The path to PDFs and $\alpha_s(m_Z)$ at N^{3}LO from a global QCD analysis

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Motivation I

Reducing PDF uncertainties entering LHC predictions requires an **in-depth understanding of the differences and similarities between PDF analysis**

ATLAS strong coupling extraction from Z p_T data at 8 TeV

	PDF set	$\alpha_s(m_Z)$	PDF uncertainty	g [GeV^2]	q [GeV^4]
baseline	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

$$\Delta_{\rm PDF}\left(\text{MSHT20 only}\right) = 0.34\,\%$$

$$\Delta_{\rm PDF}\,(\text{NNPDF4.0} - \text{CT18A}) = 1.6\,\%$$

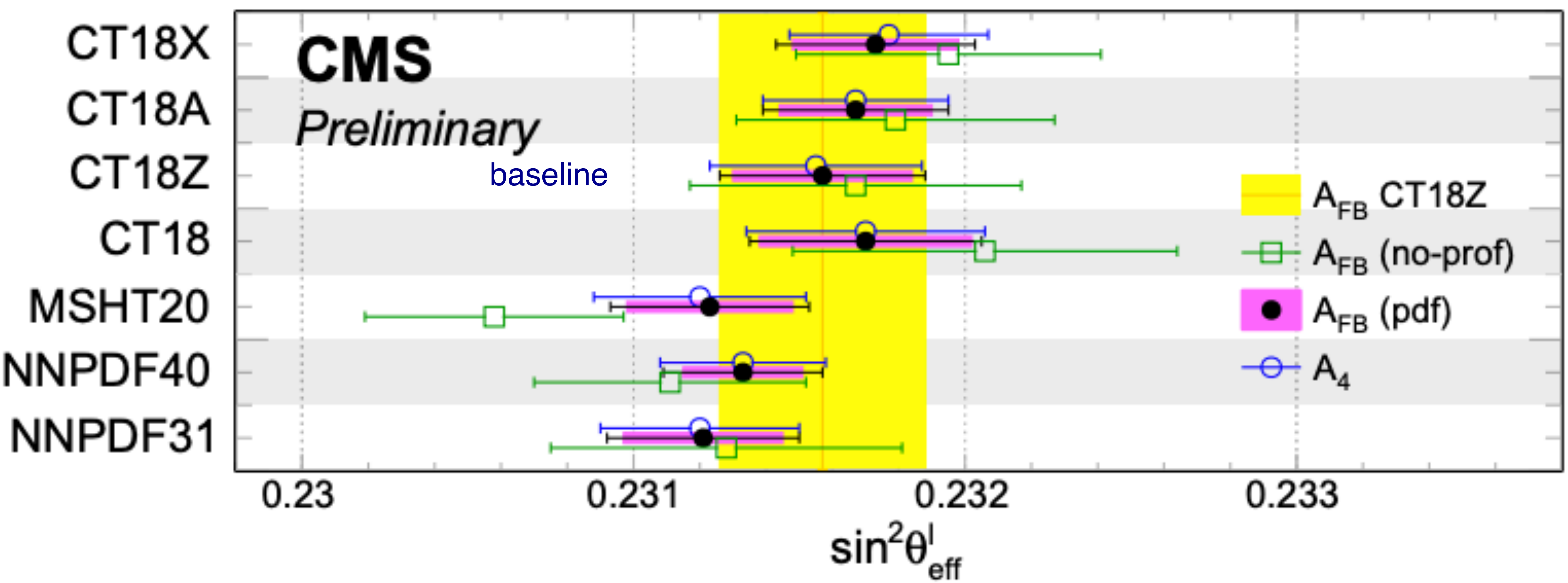
What is the ``true PDF uncertainty” that should be associated to this measurement?

How to choose ``baseline PDF” ? Is this an unbiased choice?

Motivation II

Reducing PDF uncertainties entering LHC predictions requires an **in-depth understanding of the differences and similarities between PDF analysis**

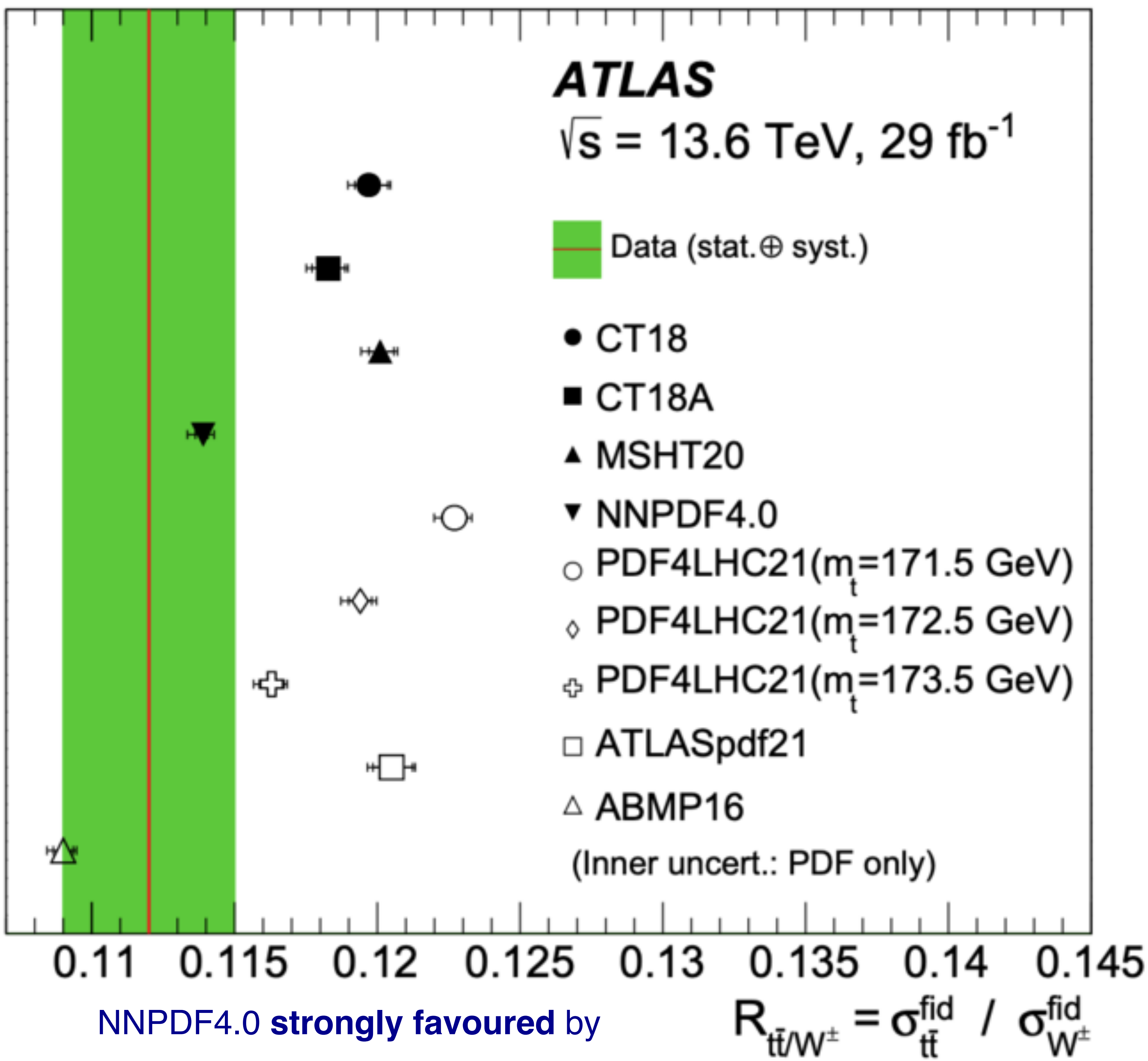
CMS determination of the weak mixing angle at 13 TeV



What is the ``true PDF uncertainty'' that should be associated to this measurement?

