aN3LO PDFs, theory uncertainties, and the impact on phenomenology

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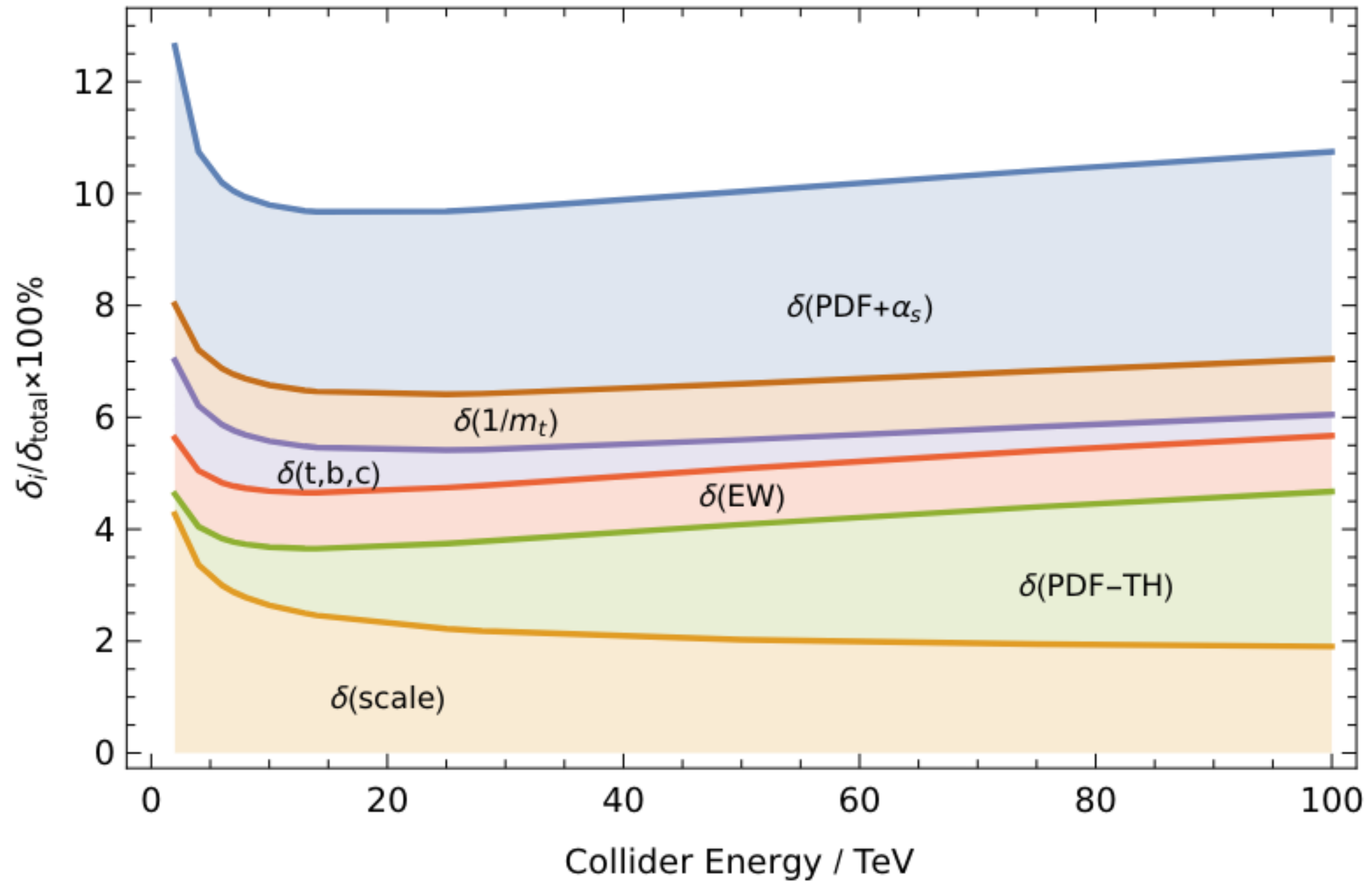
Durham, 8 April 2025

Motivation

Experiment PDF fit pQCD

$$\sigma = \sum_{ij} \boxed{f_i \otimes f_j} \otimes \boxed{\hat{\sigma}_{ij}}$$

- Predictions at particle colliders such as the LHC use two main ingredients:
  - **Matrix elements (MEs)**
  - **Parton distribution functions (PDFs)**
- Much progress has been made in the computation of MEs at N^{3}LO
- **PDF uncertainties are a bottleneck** for many LHC precision calculations
- Most widely used PDF sets are at NNLO and without theory uncertainties



Sources of uncertainty for Higgs in gluon fusion

Dulat, Lazopoulos, Mistlberger, 1802.00827

Much progress since this plot, in particular:

- NNLO top quark corrections Czakon et al., 2105.04436
- Mixed QDC-EW corrections
  Becchetti et al., 2010.09451, Bonetti, et al., 2007.09813

Motivation

$\alpha_s(m_Z)$ determination from Z_{p_T} at 8 TeV

ATLAS, 2309.12986

PDF set	$\alpha_s(m_Z)$	PDF uncertainty	g [GeV^2]	q [GeV^4]
MSHT20 [37]	0.11839	0.00040	0.44	−0.07
NNPDF4.0 [84]	0.11779	0.00024	0.50	−0.08
CT18A [29]	0.11982	0.00050	0.36	−0.03
HERAPDF2.0 [65]	0.11890	0.00027	0.40	−0.04

Δ_{PDF}(MSHT20 only) $= 4 \times 10^{-4}$

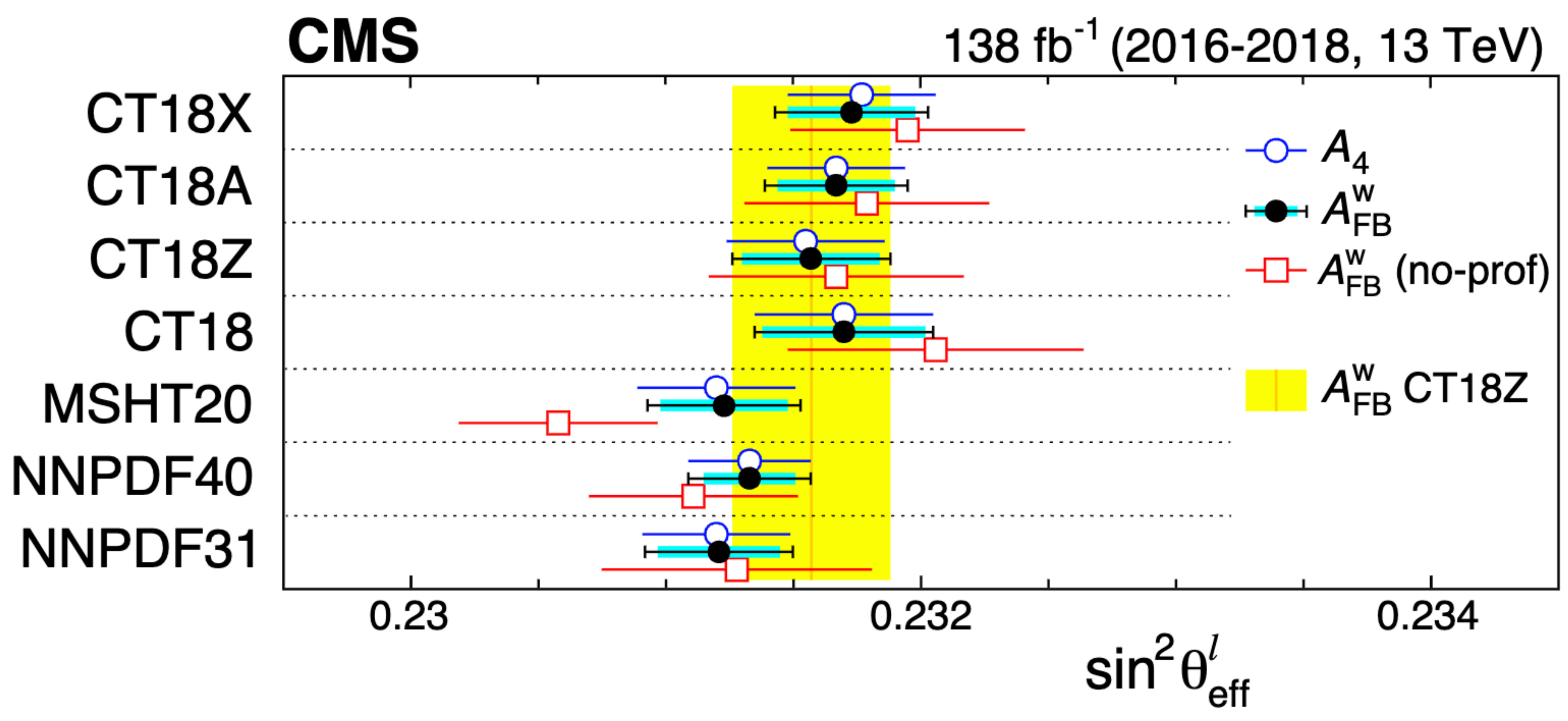
$\Delta_{PDF}(\frac{1}{2}$(CT18A-NNPDF4.0)) $= 10 \times 10^{-4}$

Final total uncertainty:

