

Approximate N³LO PDFs.

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Aproximate N³LO (and Higher Orders)

Leading source of uncertainties from Missing Higher Orders in perturbation theory. Numerous sources of this, i.e. splitting functions

$$\mathbf{P}(x, \alpha_s) = \alpha_s \mathbf{P}^{(0)}(x) + \alpha_s^2 \mathbf{P}^{(1)}(x) + \alpha_s^3 \mathbf{P}^{(2)}(x) + \alpha_s^4 \mathbf{P}^{(3)}(x) + \dots ,$$

but also heavy flavour transition matrix elements and cross-sections

$$F(x, Q^2) = \sum_{\alpha \in \{H, q, g\}} \left(C_{q,\alpha}^{\text{VF}, n_f+1} \otimes A_{\alpha i}(Q^2/m_h^2) \otimes f_i^{n_f}(Q^2) \right. \\ \left. + C_{H,\alpha}^{\text{VF}, n_f+1} \otimes A_{\alpha i}(Q^2/m_h^2) \otimes f_i^{n_f}(Q^2) \right),$$

$$\sigma_2^{had}(x_1, x_2, Q^2) = \sum_{\alpha, \beta \in \{H, q, g\}} \left(\sigma_{\alpha, \beta}^{\text{VF}, n_f+1} \otimes A_{\alpha i}(Q^2/m_h^2) \otimes f_i^{n_f}(Q^2) \right. \\ \left. \otimes A_{\beta j}(Q^2/m_h^2) \otimes f_j^{n_f}(Q^2) \right),$$

Current knowledge is up to NNLO, with full higher orders unknown. However, already significant progress in calculating at N³LO [2-13].

N³LO - What do we know?

Zero-mass structure function N³LO coefficient functions are known [2].

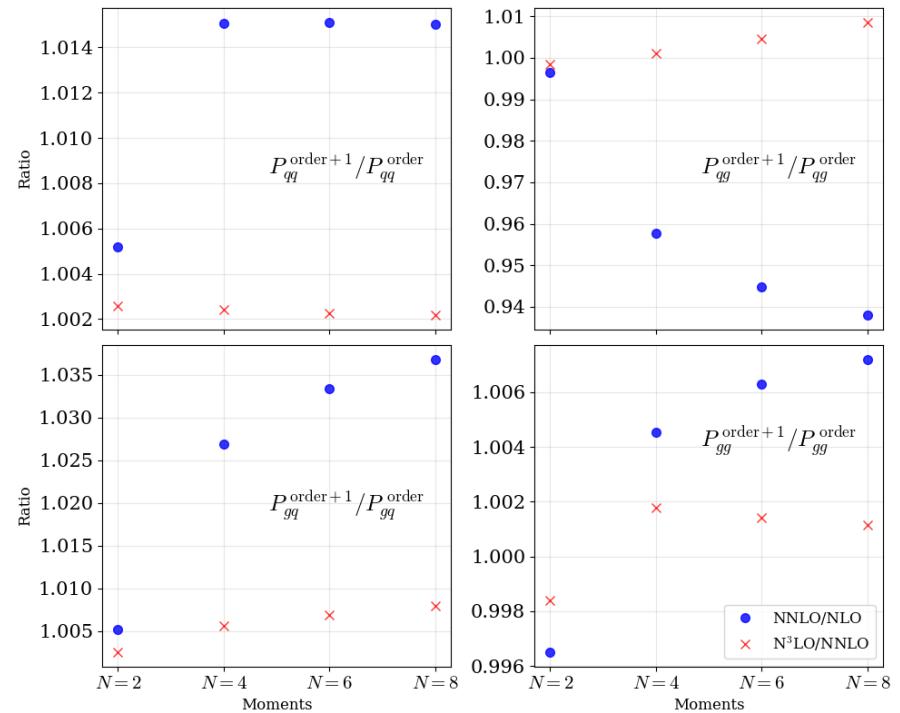
Some knowledge of leading terms in the small x and large x regime.
Unknown subleading terms weakly constrained from precedent, approx
 C_F/C_A relations, smoothness etc. Example case

$$P_{qg}^{(3)}(x) \rightarrow \frac{C_A^3}{3\pi^4} \left(\frac{82}{81} + 2\zeta_3 \right) \frac{1}{2} \frac{\ln^2 1/x}{x} + \rho_{qg} \frac{\ln 1/x}{x},$$

Some numerical constraints (Low-integer Mellin moments), until recently [3-12].

Intuition from lower orders and expectations from perturbation theory.

Very little about many cross-sections (κ -factors).



Splitting Functions at aN^3LO - MSHT [1]

N_m Mellin moments [2-6] (Moch et al.) can be used as constraints for

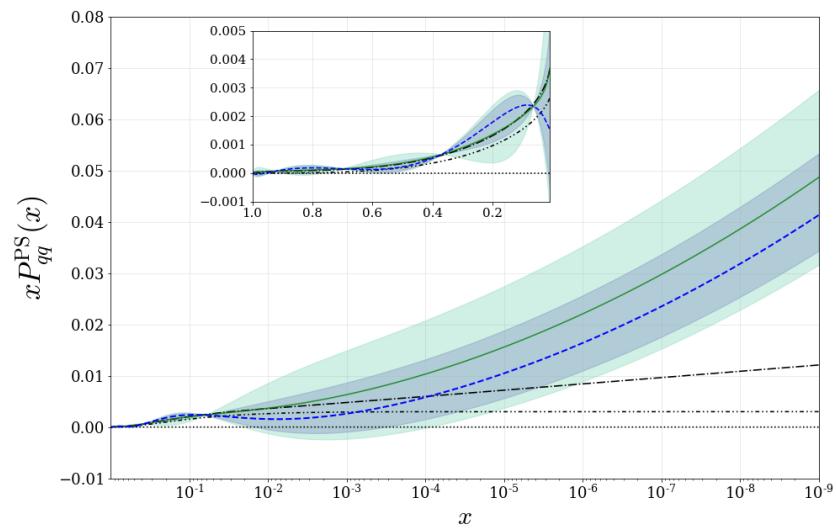
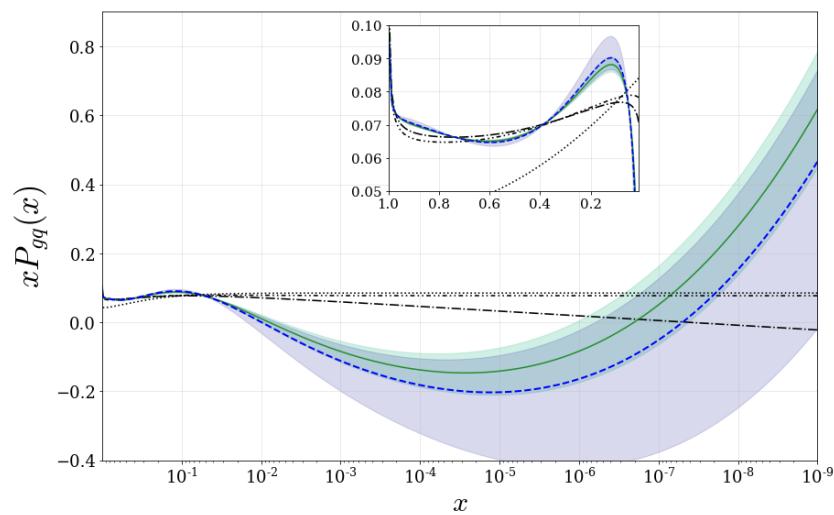
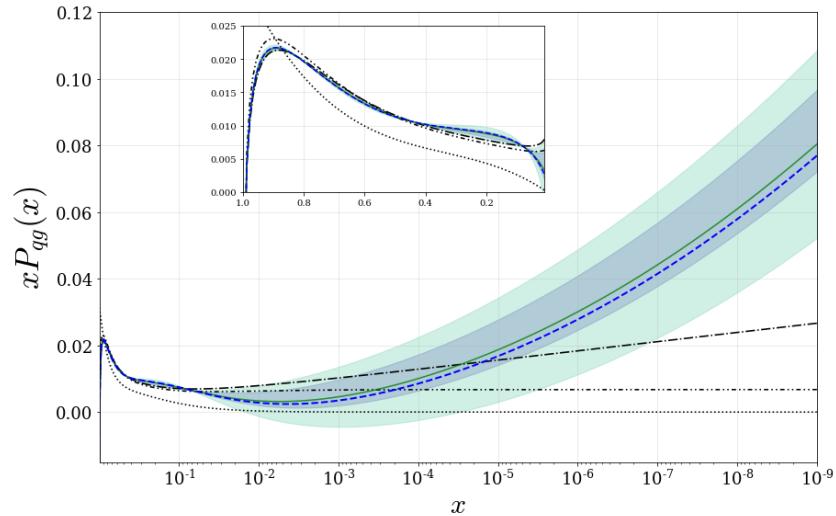
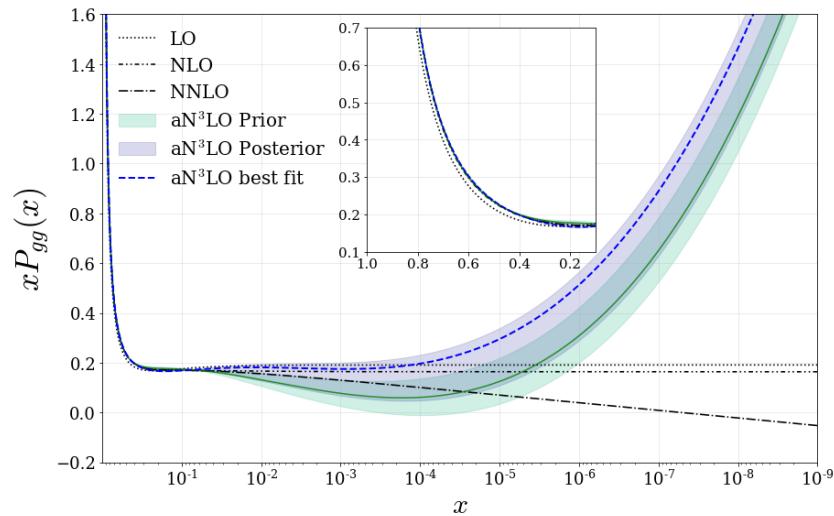
$$F(x) = \sum_{i=1}^{N_m} A_i f_i(x) + f_e(x).$$

Choose a set of relevant functions and solve for A_i .

Introduce a degree of freedom a , interpreted as a nuisance parameter allowed to vary in a PDF fit, $f_e(x) \rightarrow f_e(x, a)$. In our treatment it is the coefficient of the most divergent unknown small- x term, e.g. for $P_{qg}^{(3)}(x)$

$$\begin{aligned} f_1(x) &= \frac{1}{x} & \text{or } \ln^4 x & \text{or } \ln^3 x & \text{or } \ln^2 x, \\ f_2(x) &= \ln x, \\ f_3(x) &= 1 & \text{or } x & \text{or } x^2, \\ f_e(x, \rho_{qg}) &= \frac{C_A^3}{3\pi^4} \left(\frac{82}{81} + 2\zeta_3 \right) \frac{1}{2} \frac{\ln^2 1/x}{x} + \rho_{qg} \frac{\ln 1/x}{x}. \end{aligned}$$

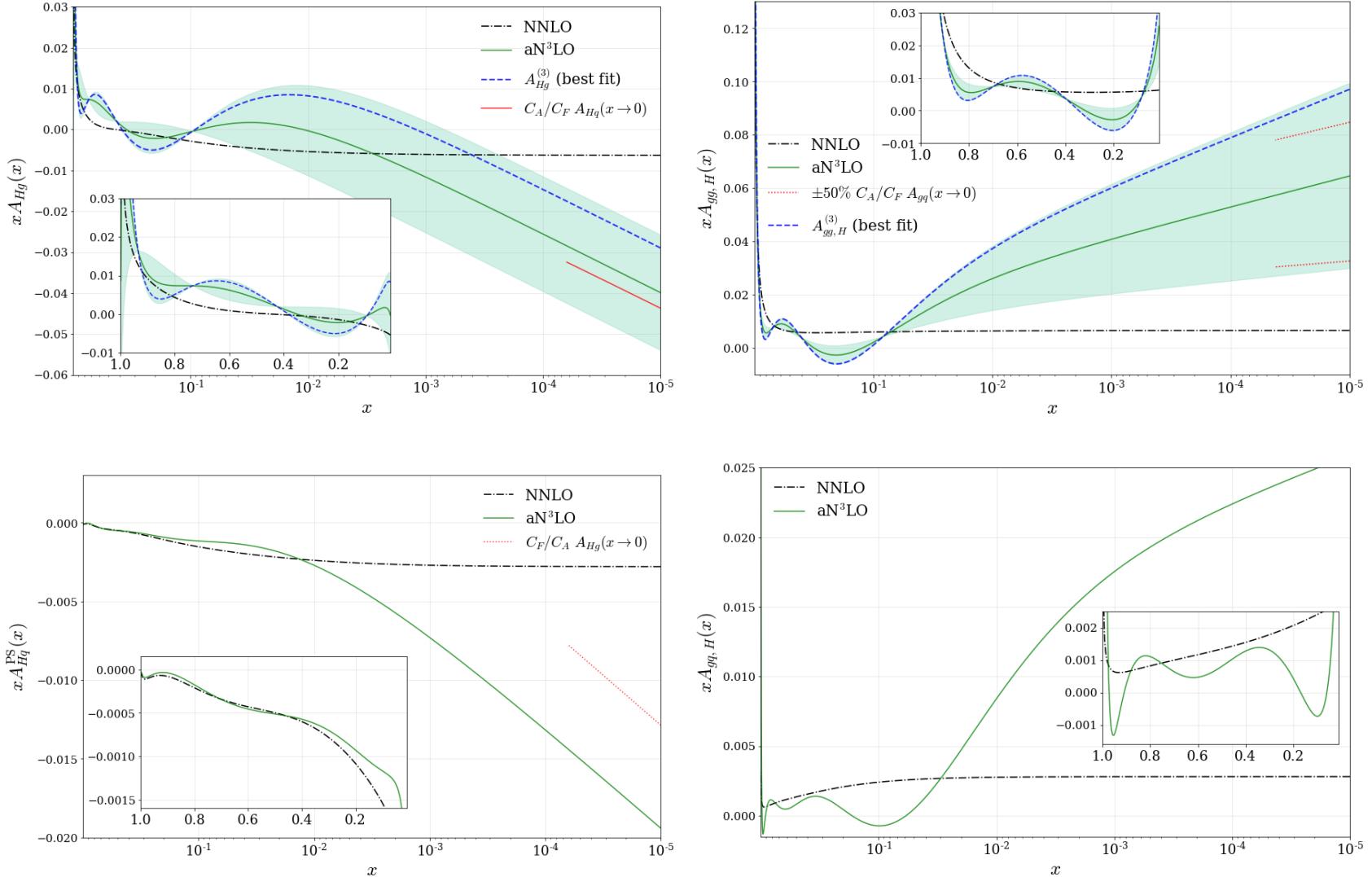
Resulting splitting functions



Uncertainty largest at small x . Best fit largely compatible with best estimate.