Is **in-situ profiling of PDFs** always justified? Back-reaction to other experiments in global fit?

Motivation III

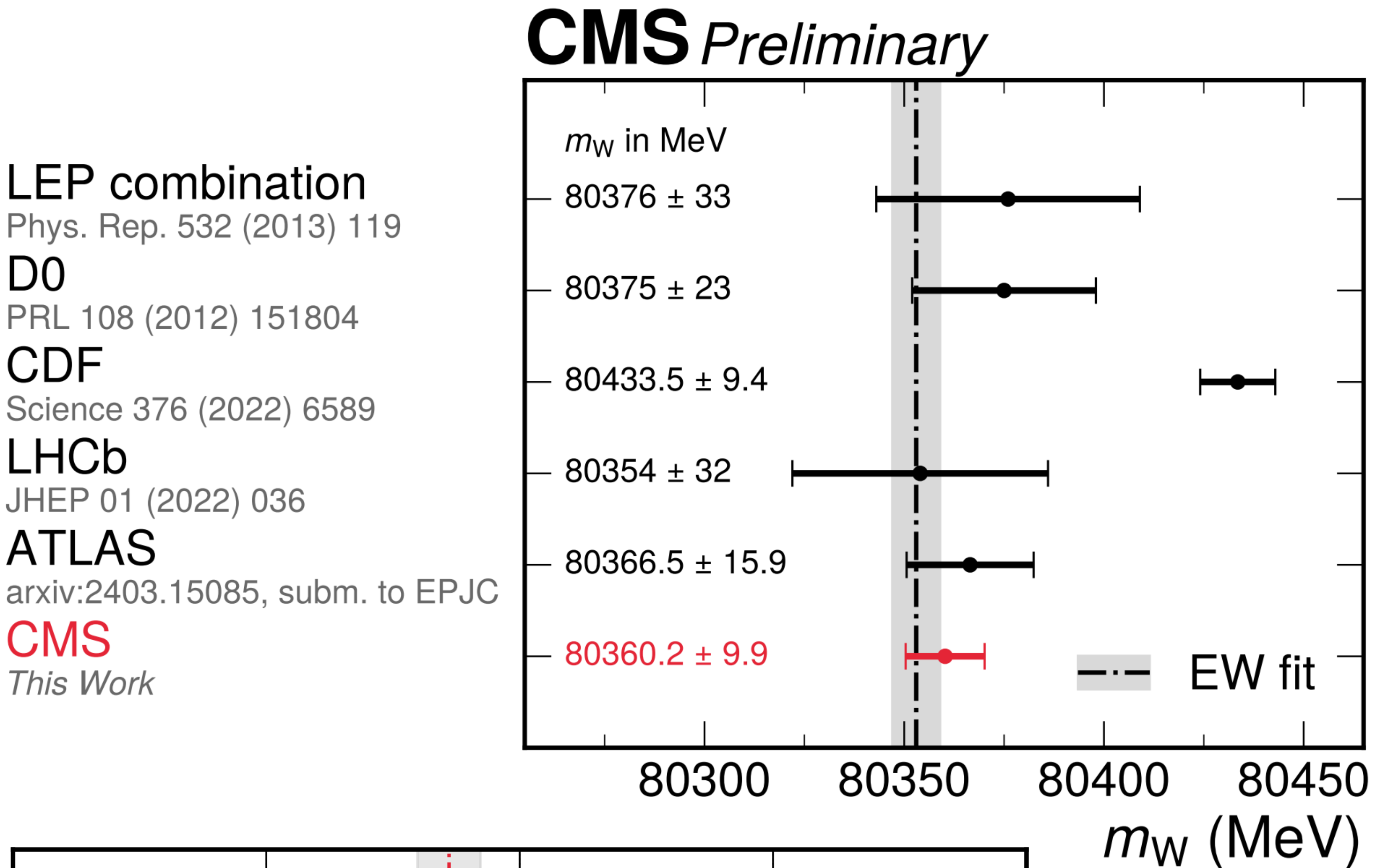


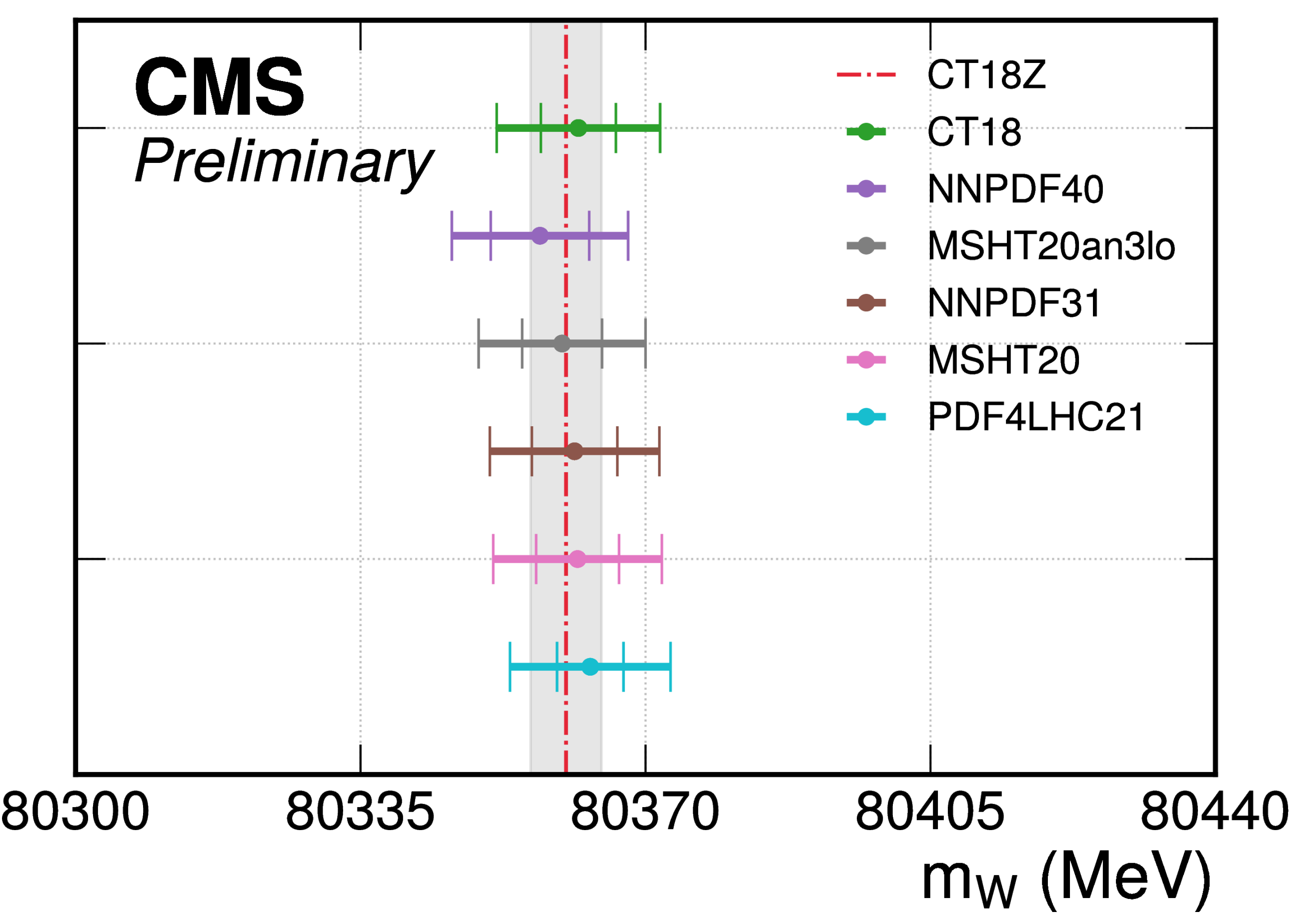
NNPDF4.0 **strongly favoured** by ATLAS data (for this observable!)