$\Delta_{TOT} = 9 \times 10^{-4}$

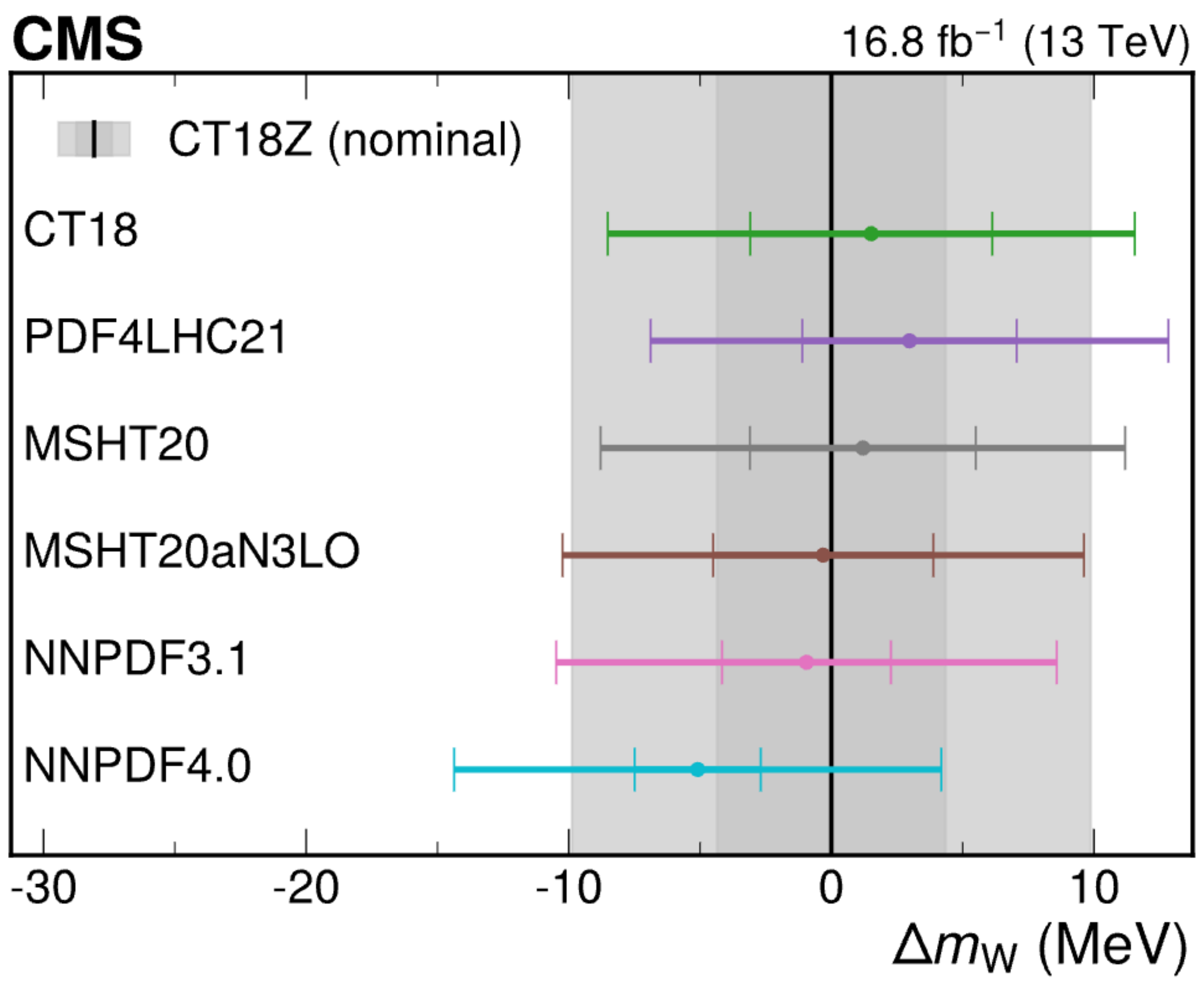
Weak mixing angle at 13 TeV

CMS, 2408.07622

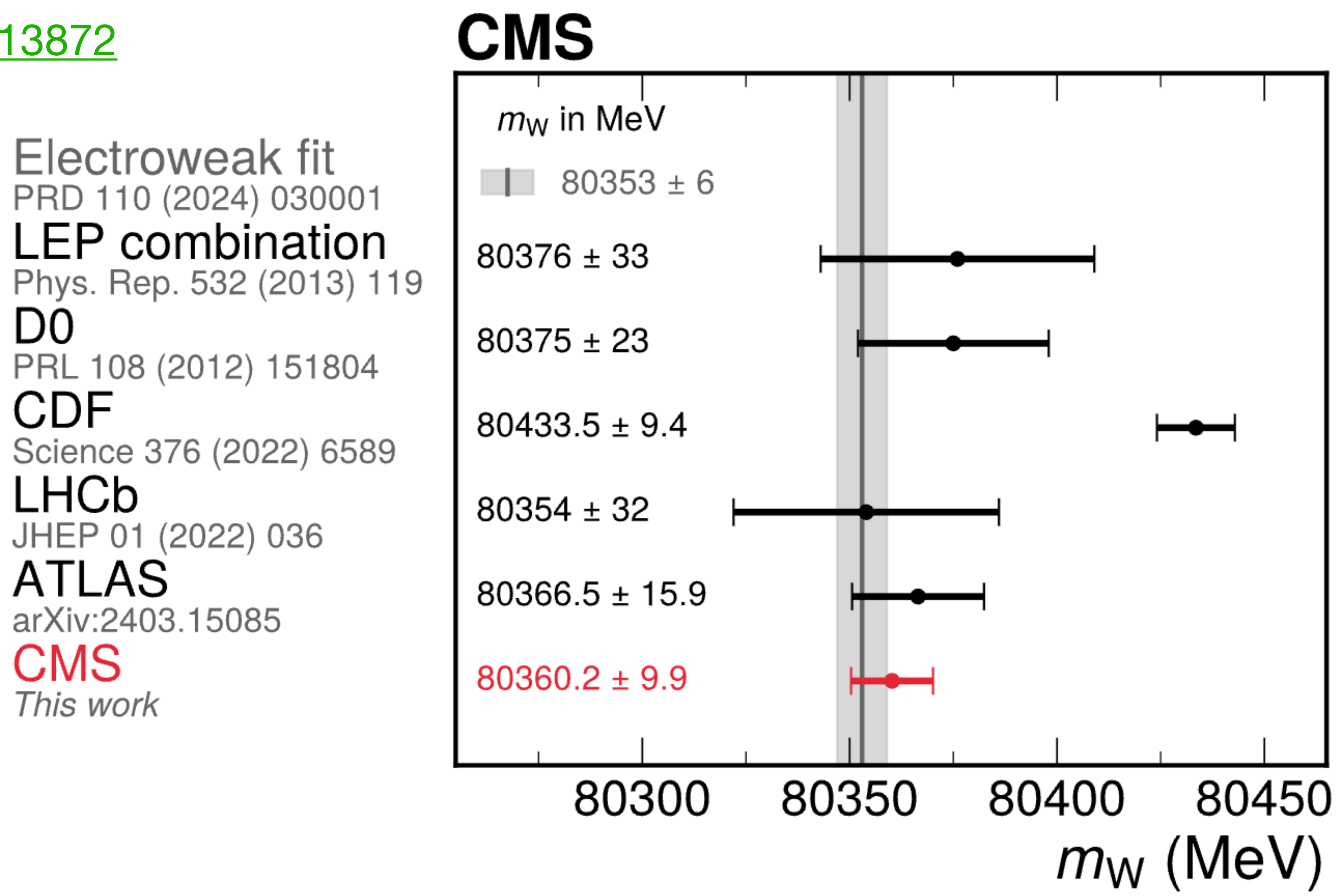


- What is the **PDF uncertainty** that should be associated with this measurement?
- How to choose the **baseline PDF**?
- Is **profiling of PDFs** justified? What is the impact on other experiments in the **global dataset**?

Motivation



[CMS, 2412.13872](https://arxiv.org/abs/2412.13872)



- W mass determination has received a lot of attention in recent years
- CMS measurement similar precision to the CDF result
- PDFs remain a major part of the theory uncertainty

PDFs used in the analysis are **rescaled** to improve agreement among them. What is the **impact on the global dataset**?

- aN3LO PDFs

What do we need for PDFs at N³LO?

A PDF fit requires several theory inputs:

- **DGLAP splitting functions**
  small-x and large-x limits
  Mellin moments
- **Matching conditions for variable flavor number schemes**
  Now exactly known but original aN3LO publications use approximations
- **DIS coefficient functions**
  Massless known, massive limits known
- **Hadronic cross-section**
  Not much is known

Strategy:

- When N³LO theory is known, it is **used**
- When partial information is available, use it while accounting for **parametrisation uncertainty**
- When it is unknown account for **missing higher order uncertainty**

N^{3}LO QCD corrections in PDF determination

Splitting Functions (information is partial)

Singlet (P_{qq}, P_{gg}, P_{gq}, P_{qg})
– large-n_f limit [NPB 915 (2017) 335; arXiv:2308.07958]
– small-x limit [JHEP 06 (2018) 145]
– large-x limit [NPB 832 (2010) 152; JHEP 04 (2020) 018; JHEP 09 (2022) 155]
– 5 (10) lowest Mellin moments [PLB 825 (2022) 136853; ibid. 842 (2023) 137944; ibid. 846 (2023) 138215]

Non-singlet ($P_{NS,v}$, $P_{NS,+}$, $P_{NS,-}$)
– large-n_f limit [NPB 915 (2017) 335; arXiv:2308.07958]
– small-x limit [JHEP 08 (2022) 135]
– large-x limit [JHEP 10 (2017) 041]
– 8 lowest Mellin moments [JHEP 06 (2018) 073]

DIS structure functions (F_L, F_2, F_3)
– DIS NC (massless) [NPB 492 (1997) 338; PLB 606 (2005) 123; NPB 724 (2005) 3]
– DIS CC (massless) [Nucl.Phys.B 813 (2009) 220]
– massive from parametrisation combining known limits and damping functions [NPB 864 (2012) 399]

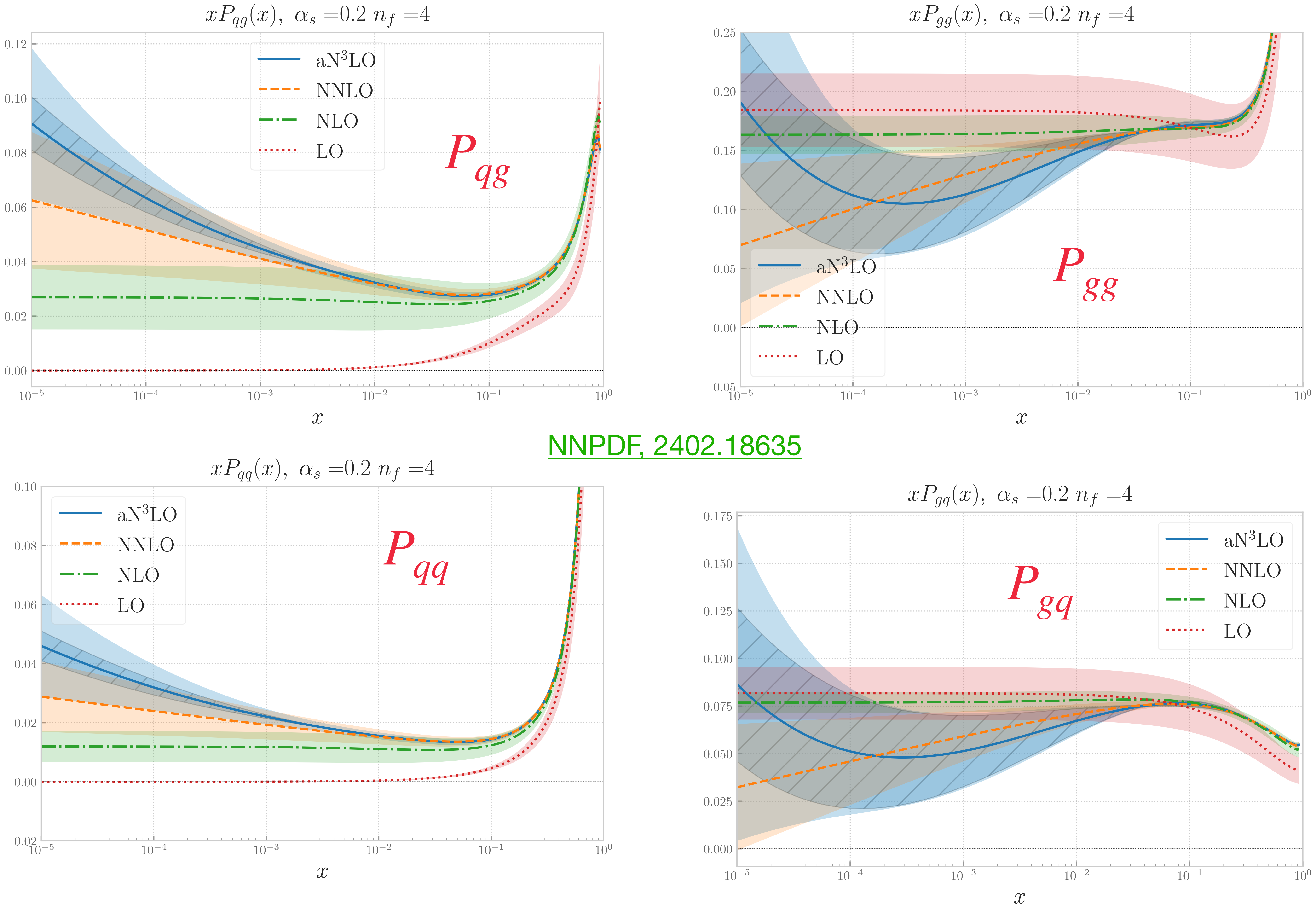
PDF matching conditions
– all known except for $a^3_{H,g}$ [NPB 820 (2009) 417; NPB 886 (2014) 733; JHEP 12 (2022) 134]

Coefficient functions for other processes
– DY (inclusive) [JHEP 11 (2020) 143]; DY (y differential) [PRL 128 (2022) 052001]

Emanuele R. Nocera (UNITO) | Progress from NNPDF | 5 August 2024 | 12 / 25

E. Nocera, Workshop on Hadron Physics and Opportunities Worldwide
Dalian, China, August 2024
(More is known today!)

Approximate N^3LO splitting functions



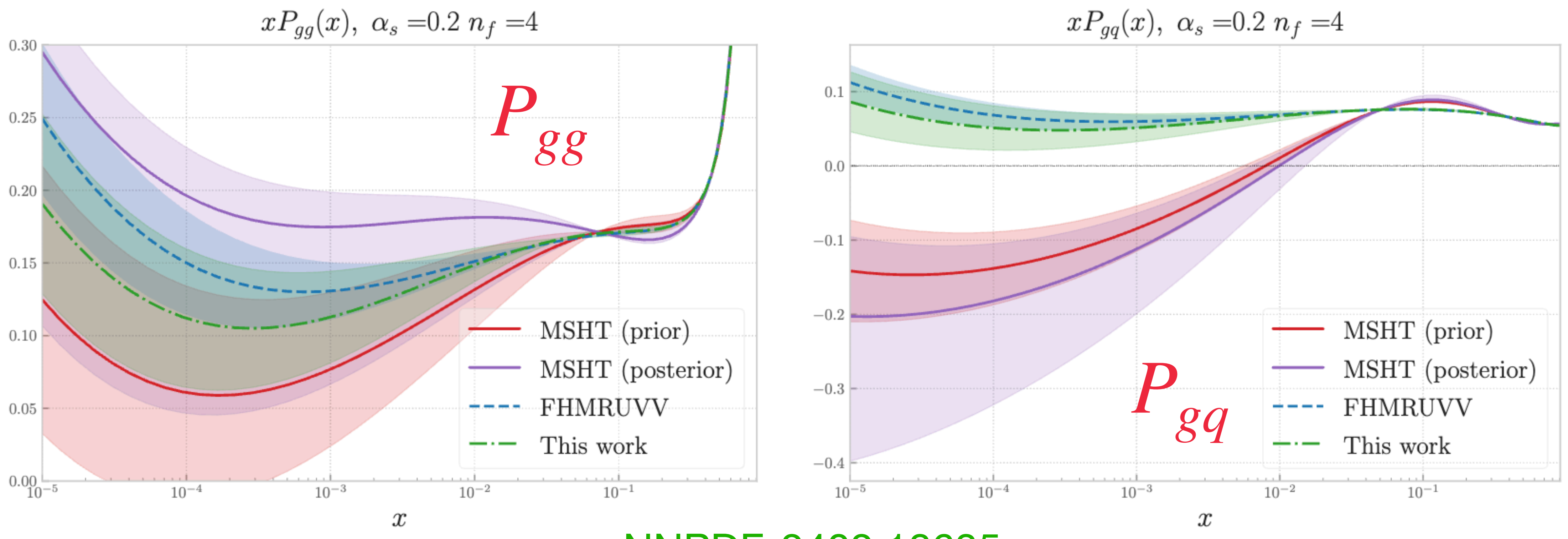
Dark blue: uncertainties due to parametrization of aN3LO contributions

Light blue: scale variations

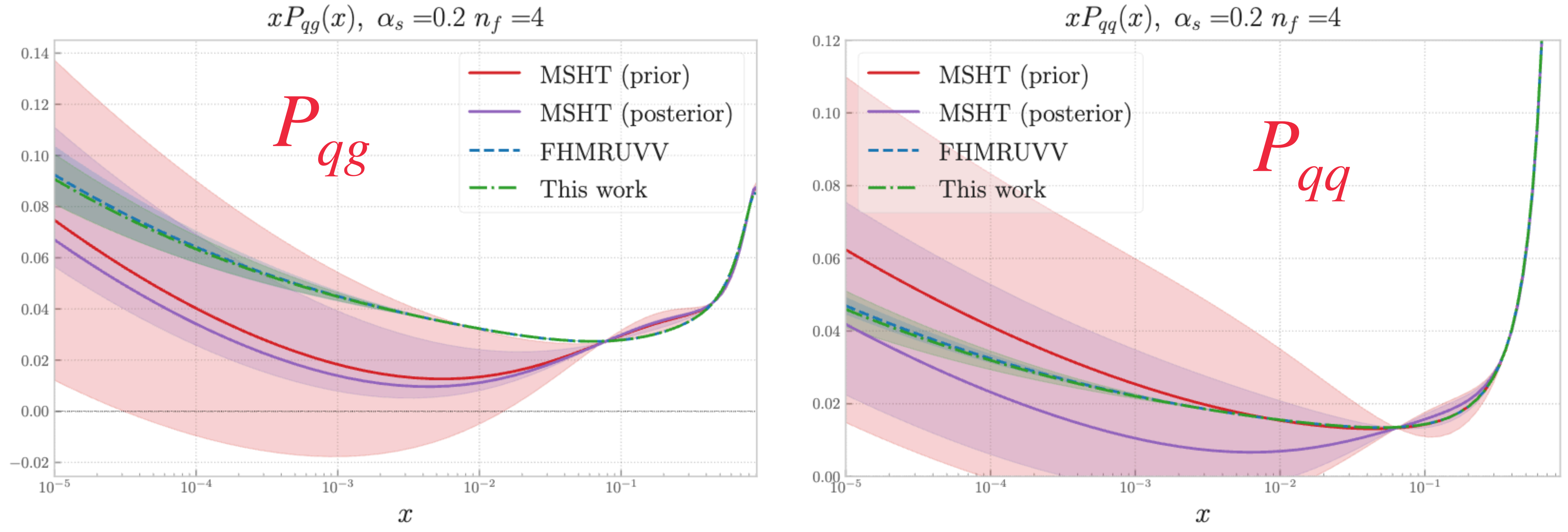
- Good **perturbative stability** within uncertainties
- **Small parametrisation uncertainty** in large range of x

Approximate does not mean poorly known!