Transition Matrix Elements at aN³LO

Following the same general procedure as for the splitting functions.



Note recent update for $A_{gg,H}$ in [22] - near to our prior at small x .

K-factors at aN³LO – Parameterise as a superposition of both NNLO and NLO K-factors.

$$K(y) = 1 + \frac{\alpha_s}{\pi} D(y) + \left(\frac{\alpha_s}{\pi}\right)^2 E(y) + \left(\frac{\alpha_s}{\pi}\right)^3 F(y) + \mathcal{O}(\alpha_s^4).$$

$$K^{\text{N}^3\text{LO}/\text{LO}} = K^{\text{NNLO}/\text{LO}} \left(1 + \alpha_s^3 \hat{a}_1 \frac{\mathcal{N}^2}{\pi} D + \alpha_s^3 \hat{a}_2 \frac{\mathcal{N}}{\pi^2} E \right).$$

Hence default is no correction at N³LO.

Correlated K-factors for each of the 5 processes: DY, Top, Jets (or Dijets), $Z p_T$ and vector boson jets and Dimuon.

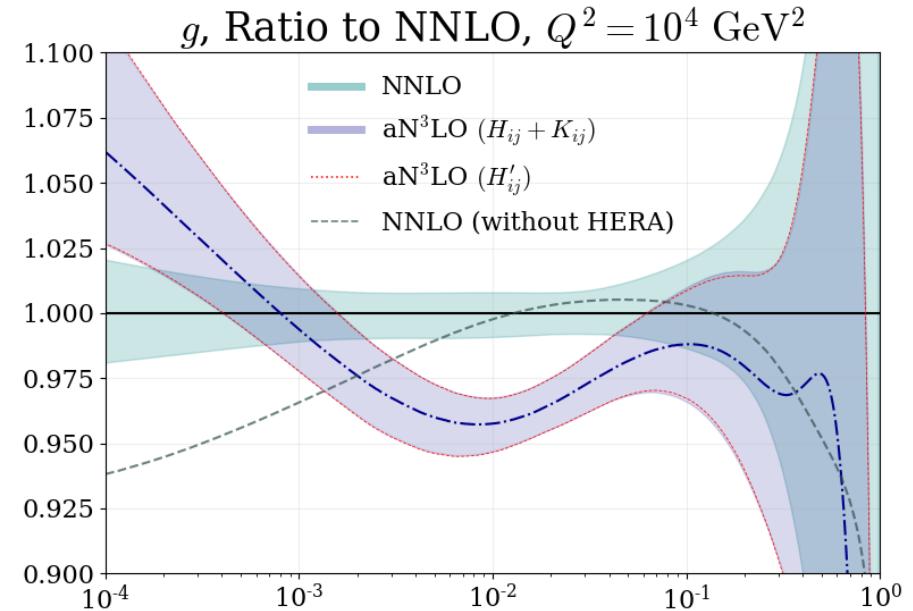
Global Fit Quality at aN³LO We see a reduction in χ^2 from NNLO across all datasets ($\Delta\chi^2 = -160$ for 20 extra parameters).

The overall χ^2 follows the general trend one may expect from perturbation theory.

	LO	NLO	NNLO	N ³ LO
$\chi^2_{N_{pts}}$	2.57	1.33	1.17	1.14

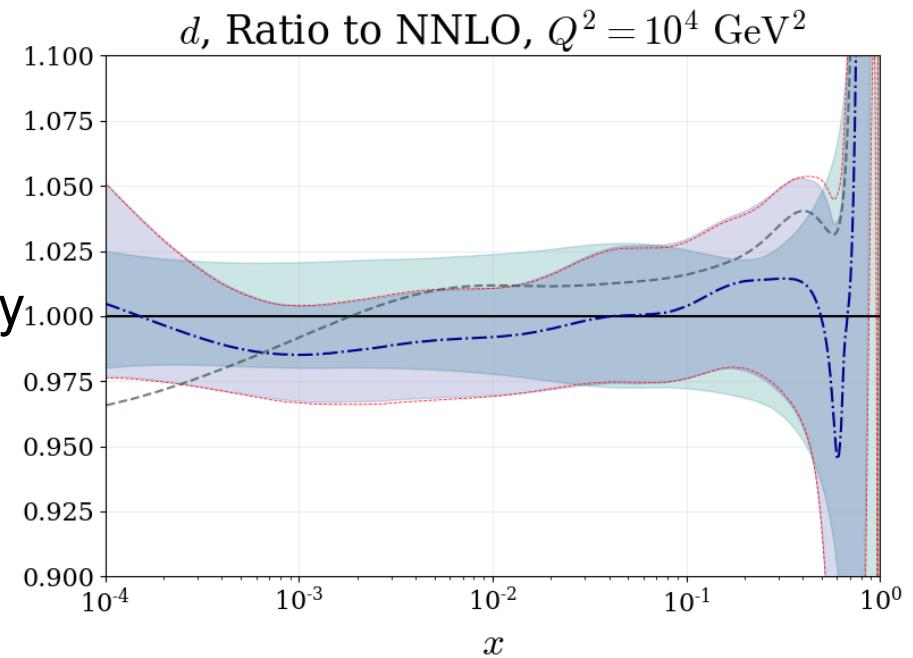
The PDFs at aN^3LO compared to NNLO - detail.

The gluon is enhanced at small- x due to the large logarithms present at higher orders.



Light quarks enhanced slightly at high x .

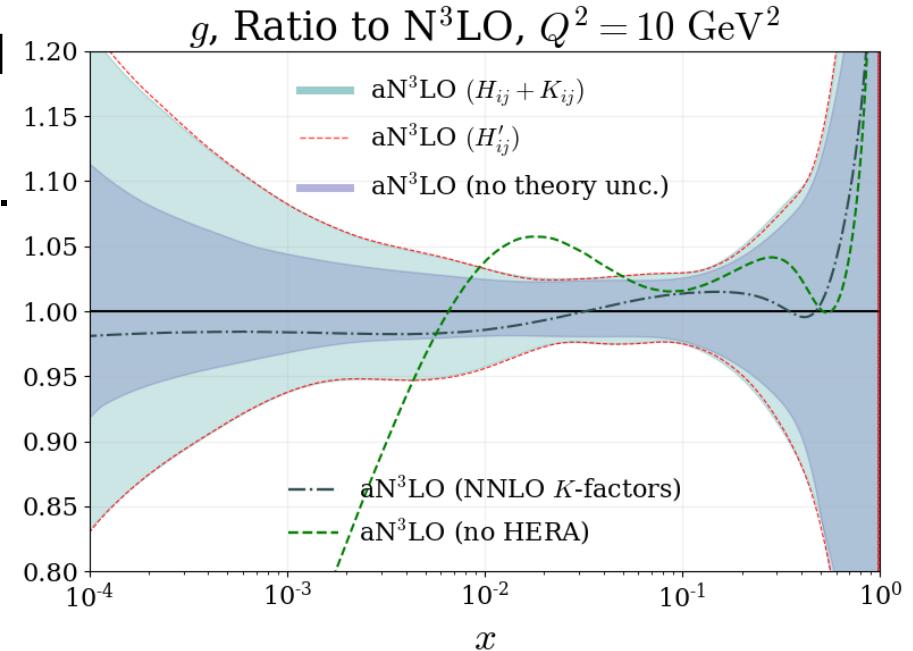
Correlated and uncorrelated K -factors show consistent uncertainty predictions.



The PDFs at aN^3LO with theoretical uncertainty.

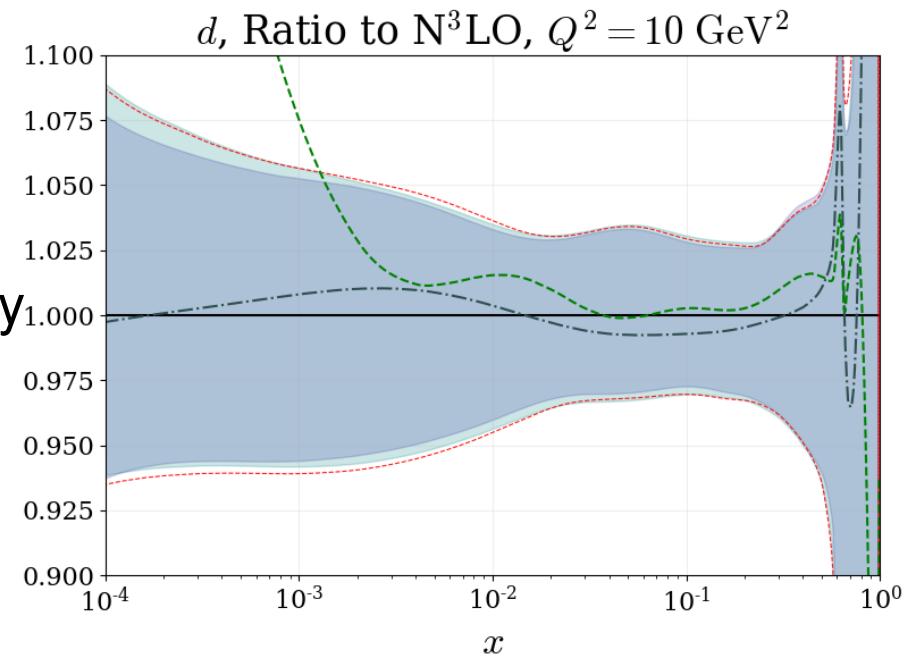
The gluon uncertainty is increased at small- x due to the large uncertainty in the splitting function.

Fit with no N^3LO K-factors leads to small changes only.

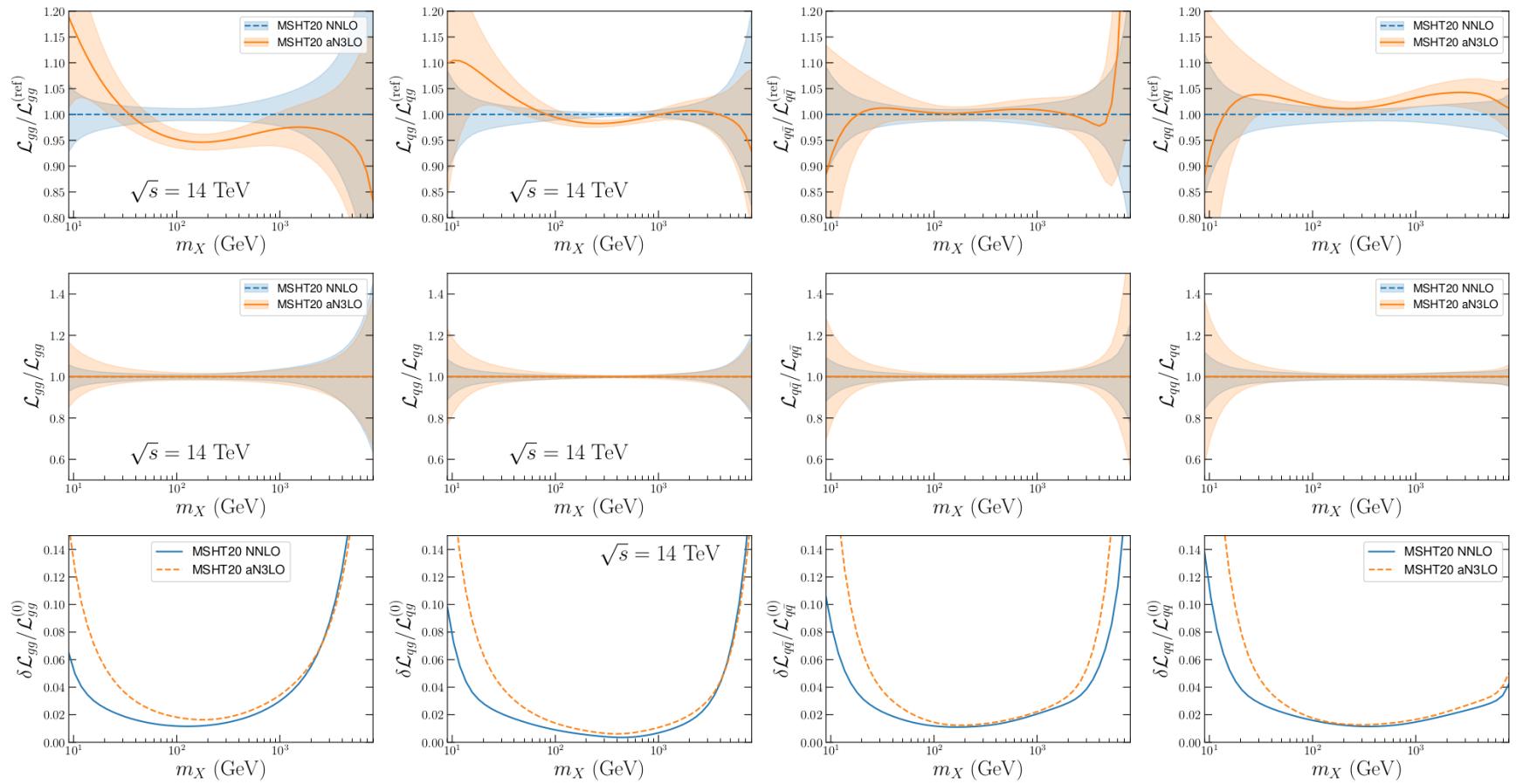


Light quark uncertainty enhanced slightly at low x .

