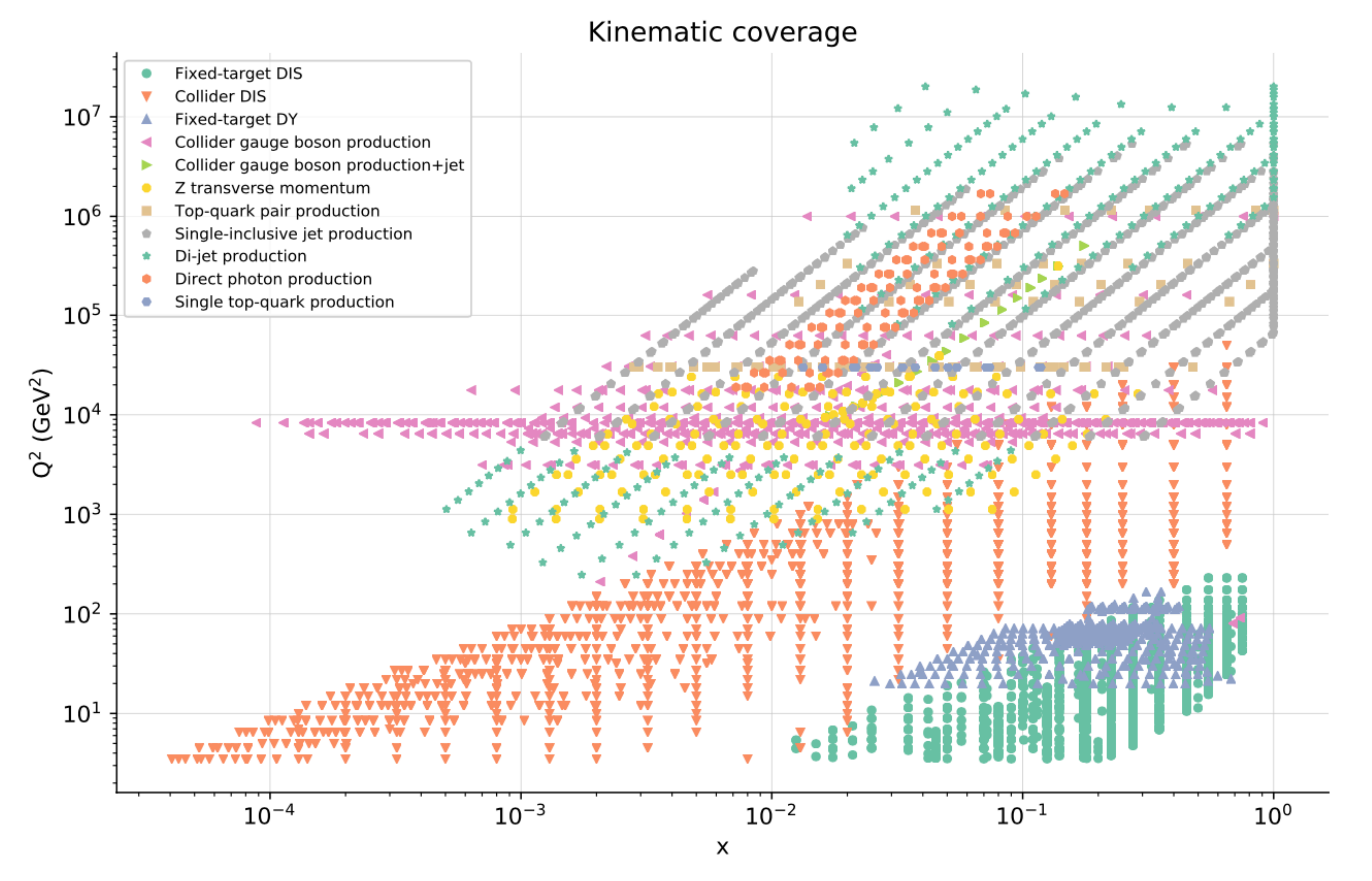
with Theory Uncertainties



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.
- **VFNS matching conditions** for each running component.
- **DIS partonic coefficients** functions, accounting for massive corrections when possible.
- **Hadronic coefficients**: which can be included mainly through *k-factors*.



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.
- **VFNS matching conditions** for each running component.
- **DIS partonic coefficients** functions, accounting for massive corrections when possible.
- **Hadronic coefficients**: which can be included mainly through *k-factors*.

➡ Construct reliable approximations from existing calculations.

➡ Determine theory uncertainties both from:

Incomplete Higher Order corrections IHOU

Missing Higher Order corrections MHOU

Not all of them are yet available at N3LO

PDF evolution @ aN3LO

Splitting functions

- Analytical calculations of the complete N3LO spitting functions are not available yet.
- At N3LO there are 7 different splitting functions to determine.
- Ideally would like to have a fast parametrisation, analytical structure too complex.

- **Non Singlet** splitting functions can be estimated with quite precise accuracy for phenomenological studies:

  Moch, Ruijl, Ueda, Vermaseren, Vogt [arXiv:1707.08315]; Davies, Vogt, Ruijl, Ueda, Vermaseren [arXiv:1610.07477]; Davies, Kom, Moch, Vogt [arXiv:2202.10362].

- **Singlet** splitting functions are more challenging and can be determined only with a finite accuracy.
  - **Large-n_f limit:** Davies, Vogt, Ruijl, Ueda, and Vermaseren. [arXiv:1610.07477]
  - **Small-x limit:** Bonvini and Marzani [arXiv:1805.06460]; Davies, Kom, Moch, Vogt. [arXiv:2202.10362]
  - **Large-x limit:** Duhr, Mistlberger, Vita [arXiv:2205.04493]; Henn, Korchemsky, Mistlberger [arXiv:1911.10174]; Soar, Moch, Vermaseren, Vogt [arXiv:0912.0369].
  - **Mellin Moments:** Moch, Ruijl, Ueda, Vermaseren, and Vogt[arXiv:2111.15561]; Falcioni, Herzog, Loch,Vogt [arXiv:2302.07593]

PDF evolution @ aN3LO
Splitting functions

$$\tilde{f}(N) = \int_0^1 x^{N-1} f(x) dx$$

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

For more details see
EKO N3LO documentation

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

1. Parametrise the difference between the *4 (10)* known moments and known limits with *4* functions $f_i(N)$.
2. Varying the sub-leading unknown $f_i(N)$ to produce a large set of parameterisation candidates (≈ 70).
3. Reduce the number of samples discarding too wiggly parameterisations and looking at the most representative cases.

- The spread among different linear combinations estimate IHOU.
- Only theoretical inputs are considered.
- All the implemented approximations respect momentum sum rules.
- Procedure tested at previous order.

For example in $P_{gg}(x)$:

1. Theoretical constraint include:
   - large-N:

$$\gamma_{gg}^{(3)}(N \to \infty) \approx A_{gg} S_1(N) + B_{gg} + \mathcal{O}\left(\frac{\ln(N)}{N}\right)$$

   - small-N pole at $N=0$, and $N=1$ *(leading contribution)*:

$$\gamma_{gg}^{(3)}(N \to 1) \approx C_4 \frac{1}{(N-1)^4} + C_3 \frac{1}{(N-1)^3} + \mathcal{O}\left(\frac{1}{(N-1)^2}\right)$$

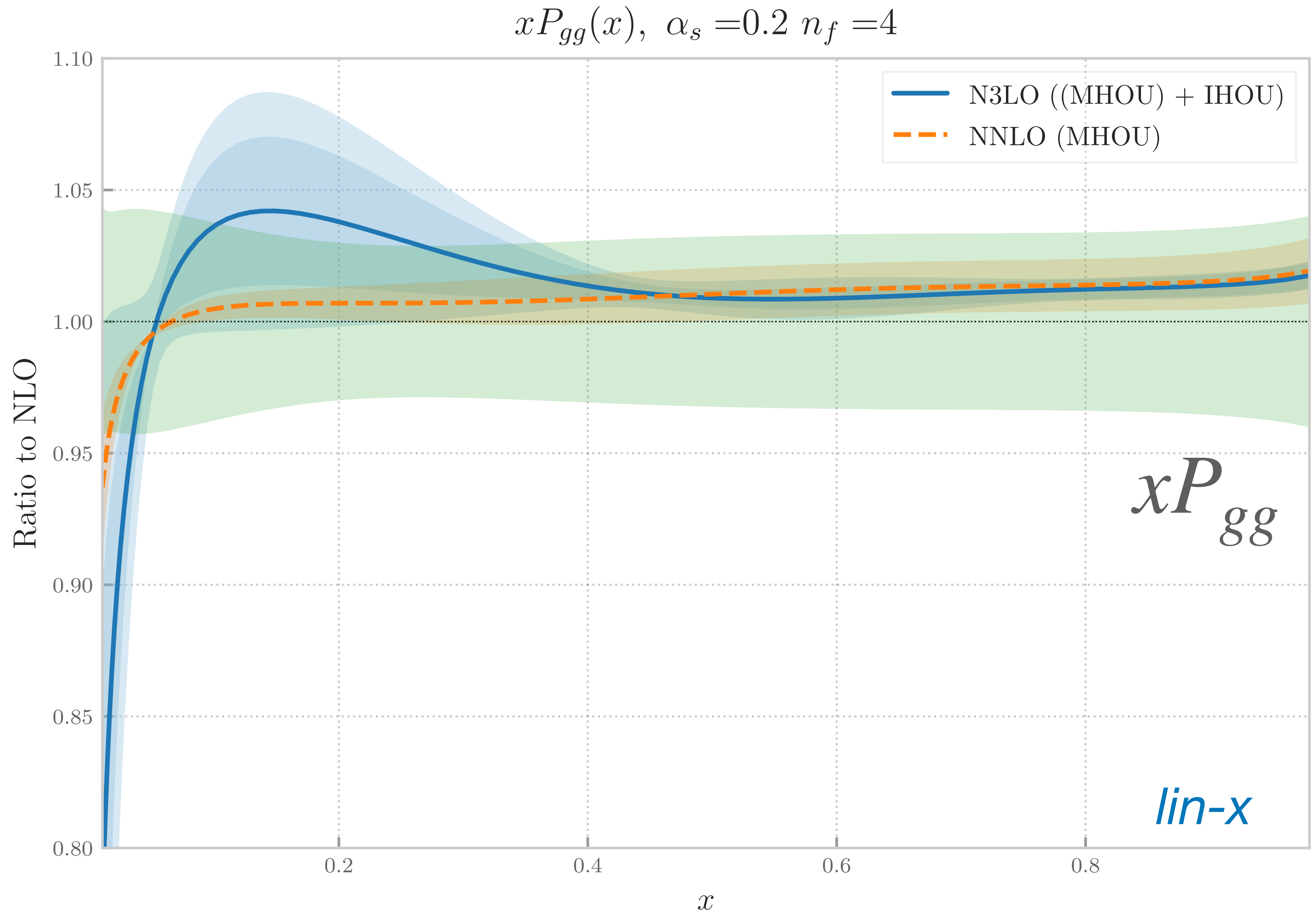
2. Solve the constraint given by the 4 known Mellin moments with many different candidates $\{f_1, f_2, f_3, f_4\}$:

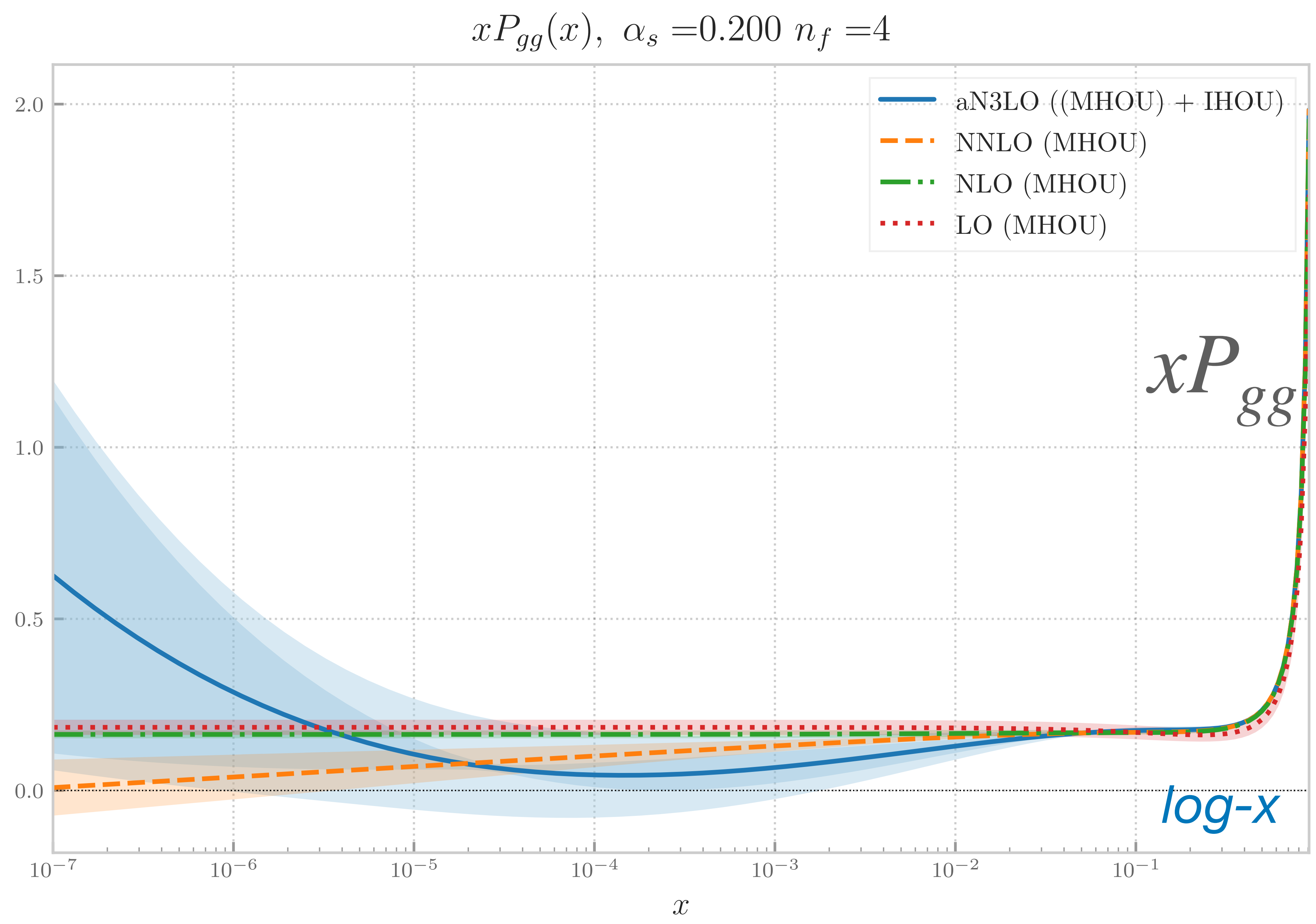
$$f_1 = \frac{S_1(N)}{N} \qquad f_3 = \left\{ \frac{1}{(N-1)}, \frac{1}{N} \right\}$$

$$f_4 = \left\{ \frac{1}{(N-1)}, \frac{1}{N^4}, \frac{1}{N^3}, \frac{1}{N^2}, \frac{1}{N}, \frac{1}{(N+1)^3}, \frac{1}{(N+1)^2}, \frac{1}{N+1}, \frac{1}{N+2}, \mathcal{M}[\ln(1-x)], \mathcal{M}[(1-x)\ln(1-x)], \frac{S_1(N)}{N^2} \right\}$$