Approximate N^{3}LO splitting functions



NNPDF, 2402.18635



Generally good agreement. MSHT was first so fewer moments known

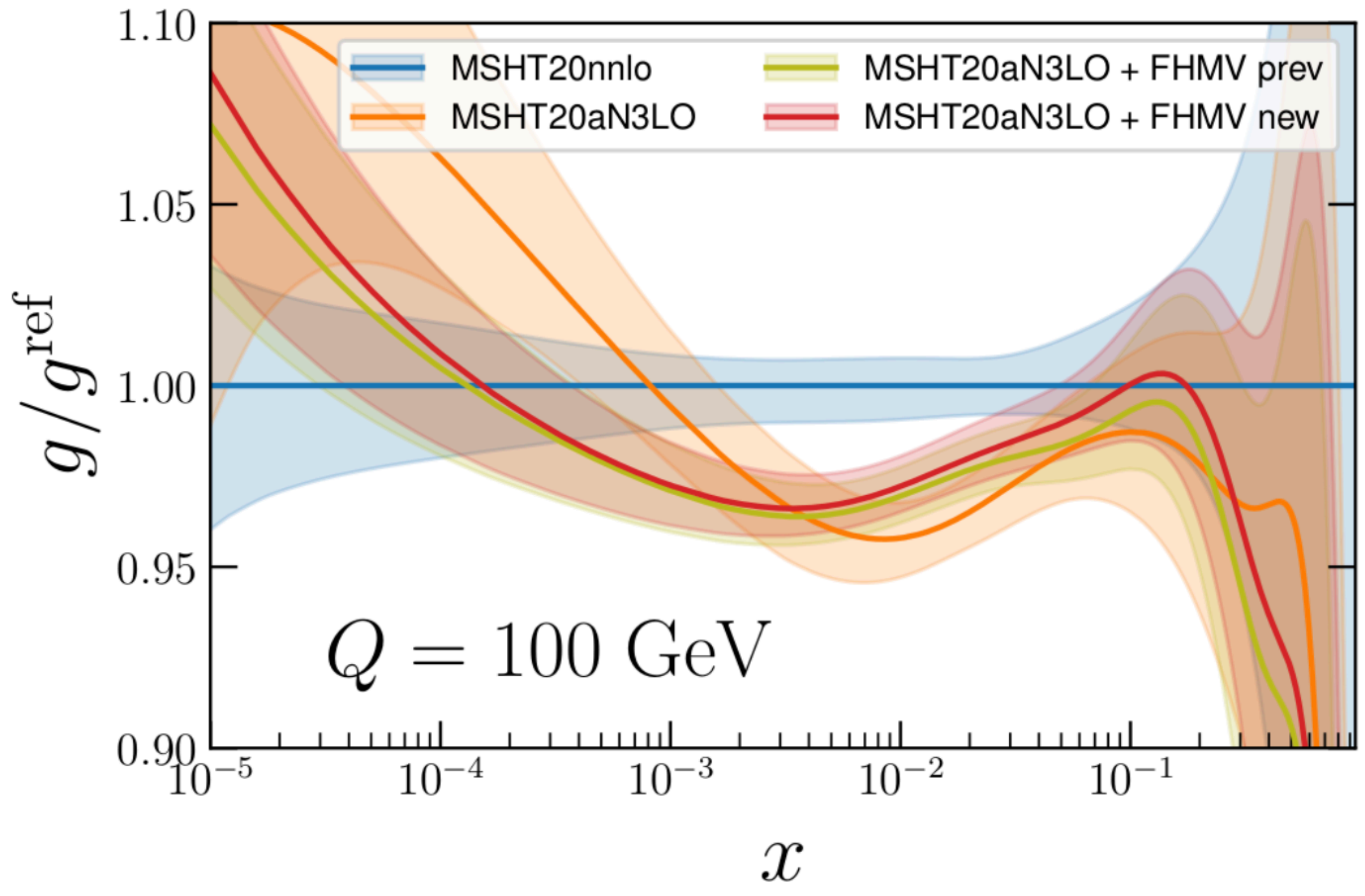
Later results are within MSHT uncertainty, except P_{gq}

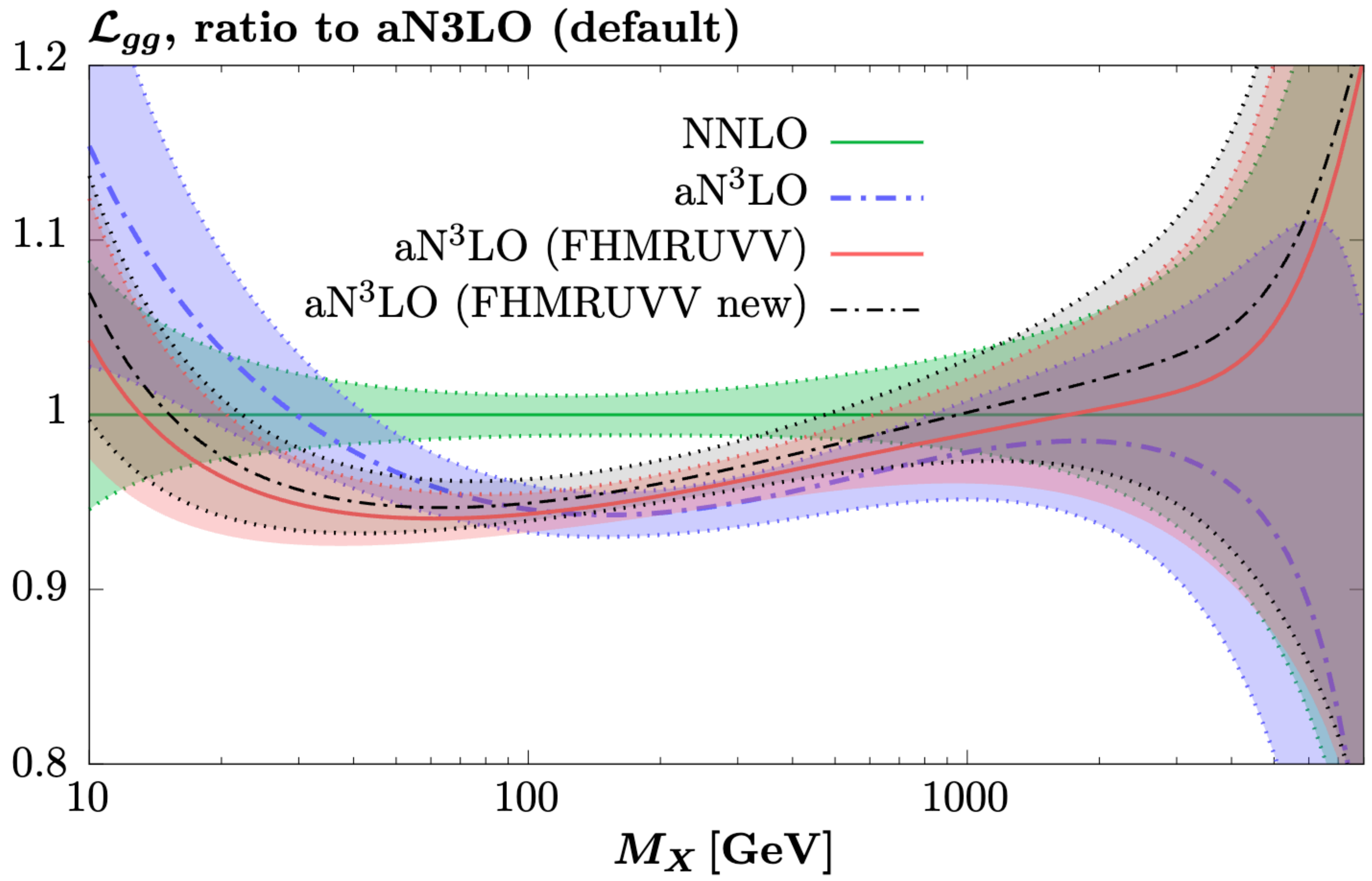
Results by Moch et al. will be the new default!

*For more info see the **Les Houches benchmark paper***
Cooper-Sarkar et al., 2406.16188

How much do Mellin moments calculated since NNPDF/MSHT releases affect aN^{3}LO PDFs?