Correlated and uncorrelated K-factors show consistent uncertainty predictions.



PDF luminosities



Big change for low masses $\sim 10\text{GeV}$, but an increase in uncertainties.

Up to 5% lowering of gluon luminosity for $\sim 100\text{GeV}$.

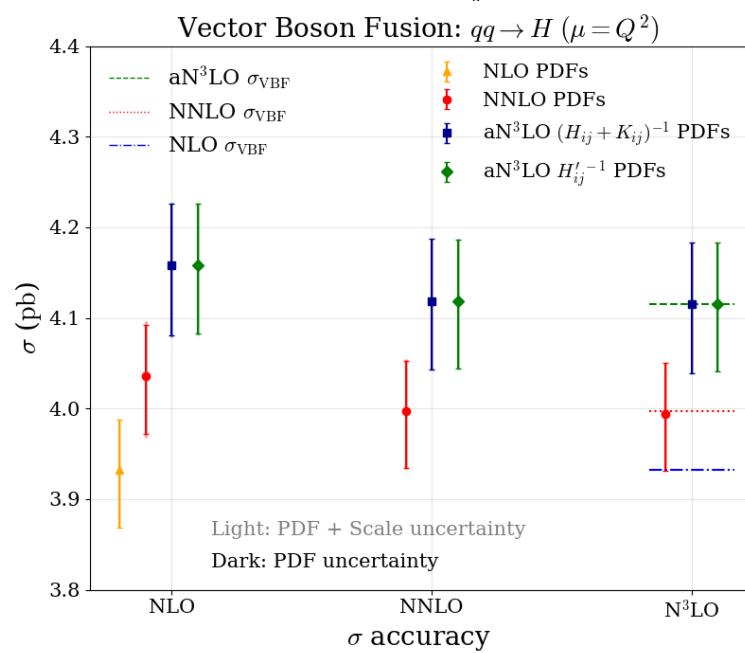
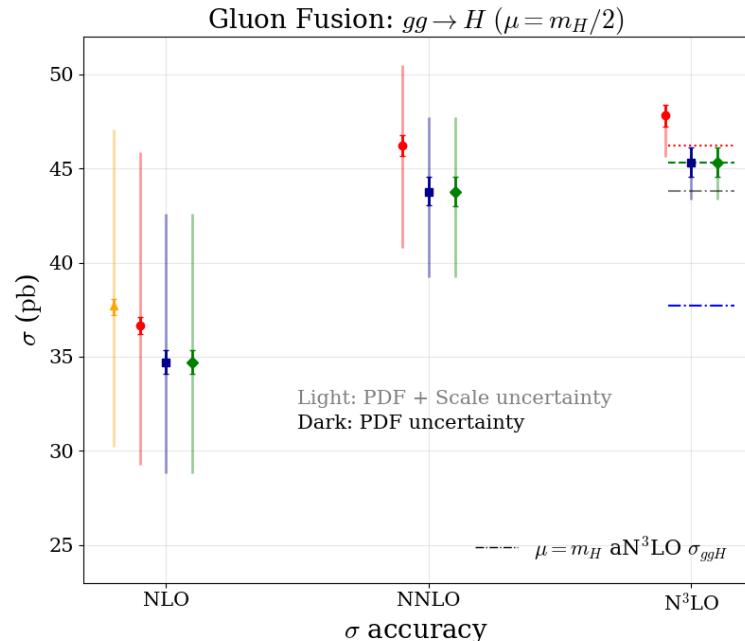
Higgs predictions at N³LO with Theoretical Uncertainty.

Good agreement between NNLO and aN³LO for gluon fusion (top).

Cancellation between N³LO cross section and PDFs not automatic.

Less cancellation for VBF (bottom).

However variation between orders is smaller for VBF cross-section.



NNPDF study also ongoing. Similar in numerous respects.

Incomplete higher order uncertainties

Approximate N³LO splitting functions as

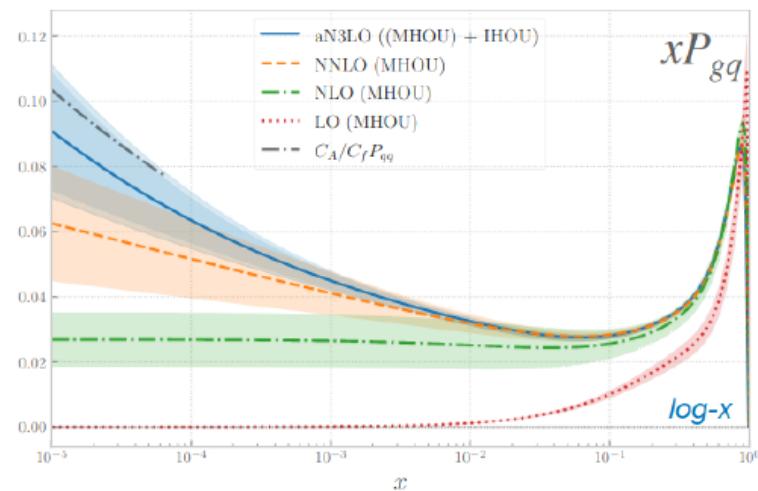
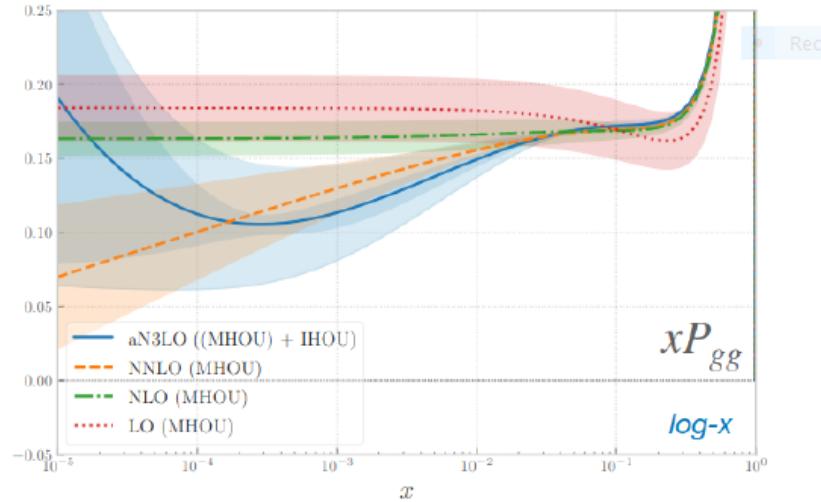
$$\gamma_{ij}^{(3)} = \gamma_{ij,n_f^3}^{(3)} + \gamma_{ij,N \rightarrow \infty}^{(3)} + \gamma_{ij,N \rightarrow 0}^{(3)} + \tilde{\gamma}_{ij}^{(3)}$$

Parametrise $\tilde{\gamma}_{ij}^{(3)} = \sum_l a_{ij}^{(l)} G_l(N)$

- G_1 for the leading unknown large- N term
- G_2 for the leading unknown small- N term
- 3 or 8 G_l for the sub-leading unknown small- and large- N contributions
- vary the functions G_l to generate a variety of approximations and estimate IHOU
- determine the coefficients $a_{ij}^{(l)}$ with known moments and momentum conservation

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

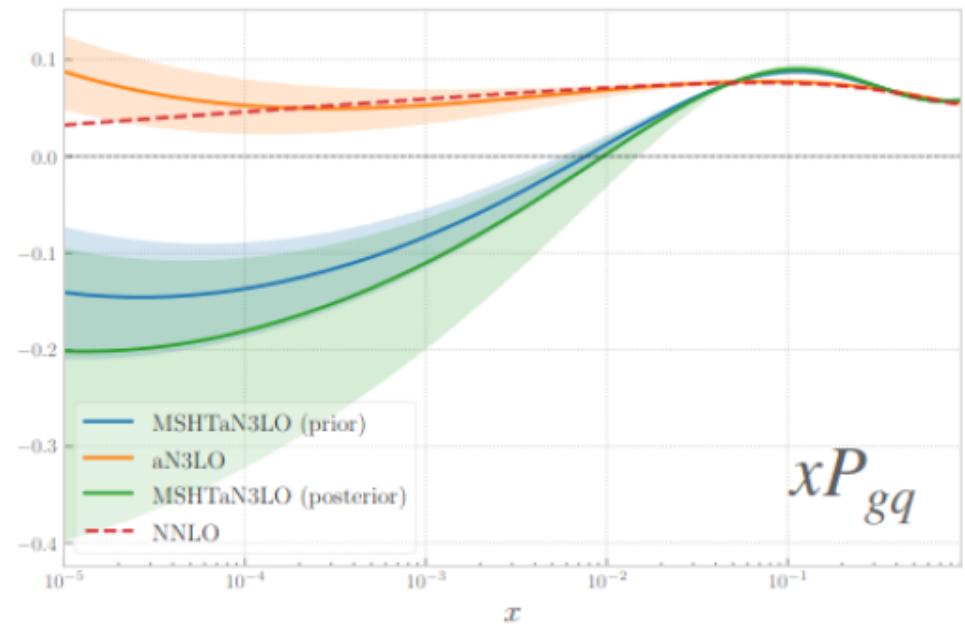
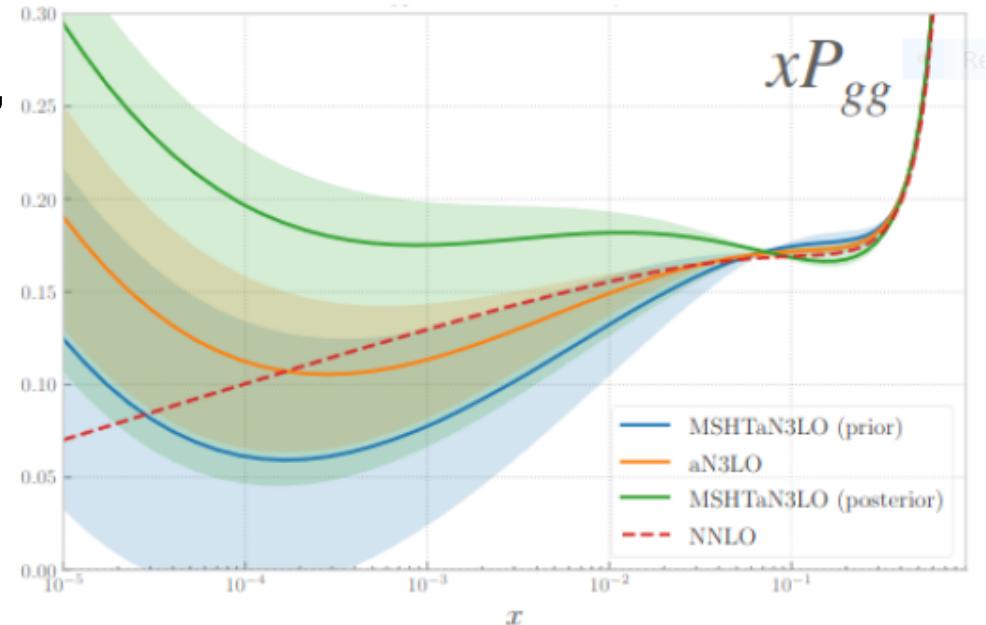
$G_1(N)$	$\mathcal{M}[(1-x) \ln^2(1-x)]$
$G_2(N)$	$-\frac{1}{(N-1)^2} + \frac{1}{N^2}$
$G_3(N)$	$\frac{1}{N^4}, \frac{1}{N^3}, \mathcal{M}[(1-x) \ln(1-x)]$ $\mathcal{M}[(1-x)^2 \ln(1-x)^2], \frac{1}{N-1} - \frac{1}{N}, \mathcal{M}[(1-x) \ln(x)]$
$G_4(N)$	$\mathcal{M}[(1-x)(1+2x)], \mathcal{M}[(1-x)x^2],$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



[arXiv:2306.15294; NNPDF, in preparation]

Largely similar splitting functions, except for P_{gq} (One extra unknown small- x divergent term in this).