- LHC precision measurements provide **discrimination power …**
- … but only their **combination into a consistent global analysis** can provide a coherent picture of the overall data vs theory comparison
- The **interpretation of precision LHC measurements** is a challenging effort pushing the limits of both theory calculations and methodological approaches

demands strong cross-talk between theory and experiment & dedicated benchmark exercises

Motivation IV





- **W mass determination** has attracted huge attention in the last years
- **CMS measurement competitive** with CDF result, agrees with SM prediction
- PDFs remain one of the leading systematic errors
- PDFs used in the analysis **``rescaled''** to improve agreement among them? Back-reaction in the global fit?

NNPDF Timeline

NNPDF timescale

☑ Sep 2021: **NNPDF4.0 (paper & code)**

☑ Aug 2022: **Intrinsic charm**

☑ Sept 2022: **PDFs & BSM searches** (A_{FB} high-mass)

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☑ Nov 2023: **IC asymmetry** study

☑ Jan 2024: NNPDF4.0 **MHOUs & QED**

☑ Feb 2024: NNPDF4.0 **aN^{3}LO**

June 2024: NNPDF4.0 **aN3LO & QED & MHOU**

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- June 2024: NNPDF4.0 **aN3LO & QED & MHOU**
- Oct 2024: GPU-based **ML hyperopt**
- WIP: combination of **aN3LO PDFs**
- June 2024: NNPDF4.0 for MC (N)NLO **event generators**
- WIP: Implications of NNPDF4.0 for LHC data
- **WIP**: alphas based on **aN3LO+QED theory**

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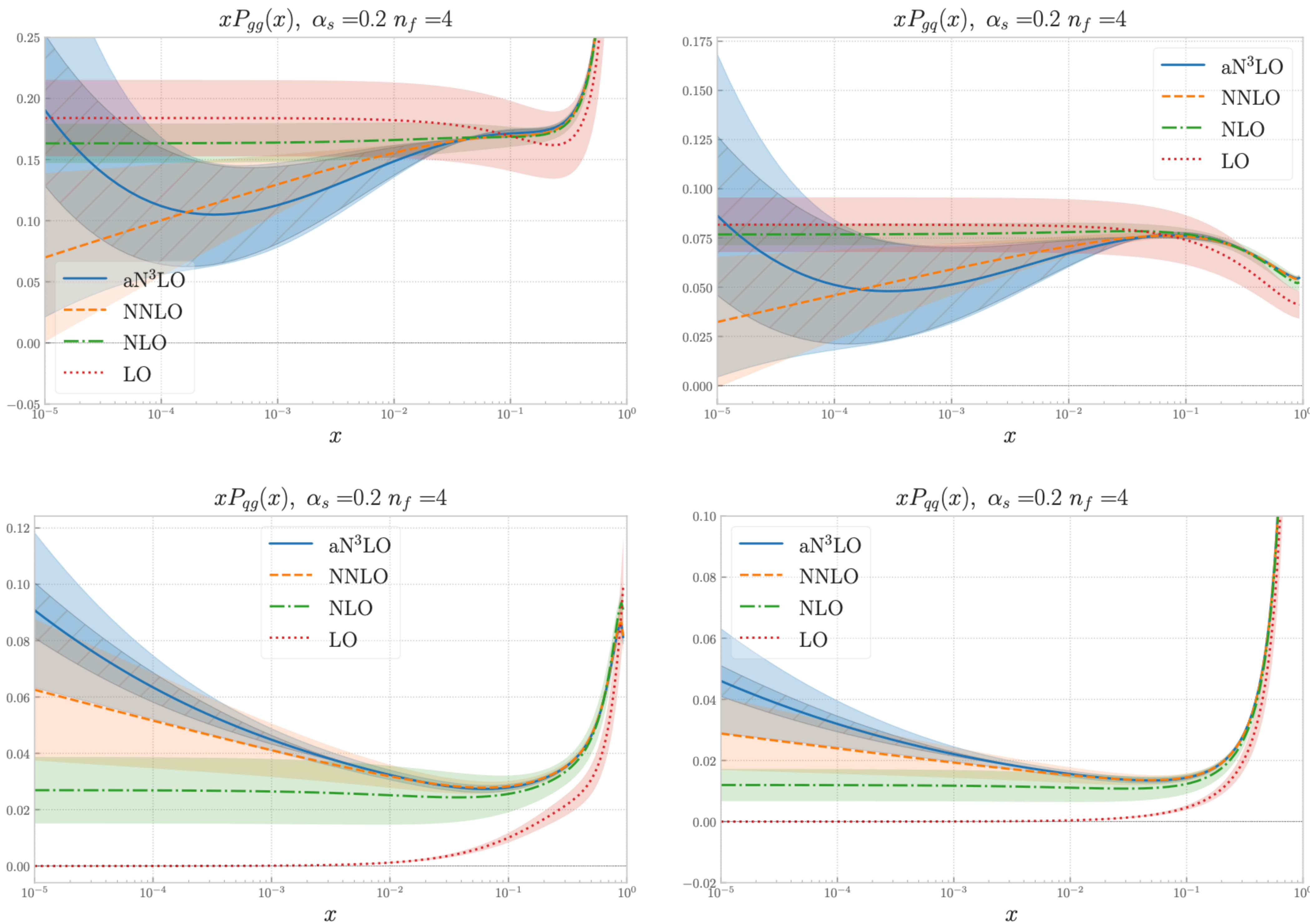
The Path to PDFs at N^3LO

aN^{3}LO splitting functions

- Approximate parametrisation for the N^{3}LO splitting functions satisfying known **exact results and limits**