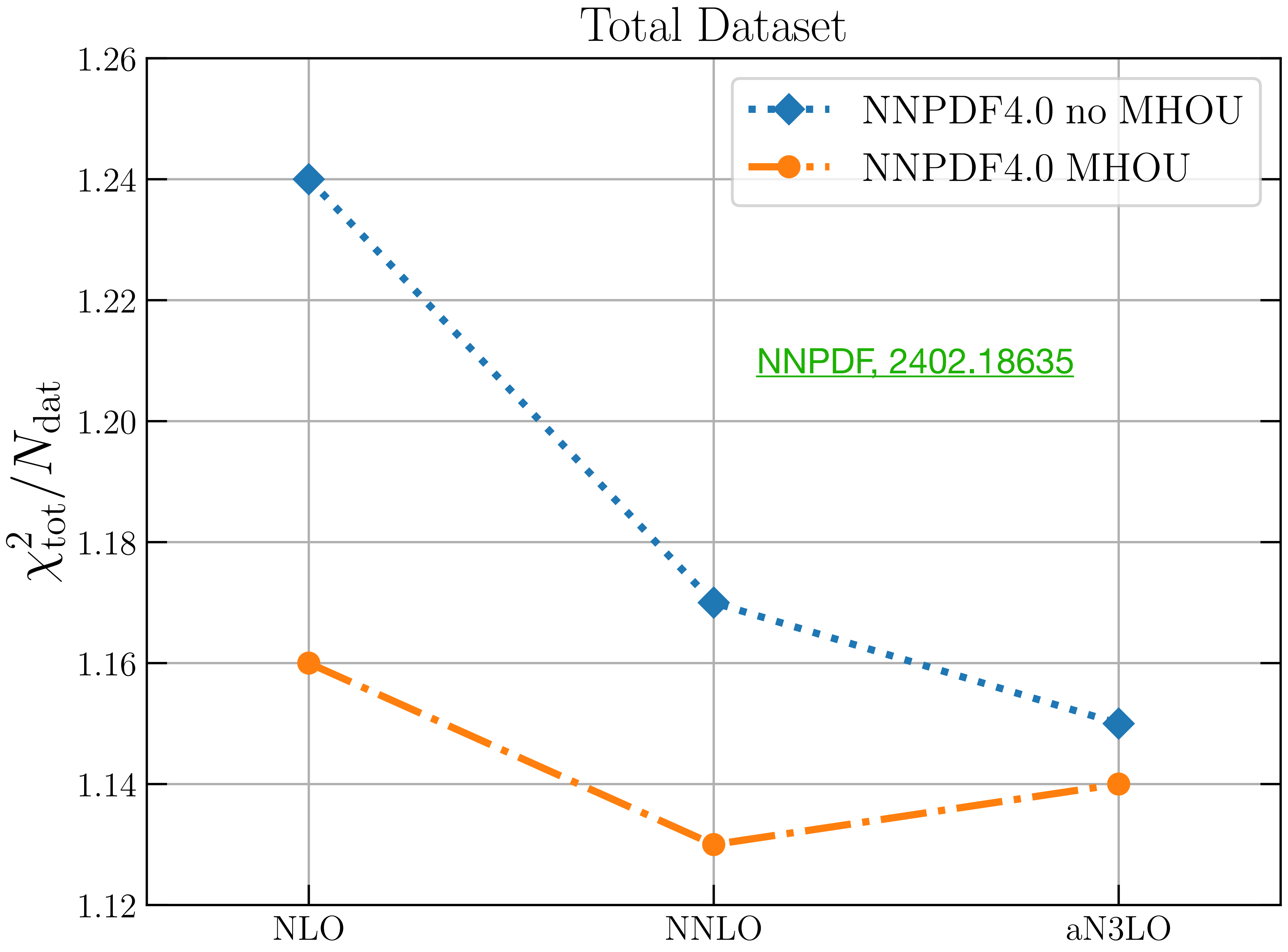
R. Thorne PDF4LHC December 2024





- Small changes in the gluon PDF
- Improved agreement between NNPDF and MSHT

Fit quality



NNPDF, 2402.18635

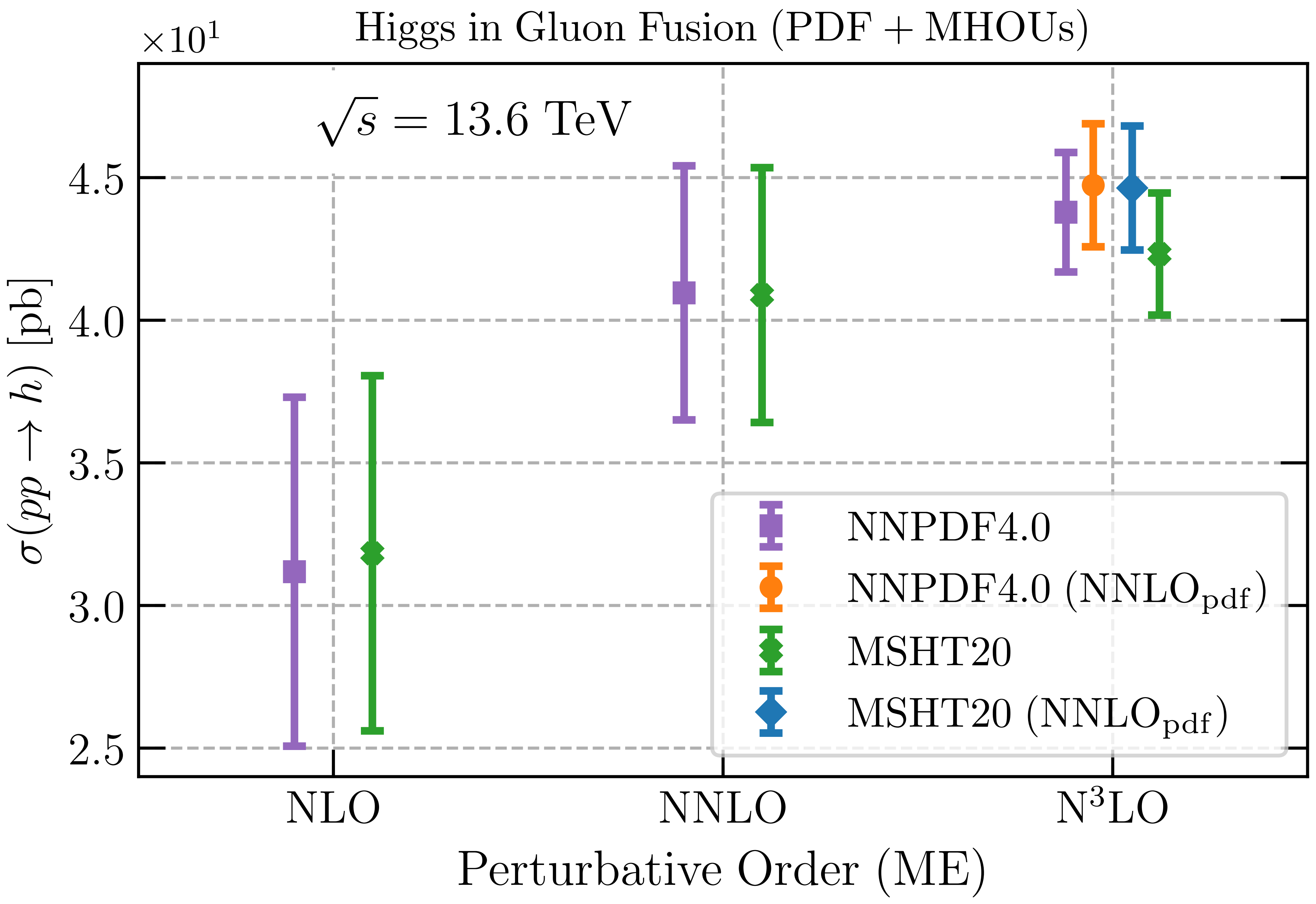
MSHT, 2207.04739

MSHT χ^2/N_{pts} (4363)	LO	NLO	NNLO	aN3LO
	2.57	1.33	1.17	1.14

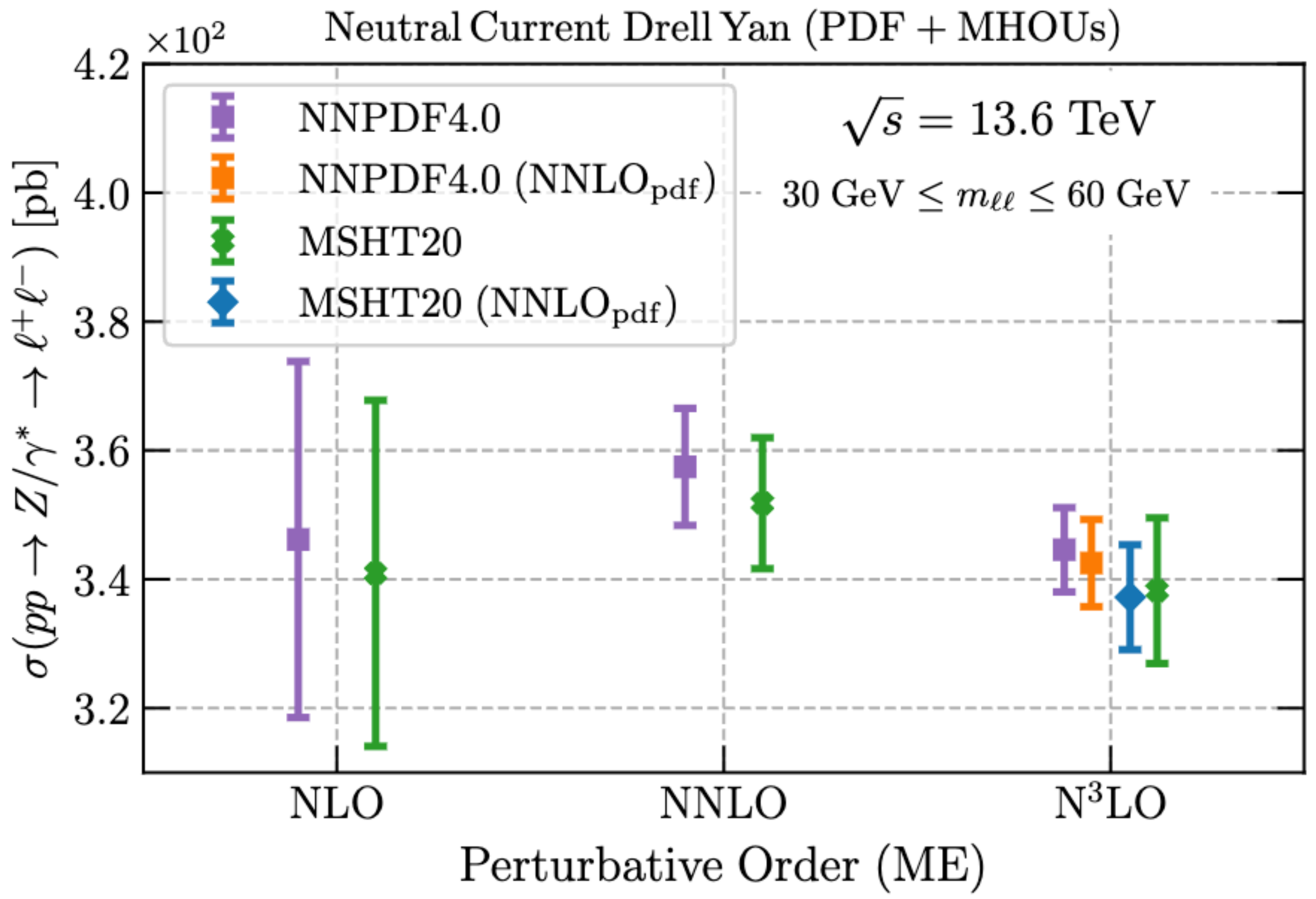
- Without MHOUs the fit improves (lower χ^2) with increasing perturbative order for both NNPDF and MSHT
- With MHOUs the fit depends only weakly on the perturbative order
- At N^{3}LO MHOUs have a small impact on the χ^2

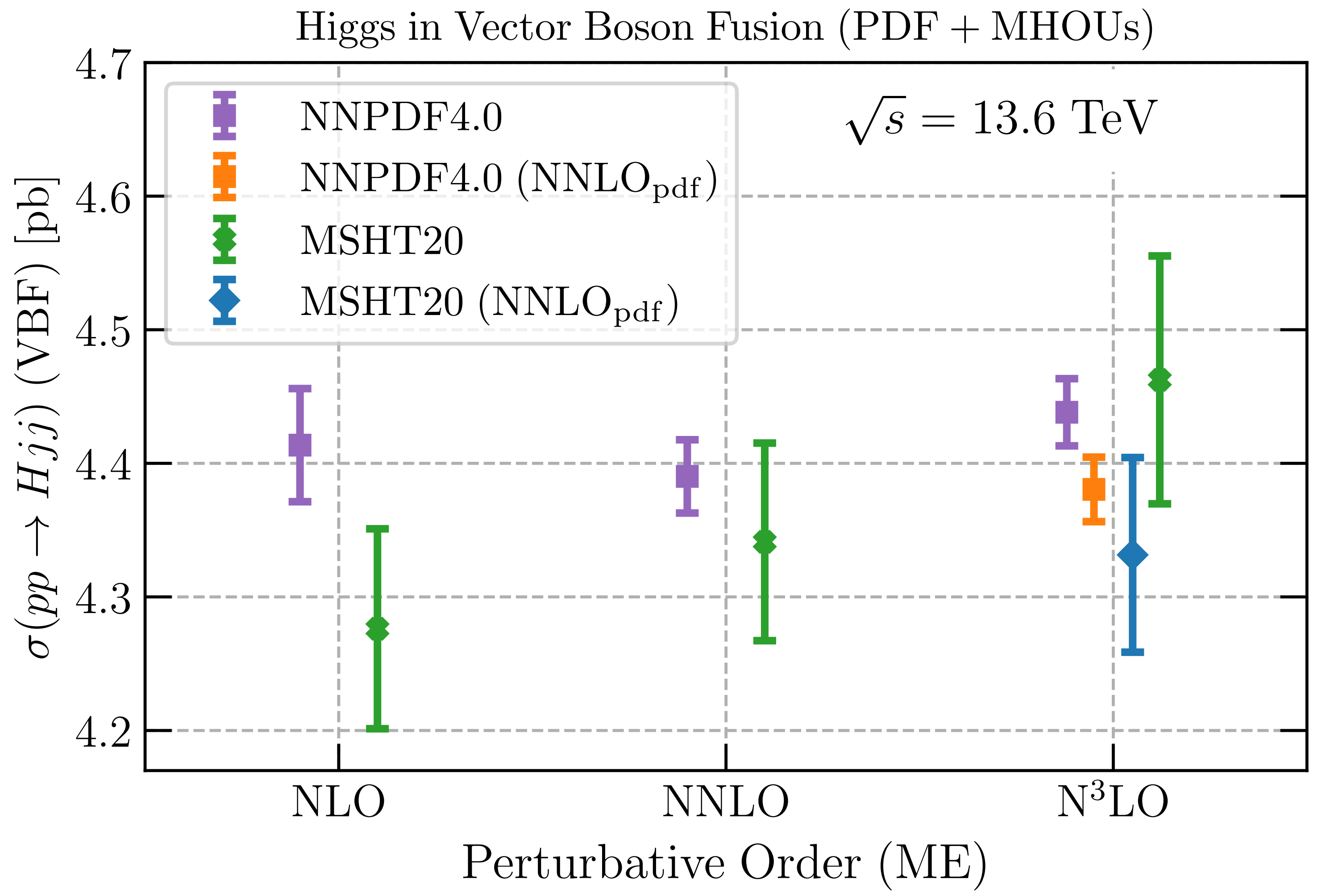
Phenomenology

[NNPDF, 2402.18635]



N^3**LO PDFs** result in a small suppression of the Higgs gluon fusion cross section compared to **NNLO PDFs**