Most recent versions include recent additional information on splitting functions.



[arXiv:2306.15294; NNPDF, in preparation]

Parts unknown at N³LO estimated using existing covariance matrix/scale variation approach. Nocera

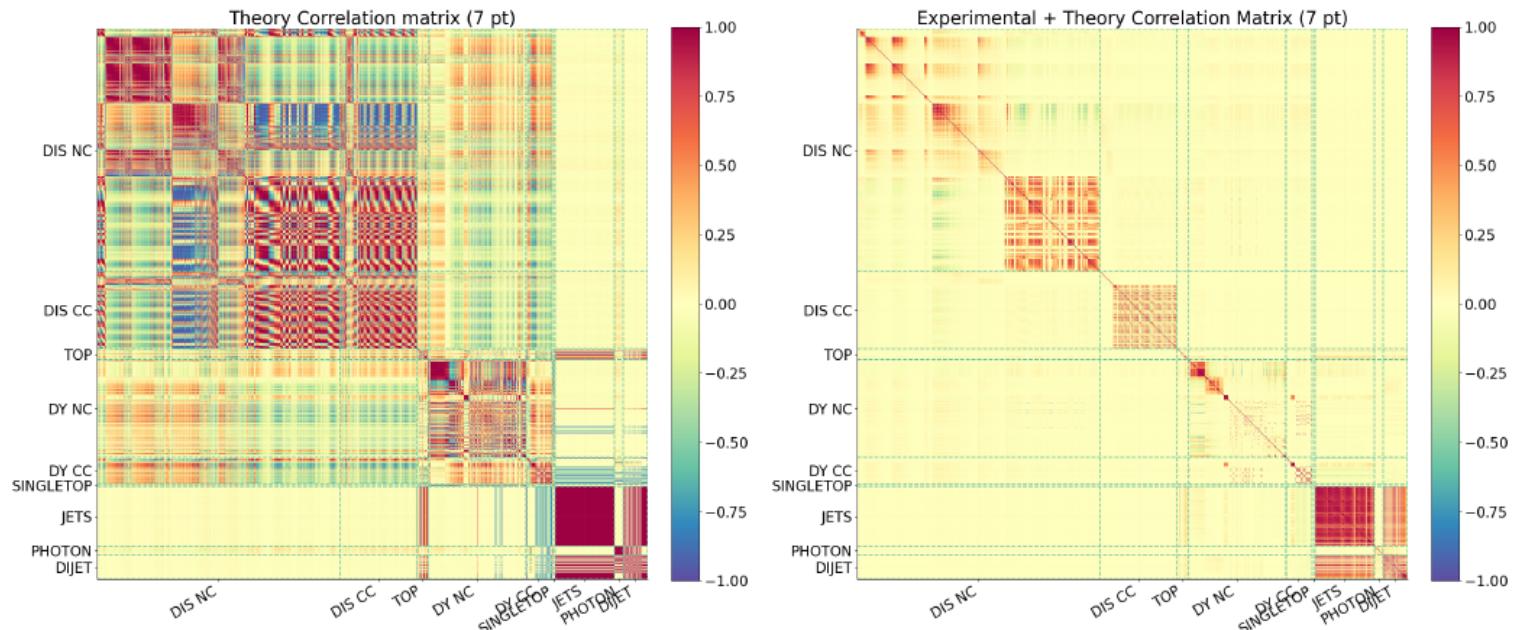
Theory uncertainties in PDF determination

Assuming that theory uncertainties are (a) Gaussian and (b) independent from experimental uncertainties, modify the figure of merit to account for theory errors

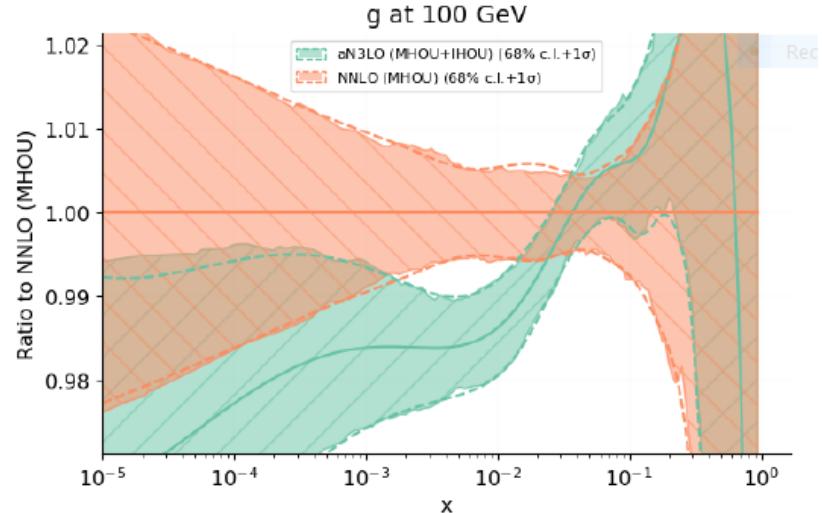
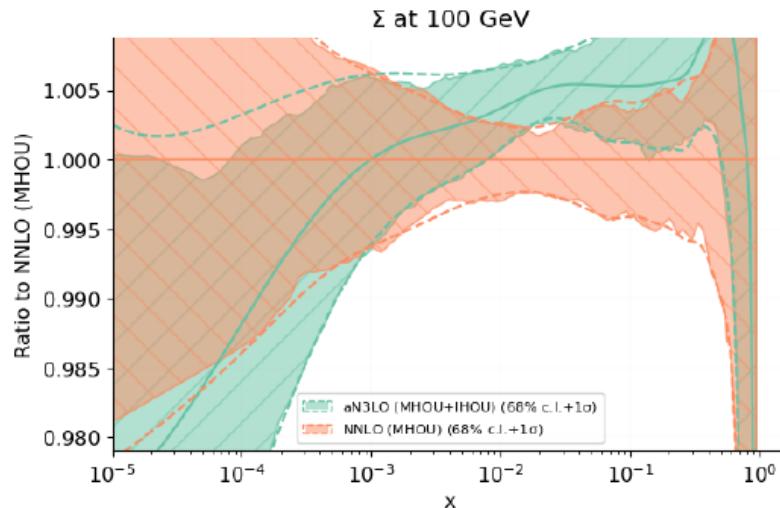
$$\chi^2 = \sum_{i,j}^{N_{\text{dat}}} (D_i - T_i)(\text{cov}_{\text{exp}} + \text{cov}_{\text{th}})^{-1}(D_j - T_j); (\text{cov}_{\text{th}})_{ij} = \frac{1}{N} \sum_k \Delta_i^{(k)} \Delta_j^{(k)}; \Delta_i^{(k)} \equiv T_i^{(k)} - T_i$$

Problem reduced to estimate the th. cov. matrix, e.g. in terms of nuisance parameters

$$\Delta_i^{(k)} = T_i(\mu_R, \mu_F) - T_i(\mu_{R,0}, \mu_{F,0}); \text{ vary scales in } \frac{1}{2} \leq \frac{\mu_F}{\mu_{F,0}}, \frac{\mu_R}{\mu_{R,0}} \leq 2$$



aN³LO PDFs — NNPDF PRELIMINARY

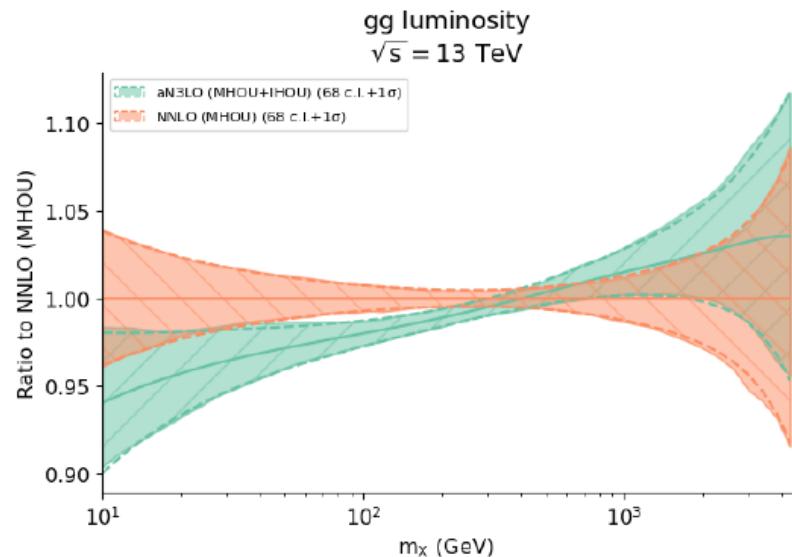


IHOU incorporated into
an independent covariance matrix
where nuisance parameters are averaged
over parametrisation variations

$$\chi^2/N_{\text{dat}} = 1.20 \text{ (NNLO (MHOU))}$$

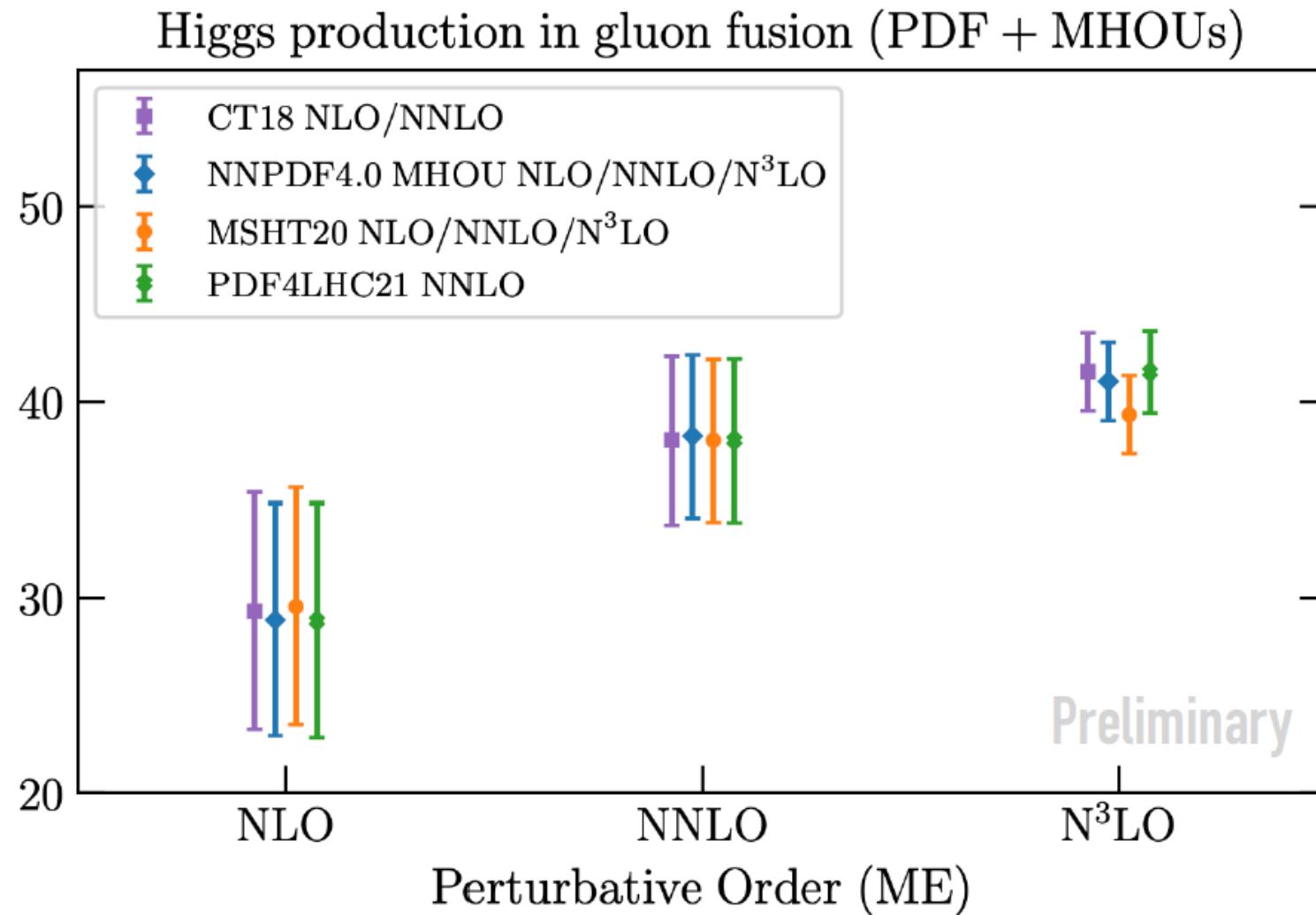
$$\chi^2/N_{\text{dat}} = 1.19 \text{ (aN}^3\text{LO (MHOU+IHOU))}$$

PDFs only affected at small x
largest effect: 2% suppression in \mathcal{L}_{gg}
around the Higgs mass



Recent presented results - smaller (but clear) change in gg luminosity.

Consequences for Higgs Cross Sections. Plot by Giacomo Magni



Changes in N^3 LO cross section relative to use of NNLO PDFs obvious.
Smaller for NNPDF than MSHT.