LO, NLO, NNLO: **MHOU (μ_F)**

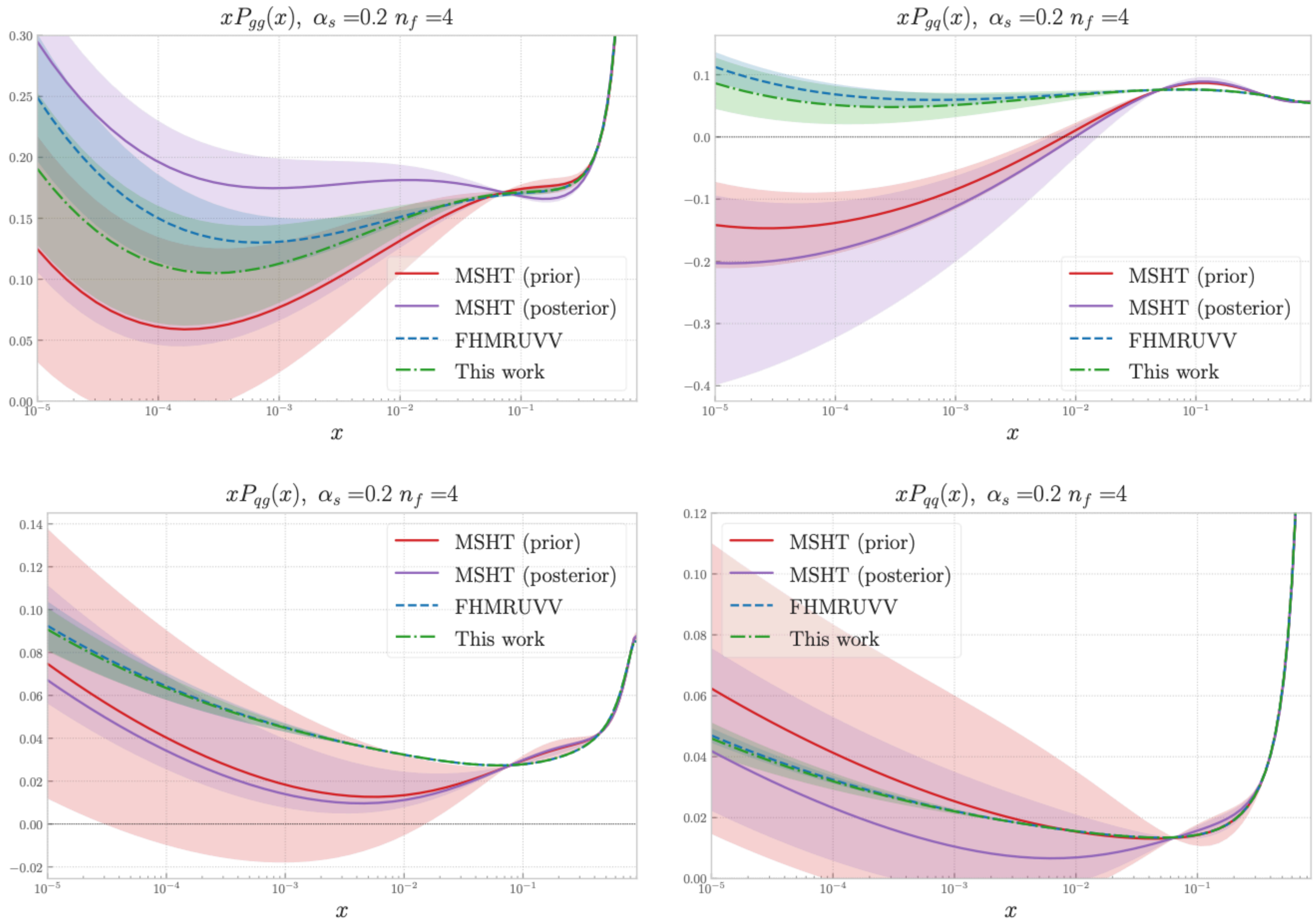
N^{3}LO: **MHOU (μ_F) + IHOUs** (dark)

Estimate **Incomplete Higher Order Uncertainties** (IHOUs) by varying interpolating functions connecting known limits

Good perturbative consistency within uncertainties

aN3LO splitting functions

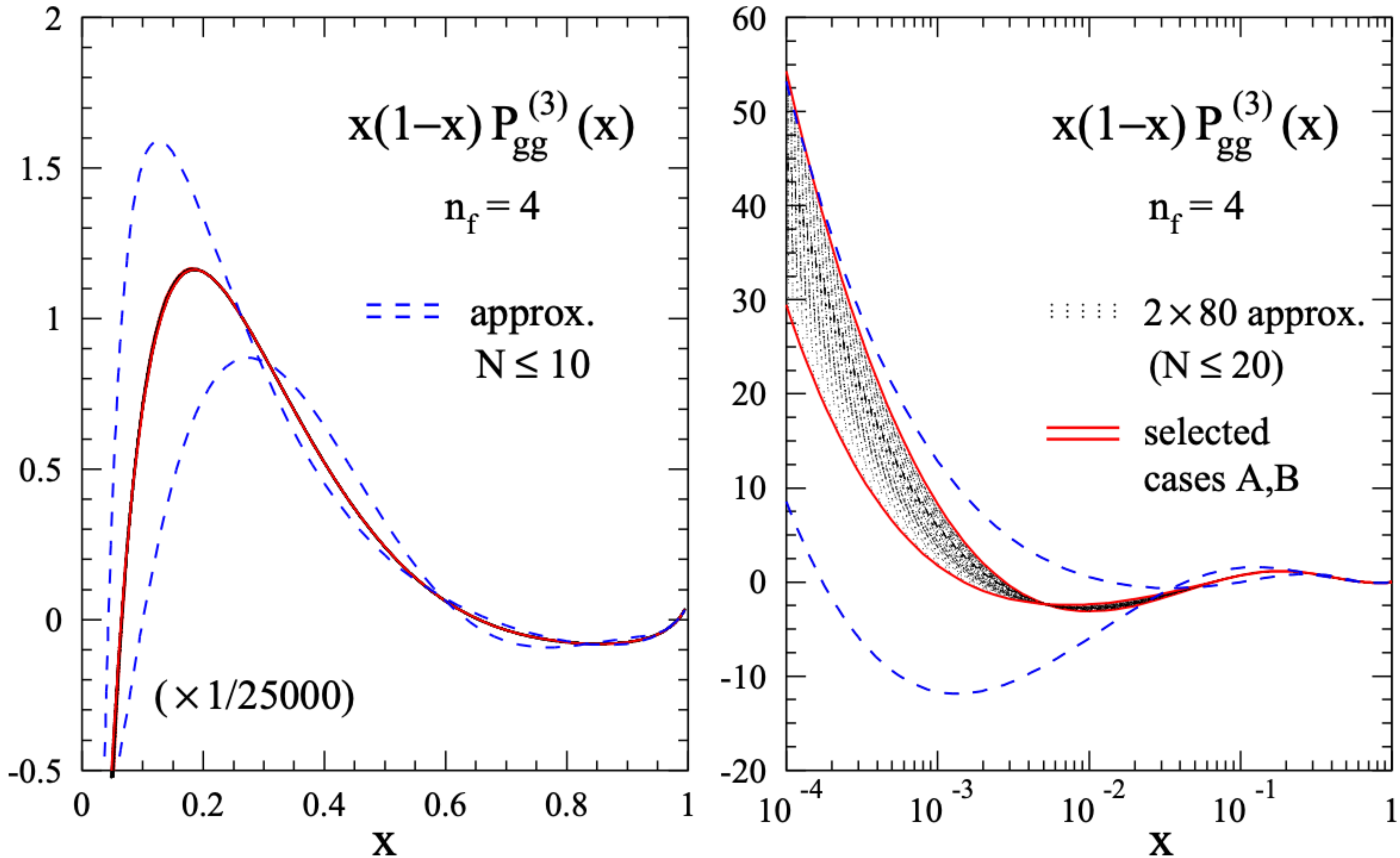
- Approximate parametrisation for the N3LO splitting functions satisfying known **exact results and limits**



Good agreement with Moch *et al.* parametrisation, IHOUs on splitting functions negligible (in data region)