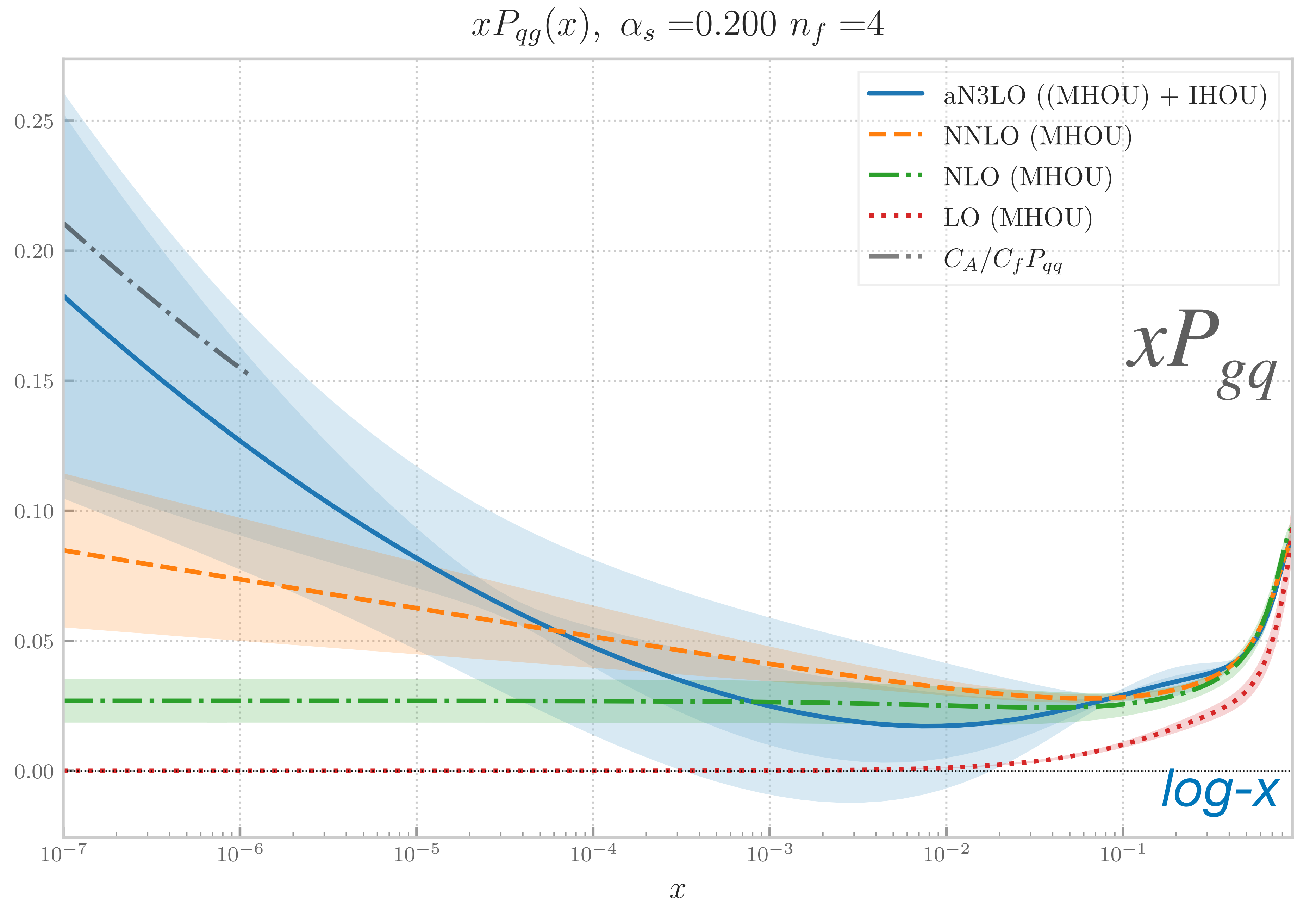
$$f_2 = \frac{1}{(N-1)^2}$$

PDF evolution @ aN3LO
Splitting functions



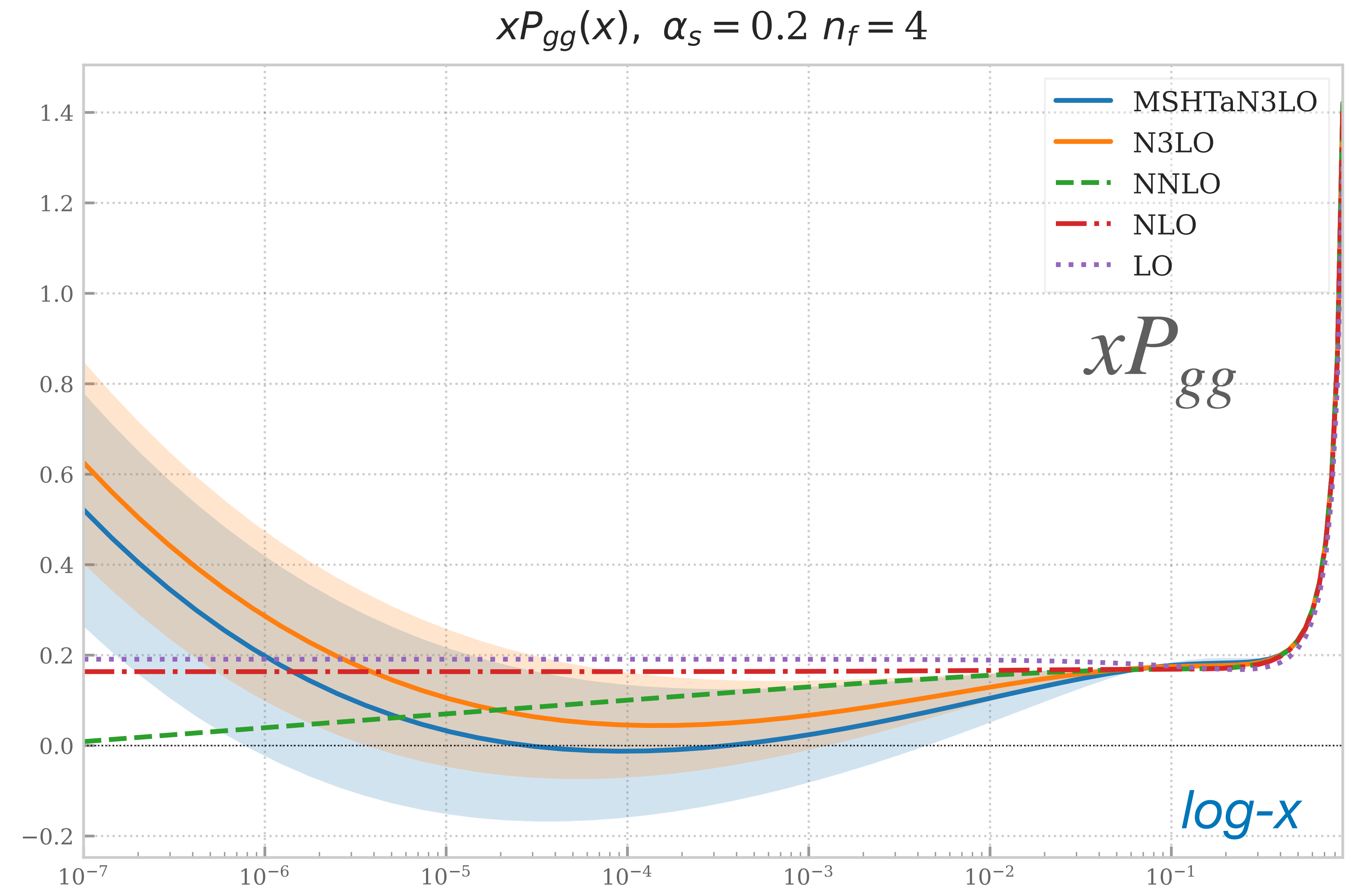


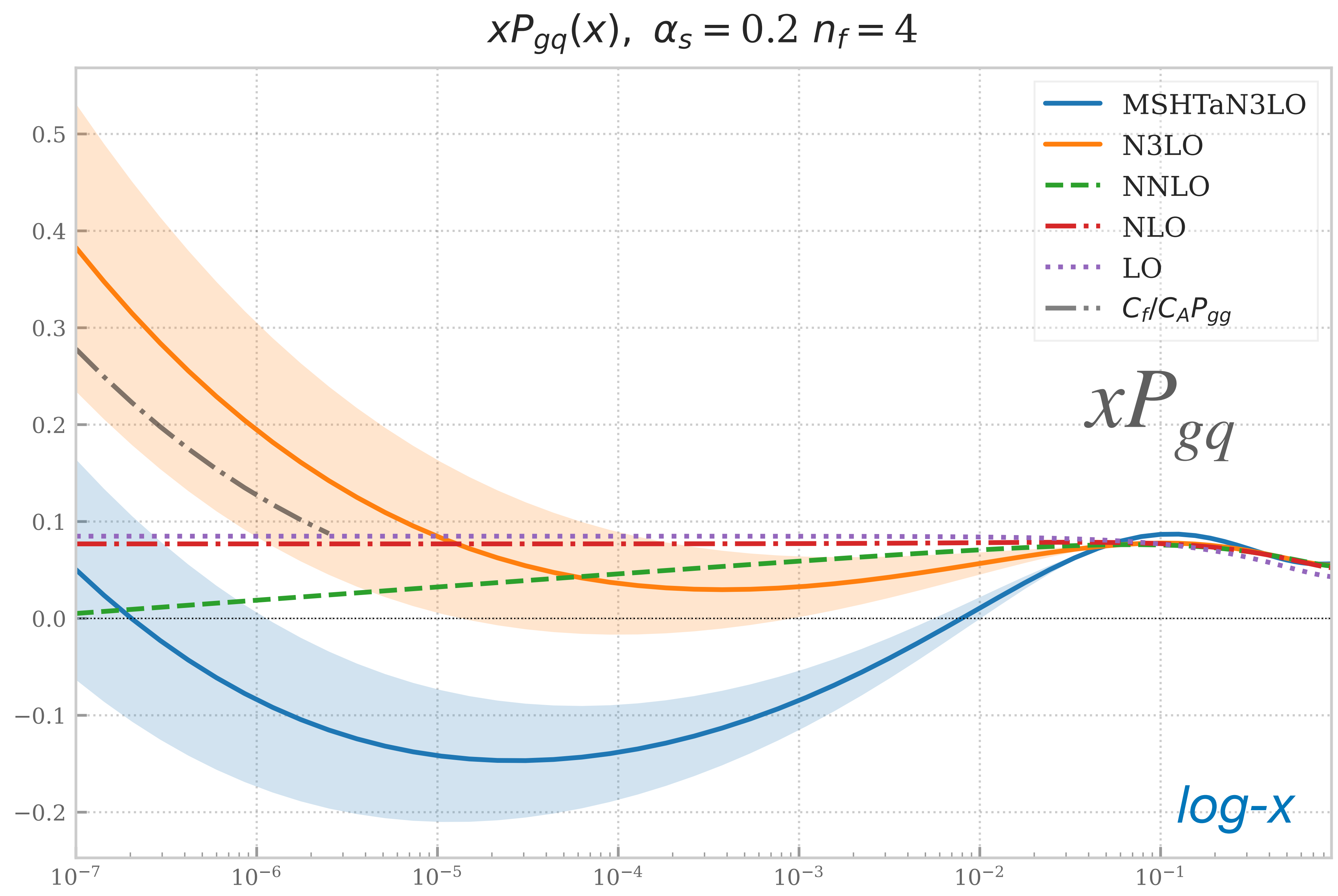
- Large logs $1/x \ln^3(x)$, $1/x \ln^2(x)$ arise at N3LO.
- NNLO MHOU are not enough in small-x region.
- IHOU are not negligible. Having 10/20 moments available would be enough to reduce IHOU.
- Off diagonal terms P_{qg}, P_{gq} are more difficult to estimate (large-N goes to 0).

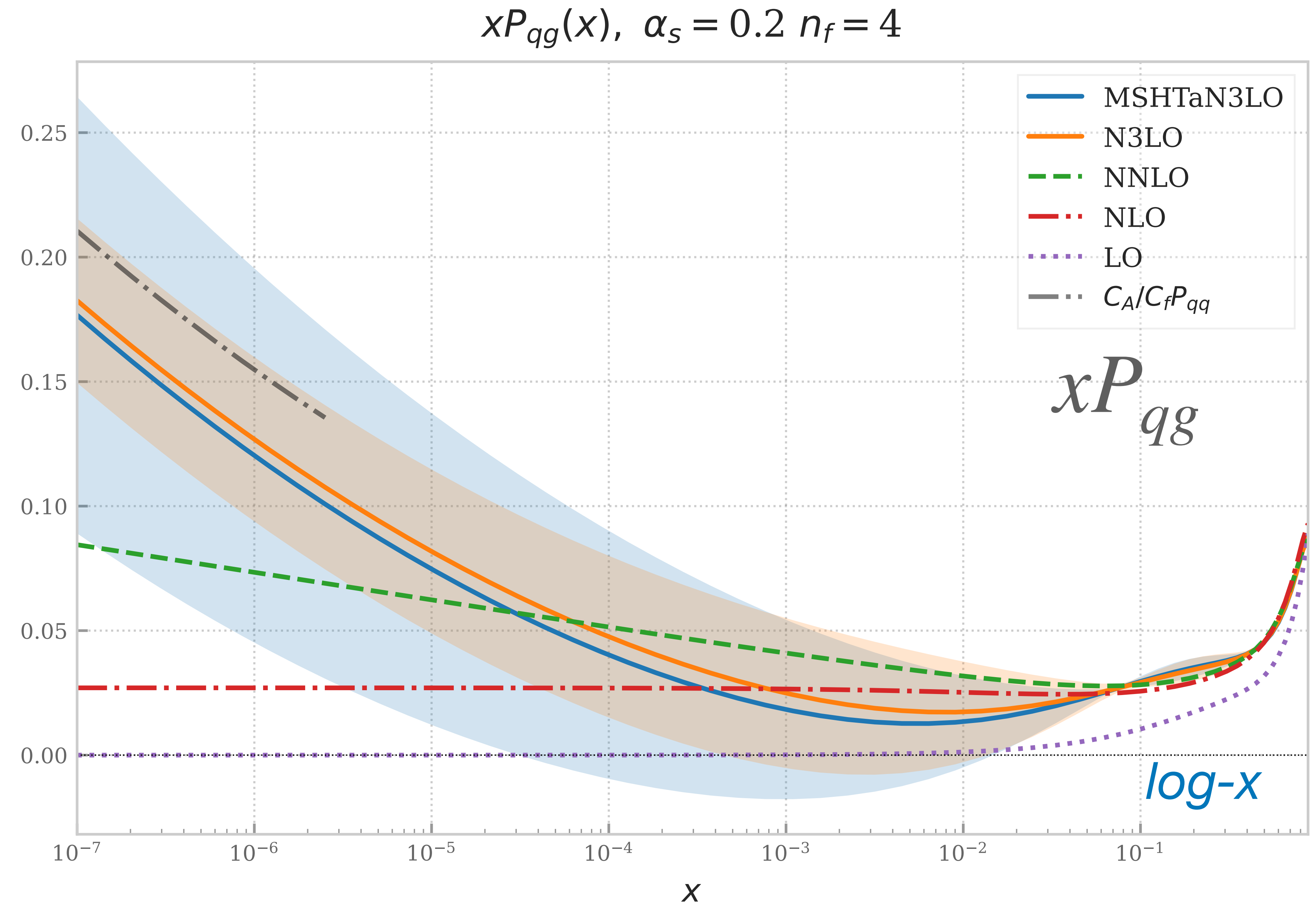


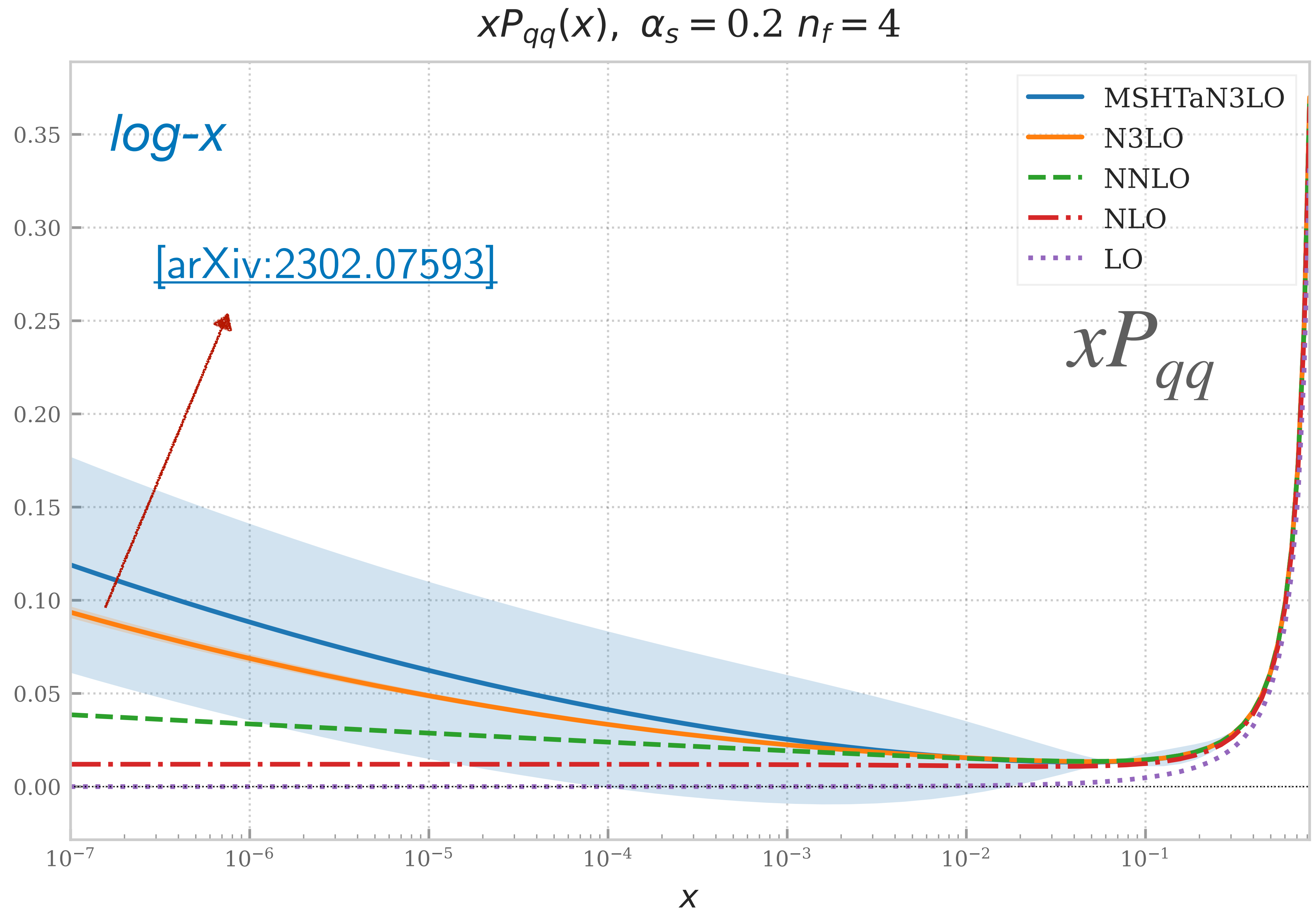
Comparison with MSHT

MSHTaN3LO: [arxiv:2207.04739]