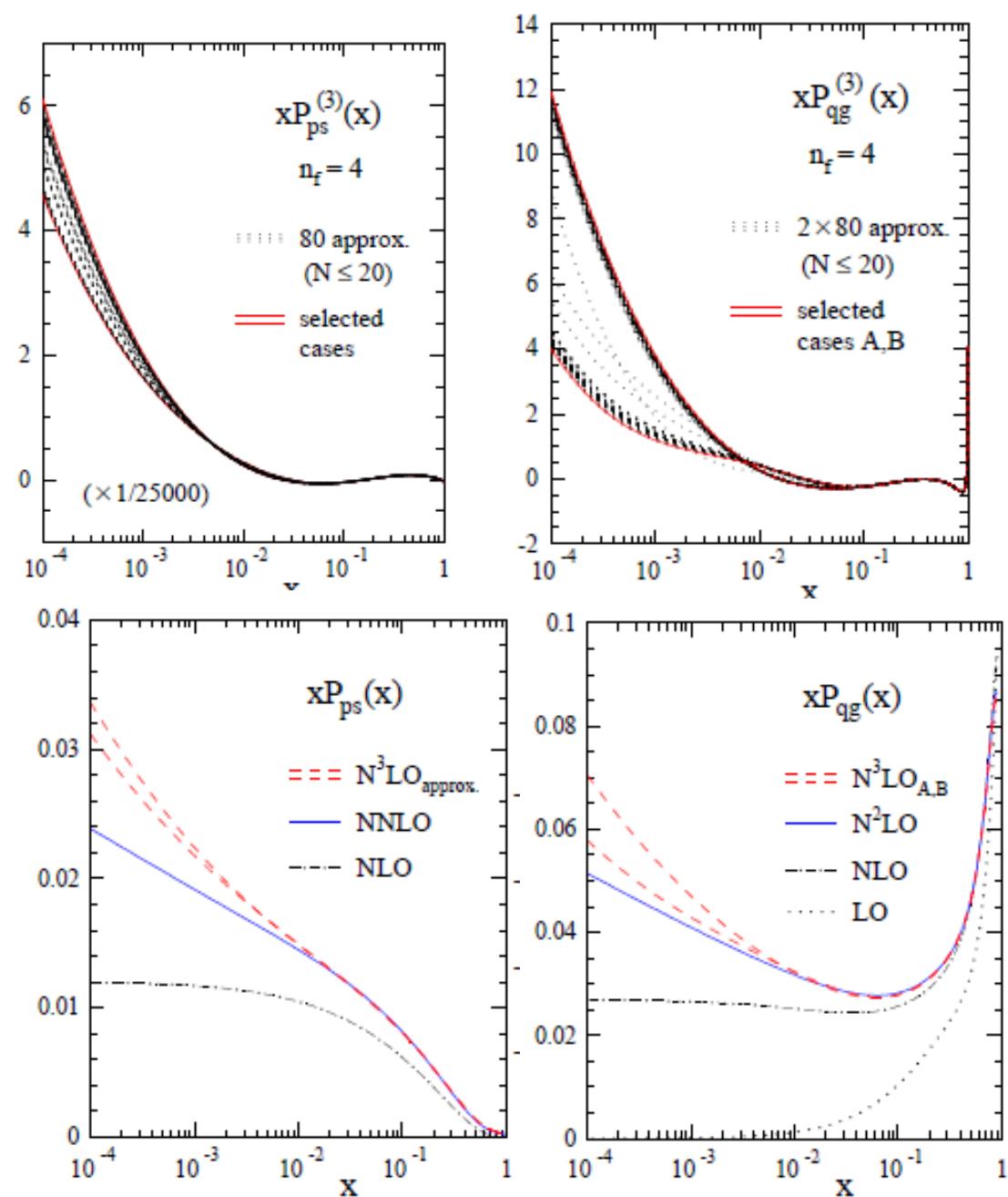
Recent improvements in knowledge of splitting functions.

Very recently [23-25] more moments have become available for splitting functions

Now 5 moments available for P_{gg} , P_{gq} . Allows improved constraint provided by [25] (Moch et al.)

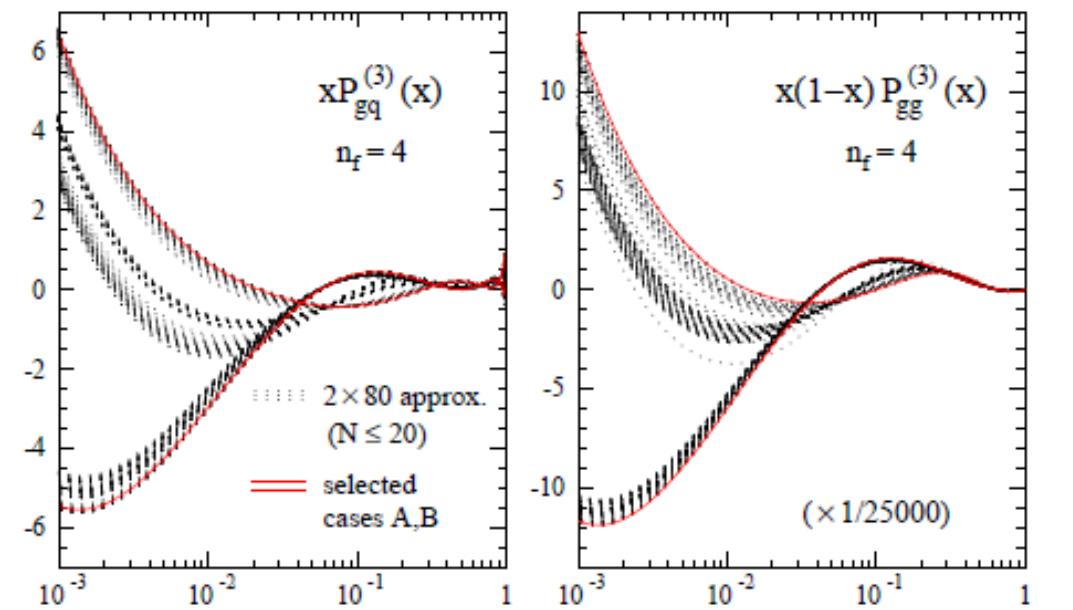
Also now 10 moments for P_{qq}^{PS} and P_{qg} . Allows much improved constraint in [24,25] (Falconi, et al.).

Range of allowed
N³LO splitting functions
using constraints.

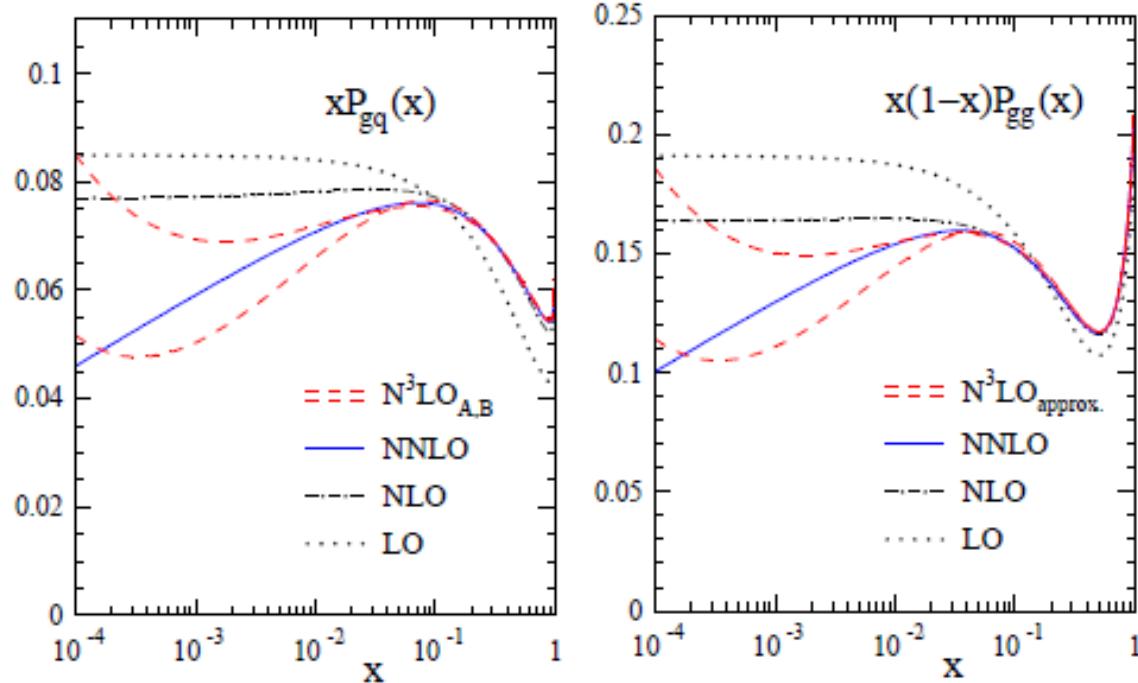


Range of allowed
total splitting splitting
functions.

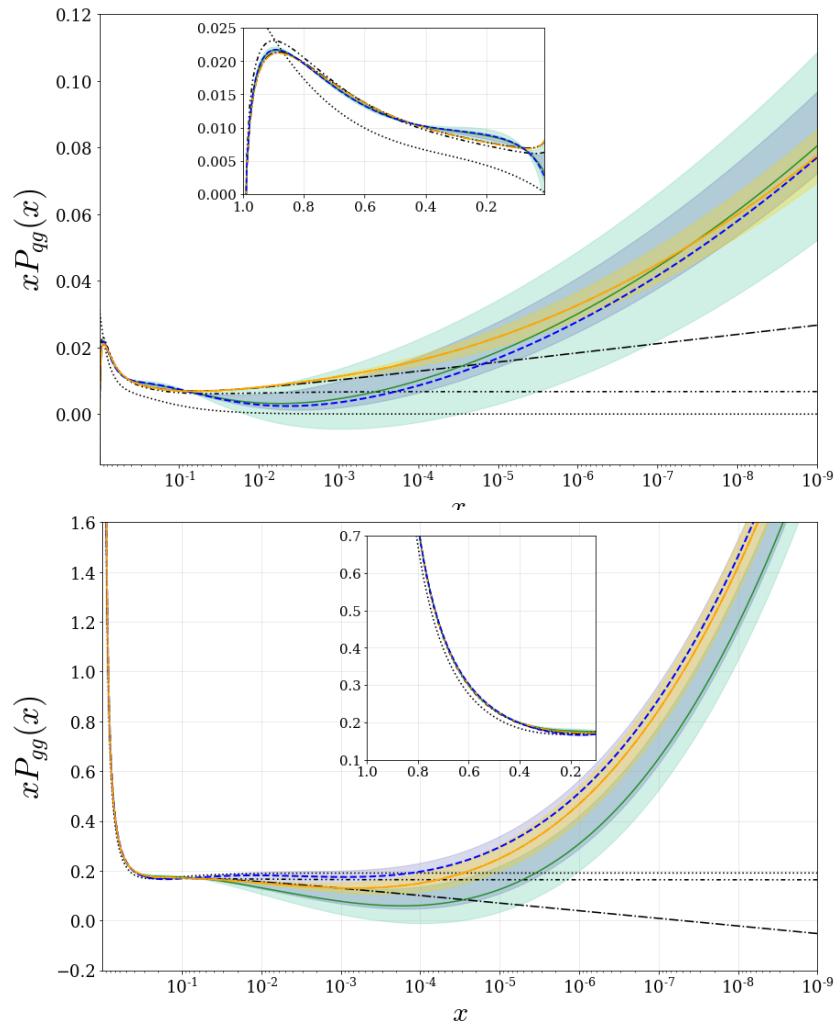
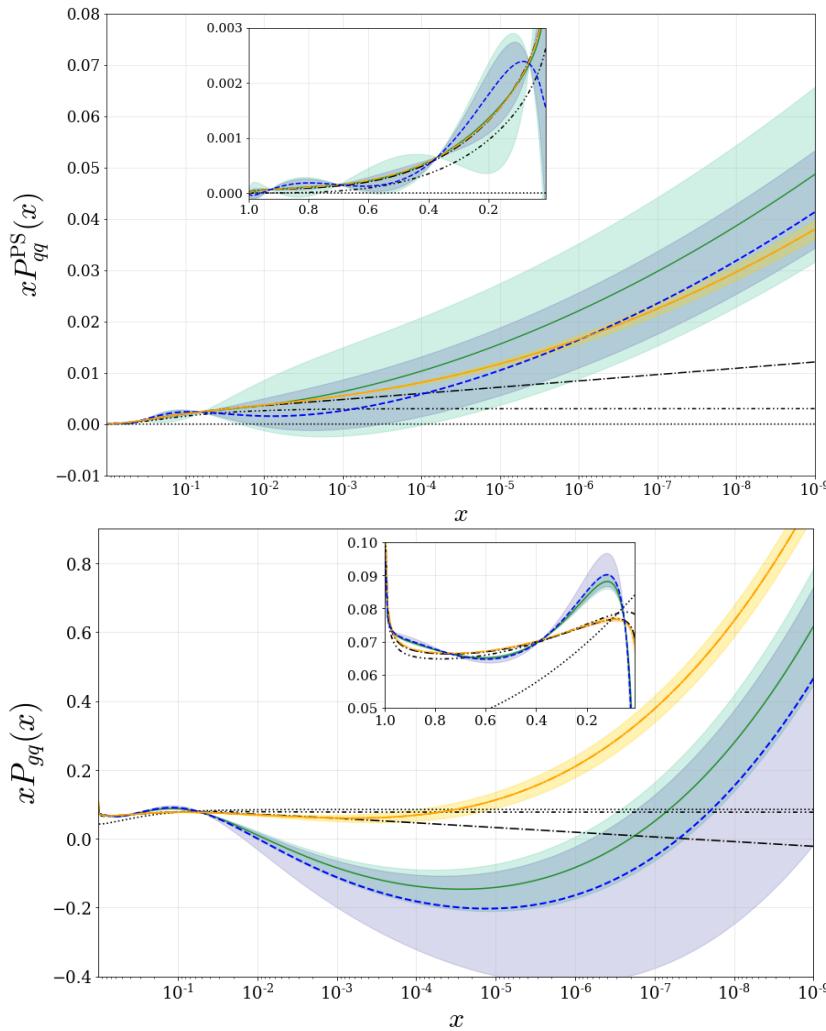
Range of allowed
N³LO splitting functions
using constraints.