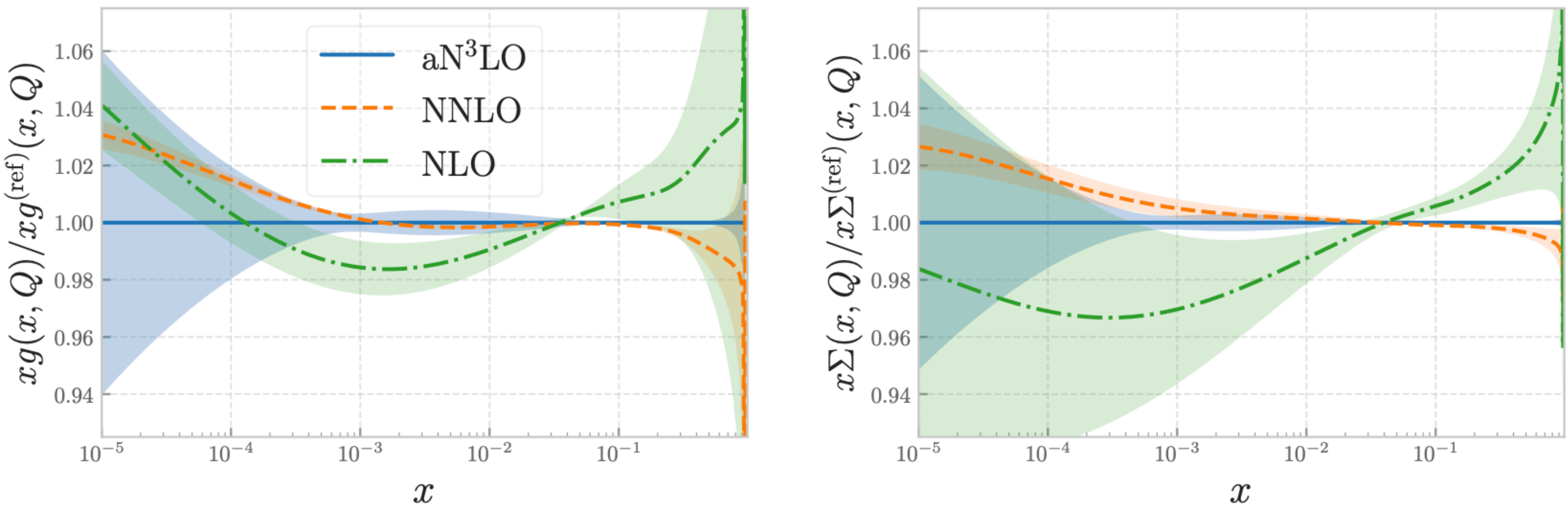
aN³LO splitting functions

- Approximate parametrisation for the N³LO splitting functions satisfying known **exact results and limits**

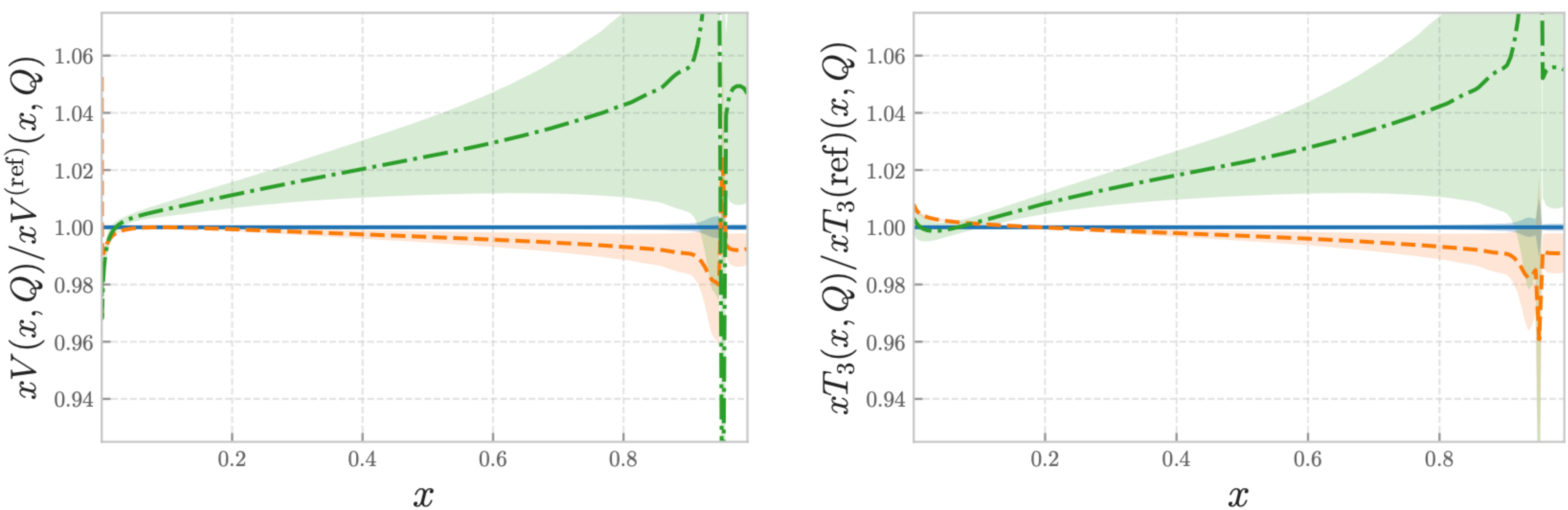


Falcioni et al, arXiv:2410.08089

Impact on PDF evolution



evolution of fixed PDF boundary condition from Q=1.65 GeV to Q=100 GeV



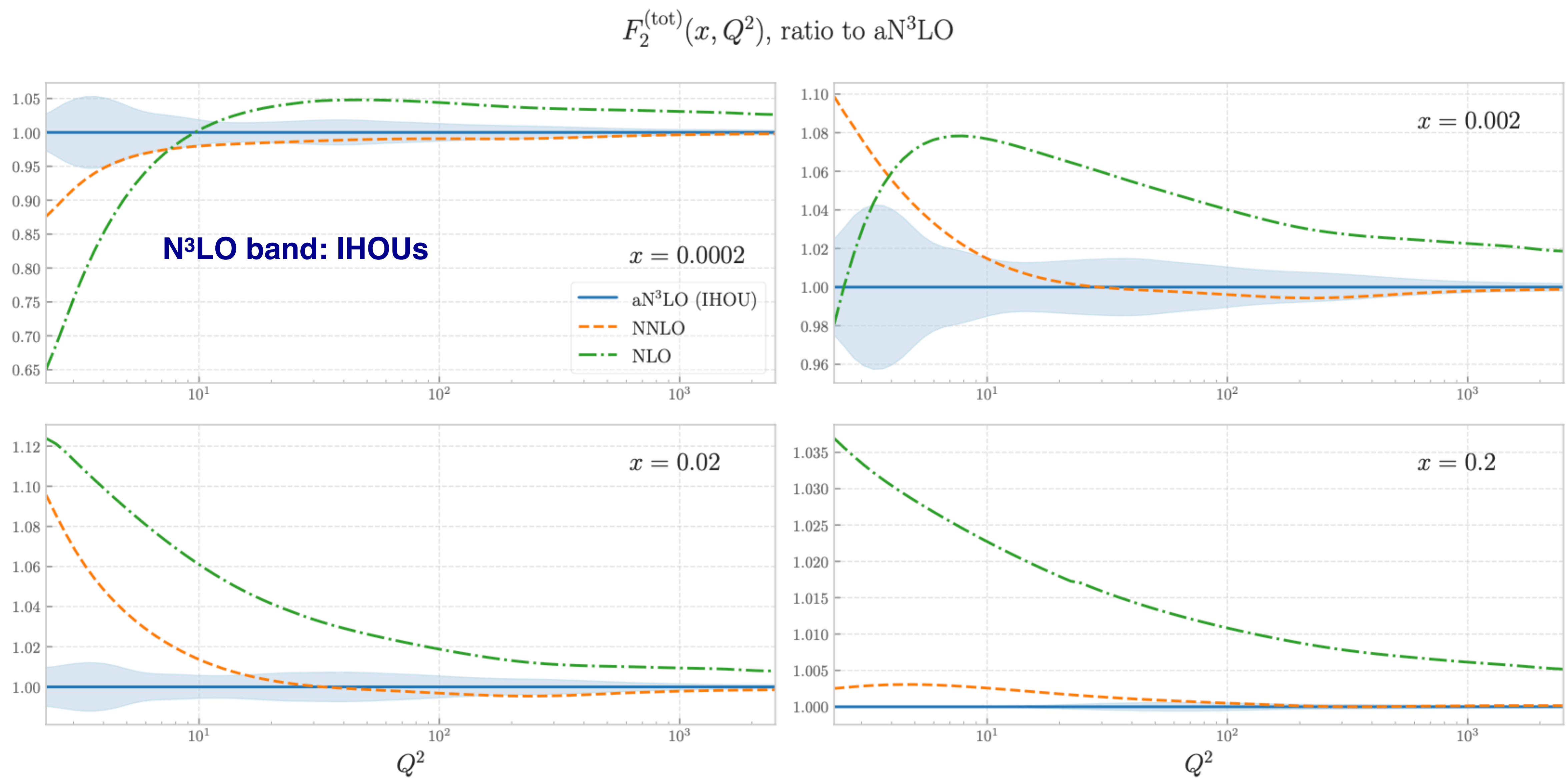
Effects of N^{3}LO corrections to DGLAP evolution **< 1%** except at small-*x* and large-*x*