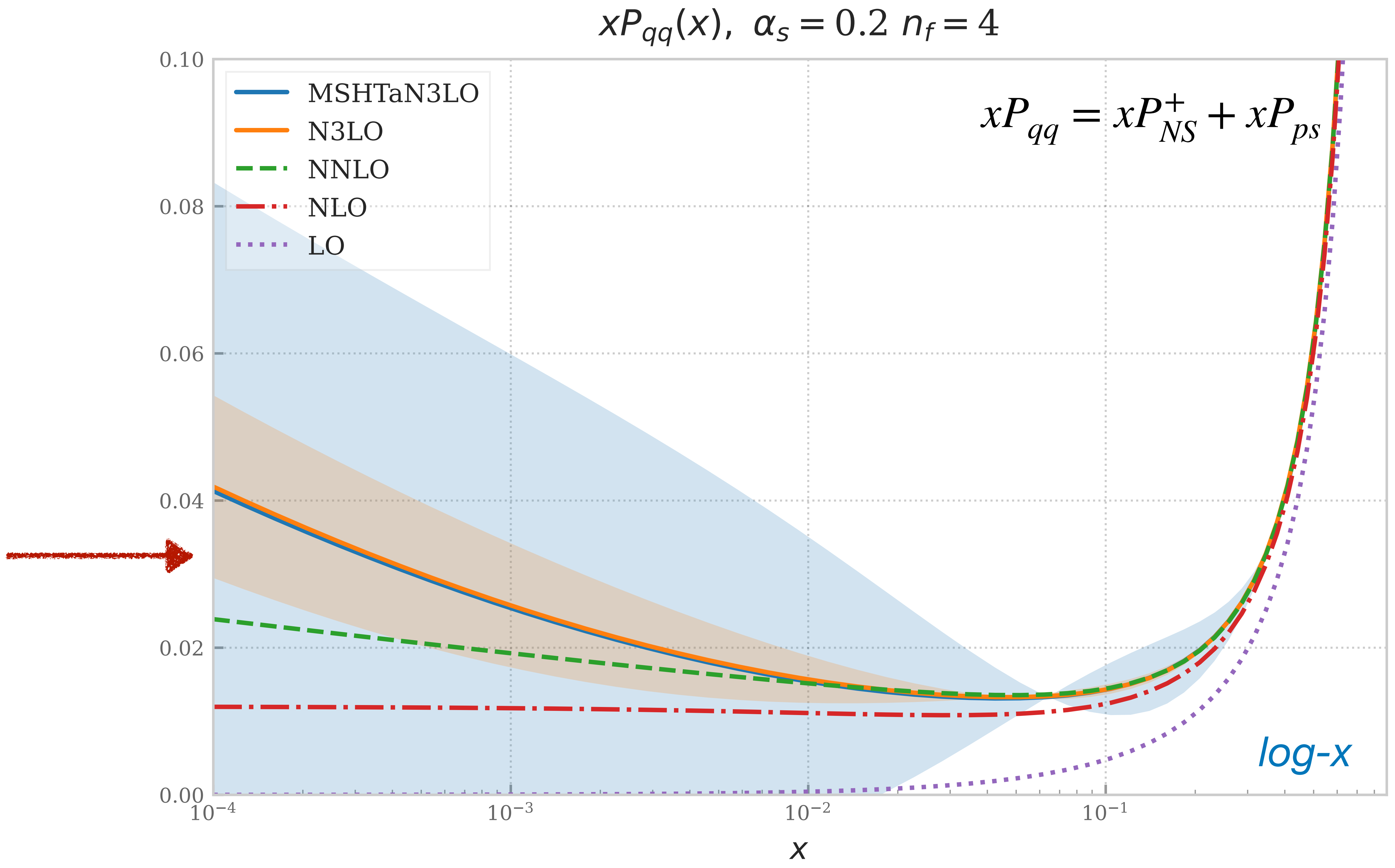




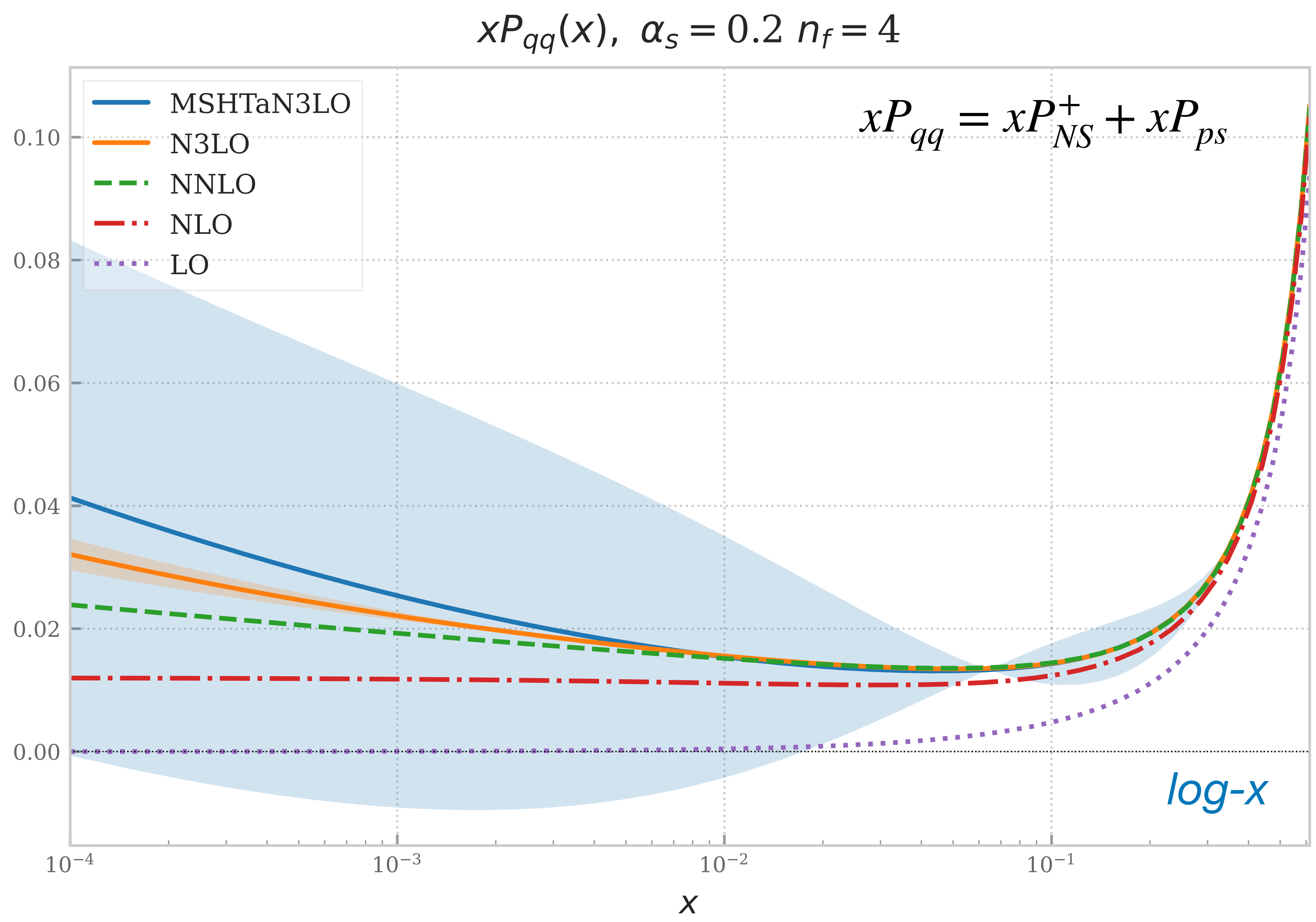


Splitting functions small-x

4 Mellin Moments only



10 Mellin Moments



DIS @ aN3LO

Structure Functions

DIS structure functions are known at N3LO in the **massless limit** 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 ($Q \to m_h^2$ and $Q \gg m_h^2$) with some damping functions.

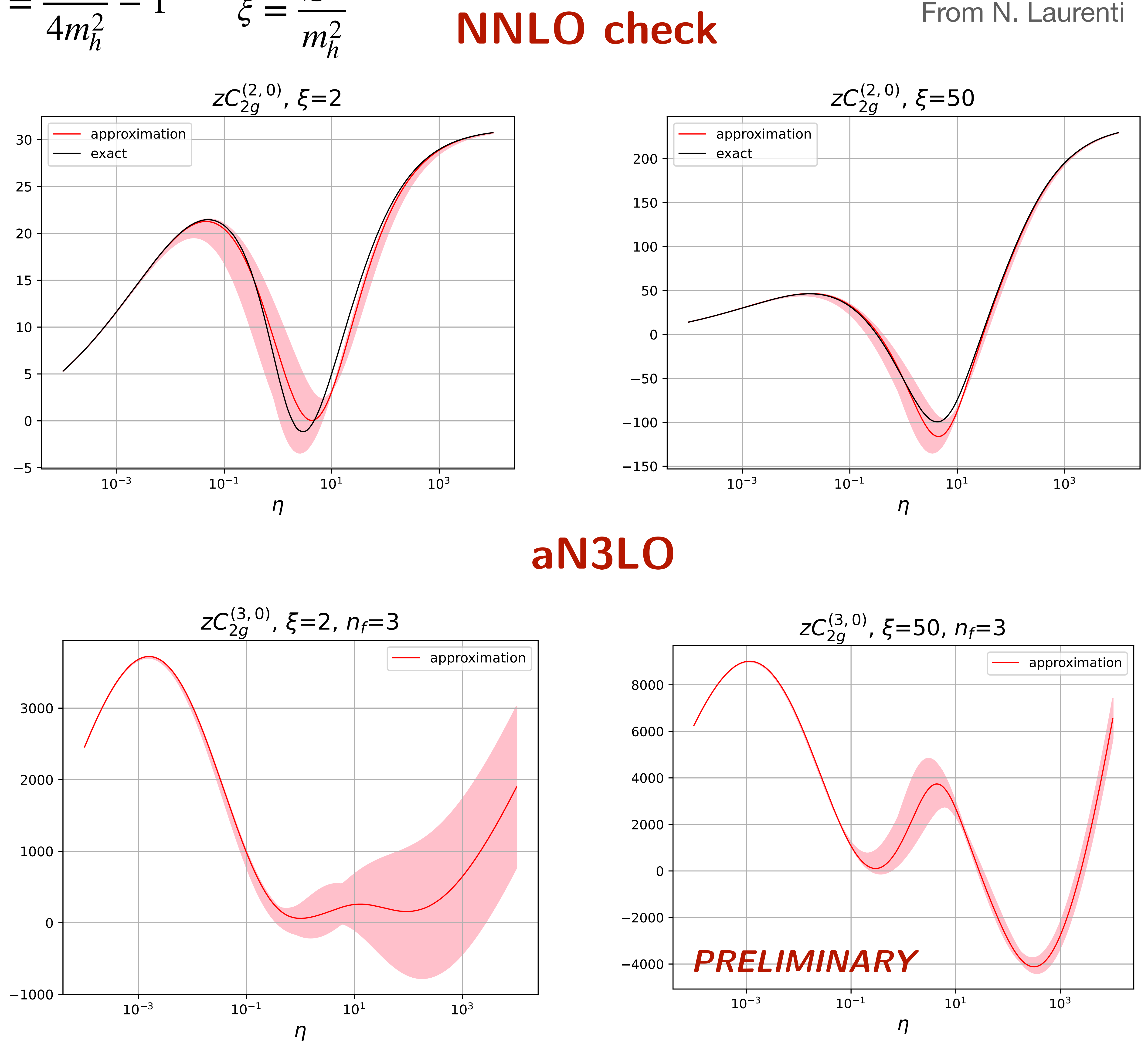
$$C^3_{g,h} = C^{(3,0)}_{g,h} + C^{(3,1)}_{g,h}\log(\frac{\mu}{m}) + C^{(3,2)}_{g,h}\log^2(\frac{\mu}{m})$$

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

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

$$\eta = \frac{s}{4m_h^2} - 1 \qquad \xi = \frac{Q^2}{m_h^2}$$

From N. Laurenti



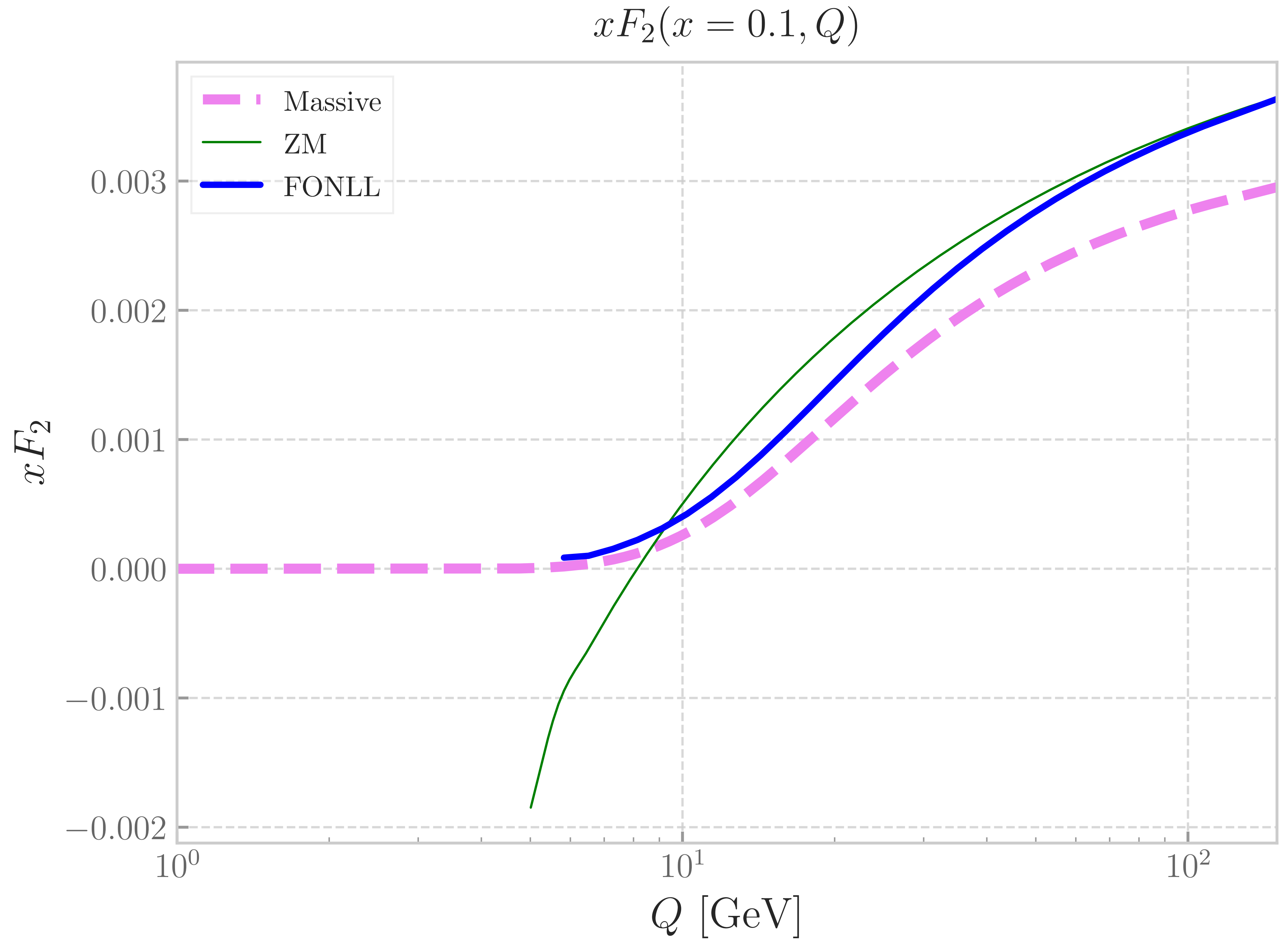
DIS @ aN3LO

Variable Flavor Number Scheme

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

During a PDF fit all these contributions needs 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)*