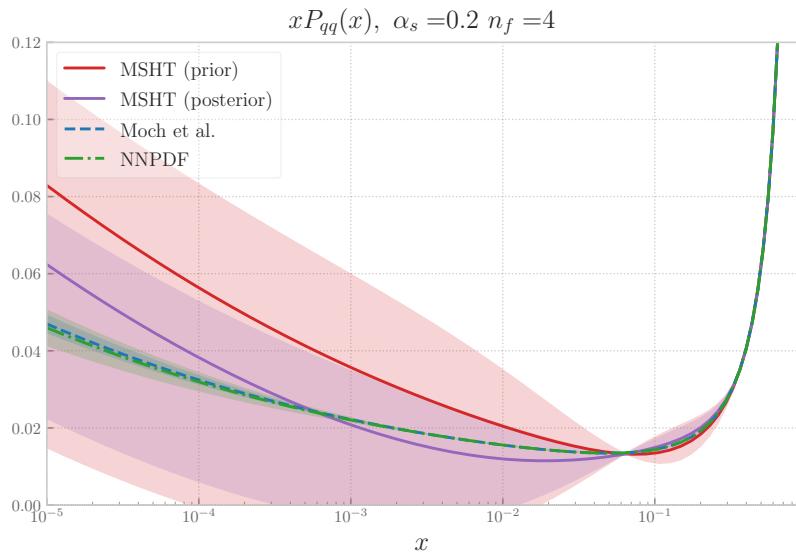
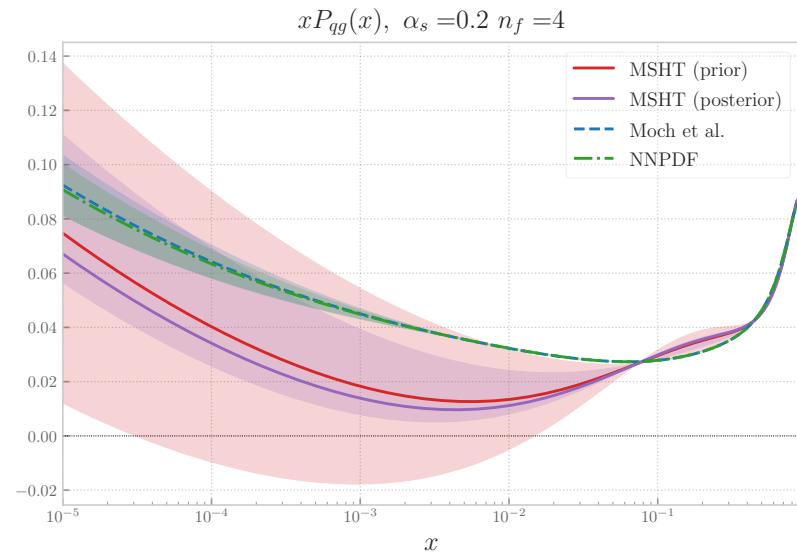
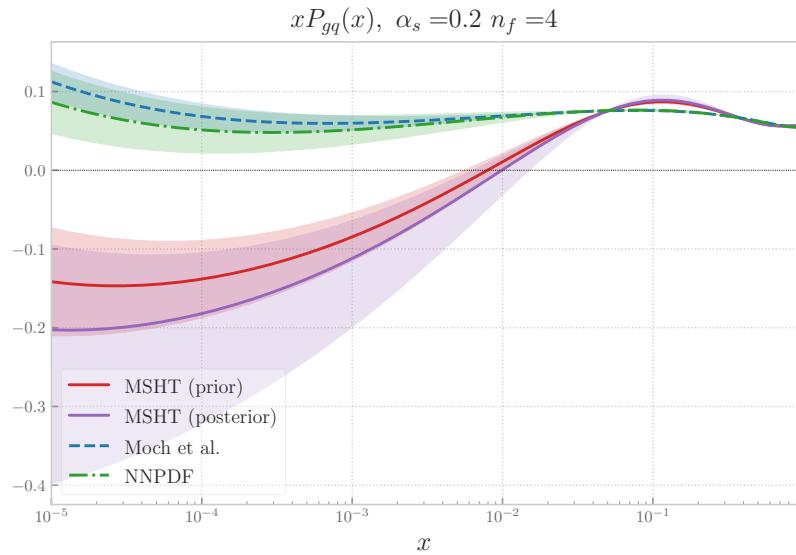
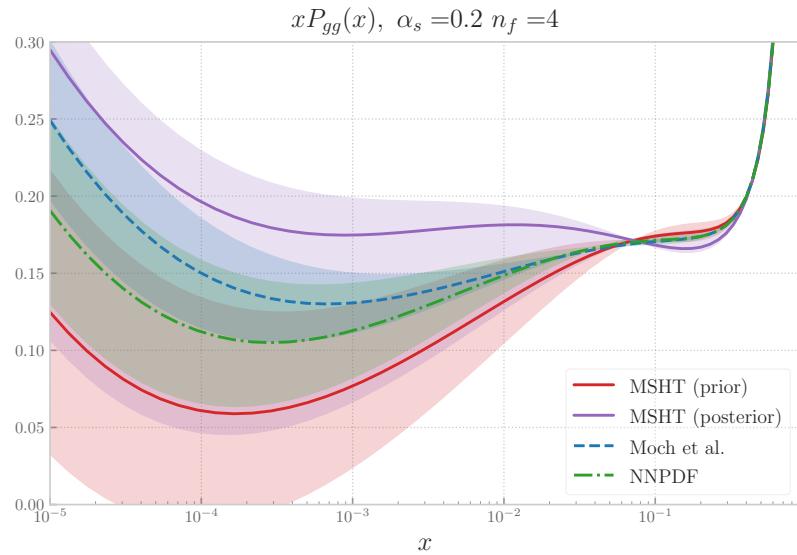
Range of allowed
total splitting splitting
functions.



Comparison with MSHT versions



Comparison with MSHT and NNPDF versions



Benchmarking PDFs at N³LO

Given seeming difference in MSHT and NNPDF results, and new results on splitting functions desire for this.

Check consistency of PDF evolution, and of effect of N³LO specifically on evolution.

$$\begin{aligned} xu_v(x, \mu_{f,0}^2) &= 5.107200 x^{0.8} (1-x)^3 \\ xd_v(x, \mu_{f,0}^2) &= 3.064320 x^{0.8} (1-x)^4 \\ xg(x, \mu_{f,0}^2) &= 1.700000 x^{-0.1} (1-x)^5 \\ xd(x, \mu_{f,0}^2) &= .1939875 x^{-0.1} (1-x)^6 \\ xu(x, \mu_{f,0}^2) &= (1-x) xd(x, \mu_{f,0}^2) \\ xs(x, \mu_{f,0}^2) &= xs(x, \mu_{f,0}^2) = 0.2 x(u+d)(x, \mu_{f,0}^2) \end{aligned}$$

Following outline of previous benchmarking up to NNLO in [arXiv:hep-ph/0511119](https://arxiv.org/abs/hep-ph/0511119).

Evolve specific PDF inputs at $Q_0^2 = 2\text{GeV}^2$ up to higher scales using FFNS ($n_f = 4$) and VFNS.

Ongoing study to be written up for Les Houches proceedings.

Check output of various PDF flavours at $Q^2 = 10^4 \text{ GeV}^2$.

first check consistency between groups and previous results at **NNLO**.

NNPDF reproduce results at small fractions of a percent.

Table 15: As Table 14, but for the variable- N_f evolution using the flavour matching conditions of Ref. [156, 158, 159]. The corresponding values for the strong coupling $\alpha_s(\mu_r^2 = 10^4 \text{ GeV}^2)$ are given by 0.115818, 0.115605 and 0.115410 for $\mu_r^2/\mu_f^2 = 0.5, 1$ and 2, respectively. For brevity the small, but non-vanishing valence distributions s_v, c_v and b_v are not displayed.

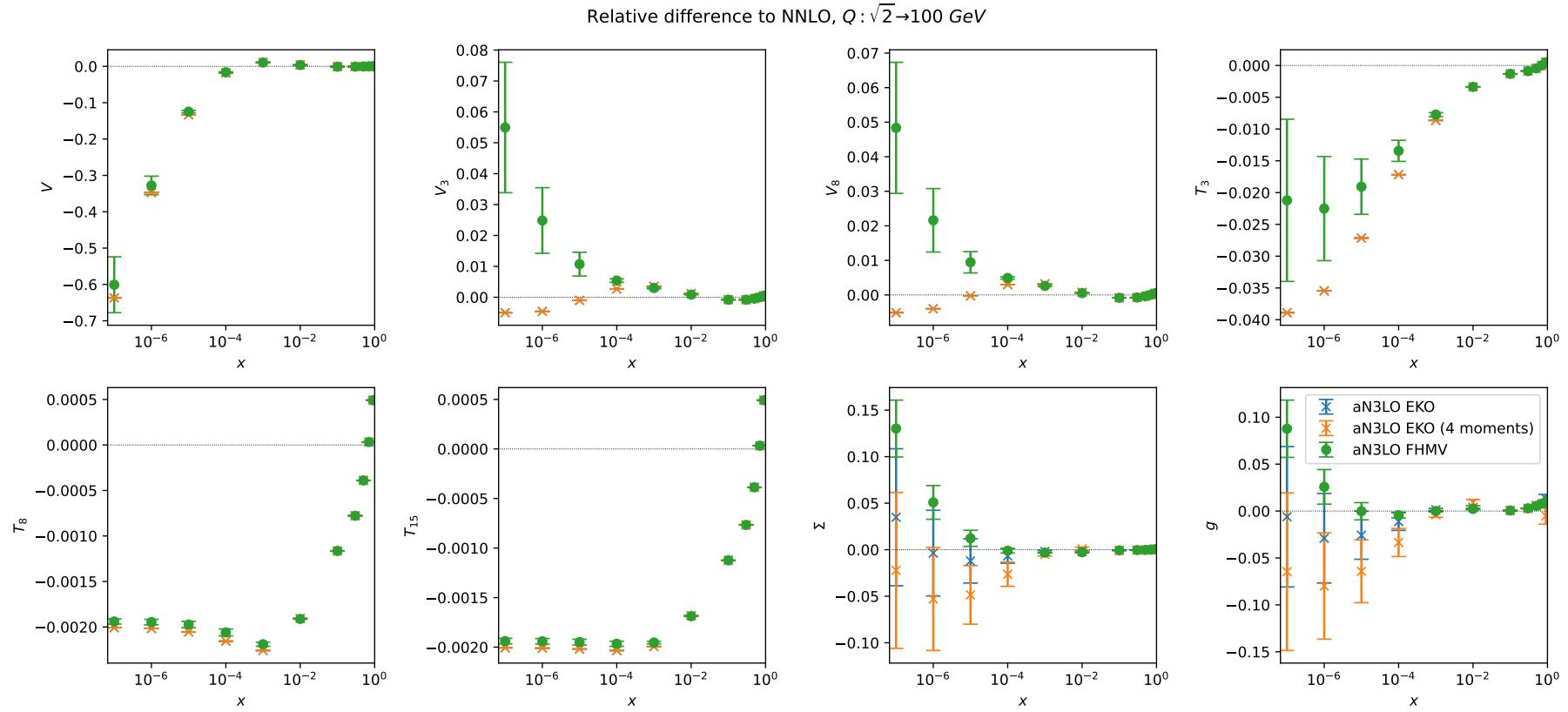
NNLO, $N_f = 3 \dots 5, \mu_f^2 = 10^4 \text{ GeV}^2$								
$\mu_r^2 = \mu_f^2$								
$\mu_r^2 = 2\mu_f^2$								
$\mu_r^2 = 1/2\mu_f^2$								

Sheet3

	% Diff															
q2	10 -7	100	100	100	10 -5	100	100	100	10 -3	100	100	100	100	100	100	100
x	10 -7	10 -6	100	10 -5	10 -4	100	100	100	10 -2	100	100	100	100	100	100	100
xuv	6.724777805	1.454466004	0.318978085	0.060889348	0.004290249	0.001781482	0.001489646	0.005107935	0.003415103	0.004782076	0.002872995					
xdv	957.6335728	1.298917918	0.304533463	0.059361691	0.003524803	0.00325544	0.003738674	0.002895372	0.001302436	0.005432174	0.29210766					
xL-	5.521662538	1.012778192	0.180796357	0.027580135	0.003328673	0.003819014	0.005341067	0.001439285	0.009377039	0.076507725	2.261210857					
2xL+	0.049860097	0.018875605	0.004304481	0.005281659	0.015566098	0.016314224	0.020964573	0.032699221	0.033842586	0.035408441	0.260661713					
xs+	0.048674074	0.020513593	0.006189168	0.008904641	0.016824242	0.023365487	0.034818614	0.061531196	0.082927462	0.101422762	2.729164926					
xc+	0.038311983	0.007735995	0.016949668	0.03152775	0.050991358	0.079843716	0.16641915	0.291197955	0.186763124	1.352281881	35.11659333					
xb+	0.060199384	0.028298568	0.008972637	0.005748467	0.02104596	0.040932376	0.084744199	0.160580891	0.06762597	0.933216499	21.37352777					
xg	89.99308504	0.037556155	0.018420186	0.00662357	0.002179872	0.003327432	0.006718046	0.025870709	0.043835672	0.037651874	0.367129326					