Excellent **perturbative convergence of PDF evolution**, may be improved with small-*x* or large-*x* resummations

Structure functions

- Exact (approximate) massless (massive) deep-inelastic coefficient functions at N³LO accuracy & extension of the **FONLL general -mass scheme at N³LO**

- Relies on parametrisation of massive DIS coefficients reproducing known results



- **N³LO corrections to** DIS inclusive structure functions become significant at low-*Q*

- IHOUs associated to **N³LO massive coefficient functions** deweight the impact of HERA low-*Q* data

Fit settings

- Same methodology, dataset, and **pipeline for theory calculations** as in NNPDF4.0 MHOU & QED sets
- Produce fit variants with and without theory uncertainties (using the theory covariance matrix)

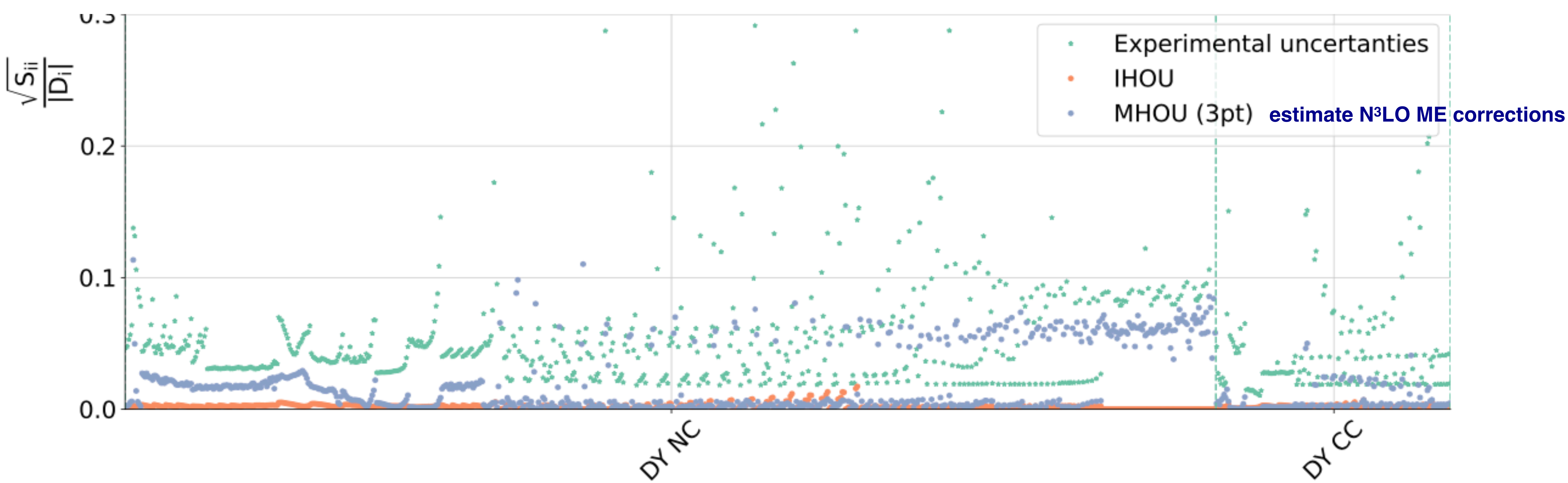
$$\Delta_i(\rho_f, \rho_r) \equiv T_i(\rho_f, \rho_r) - T_i(0,0),$$

Shift wrt central theory on the physical observables due to theory variations (e.g. scales)

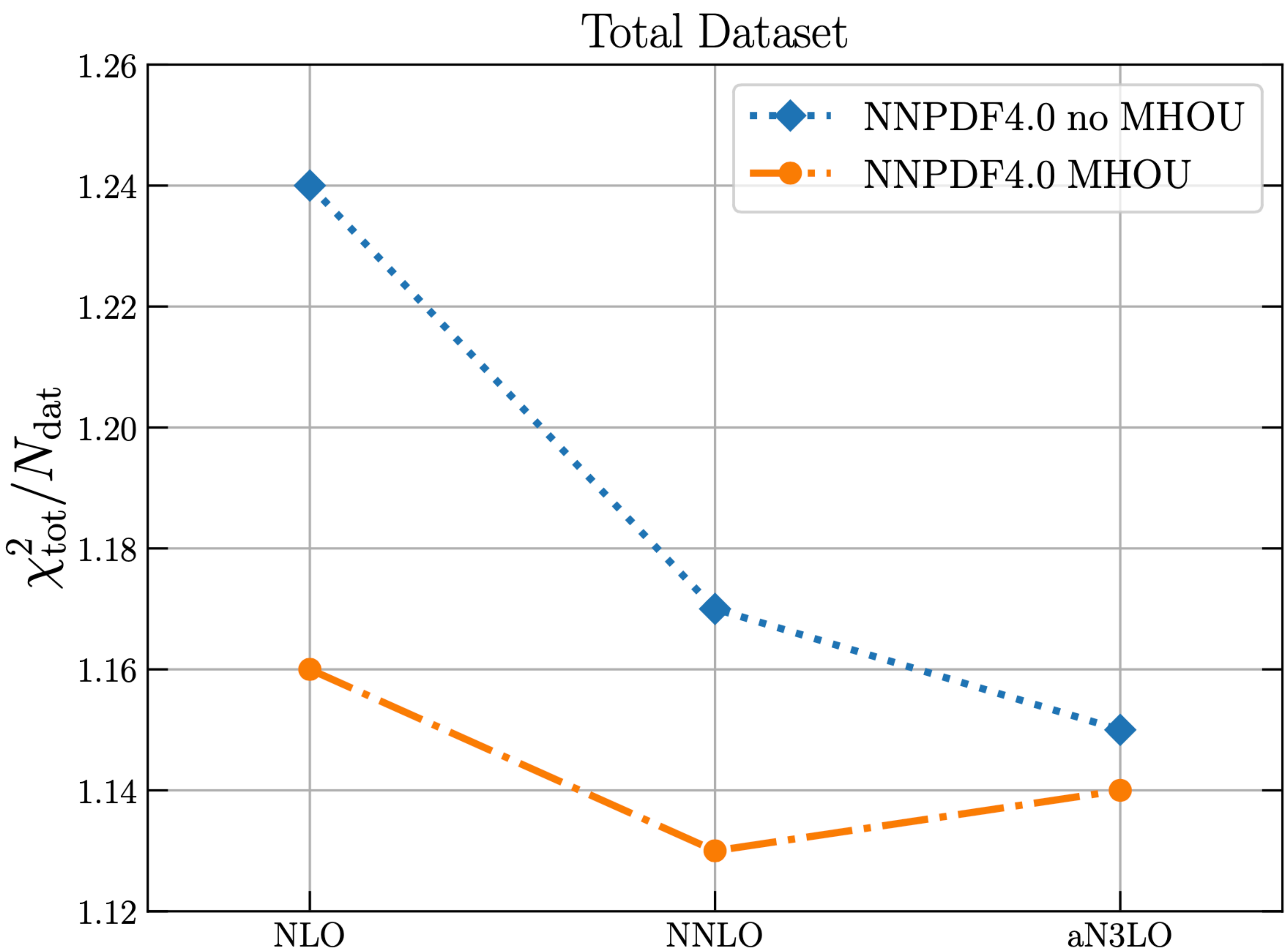
$$S_{ij} = n_m \sum_{V_m} \Delta_i(\rho_f, \rho_{r_i}) \Delta_j(\rho_f, \rho_{r_j}),$$