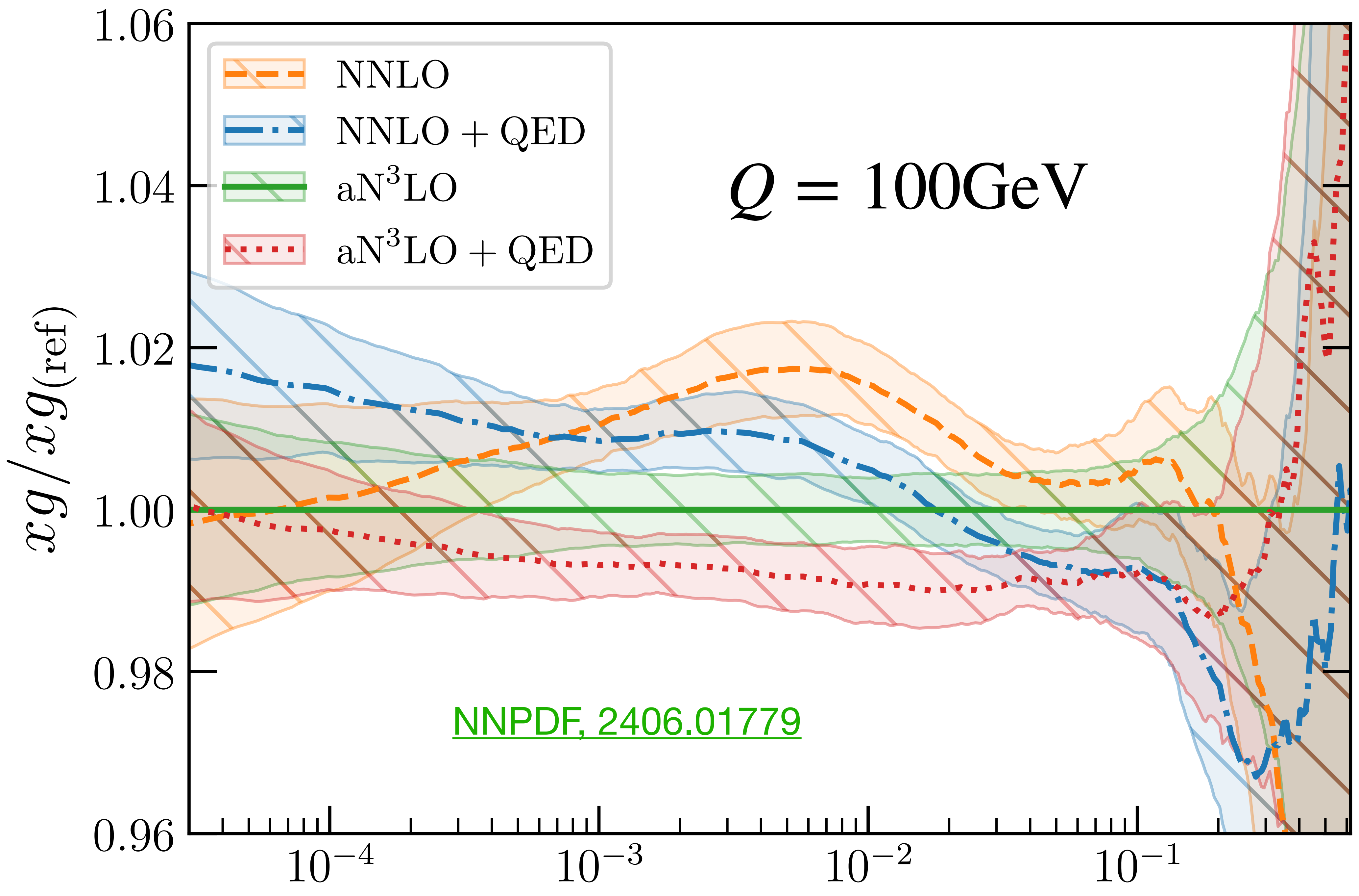


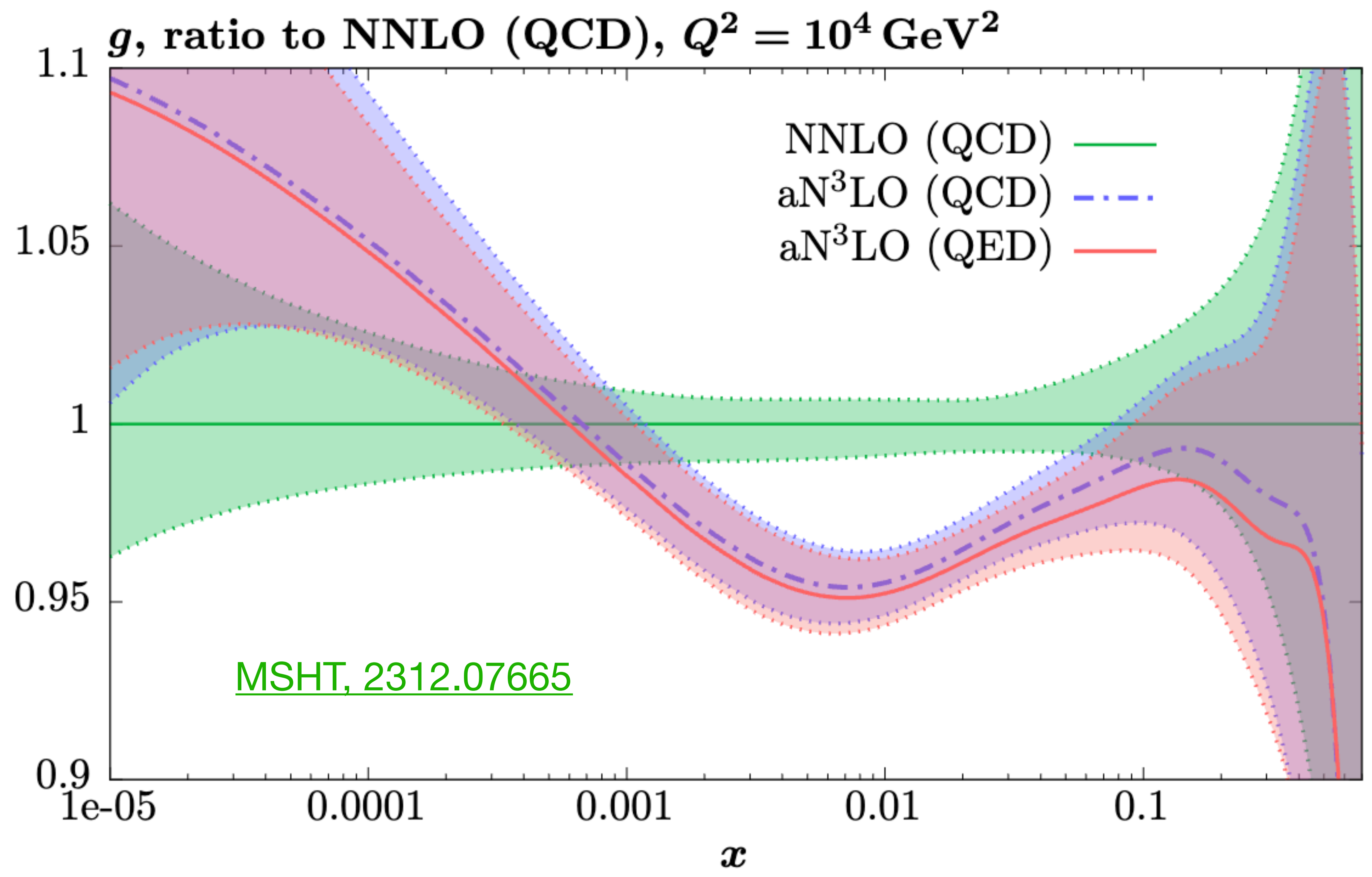
Generally perturbative convergence for Higgs in VBF and Drell-Yan

$N^3LO/NNLO$ ratio is similar for NNPDF and MSHT

QED corrections and photon PDF

PDFs at $\mathrm{aN^3LO_{QCD}} \otimes \mathrm{NLO_{QED}}$ with photon PDF is available from both NNPDF and MSHT representing the **most accurate PDFs**





- Photon subtracts momentum from the gluon PDF
- NNPDF: QED effect similar in magnitude to aN3LO corrections
- MSHT: larger aN3LO but smaller QED correction

- # MSHT+NNPDF aN3LO(+QED) combination

MSHT&NNPDF, 2411.05373

MSHT+NNPDF aN3LO combination

- Same approach as PDF4LHC: 100 replicas from NNPDF and 100 replicas from MSHT
- Both for aN3LO QCD and aN3LO + QED, together with NNLO baseline
- Usual differences in theory, methodology, and experiment remain ⇒ conservative
- Can be extended if other PDFs at the same accuracy become available

PDF set	pert. order (PDF)
`PDF4LHC21_mc`	$\mathrm{NNLO_{QCD}}$
`MSHT20xNNPDF40_nnlo`	$\mathrm{NNLO_{QCD}}$
`MSHT20xNNPDF40_nnlo_qed`	$\mathrm{NNLO_{QCD}} \otimes \mathrm{NLO_{QED}}$
`MSHT20xNNPDF40_an3lo`	$\mathrm{aN^3LO_{QCD}}$
`MSHT20xNNPDF40_an3lo_qed`	$\mathrm{aN^3LO_{QCD}} \otimes \mathrm{NLO_{QED}}$
`NNPDF40_an3lo_as_01180_mhou`	$\mathrm{aN^3LO_{QCD}}$
`NNPDF40_an3lo_as_01180_qed_mhou`	$\mathrm{aN^3LO_{QCD}} \otimes \mathrm{NLO_{QED}}$
`MSHT20an3lo_as118`	$\mathrm{aN^3LO_{QCD}}$
`MSHT20qed_an3lo`	$\mathrm{aN^3LO_{QCD}} \otimes \mathrm{NLO_{QED}}$

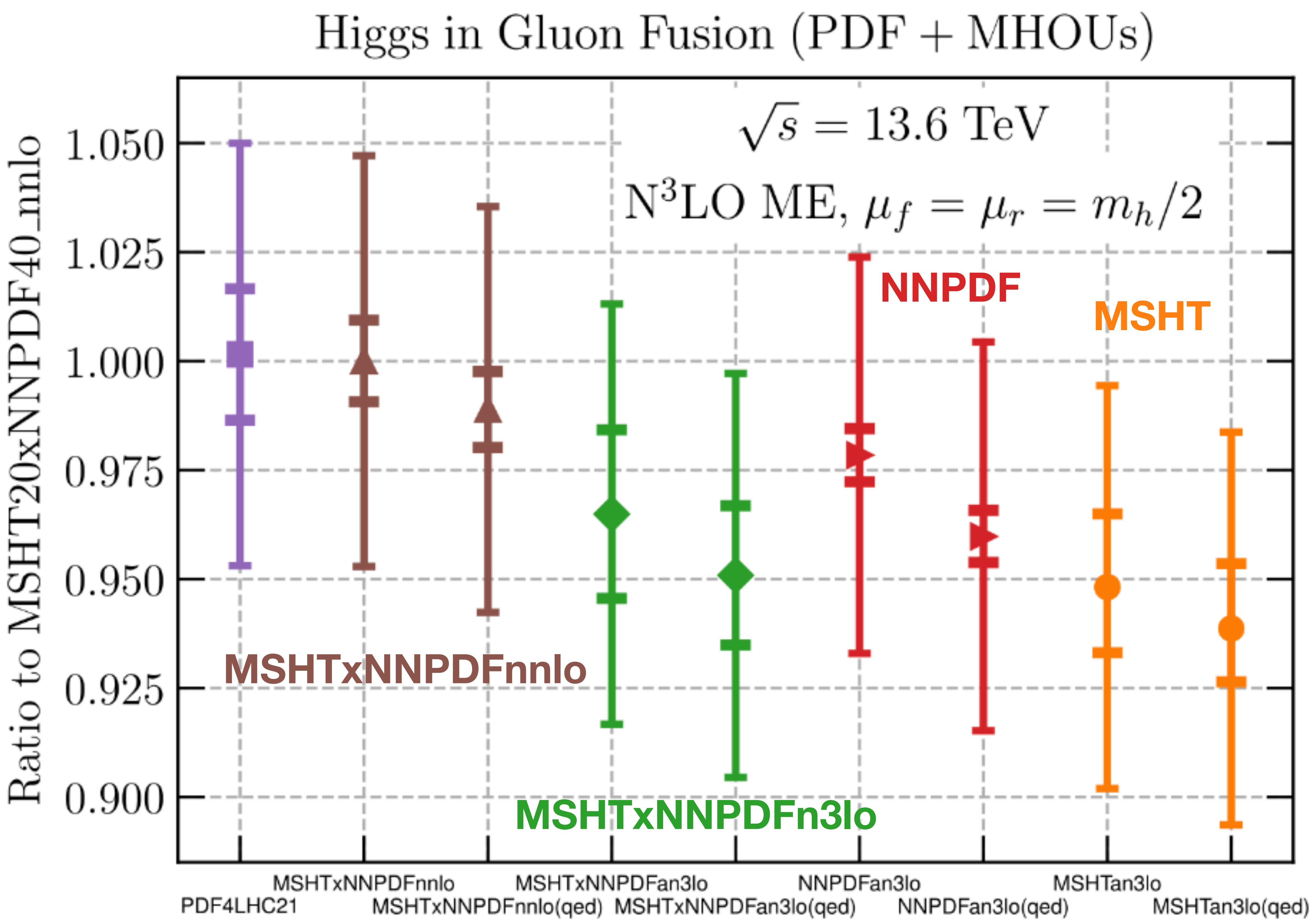
Higgs production

Inner error bars: PDF unc.

Outer error bars: PDF unc. + MHOU

For the combination:

- aN3LO correction -3%
- aN3LO+QED correction -5%



Higgs production

Without N3LO PDFs, uncertainty is **approximated**

$$\Delta^{\text{app}}_{\text{NNLO}} \equiv \frac{1}{2}\left|\frac{\sigma^{\text{NNLO}}_{\text{NNLO-PDF}} - \sigma^{\text{NNLO}}_{\text{NLO-PDF}}}{\sigma^{\text{NNLO}}_{\text{NNLO-PDF}}}\right|$$

How does this compare to the **exact N3LO shift**?

$$\Delta^{\text{exact}}_{\text{NNLO}} \equiv \left|\frac{\sigma^{\text{N}^3\text{LO}}_{\text{N}^3\text{LO-PDF}} - \sigma^{\text{N}^3\text{LO}}_{\text{NNLO-PDF}}}{\sigma^{\text{N}^3\text{LO}}_{\text{N}^3\text{LO-PDF}}}\right|$$

	ggF	VBF
Δexact	3.3%	2.3%
Δapprox	0.9%	0.5%

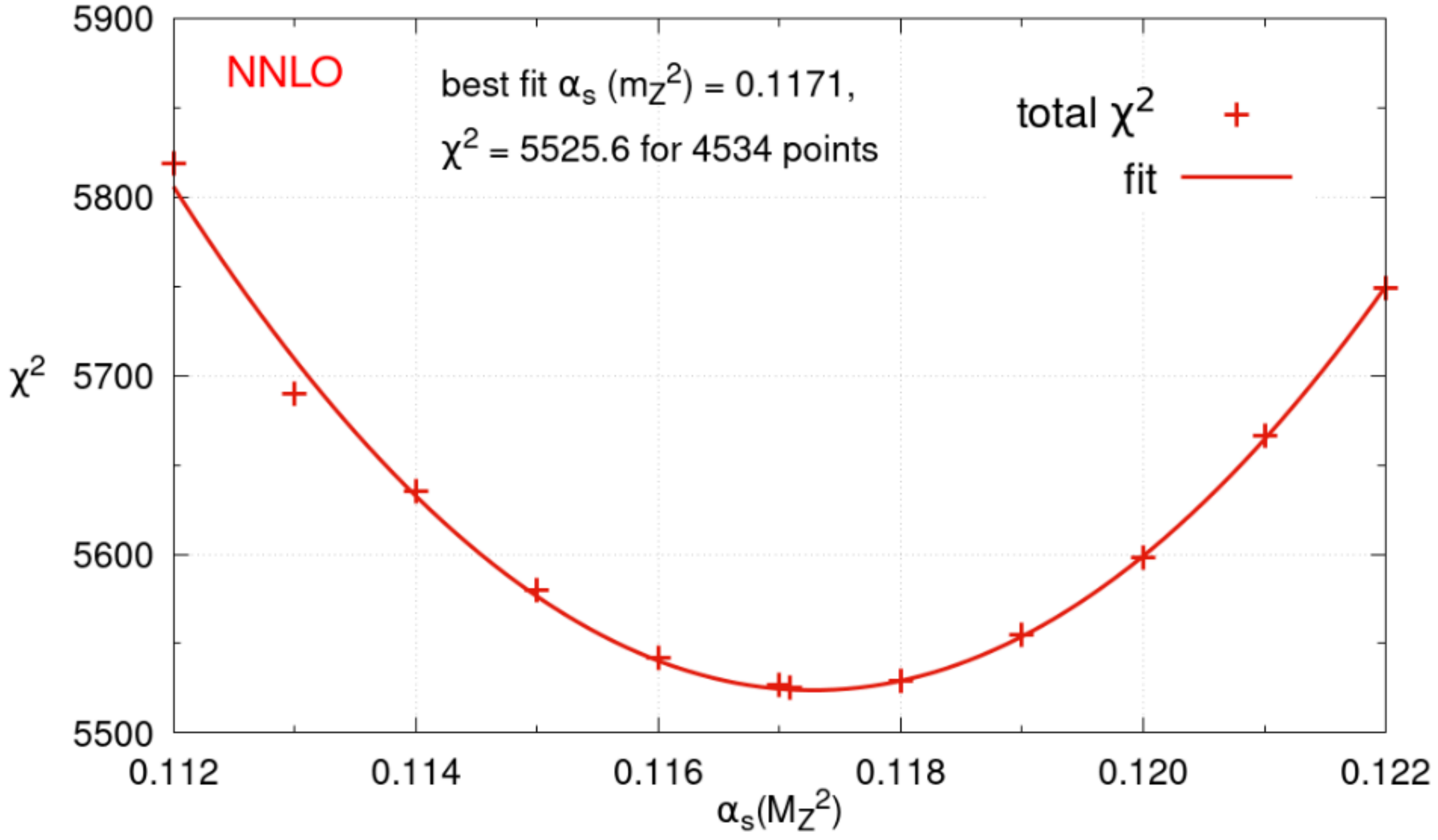
Previous estimates of the N3LO mismatch were underestimated