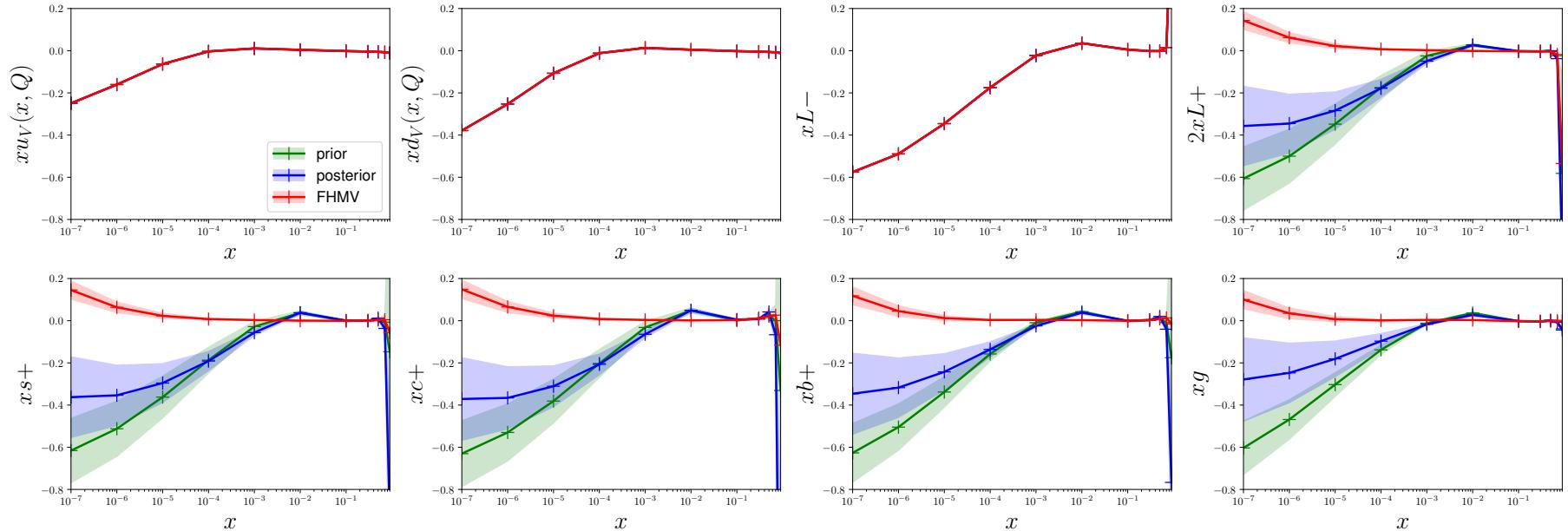
MSHT similar except at very high x , and low x , mainly in extrapolation region of grids.

NNPDF evolution at N³LO compared to NNLO for various splitting function choices. **Preliminary**



Some difference in own versions, particularly when based on less information than most up-to-date versions, at very small x .

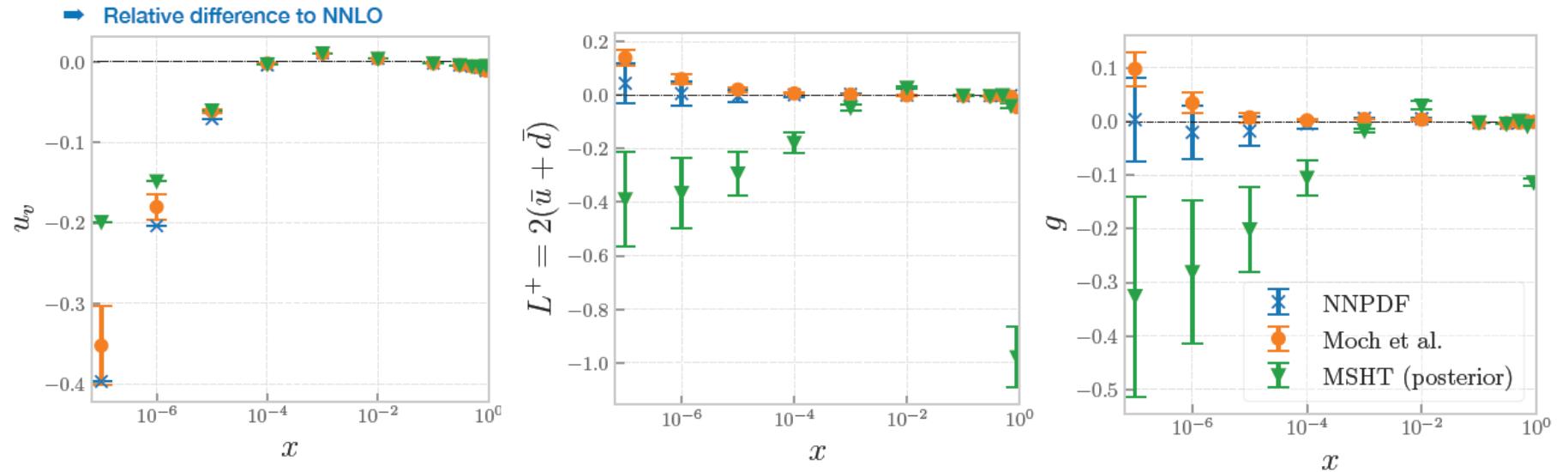
MSHT evolution at N³LO compared to NNLO for various splitting function choices. **Preliminary**



Therefore good agreement with **NNPDF** for most up-to-date splitting functions provided externally from groups.

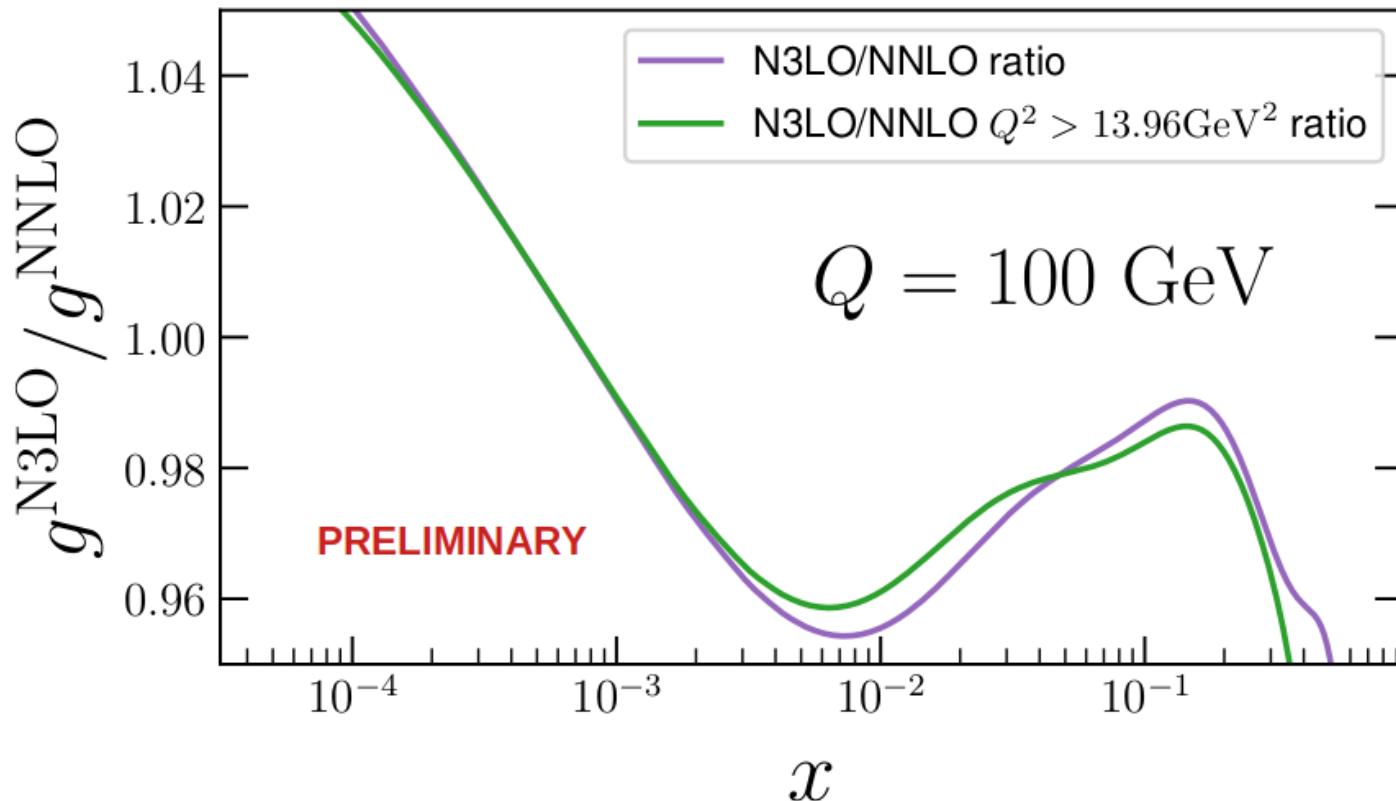
More difference in own versions based on less information, and different to **NNPDF**, but mainly at very small x .

MSHT and NNPDF evolution at $N^3\text{LO}$ compared to NNLO . Preliminary



Good agreement for Moch et al. splitting functions except for extremely low non-singlet distributions where different approximations for unknown $P_{q\bar{q}}^{NS}$ have been made.

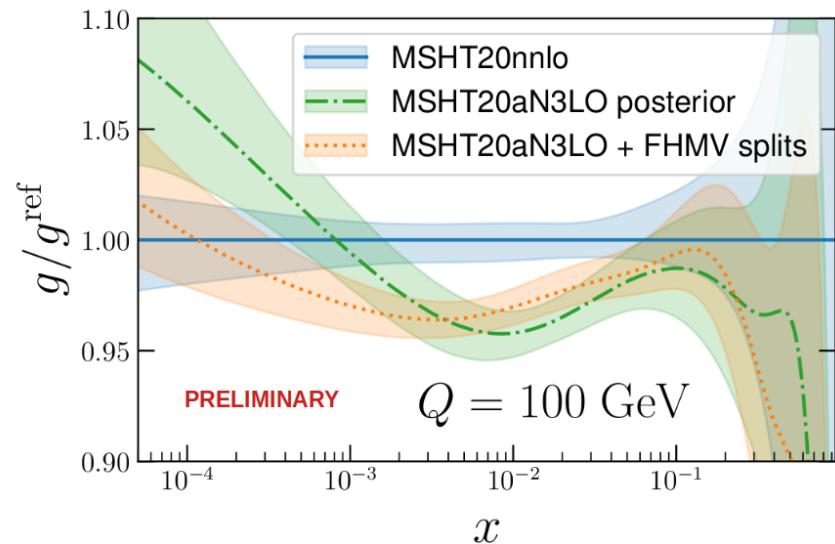
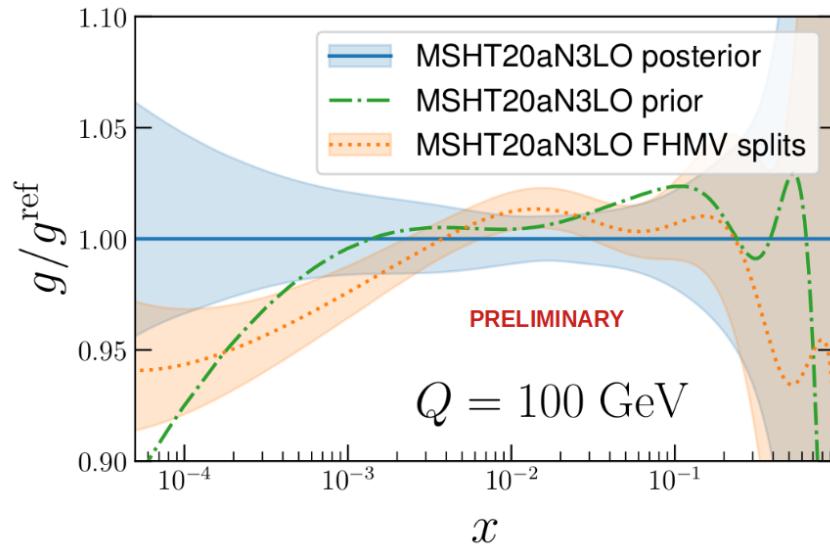
Effect of MSHT fitting with NNPDF cuts.



Raising the cuts in the MSHT fit to make them equivalent to the NNPDF choice (enabling upward and downwards scale variation).

Changes the effect of N³LO compared to NNLO to make the change between orders in MSHT slight less for gluon near $x = 0.01$.

Effect of MSHT fits with improved splitting functions.