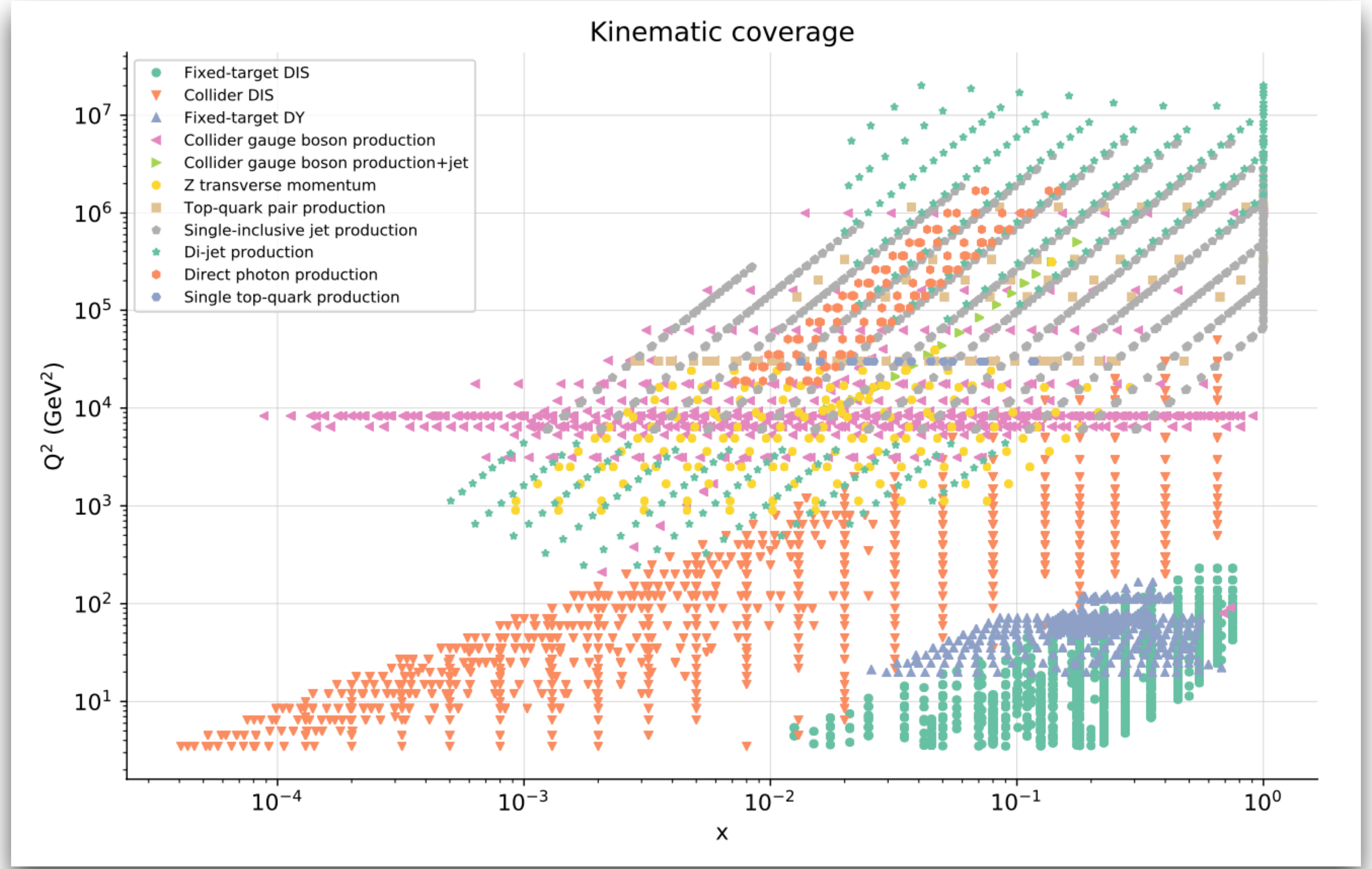
DIS structure functions are computed in the **FONLL** procedure [arxiv:1001.2312]:

- Up to N3LO for the Heavy structure functions F_{heavy}
- Up to NNLO for F_{light} + Massless N3LO contributions.

Preliminary aN3LO PDFs fits

What do we include in a global aN3LO ?

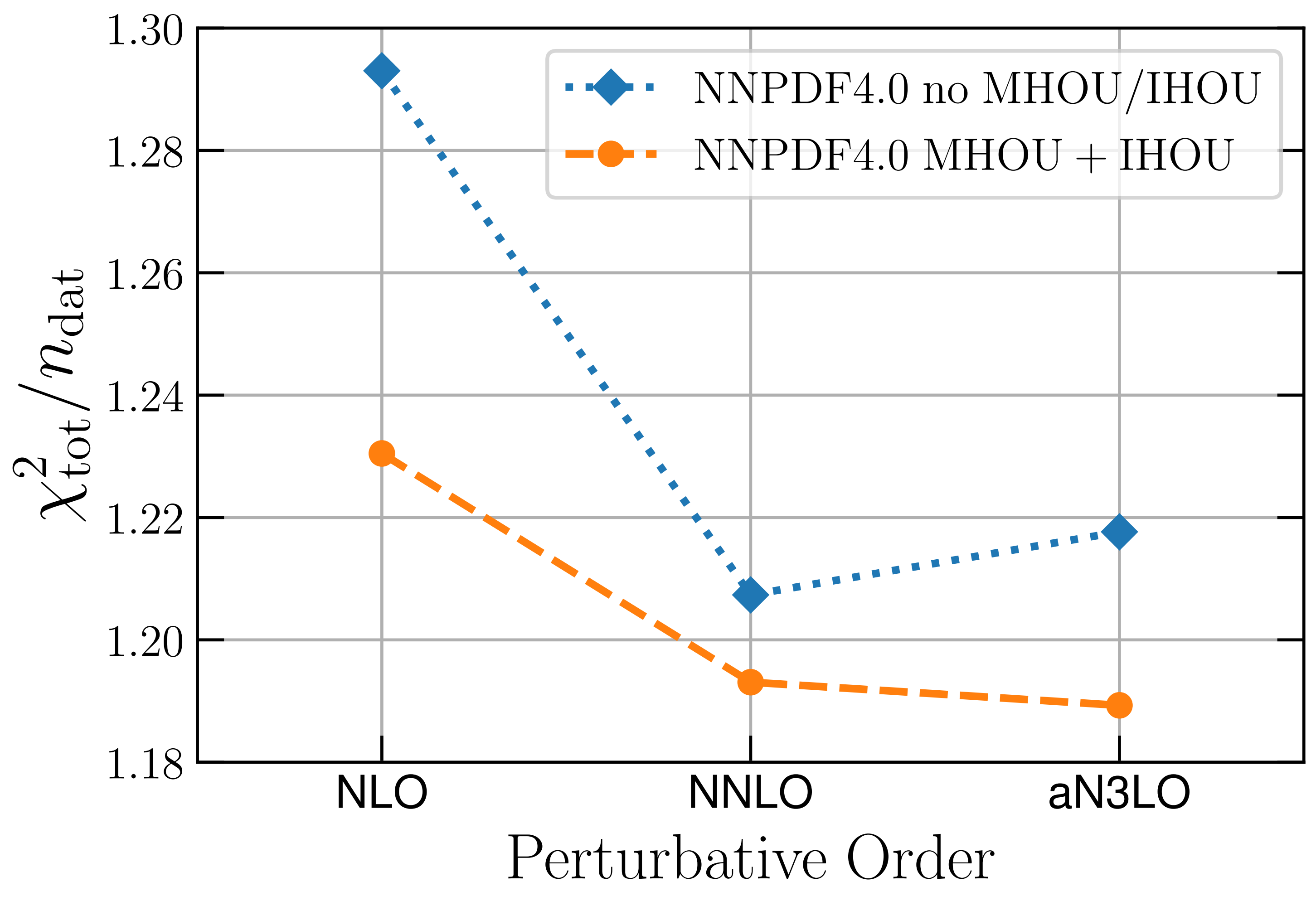
- **VFNS Evolution at aN3LO** for all datasets with IHOU.
- **DIS dataset for CC and NC**, with IHOU for massive calculations.
- Hadronic dataset all at NNLO with some K-factors for DY inclusive and rapidity distributions (not done yet)
- Datasets which do not contain aN3LO are included only if MHOU are considered.



Impact of IHOU theory uncertainties

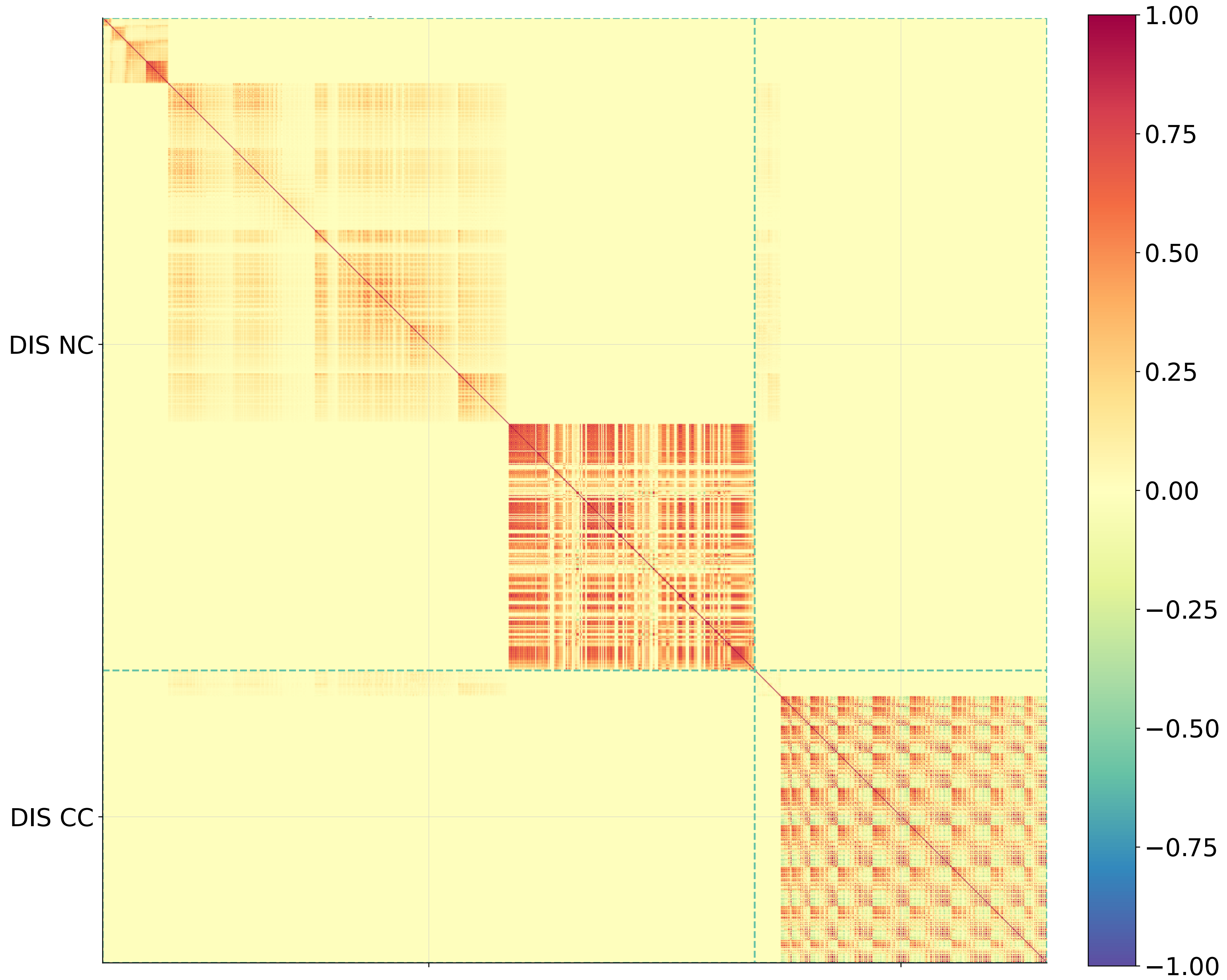
- Construct a theory covariance matrix by varying one single splitting function (during the DGLAP evolution) at the time.
- Variations in the heavy DIS coefficients functions are also taken into account.
- Produce an ≈ 70 point prescription theory covariance assuming that each variation is not correlated to the others.
- This source of uncertainty can added to the MHOU theory covariance mat obtained with scale variations:

$$Cov_{th} = Cov_{MHOU} + Cov_{IHOU}$$

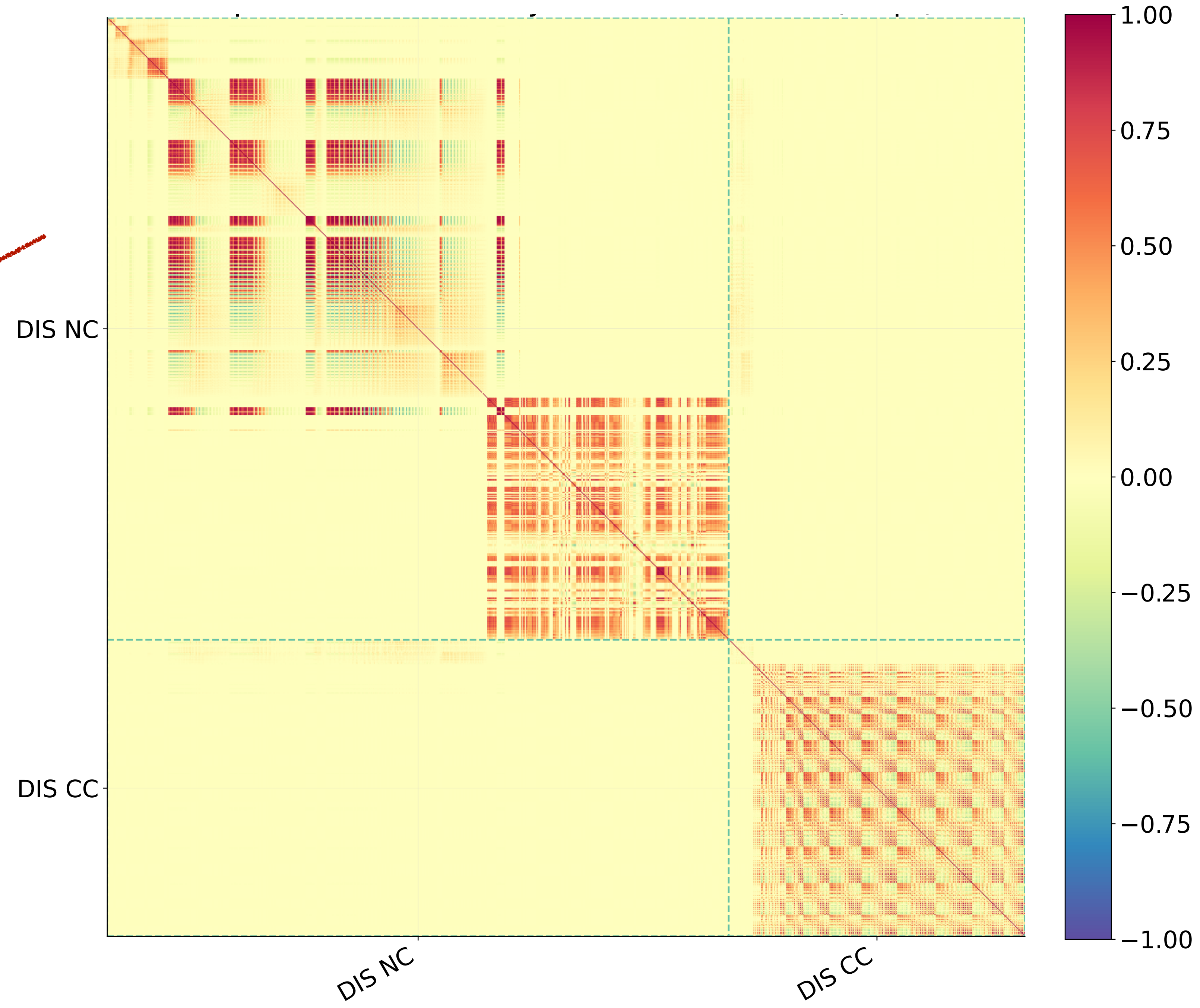


IHOU have larger effect on the small-x HERA data

Exp correlations

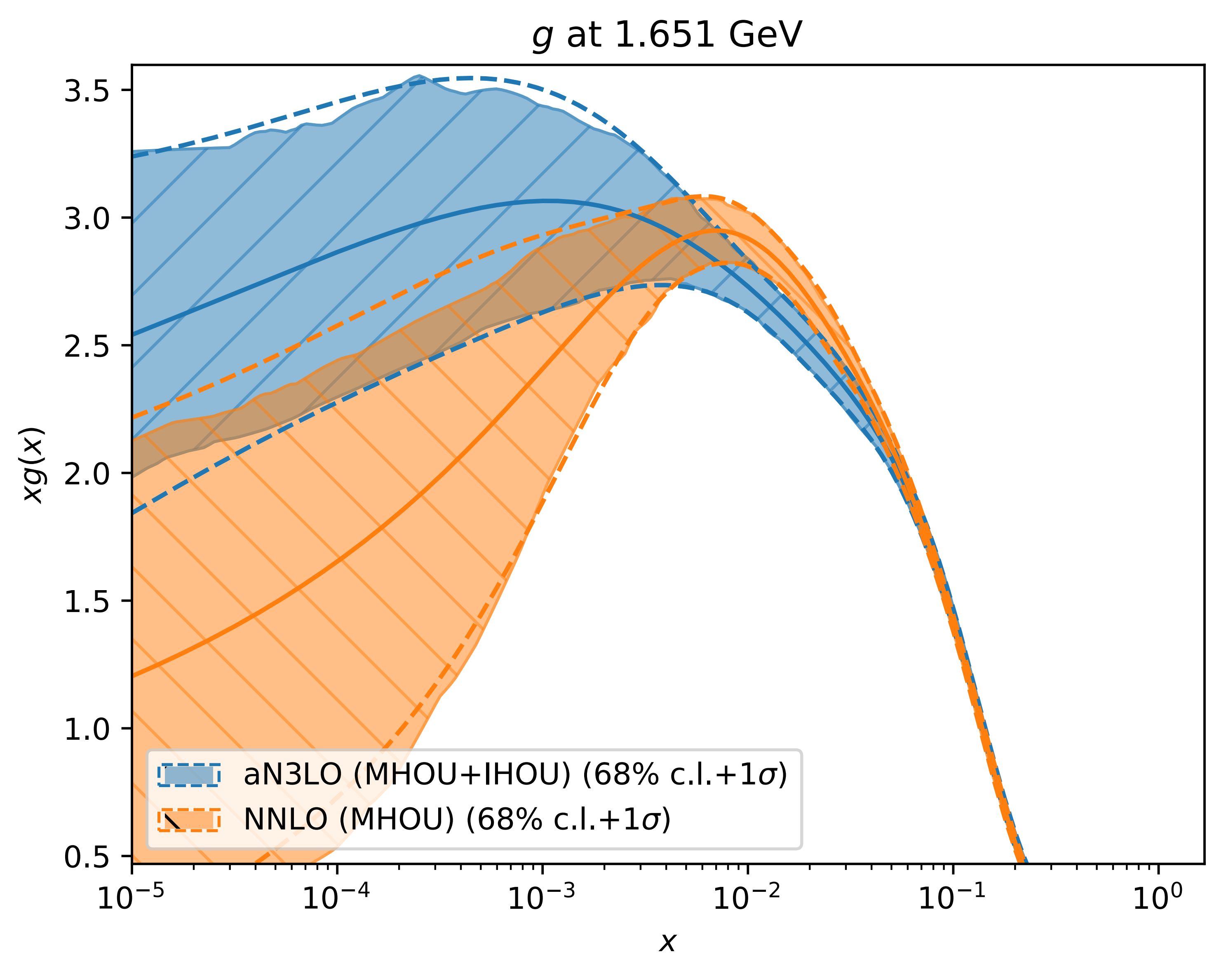


Exp + IHOU correlations **aN3LO**

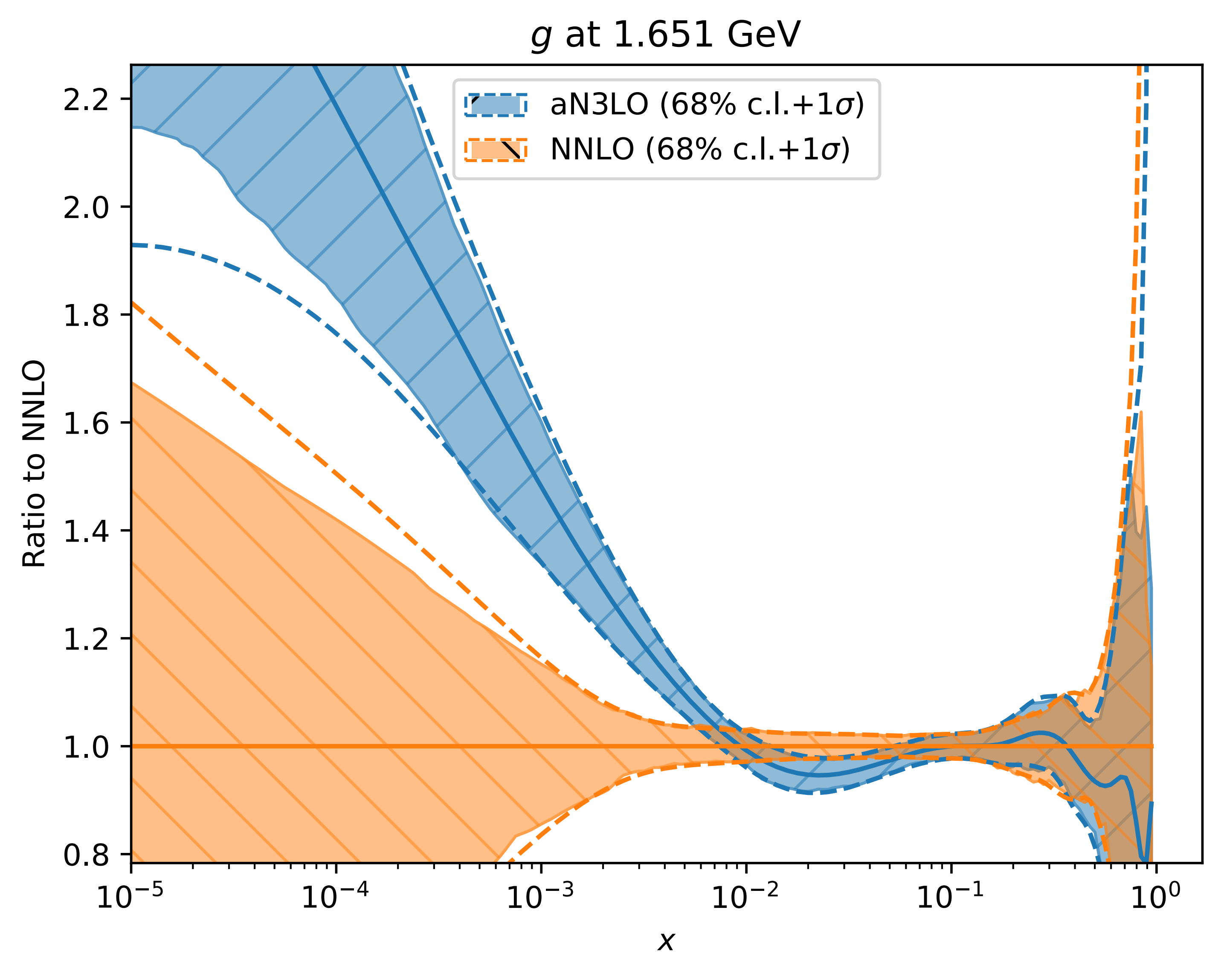


Preliminary aN3LO PDFs fits

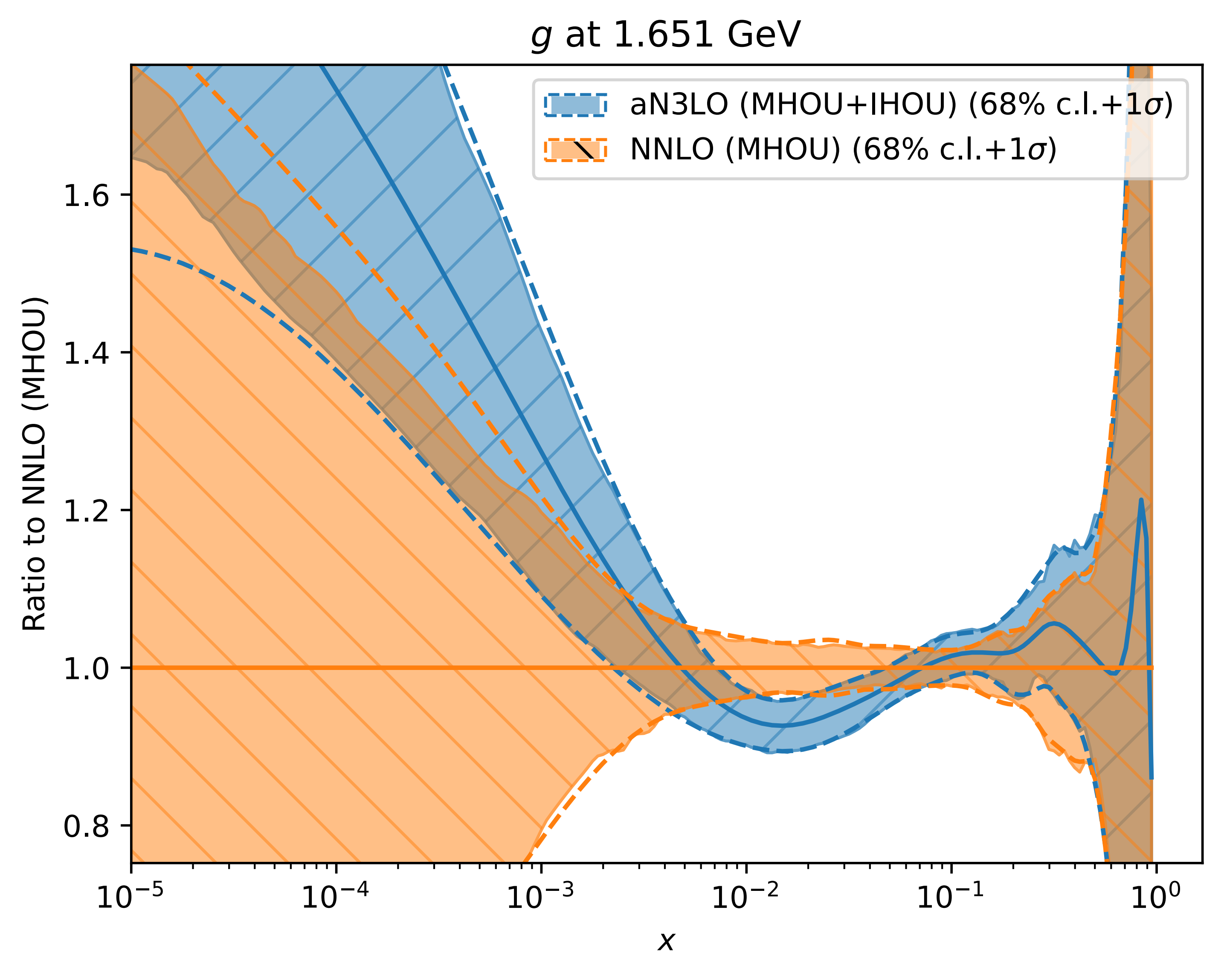
- First runs of **aN3LO** fits show a quite visible impact of N3LO corrections in the **small-x** region for gluon g and Singlet Σ.
- At large-x PDFs are compatible within one sigma with NNLO.
- Theory uncertainties reduce tensions with NNLO pdfs also in the small-x region.



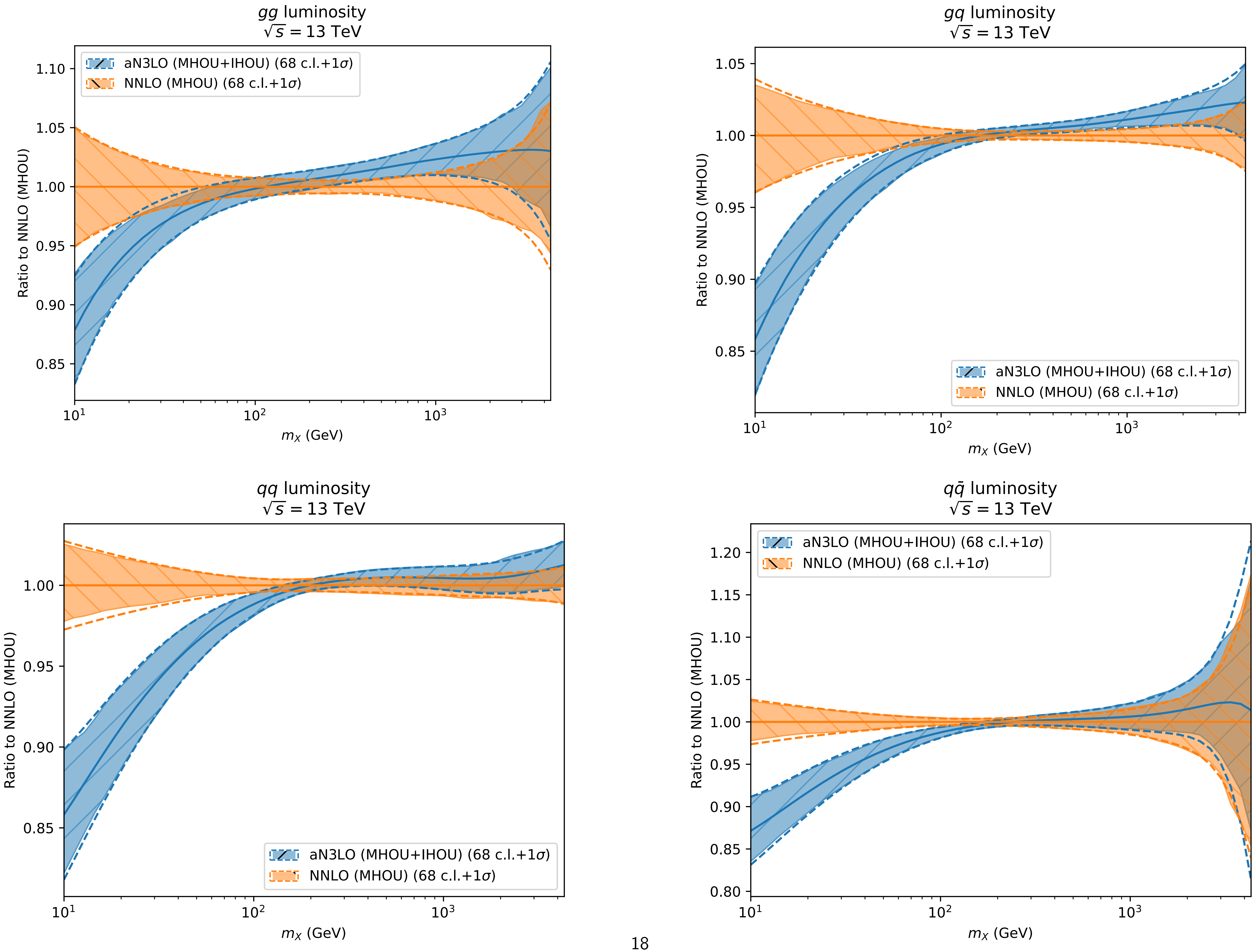
w/o Theory Uncertainties



with Theory Uncertainties



Preliminary aN3LO PDFs fits



Summary

- Approximate N3LO PDFs determination must take into account that not all the contributions are not fully available.
- Theory uncertainties do have different pattern from experimental ones.
- For an aN3LO we need to estimate both IHOU and MHOU.

From our preliminary results…

- Theory uncertainties have a visible impact on PDFs fits.
- First aN3LO results do not show large tensions with NNLO, especially if theory uncertainties are taken into account

TODO list

- Inclusion of N3LO for DY rapidity distributions.
- What about N3LO in DY pT distribution ?
- And single t and $t\bar{t}$?
- Can we benchmark our aN3LO inputs and eventually PDFs with MSHT ?