- $\alpha_s(m_Z)$ extractions

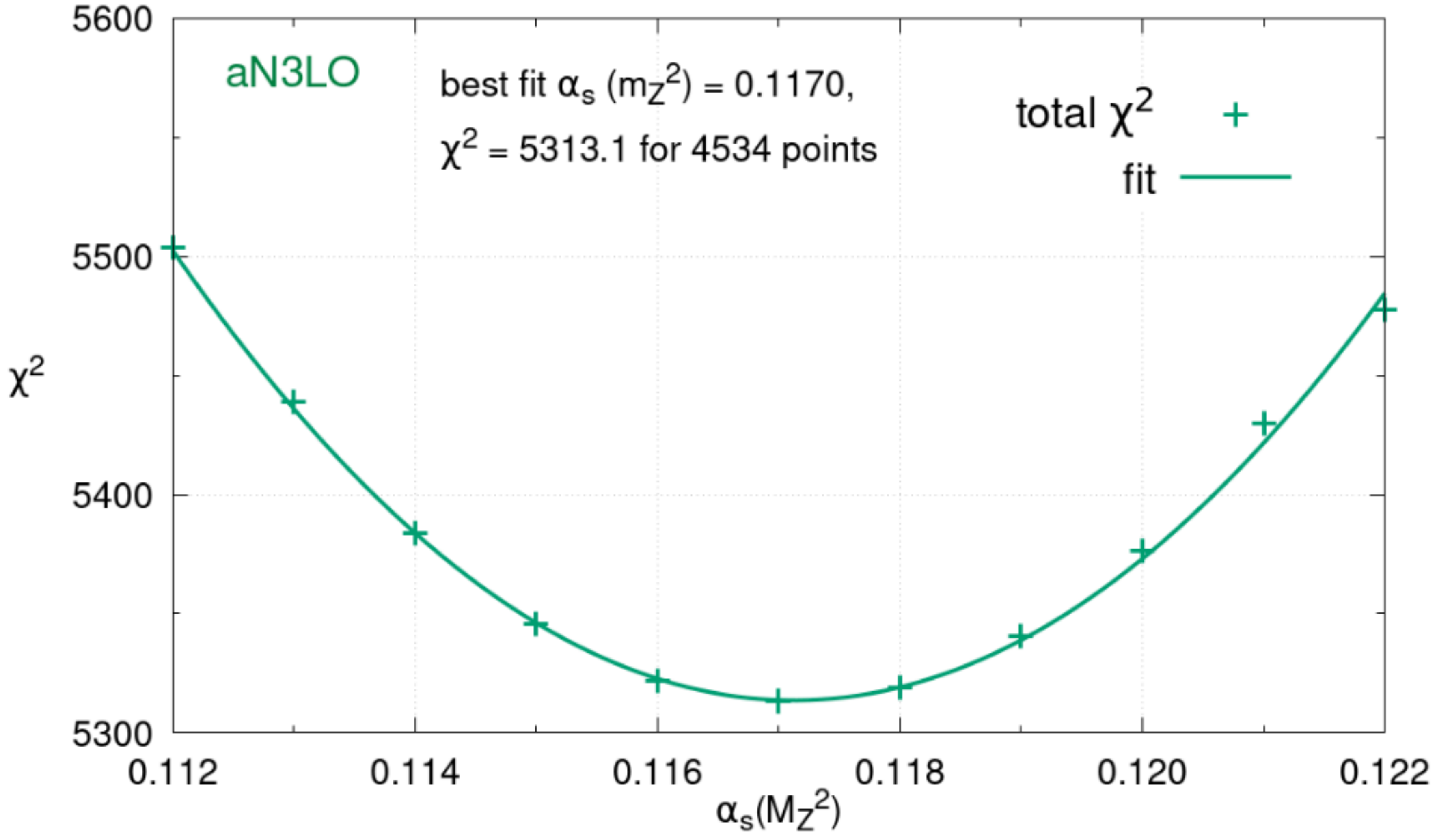
$\alpha_s(m_Z)$ at aN3LO in MSHT

MSHT, 2404.02964

$$\alpha_s(m_Z)_{\text{NNLO}} = 0.1170(16)$$



$$\alpha_s(m_Z)_{\text{aN}^3\text{LO}} = 0.1171(14)$$

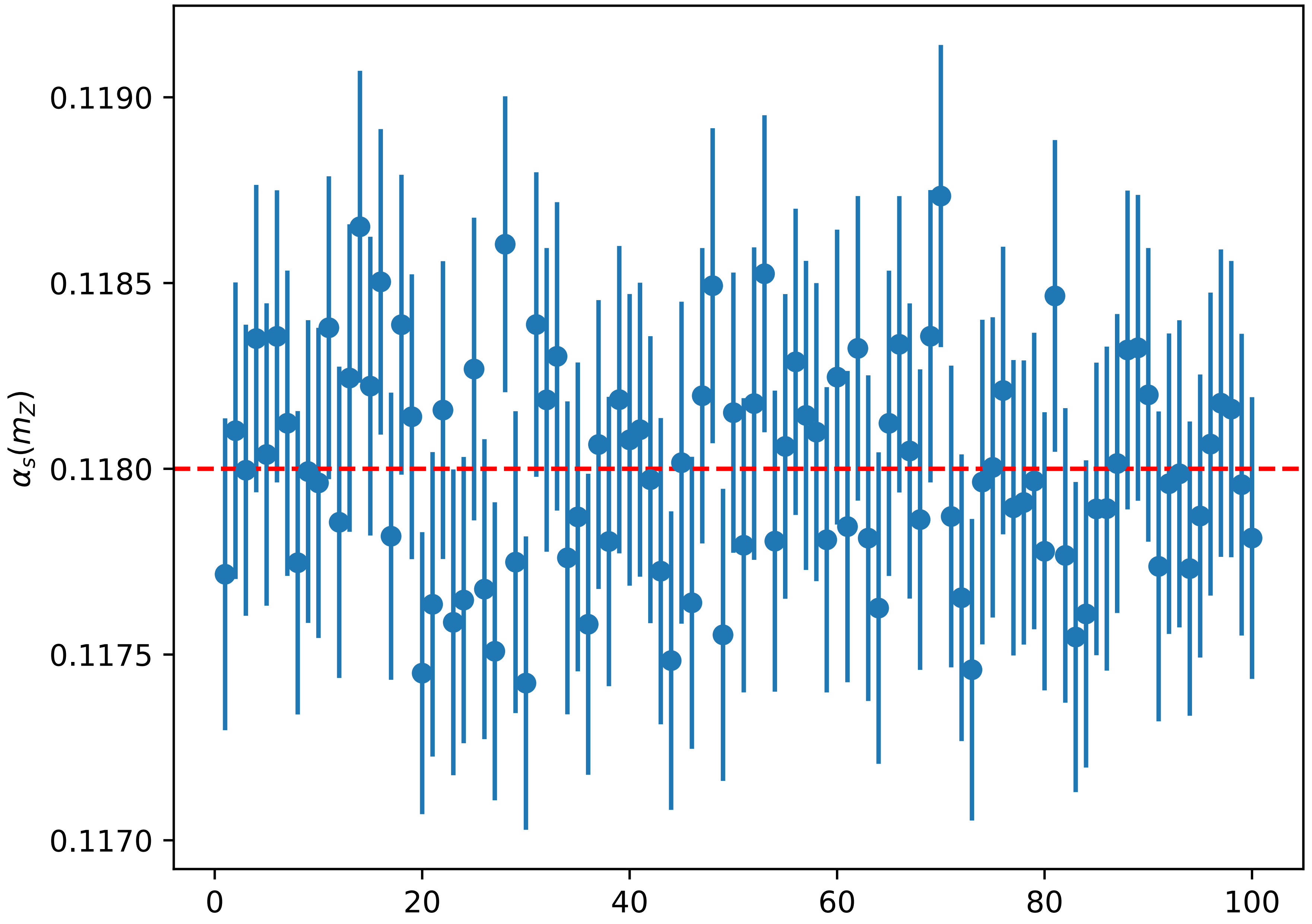


- First PDF $\alpha_s(m_Z)$ determination at aN³LO!
- Consistent with NNLO result

$\alpha_s(m_Z)$ in NNPDF - closure test

Work in progress

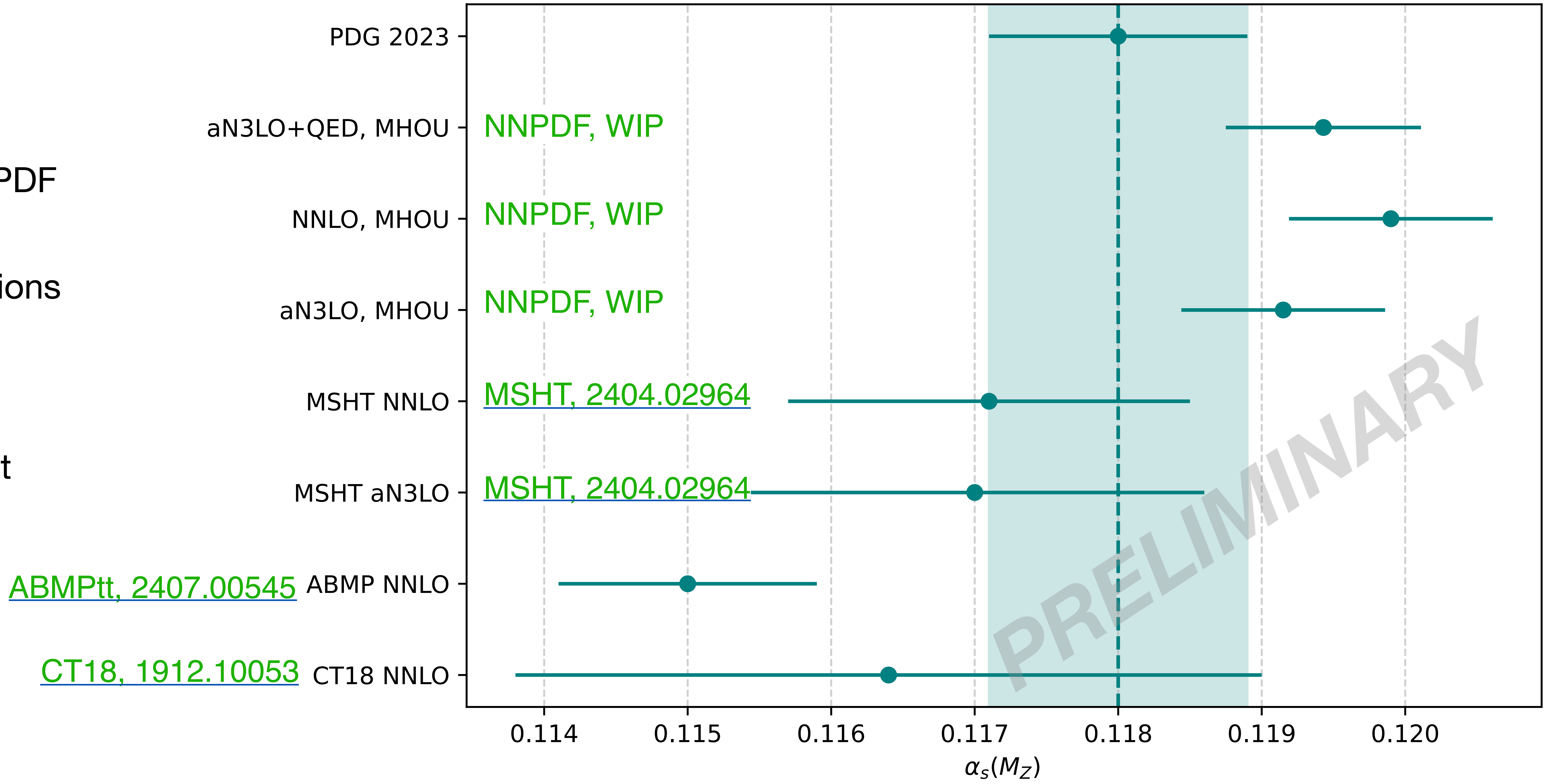
- Generate data from theory predictions at $\alpha_s(m_Z)_{\text{pseudodata}} = 0.118$
- Verify that is is correctly reproduced in two independent fitting methodologies
- Discovered ``plausible” methodologies that fail the closure test



$\alpha_s(m_Z) = 0.11800(4)$ ✓

$\alpha_s(m_Z)$ determinations

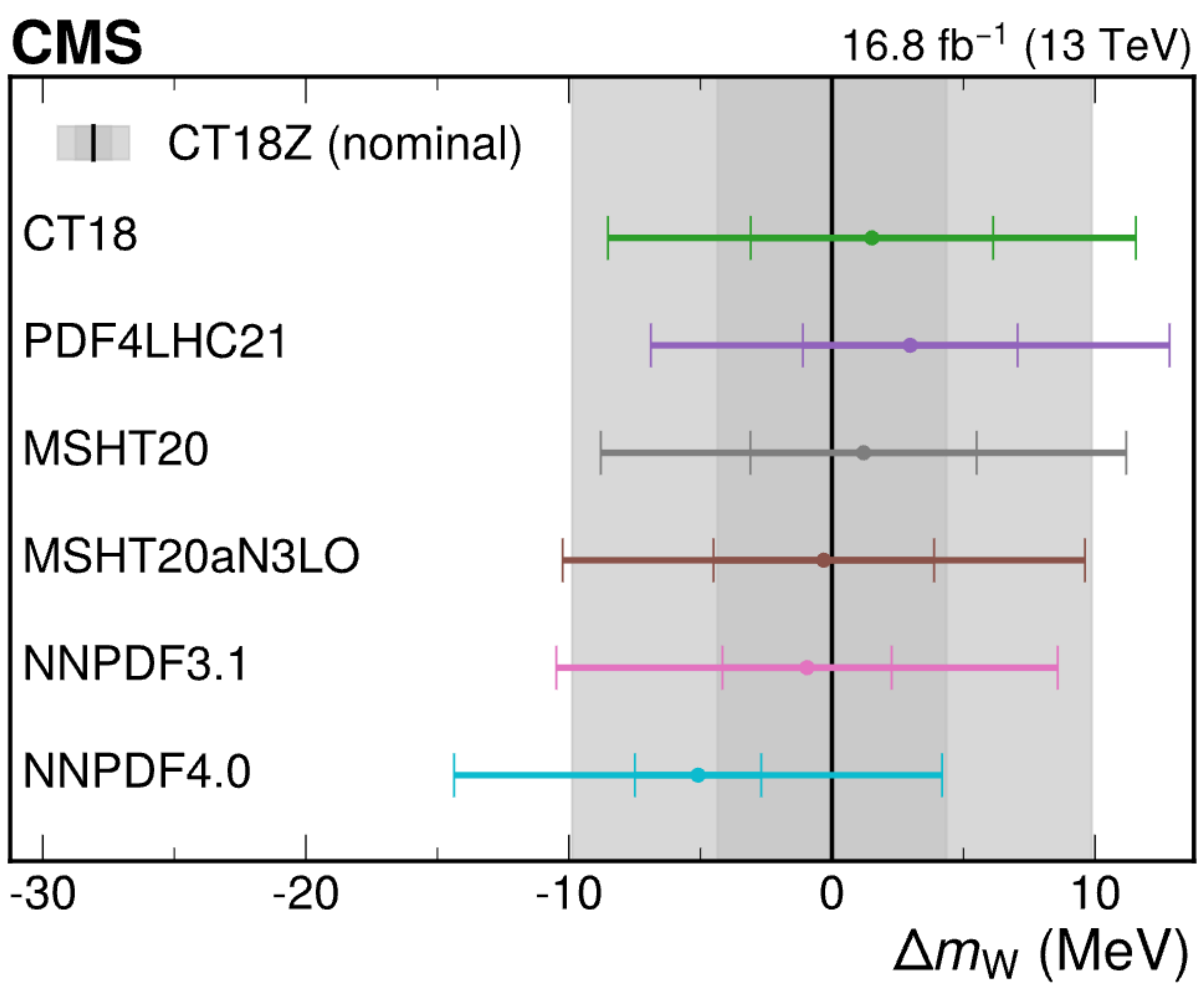
- Perturbative stability between NNLO and aN^{3}LO (NNPDF and MSHT)
- At aN^{3}LO only small upward shift due to QED corrections and photon PDF
- $\alpha_s(M_Z)^{\text{aN3LO,QED,MHOU}} = 0.1194(7)$
- Different groups use different data, theory, experiment (as in standard PDF fits), leading to **differences in extracted** $\alpha_s(m_Z)$



Summary

- aN^3LO PDFs enable consistent N3LO calculations
- aN^3LO evolution is close to exact
- N^3LO cross sections are a long term goal
- Both N^3LO QCD and NLO QED correction are relevant for Higgs in gluon fusion
- aN^3LO+QED represents the most accurate PDFs currently available (NNPDF and MSHT)

- How should we deal with **differences between PDFs**?
- **Missing higher order uncertainties** are computed via scale variations or NNLO-NLO shifts. Is there a better way?