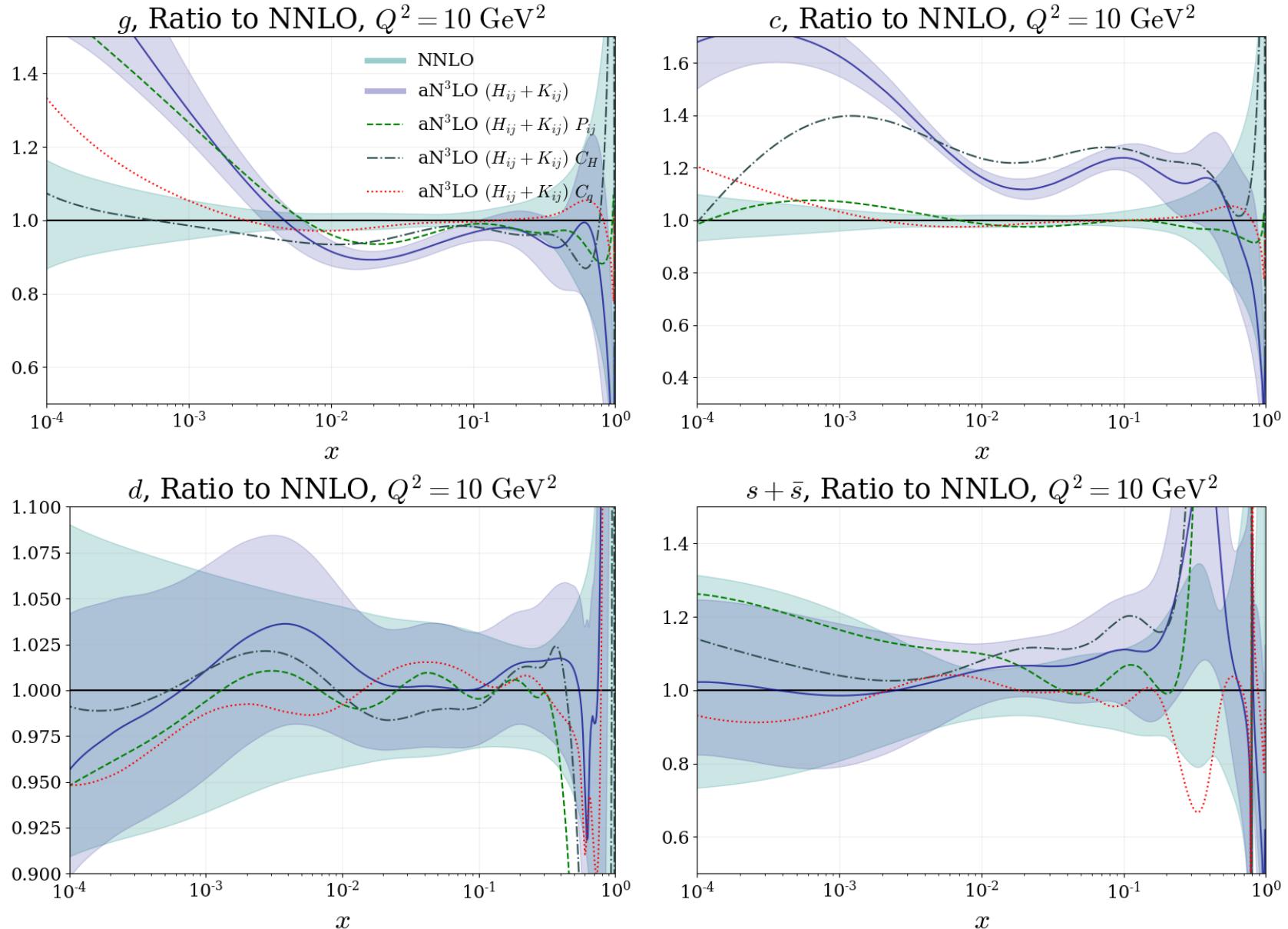
Note - no uncertainties used for improved splitting functions - only central value. Now almost exclusively at small x .

$\chi^2 \sim 50$ worse than before (over 100 lower than NNLO) very largely at small x - would improve at some level once uncertainty accounted for.

Use of (central value of) improved N³LO splitting functions changes N³LO gluon a little compared to published MSHT PDFs, raising 1.5% near $x = 0.01$.

Main features of N³LO comparison to NNLO remain the same.

Effect of each individual N^3LO change.



Not only splitting functions responsible for change in PDFs.

Conclusions

Approximate **N³LO** PDFs are available and we encourage their use.

Designed so that theoretical uncertainties represent the missing parts of **N³LO**, i.e. assume this is the dominant source of missing higher order corrections. Approaches to this differ.

Better precision, control of uncertainties, and better fit quality.

MSHT PDFs available as **LHAPDF** grids at www.hep.ucl.ac.uk/msht/ [1]. **NNPDF** versions soon.

Some apparent differences between **MSHT** and preliminary **NNPDF** versions.

Benchmarking exercise underway. Shows evolution consistent when same splitting functions used. Differences in evolution from the applied splitting functions – recent updates have led to significant improvements.

Indications from fits with more similar splitting functions and further analyses (e.g. cuts) reveal convergence and/or understanding of differences.

References

- [1] - J. McGowan, T. Cridge, L. A. Harland-Lang and R. S. Thorne, Eur. Phys. J. C83 (2023) no.3, 185.
- [2] - J. Vermaseren, A. Vogt, and S. Moch, Nuclear Physics B, 724, 3182 (2005)
- [3] - S. Moch, B. Ruijl, T. Ueda, J. A. M. Vermaseren, and A. Vogt, Journal of High Energy, 1653, Physics, 2017, (2017)
- [4] - A. Vogt et al., PoS LL2018, 050 (2018), 1808.08981
- [5] - S. Moch, B. Ruijl, T. Ueda, J. A. M. Vermaseren, and A. Vogt, (2021), 2111.15561
- [6] - S. Moch, B. Ruijl, T. Ueda, J. A. M. Vermaseren, and A. Vogt, Journal of High Energy, 1664, Physics, 2017, (2017)
- [7] - I. Bierenbaum, J. Blumlein, and S. Klein, Nuclear Physics B, 820, 417 (2009)
- [8] - M. Bonvini and S. Marzani, Journal of High Energy Physics, 2018, (2018)
- [9] - J. Ablinger et al., Nucl. Phys. B, 886, 733 (2014), 1406.4654.
- [10] - J. Ablinger et al., Nuclear Physics B, 890, 48151 (2015)
- [11] - J. Ablinger et al., Nuclear Physics B, 882, 263288 (2014)
- [12] - H. Kawamura, N. A. Lo Presti, S. Moch, and A. Vogt, Nucl. Phys. B, 864, 399 (2012), 1689
- [13] - J. Blumlein et al., PoS, QCDEV2017, 031 (2017), 1711.07957
- [14] - NNPDF coll. Eur. Phys. J. C 79 838 (2019)
- [15] - Z. Kassabov, M. Ubiali and C Voisey, 2207.07616
- [16] - F. Tackmann, SCET 2019 Workshop (2019)
- [17] - R. D. Ball and R. L. Pearson, The European Physical Journal C, 81, (2021)
- [18] - H. Kawamura, N. Lo Presti, S. Moch, and A. Vogt, Nuclear Physics B, 864, 399468, 1682, (2012).

- [19] - X. Chen et al., Phys.Rev.Lett. 128 (2022) 5, 052001, 2107.09085
- [20] - N. Kidonakis, 2109.14102
- [21] - J. Baglio et al., JHEP 12 (2022) 066, 2209.06138
- [22] - J. Ablinger et al., JHEP 12 (2022) 134, 2211.05462
- [23] G. Falcioni, F. Herzog, S. Moch and A. Vogt, Phys. Lett. B 842 (2023), 2302.07593.
- [24] G. Falcioni, F. Herzog, S. Moch and A. Vogt, Phys. Lett. B 846 (2023), 2307.04158.
- [25] S. Moch, B. Ruijl, T. Ueda, J. Vermaseren and A. Vogt, 2310.05744.

Back-up

Uncertainties as Nuisance Parameters.

Theoretical uncertainties in PDFs have been addressed via scale variations [14,15]. Do not use extensive available N^3LO information.

Do we need to wait for a full description of the next order to be able to use the knowledge we have?

Usual probability distribution

$$P(T|D) \propto \exp\left(-\frac{1}{2}(T - D)^T H_0(T - D)\right)$$

Can attempt to parameterise the higher order effects with a nuisance parameter defined by a prior probability distribution [16], see also [17].

Allow the fit to move these N^3LO parameters (with a penalty attached to ensure we stay close to the behaviour already known). $T \rightarrow T + \theta u$, where most probable prior value of $\theta = t$ and of N^3LO theory is $T' = T + tu$.

$$T \rightarrow T' + (\theta - t)u = T + tu + (\theta - t)u.$$

Defining $\theta' = \theta - t$ and

$$P(\theta') = \frac{1}{\sqrt{2\pi}\sigma_{\theta'}} \exp(-\theta'^2/2\sigma_{\theta'}^2).$$

Then

$$\begin{aligned} P(T|D\theta) &\propto \exp\left(-\frac{1}{2}(T + tu + \frac{(\theta-t)}{\sigma_{\theta'}}u - D)^T H_0 (T + tu + \frac{(\theta-t)}{\sigma_{\theta'}}u - D)\right) \\ P(T'|D\theta') &\propto \exp\left(-\frac{1}{2}(T' + \frac{\theta'}{\sigma_{\theta'}}u - D)^T H_0 (T' + \frac{\theta'}{\sigma_{\theta'}}u - D)\right) \end{aligned}$$

Overall we obtain

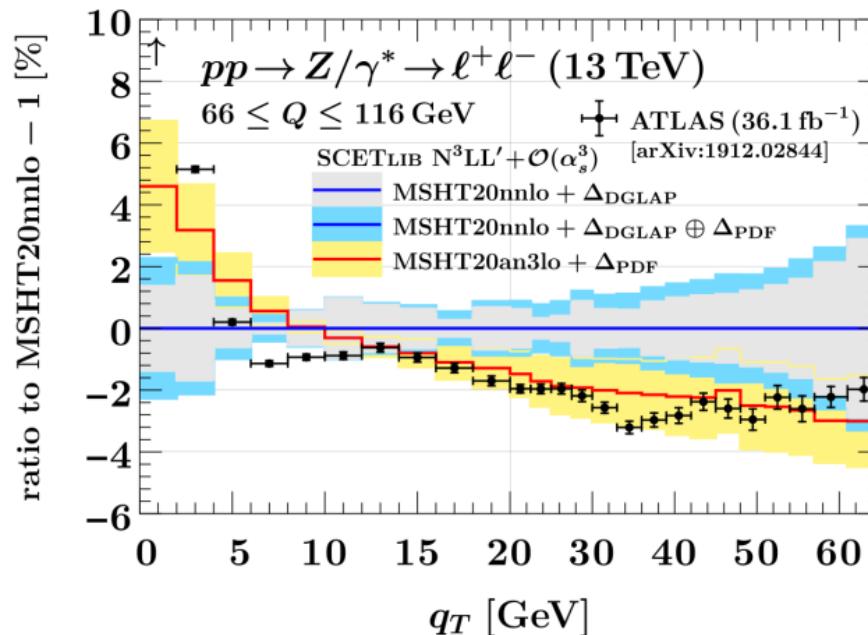
$$P(T'|D) \propto \int d\theta \exp\left(-\frac{1}{2}\left[(T' + \frac{\theta'}{\sigma_{\theta'}}u - D)^T H_0 (T' + \frac{\theta'}{\sigma_{\theta'}}u - D) + \theta'^2/\sigma_{\theta'}^2\right]\right).$$

With these alterations, we follow the same practice as set out in the **MSHT20 NNLO** PDF fit - the exact same global fit is done to approximate **N³LO** (aN³LO).

Application of aN³LO PDFs.

aN3LO PDFs for Zp_T at low q_T :

- MSHT20aN3L0 PDFs already starting to be used by theory community
 - e.g. resummed (+ fixed order) predictions for Zp_T spectrum at low transverse momenta:



- aN3LO PDFs fit the measured ATLAS data better, likely due to indirect effects of gluon shape change.... need to look into this more!

Figure Credit: SCETlib - Georgios Billis, shown by Johannes Michel at LHC EW WG Sep 2022.

A selection of other references not directly mentioned but used for these results:

- [] - G. Altarelli and G. Parisi, Nucl. Phys. B, 126, 298 (1977)
- [] - E. G. Floratos, D. A. Ross, and C. T. Sachrajda, Nucl. Phys. B, 152, 493 (1979)
- [] - A. Gonzalez-Arroyo and C. Lopez, Nucl. Phys. B, 166, 429 (1980)
- [] - W. Furmanski and R. Petronzio, Phys. Lett. B, 97, 437 (1980)
- [] - E. G. Floratos, C. Kounnas, and R. Lacaze, Nucl. Phys. B, 192, 417 (1981)
- [] - S. Moch, J. Vermaseren, and A. Vogt, Nuclear Physics B, 688, 101134 (2004)
- [] - A. Vogt, S. Moch, and J. Vermaseren, Nuclear Physics B, 691, 129181 (2004)
- [] - M. Buza, Y. Matiounine, J. Smith, and W. L. van Neerven, The European Physical Journal C, 1, 301320 (1998).
- [] - M. Buza, Y. Matiounine, J. Smith, and W. van Neerven, Nuclear Physics B, 485, 1670, 420456 (1997).
- [] - S. Catani, M. Ciafaloni, and F. Hautmann, Nucl. Phys. B, 366, 135 (1991).
- [] - . Laenen and S.-O. Moch, Phys. Rev. D, 59, 034027 (1999), hep-ph/9809550