Backup slides

Pineline

A new tool chain for PDFs theory predictions

Barontini, Candido, Cruz-Martinez, Hekhorn, Schwan
[arxiv:2302.12124]

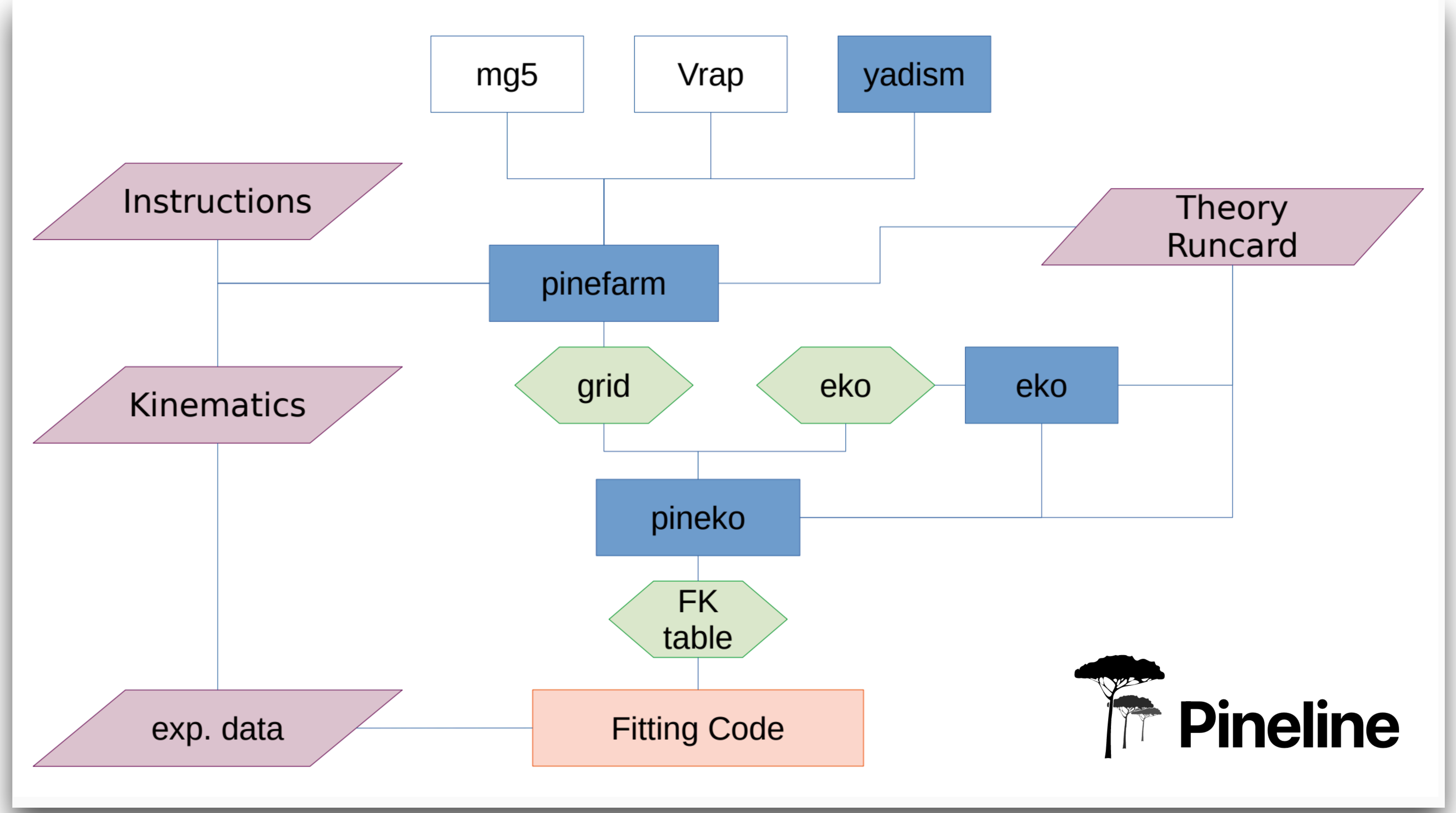
The code infrastructure needed to compute theory predictions has been completely rewritten and is now fully **open source**

One program, one job.

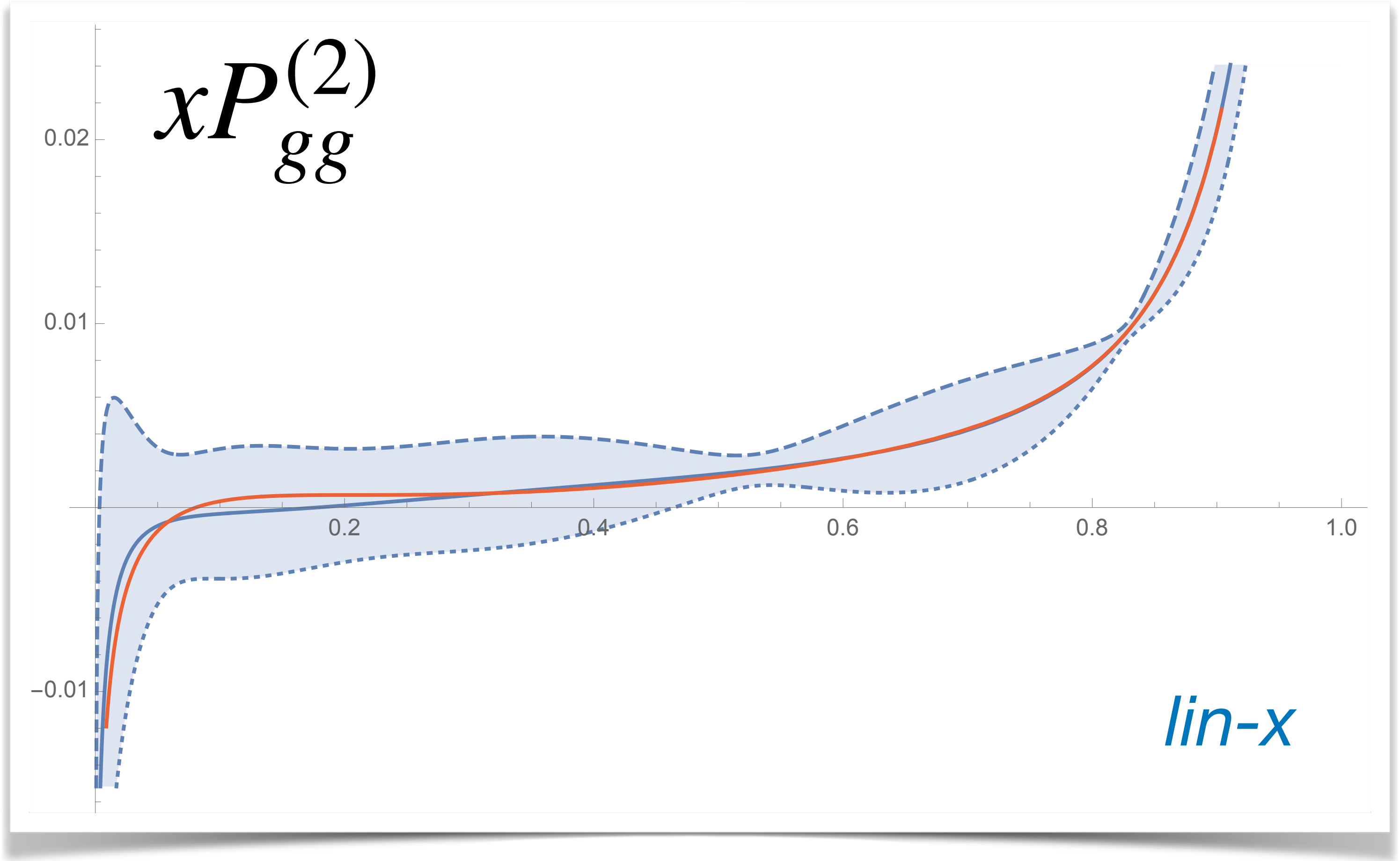
Easier to maintain. Mainly python written. Open-source

https://nnpdf.github.io/pineline/

https://github.com/NNPDF



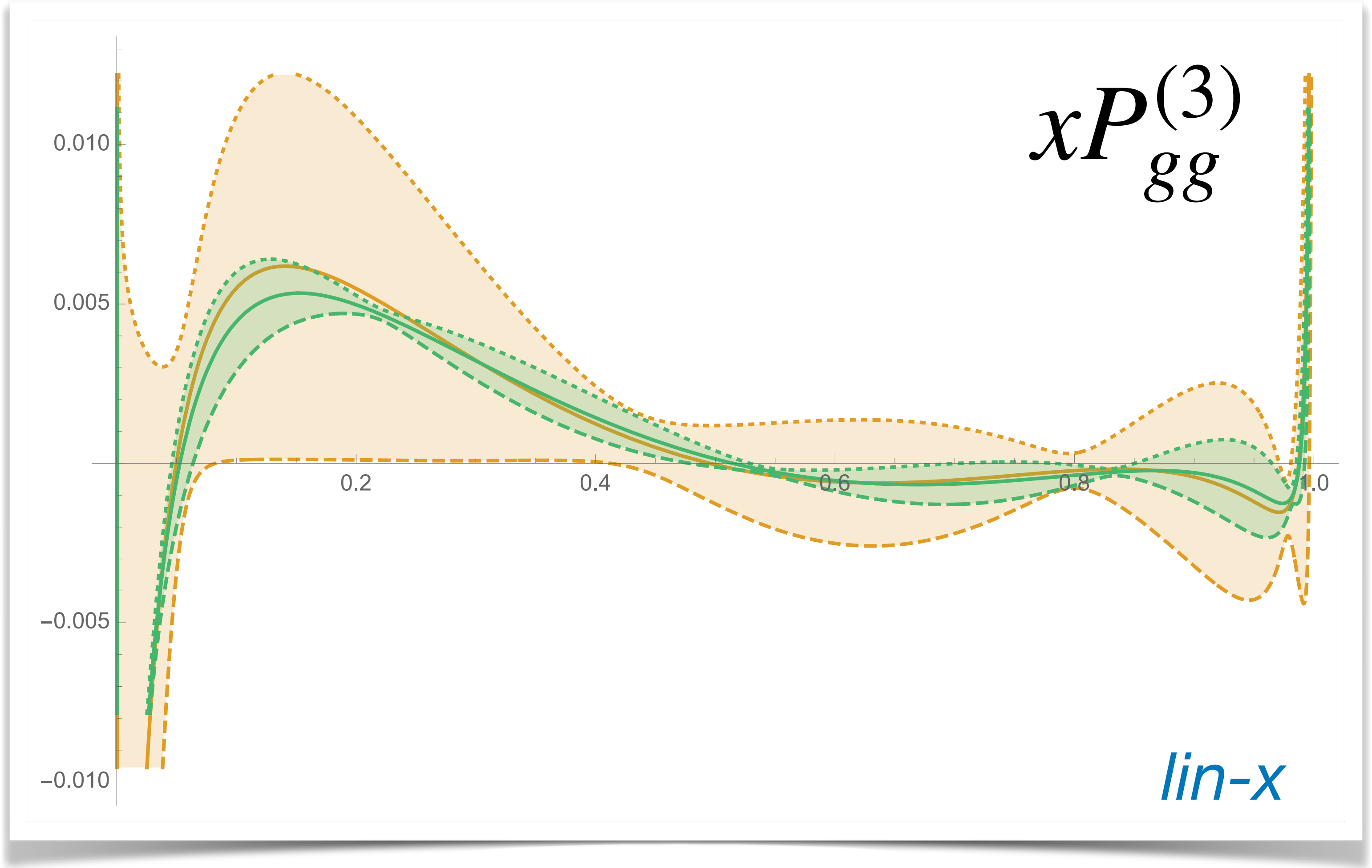
Splitting functions approximations tests