Theory covariance matrix: combine all shifts, keeping into account their correlations

- The theory covariance matrix includes contributions from **MHOUs** (μ_F and μ_R variations) and **IHOUs**
- Hadronic data is fitted **using aN³LO evolution and NNLO matrix elements**, supplemented by MHOUs associated to μ_R variations to account for missing K-factors



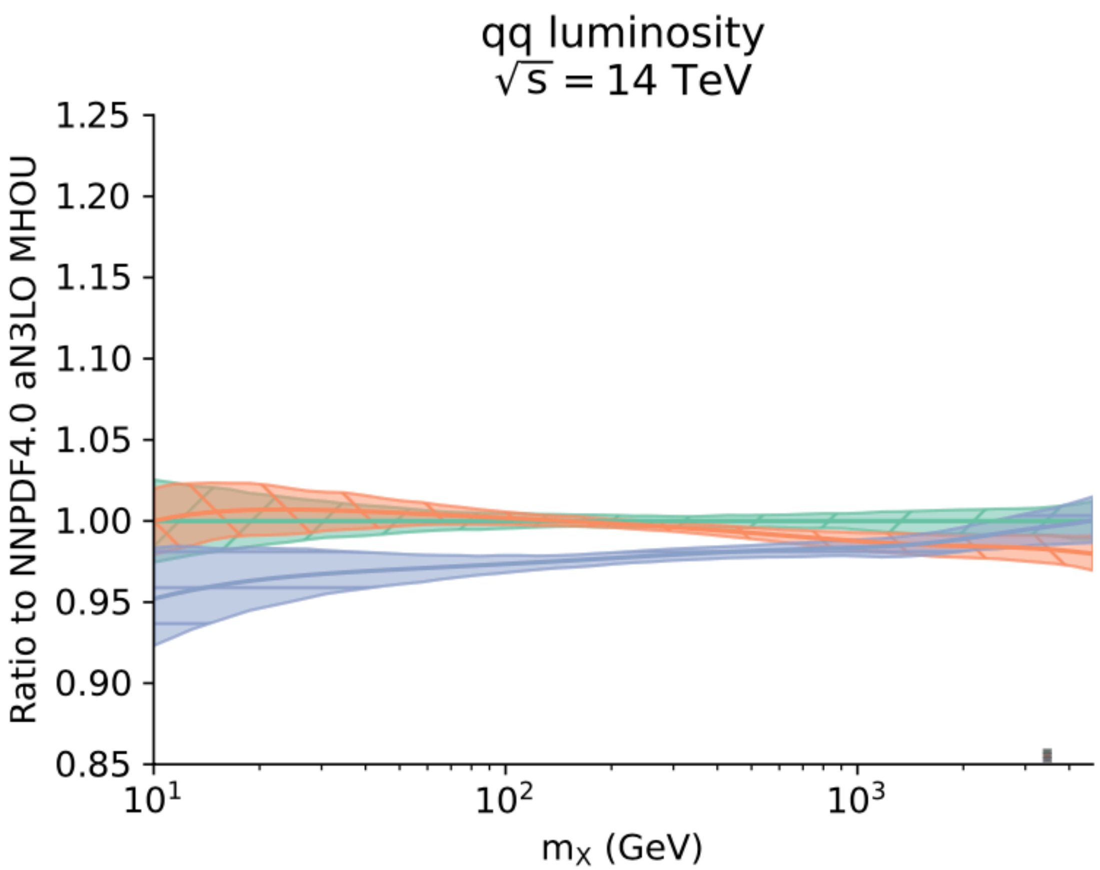
Results: Fit quality

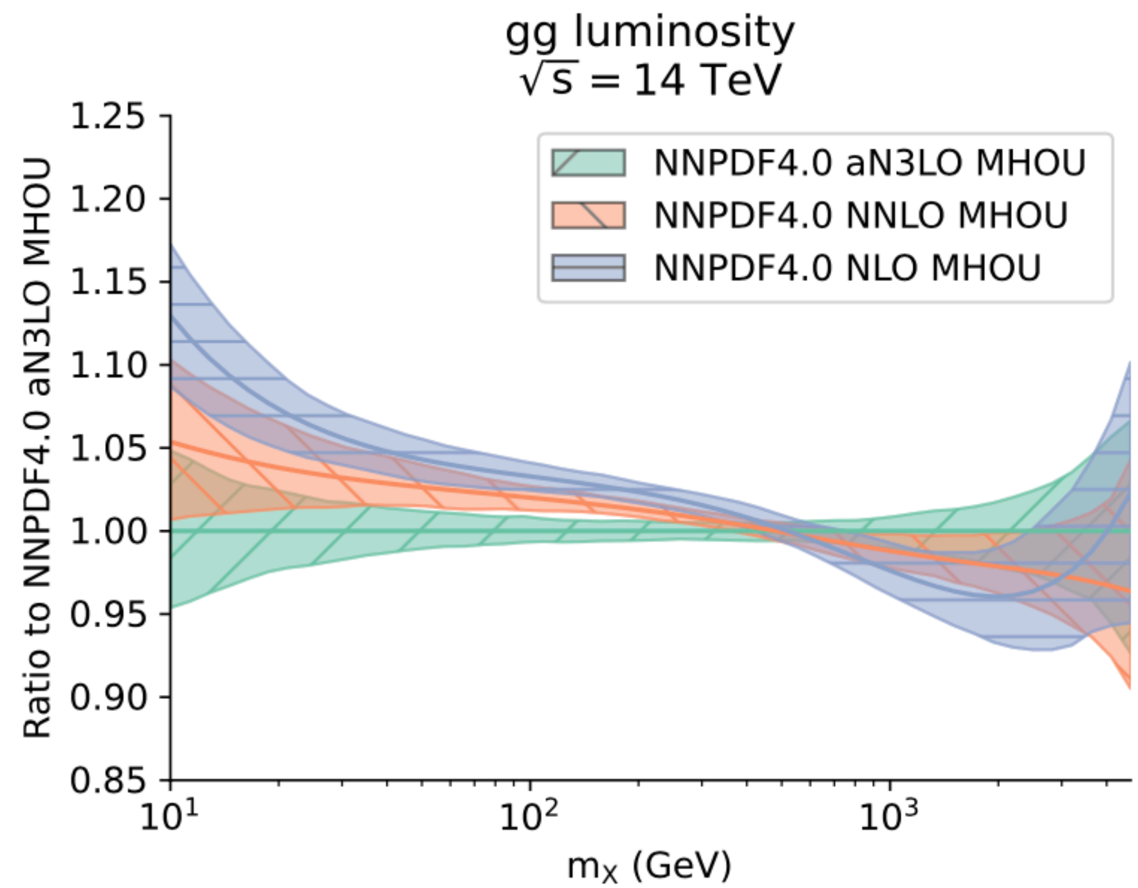