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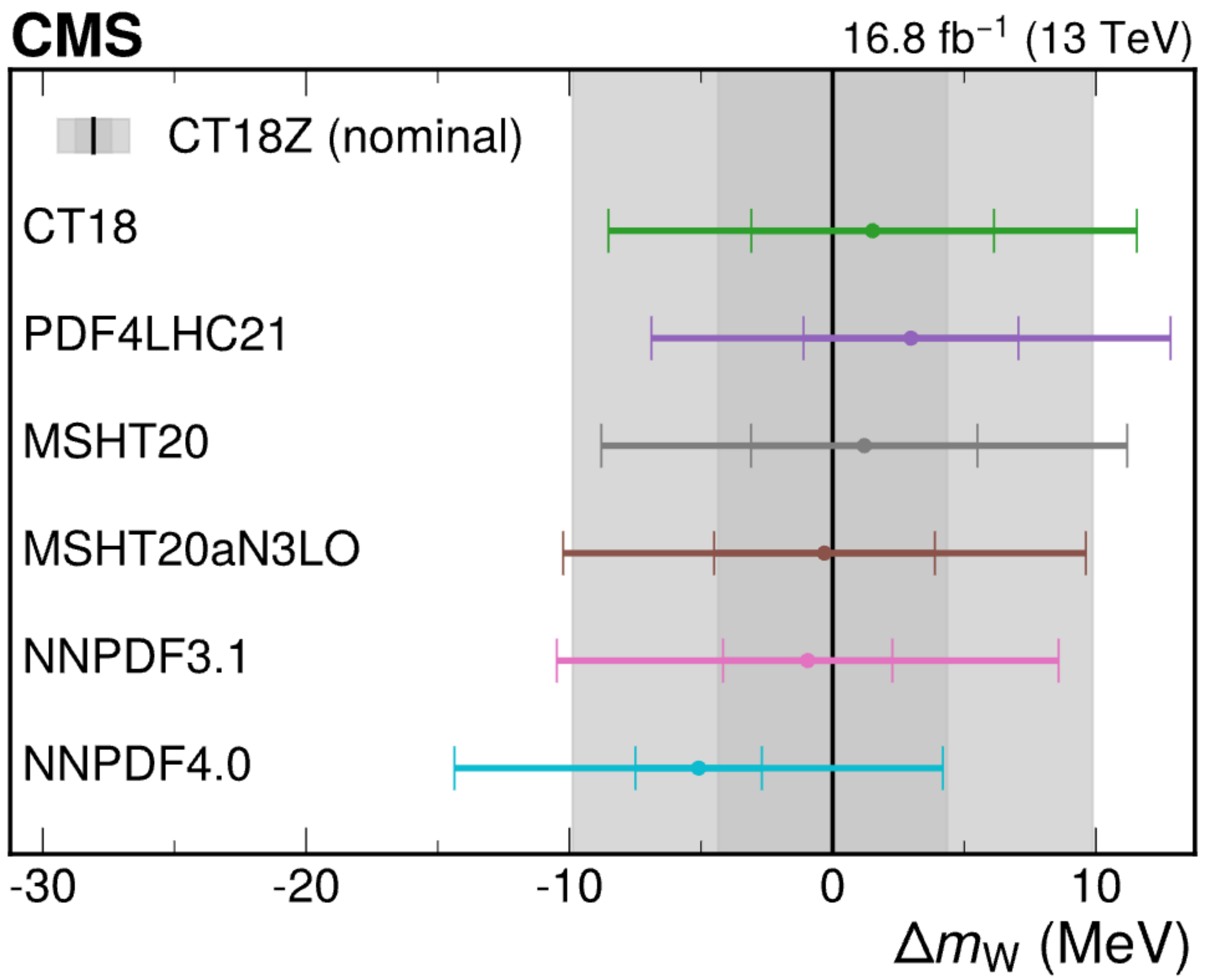
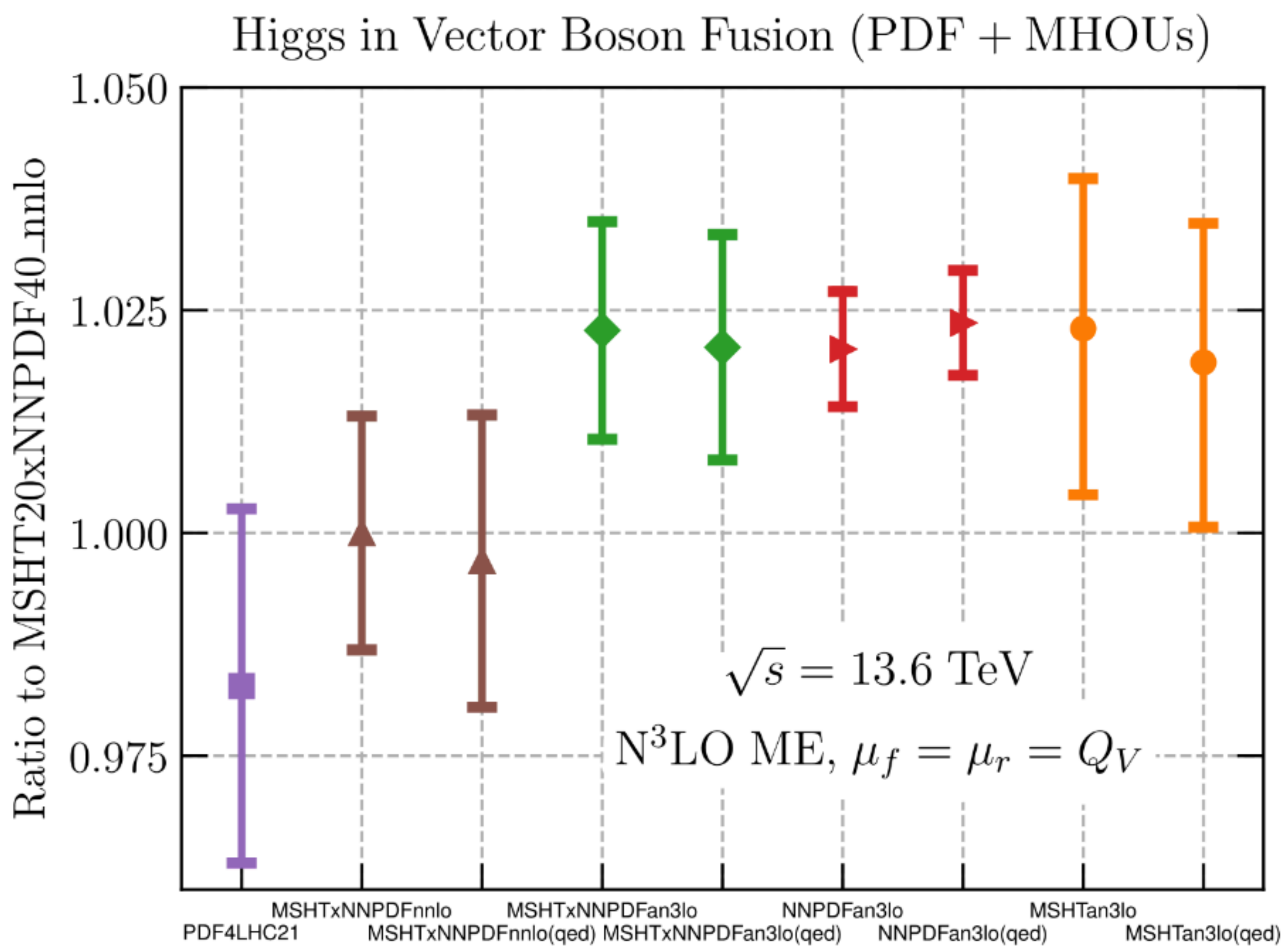
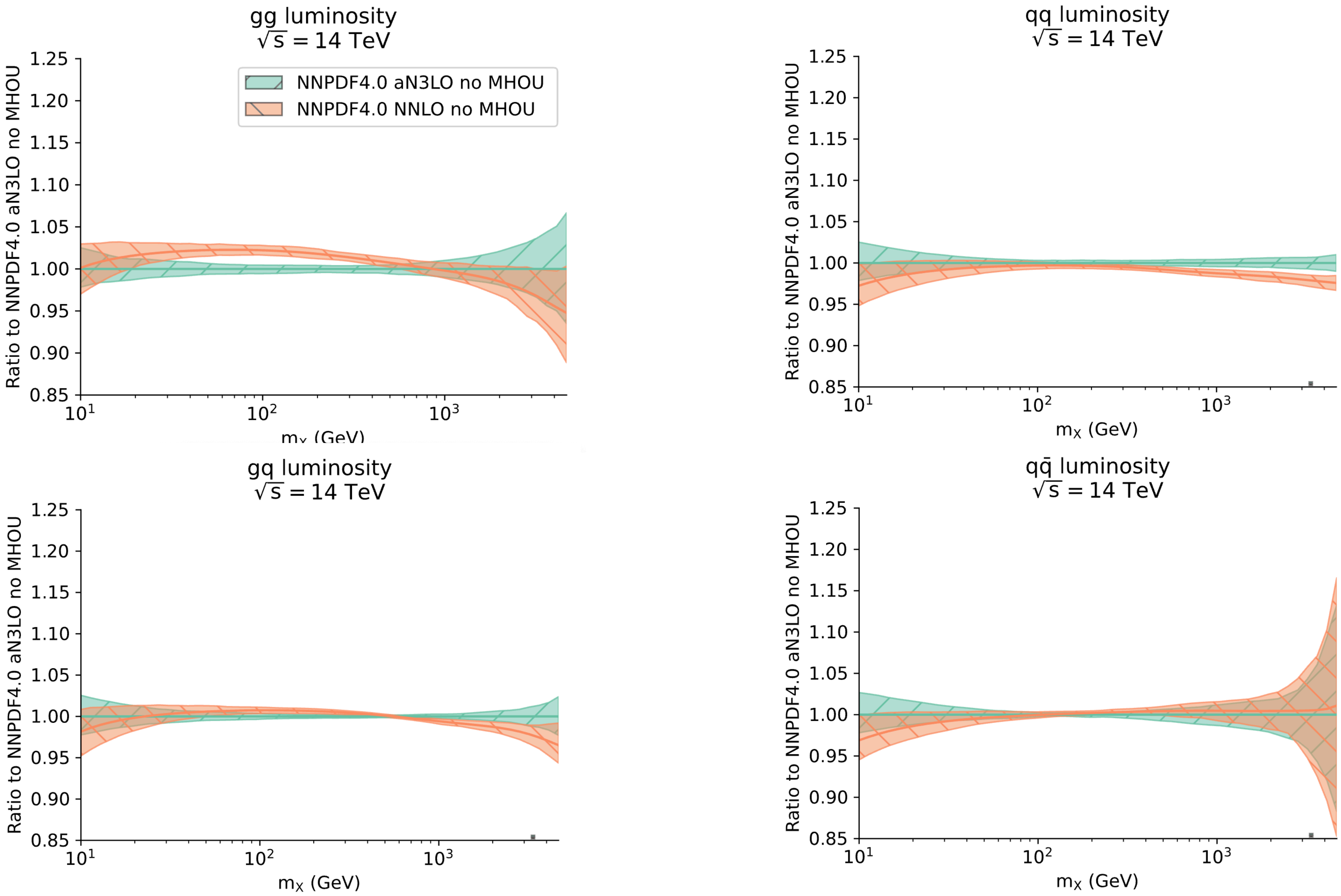


Thank you for your attention!