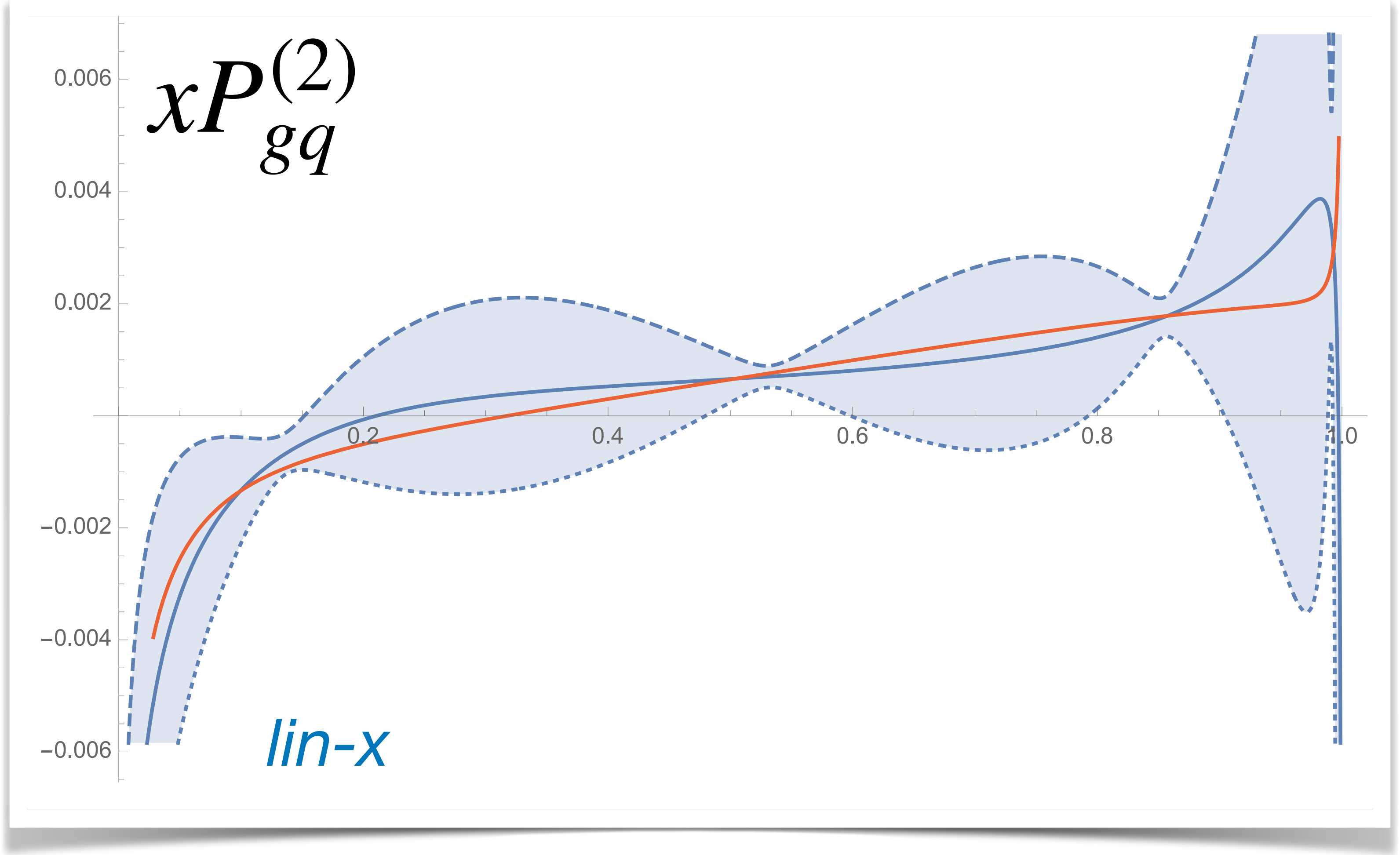


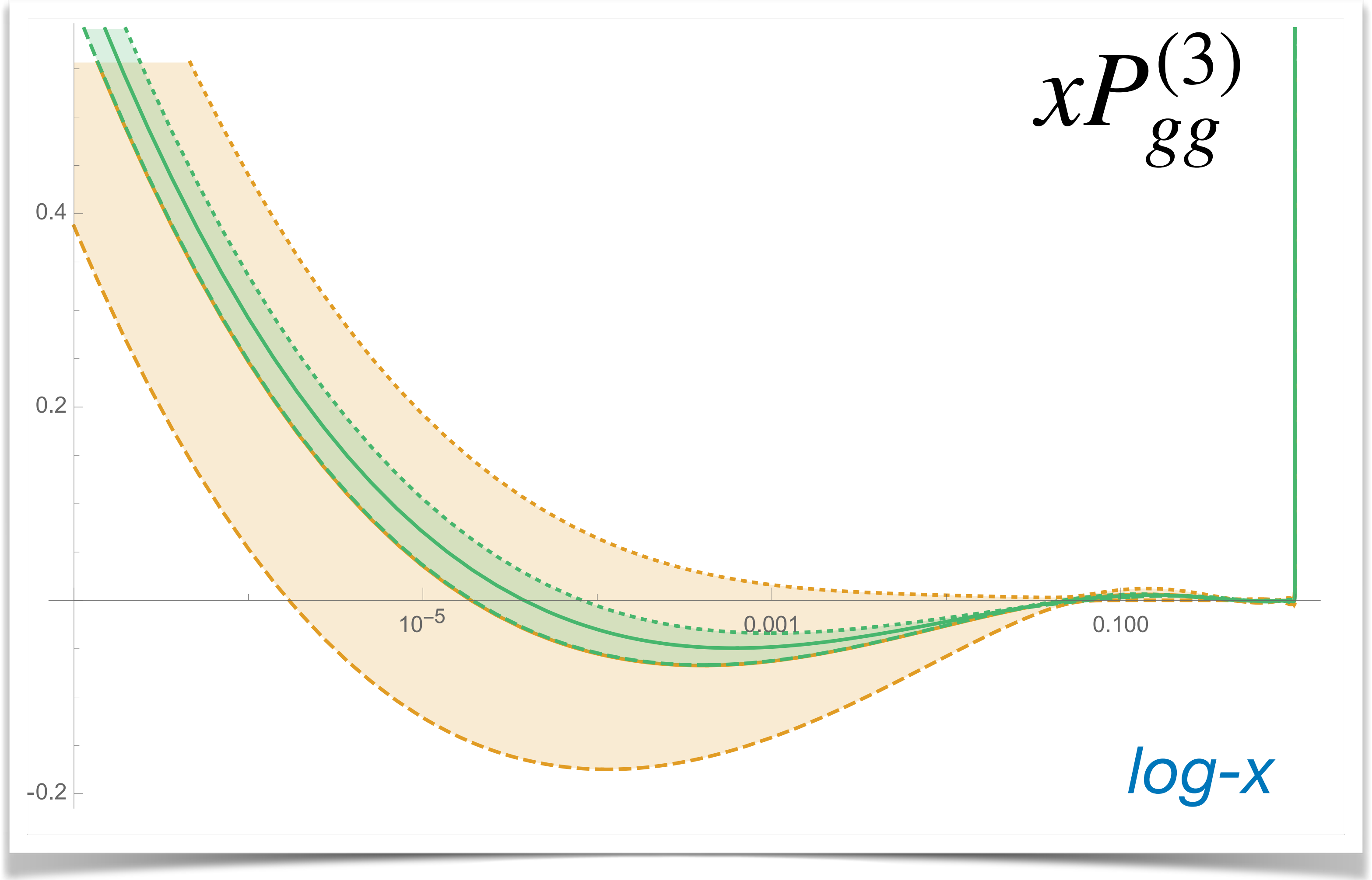
Approx

Analytic

1. A possible way to validate the procedure is to **reproduce the known NNLO** singlet splitting functions using the very similar constrain that we have right now on the N3LO ones.







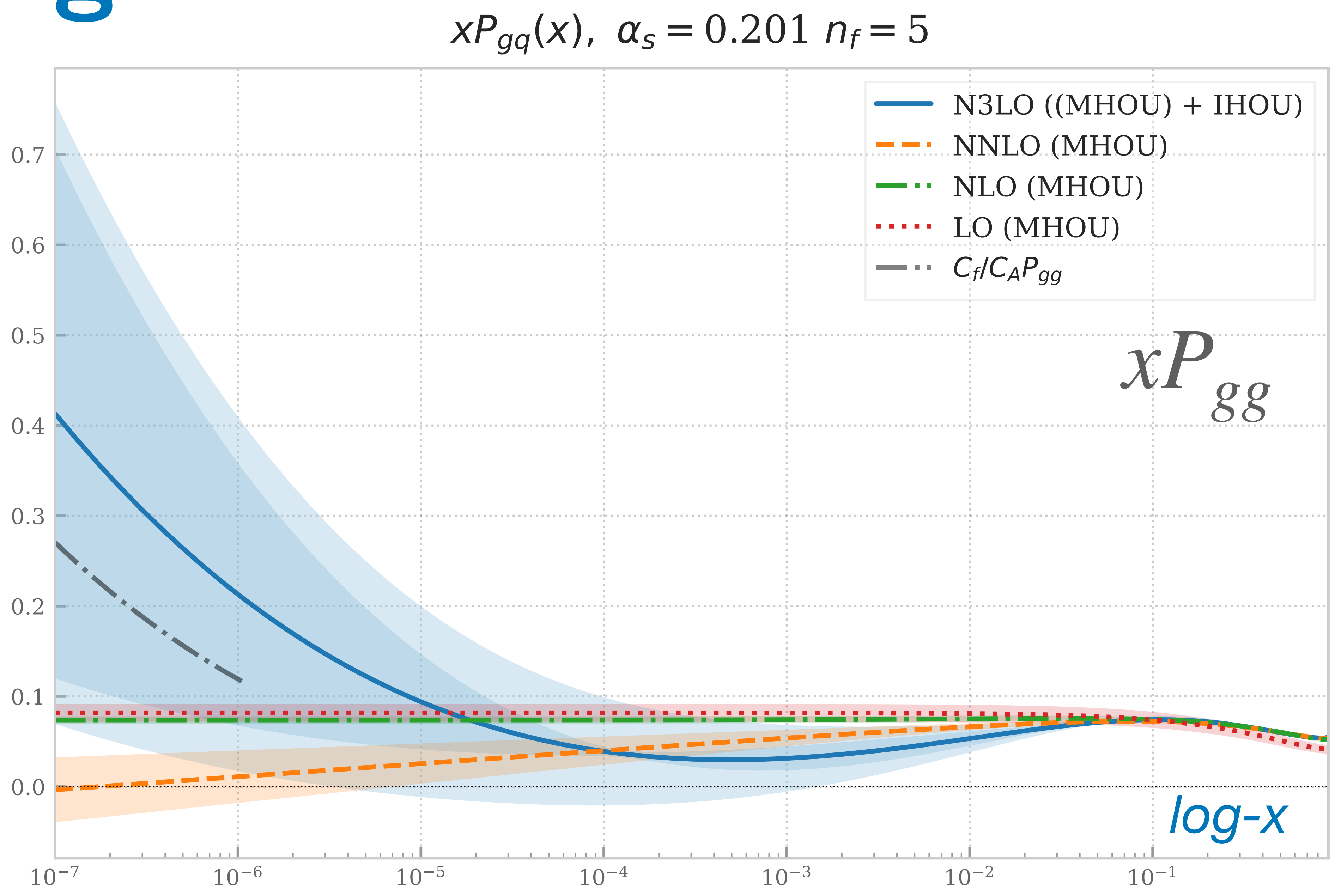
4 Moments fixed

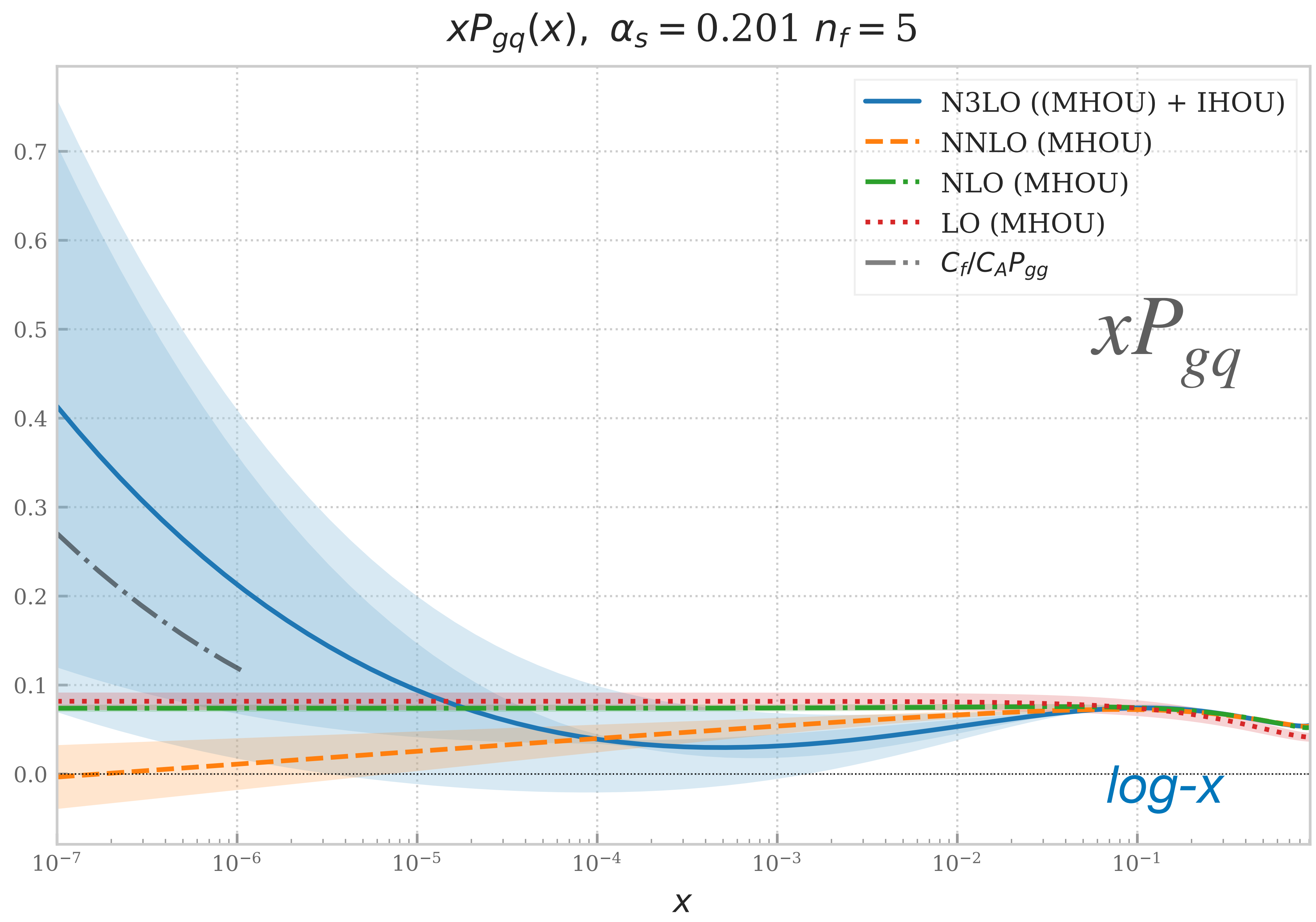
+ N=3 fixed

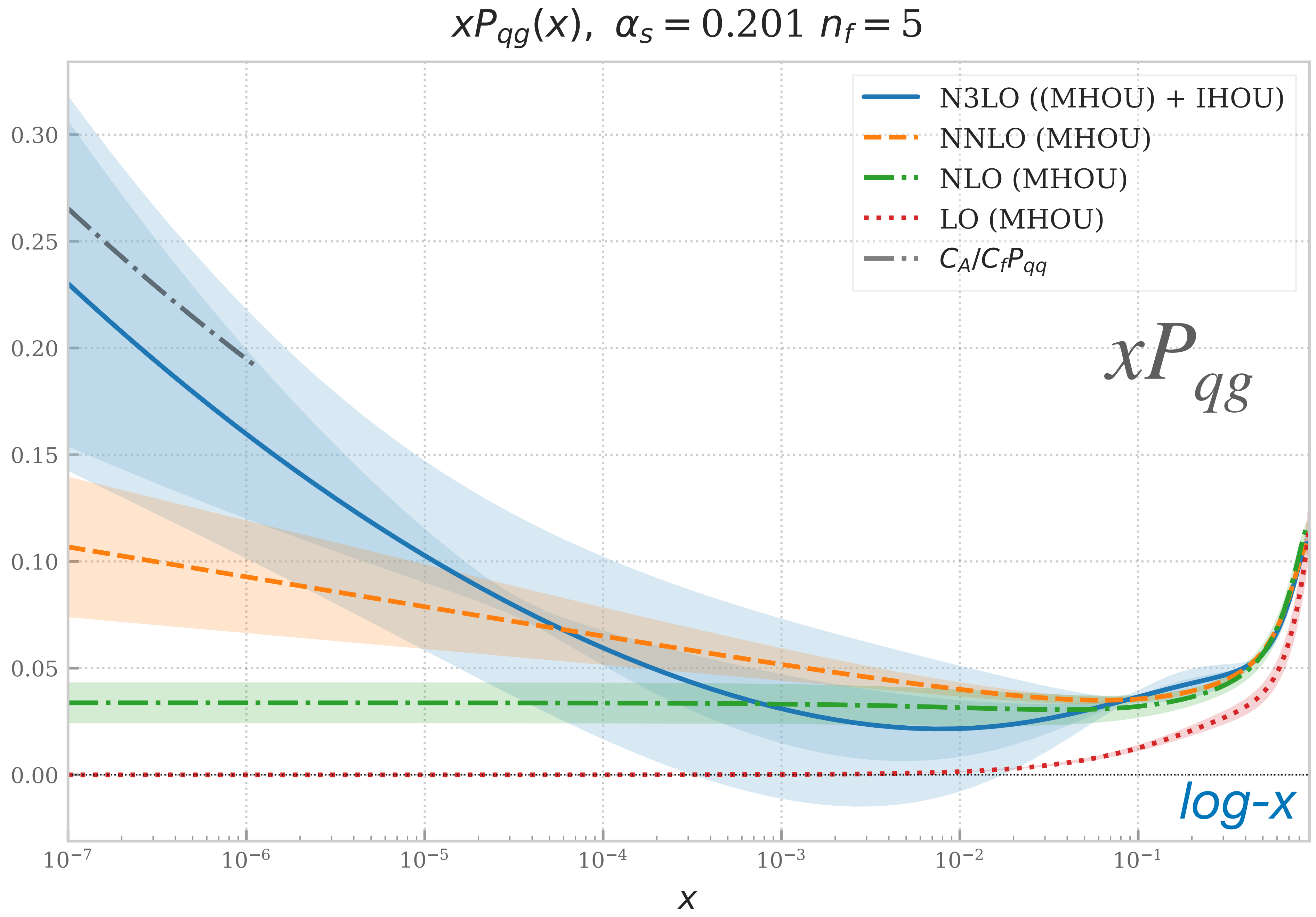
2. Another way to validate the results is to **interpolate the known moments**, and construct a more constrained parametrisation now including 5/6 moments.
If the procedure is working (the samples are varied enough) the uncertainty band obtained in this way should be small than the default one.

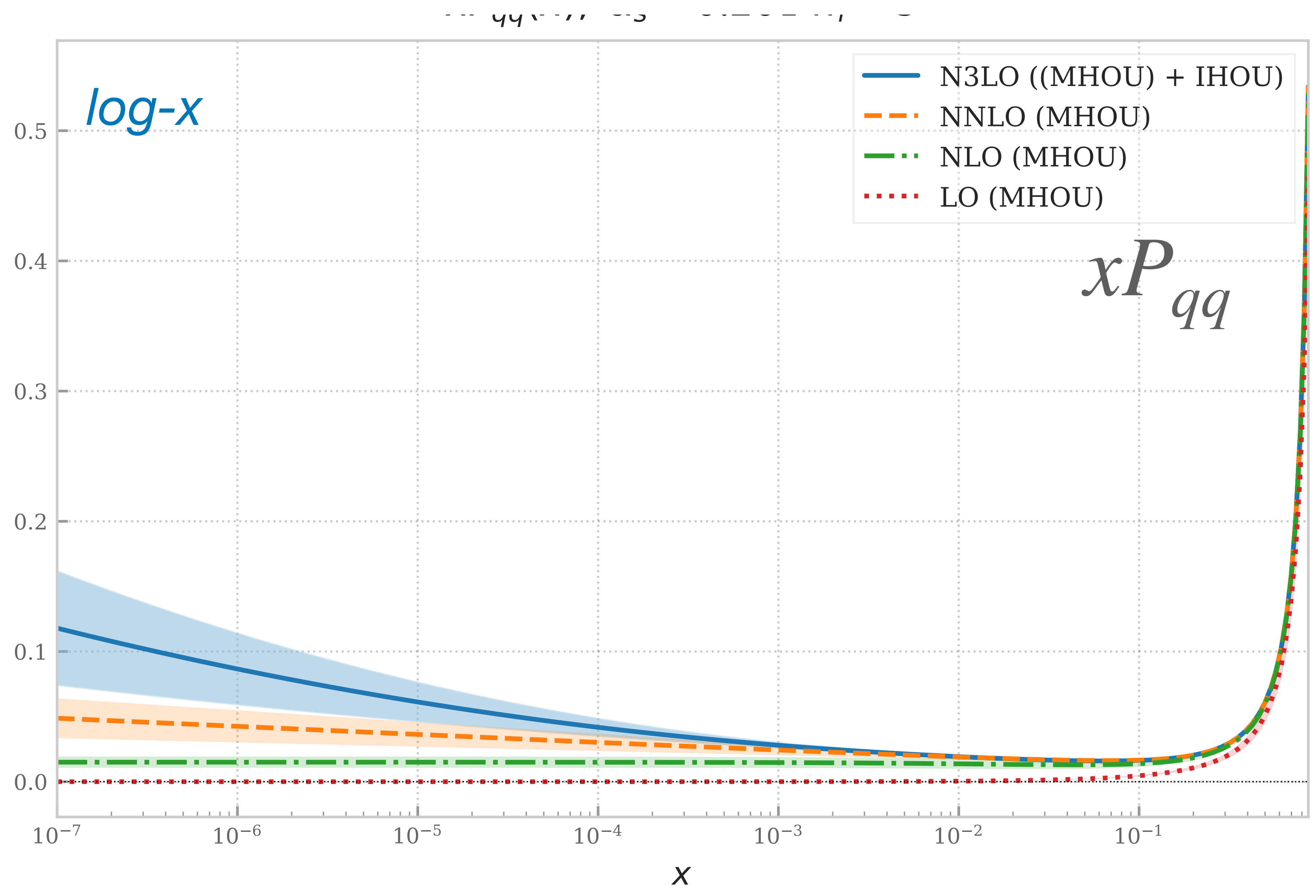
Splitting functions small-x

PRELIMINARY RESULTS



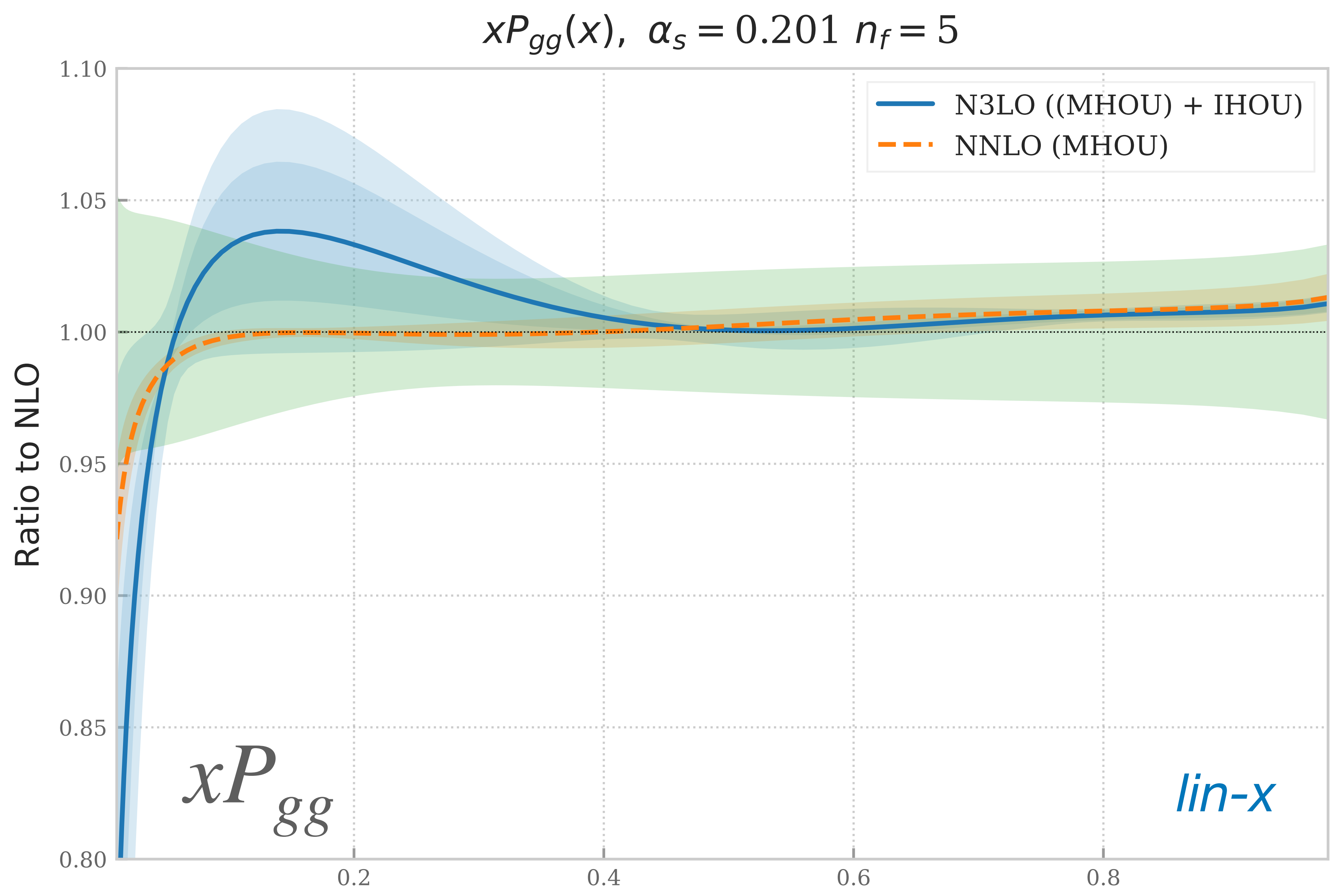


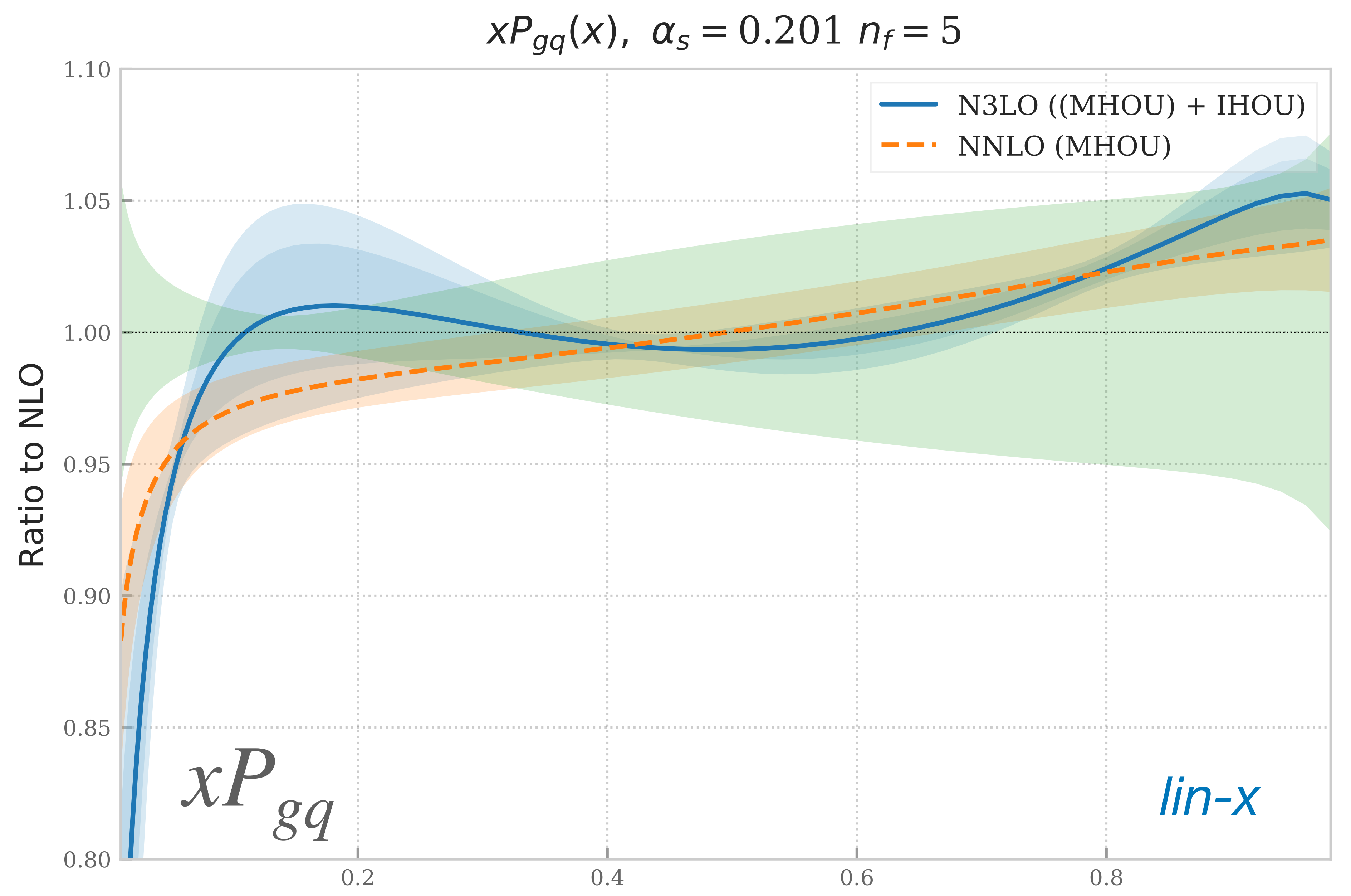


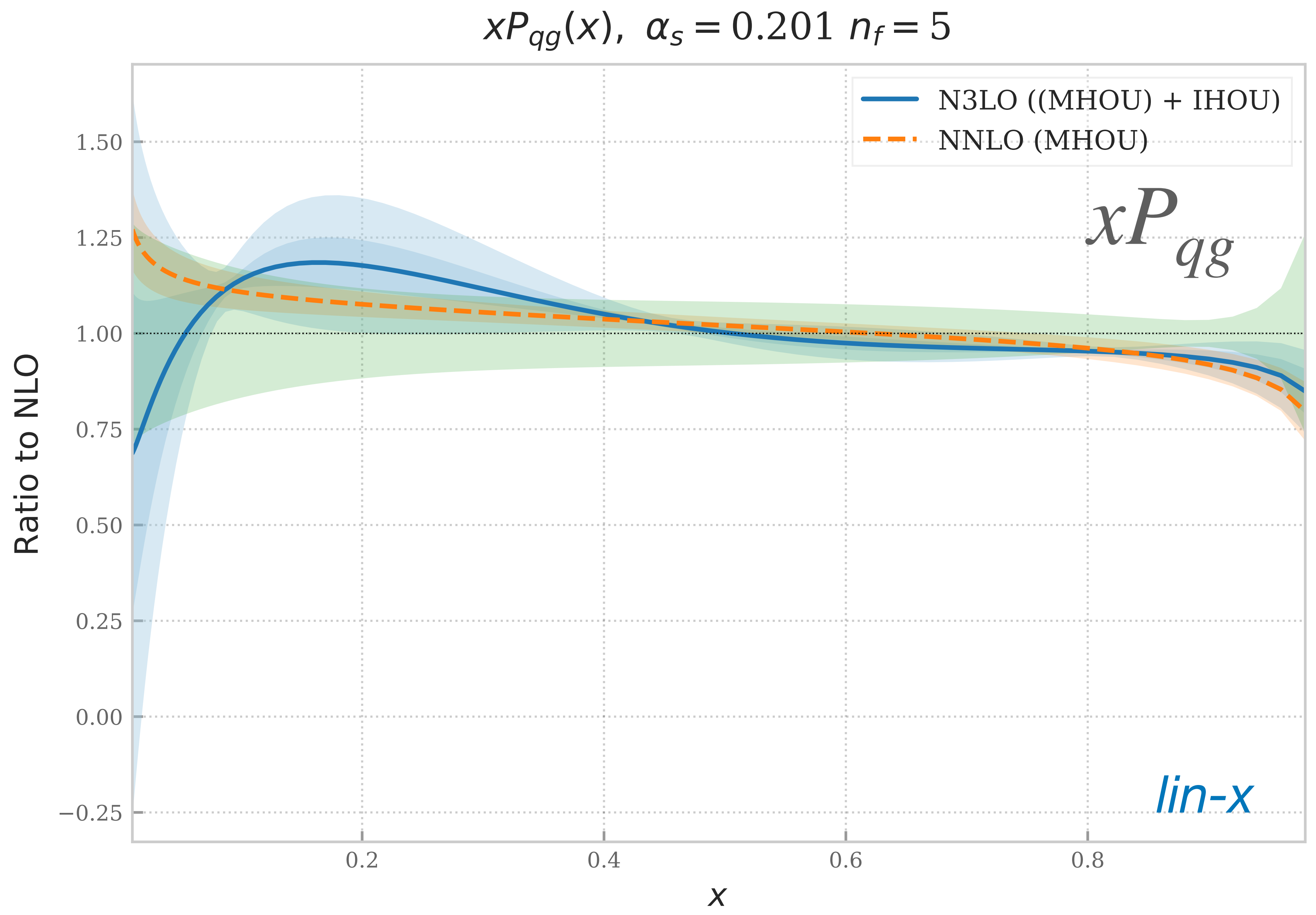


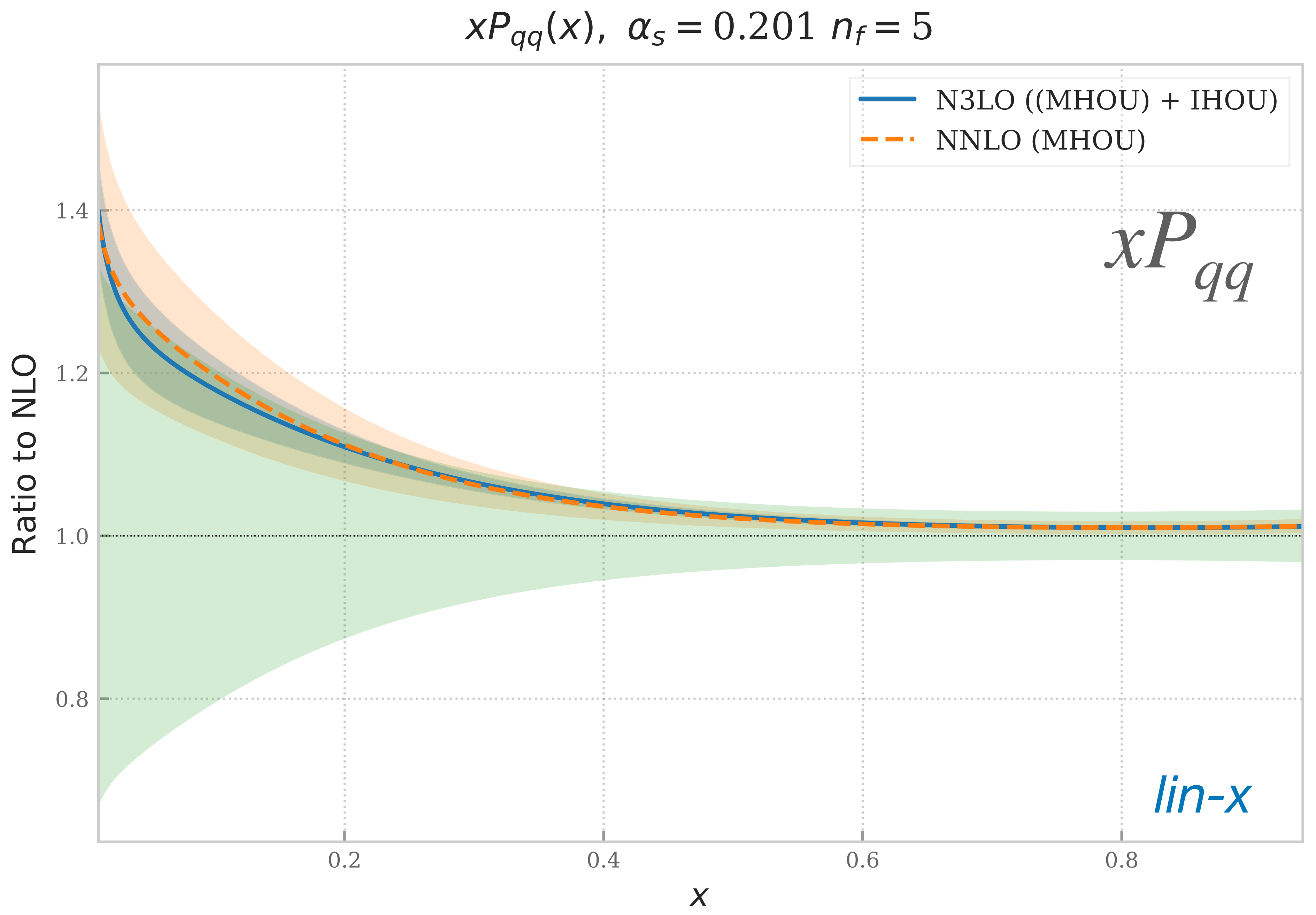
Splitting functions large-x

PRELIMINARY RESULTS









Comparison with MSHT large-x

MSHTaN3LO: [arxiv:2207.04739]

PRELIMINARY RESULTS