Backup slides

Higgs production in VBF




gg luminosity
$\sqrt{s} = 14$ TeV
NNPDF4.0 aN3LO no MHOU
NNPDF4.0 NNLO no MHOU
Ratio to NNPDF4.0 aN3LO no MHOU
1.25
1.20
1.15
1.10
1.05
1.00
0.95
0.90
0.85
10^1
10^2
10^3
m_X (GeV)
qq luminosity
$\sqrt{s} = 14$ TeV
gq luminosity
$\sqrt{s} = 14$ TeV
$q\bar{q}$ luminosity
$\sqrt{s} = 14$ TeV

QED corrections and photon PDF

- So far we considered only QCD evolution, but $\mathcal{O}(\alpha_s^2) \approx \mathcal{O}(\alpha_{em})$ so also **photon initiated contributions** may be relevant
- Modify the DGLAP running to **account for QED corrections**:

$$P = P_{QCD} + P_{QCD\otimes QED}$$

$$P_{QCD\otimes QED} = \alpha_{em} P^{(0,1)} + \alpha_{em}\alpha_s P^{(1,1)} + \alpha_{em}^2 P^{(0,2)}$$

- Data does not provide strong constraints on the photon, but the **photon PDF** can be computed from DIS structure functions: **Manohar, Nason, Salam, Zanderighi, [arXiv:1607.04266], [arXiv:1708.01256]**

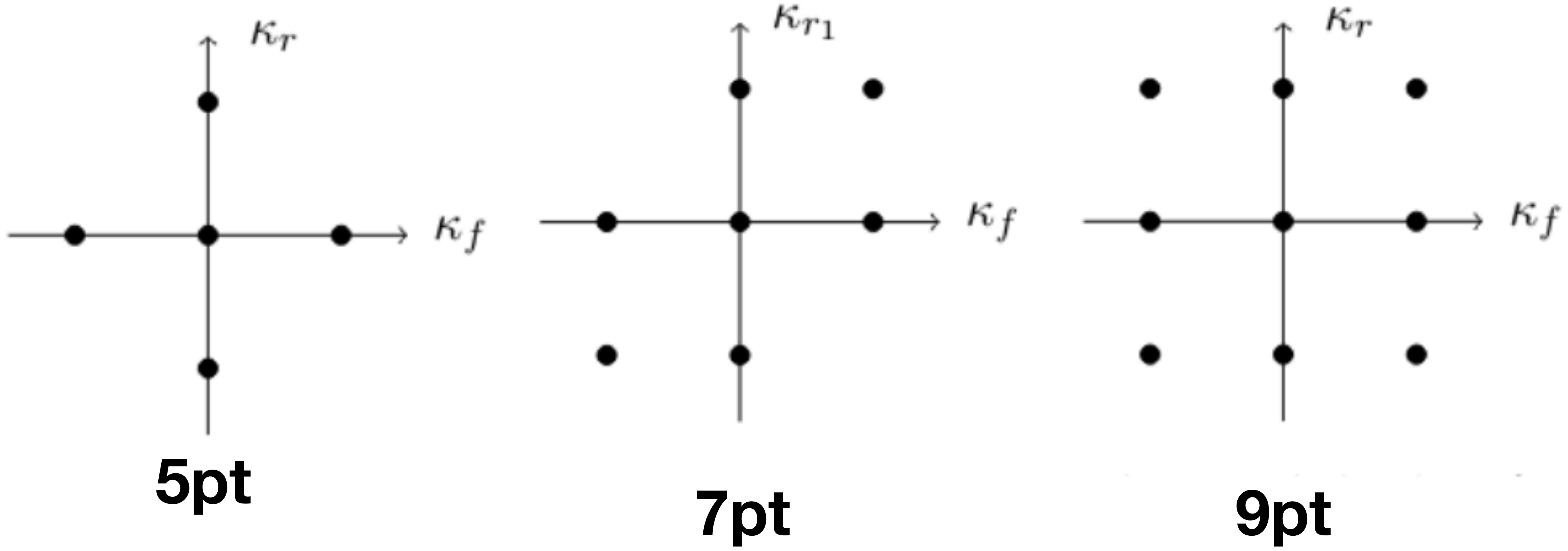
$$x\gamma\left(x,\mu^2\right) = \frac{2}{\alpha\left(\mu^2\right)} \int_x^1 \frac{dz}{z} \left\{ \int_{\frac{m_p^2 x^2}{1-z}}^{\frac{\mu^2}{1-z}} \frac{dQ^2}{Q^2} \alpha^2(Q^2) \left[-z^2 F_L\left(x/z, Q^2\right) + \left(z P_{\gamma q}(z) + \frac{2x^2 m_p^2}{Q^2} \right) F_2\left(x/z, Q^2\right) \right] - \alpha^2\left(\mu^2\right) z^2 F_2\left(x/z,\mu^2\right) \right\}$$

- The **momentum sum rule** needs to account for the photon PDF:

$$\sum_{i=q,\bar{q},g,\gamma} \int_0^1 dx x f_i\left(x, Q^2\right) = 1.$$

Theory uncertainties in PDFs

Missing higher order uncertainties (MHOUs) are estimated through 7 point scale variations



- In a fit we minimize the χ^2:

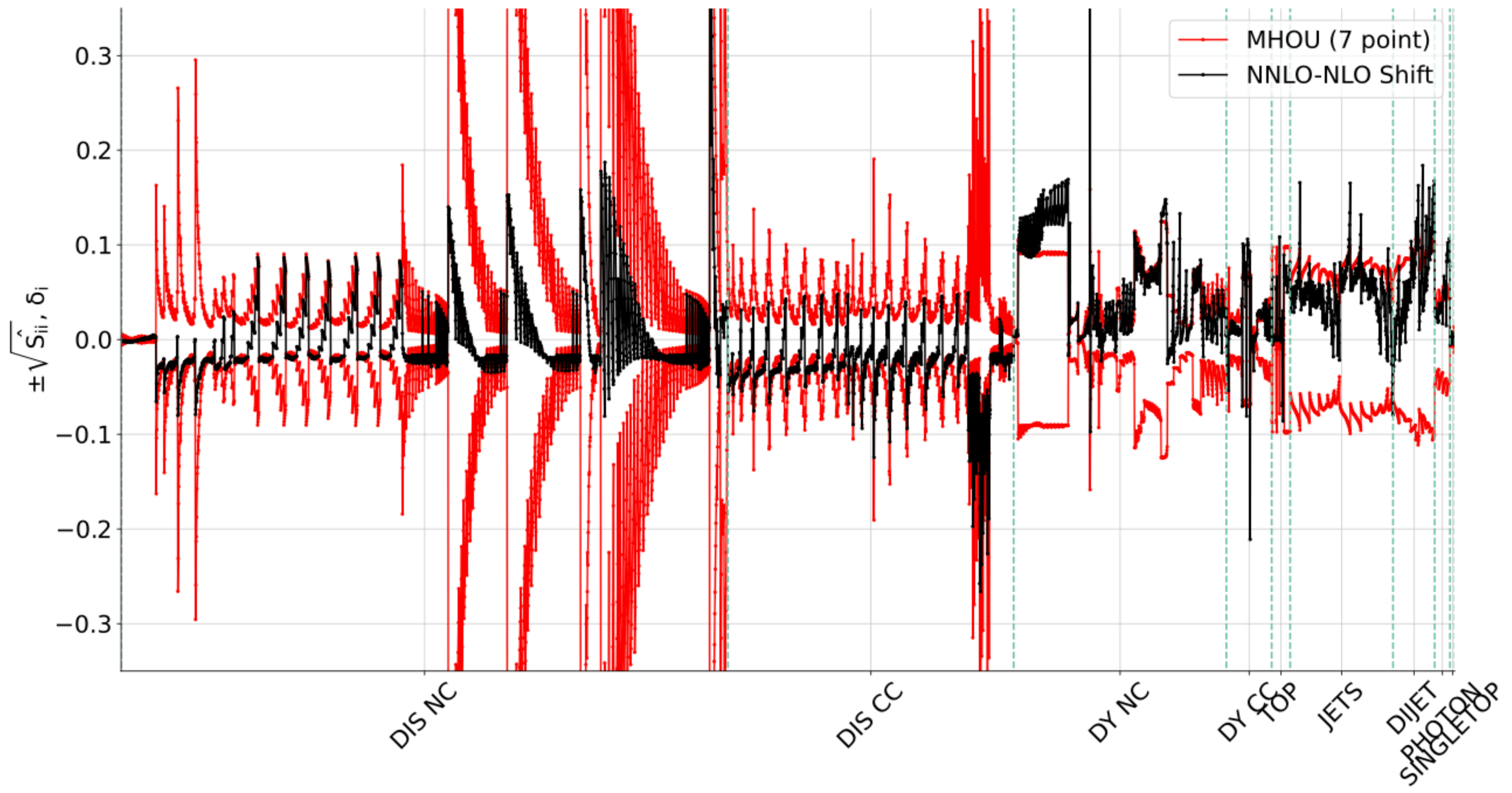
$$P(T \mid D\lambda) \propto \exp\left(-\frac{1}{2}(T-D)^T C^{-1}(T-D)\right) \equiv \exp\left(\chi^2\right)$$

- To account for MHOUs we treat the theory covmat on the same footing as the experimental covmat: $C = C_{\mathrm{exp}} + C_{\mathrm{MHOU}}$

$$C_{\mathrm{MHOU},ij} = n_m \frac{1}{V_m} \sum \left(T_i(\kappa_f, \kappa_r) - T_i(0,0)\right)\left(T_j(\kappa_f, \kappa_r) - T_j(0,0)\right)$$

Validating the MHOU covmat

The MHOU covmat is validated by comparing the **shifts from scale variations at NLO** to the known **NNLO-NLO shifts**



Data

Data set	Ref.	NNPDF3.1	NNPDF4.0	ABMP16	CT18	MSHT20
ATLAS W, Z 7 TeV ($\mathcal{L} = 35$ pb^{-1})	[53]	✓	✓	✓	✓	✓
ATLAS W, Z 7 TeV ($\mathcal{L} = 4.6$ fb^{-1})	[54]	✓	✓	✗	(✓)	✓
ATLAS low-mass DY 7 TeV	[55]	✓	✓	✗	(✓)	✗
ATLAS high-mass DY 7 TeV	[56]	✓	✓	✗	(✓)	✓
ATLAS W 8 TeV	[81]	✗	(✓)	✗	✗	✓
ATLAS DY 2D 8 TeV	[80]	✗	✓	✗	✗	✓
ATLAS high-mass DY 2D 8 TeV	[79]	✗	✓	✗	(✓)	✓
ATLAS $\sigma_{W,Z}$ 13 TeV	[83]	✗	✓	✓	✗	✗
ATLAS W+jet 8 TeV	[95]	✗	✓	✗	✗	✓
ATLAS Z p_T 7 TeV	[274]	(✓)	✗	✗	(✓)	✗
ATLAS Z p_T 8 TeV	[65]	✓	✓	✗	✓	✓
ATLAS $W + c$ 7 TeV	[85]	✗	✓	✗	(✓)	✗
ATLAS $\sigma_{tt}^{\rm tot}$ 7, 8 TeV	[67]	✓	✓	✓	✗	✗
ATLAS $\sigma_{tt}^{\rm tot}$ 7, 8 TeV	[275–280]	✗	✗	✓	✗	✗
ATLAS $\sigma_{tt}^{\rm tot}$ 13 TeV ($\mathcal{L} = 3.2$ fb^{-1})	[68]	✓	✗	✓	✗	✗
ATLAS $\sigma_{tt}^{\rm tot}$ 13 TeV ($\mathcal{L} = 139$ fb^{-1})	[136]	✗	✓	✗	✗	✗
ATLAS $\sigma_{tt}^{\rm tot}$ and Z ratios	[281]	✗	✗	✗	✗	(✓)
ATLAS $t\bar{t}$ lepton+jets 8 TeV	[69]	✓	✓	✗	✓	✓
ATLAS $t\bar{t}$ dilepton 8 TeV	[91]	✗	✓	✗	✗	✓
ATLAS single-inclusive jets 7 TeV, R=0.6	[75]	✓	(✓)	✗	✓	✓
ATLAS single-inclusive jets 8 TeV, R=0.6	[88]	✗	✓	✗	✗	✗
ATLAS dijets 7 TeV, R=0.6	[148]	✗	✓	✗	✗	✗
ATLAS direct photon production 8 TeV	[102]	✗	(✓)	✗	✗	✗
ATLAS direct photon production 13 TeV	[103]	✗	✓	✗	✗	✗
ATLAS single top R_t 7, 8, 13 TeV	[96, 98, 100]	✗	✓	✓	✗	✗
ATLAS single top diff. 7 TeV	[96]	✗	✓	✗	✗	✗
ATLAS single top diff. 8 TeV	[98]	✗	✓	✗	✗	✗

Data set	Ref.	NNPDF3.1	NNPDF4.0	ABMP16	CT18	MSHT20
CMS W asym. 7 TeV ($\mathcal{L} = 36$ pb^{-1})	[282]	✗	✗	✗	✗	✓
CMS Z 7 TeV ($\mathcal{L} = 36$ pb^{-1})	[283]	✗	✗	✗	✗	✓
CMS W electron asymmetry 7 TeV	[57]	✓	✓	✗	✓	✓
CMS W muon asymmetry 7 TeV	[58]	✓	✓	✓	✓	✗
CMS Drell-Yan 2D 7 TeV	[59]	✓	✓	✗	(✓)	✓
CMS Drell-Yan 2D 8 TeV	[284]	(✓)	✗	✗	✗	✗
CMS W rapidity 8 TeV	[60]	✓	✓	✓	✓	✓
CMS W, Z p_T 8 TeV ($\mathcal{L} = 18.4$ fb^{-1})	[285]	✗	✗	✗	(✓)	✗
CMS Z p_T 8 TeV	[66]	✓	✓	✗	(✓)	✗
CMS $W + c$ 7 TeV	[78]	✓	✓	✗	(✓)	✓
CMS $W + c$ 13 TeV	[86]	✗	✓	✗	✗	(✓)
CMS single-inclusive jets 2.76 TeV	[77]	✓	✗	✗	✗	✓
CMS single-inclusive jets 7 TeV	[147]	✓	(✓)	✗	✓	✓
CMS dijets 7 TeV	[76]	✗	✓	✗	✗	✗
CMS single-inclusive jets 8 TeV	[89]	✗	✓	✗	✓	✓
CMS 3D dijets 8 TeV	[149]	✗	(✓)	✗	✗	✗
CMS $\sigma_{tt}^{\rm tot}$ 5 TeV	[90]	✗	✓	✗	✗	✗
CMS $\sigma_{tt}^{\rm tot}$ 7, 8 TeV	[146]	✓	✓	✗	✗	✗
CMS $\sigma_{tt}^{\rm tot}$ 8 TeV	[286]	✗	✗	✗	✗	✓
CMS $\sigma_{tt}^{\rm tot}$ 5, 7, 8, 13 TeV	[70, 287–295]	✗	✗	✓	✗	✗
CMS $\sigma_{tt}^{\rm tot}$ 13 TeV	[71]	✓	✓	✓	✗	✗
CMS $t\bar{t}$ lepton+jets 8 TeV	[72]	✓	✓	✗	✗	✓
CMS $t\bar{t}$ 2D dilepton 8 TeV	[92]	✗	✓	✗	✓	✓
CMS $t\bar{t}$ lepton+jet 13 TeV	[93]	✗	✓	✗	✗	✗
CMS $t\bar{t}$ dilepton 13 TeV	[94]	✗	✓	✗	✗	✗
CMS single top $\sigma_t + \sigma_{\bar{t}}$ 7 TeV	[97]	✗	✓	✓	✗	✗
CMS single top R_t 8, 13 TeV	[99, 101]	✗	✓	✓	✗	✗
CMS single top 13 TeV	[296, 297]	✗	✗	✗	✗	(✓)