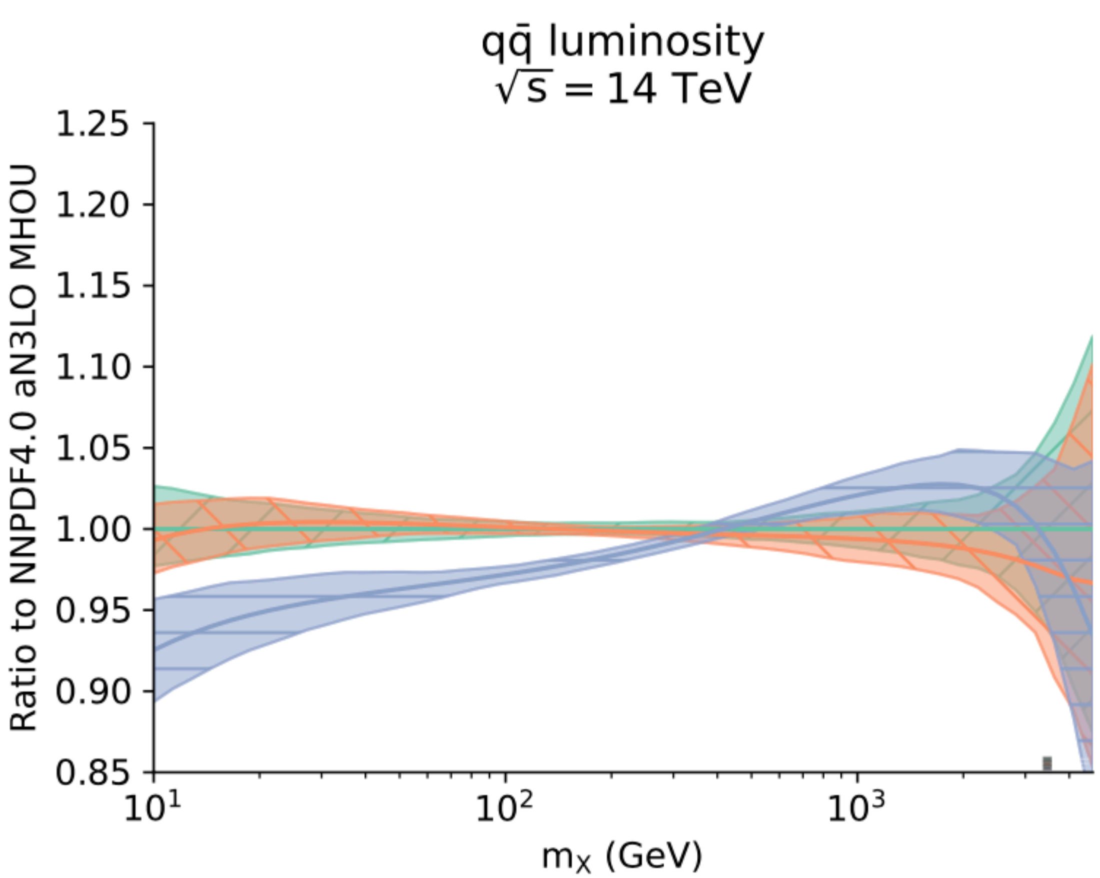
- Without MHOUs, the **χ^2 improves with the perturbative accuracy** of the PDF fit
- With MHOUs, the **χ^2** becomes **feebly dependent on the perturbative accuracy**
- At aN^{3}LO impact of MHOUs is small (also at PDF level) but non negligible

N^{3}LO corrections required for perturbative convergence at the PDF fit level!

Results: perturbative convergence

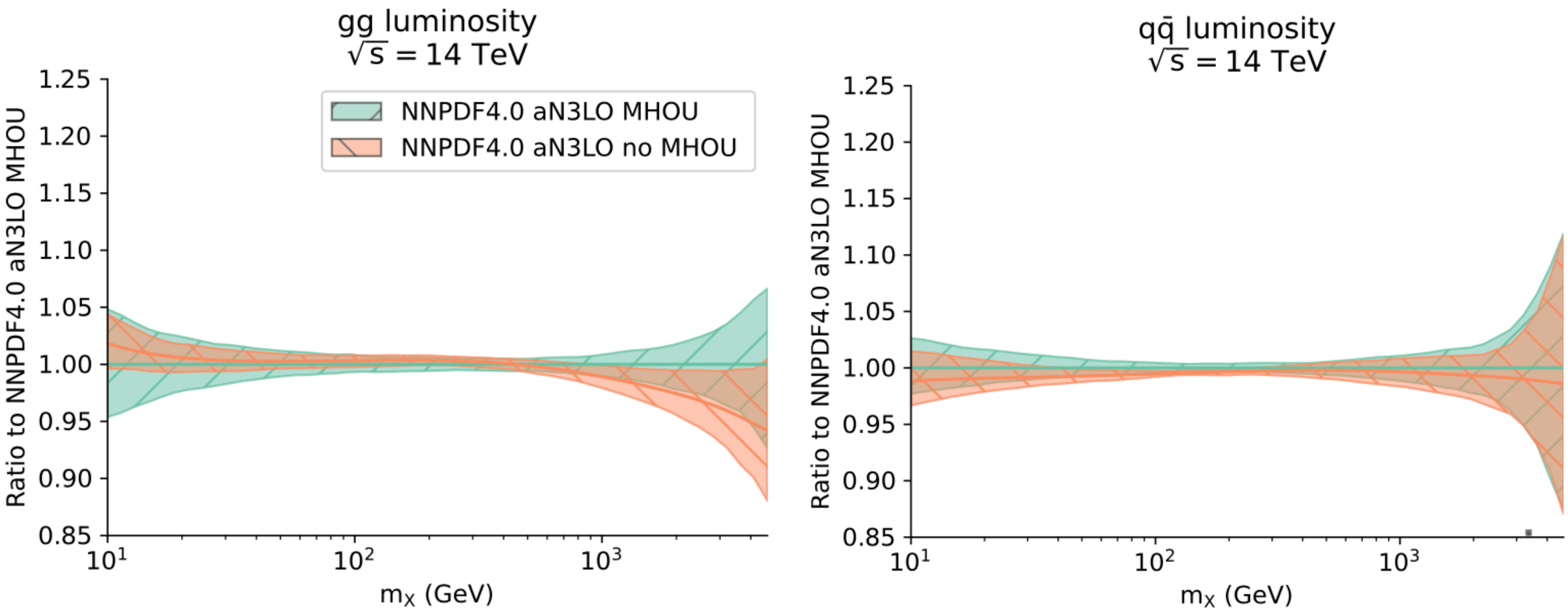






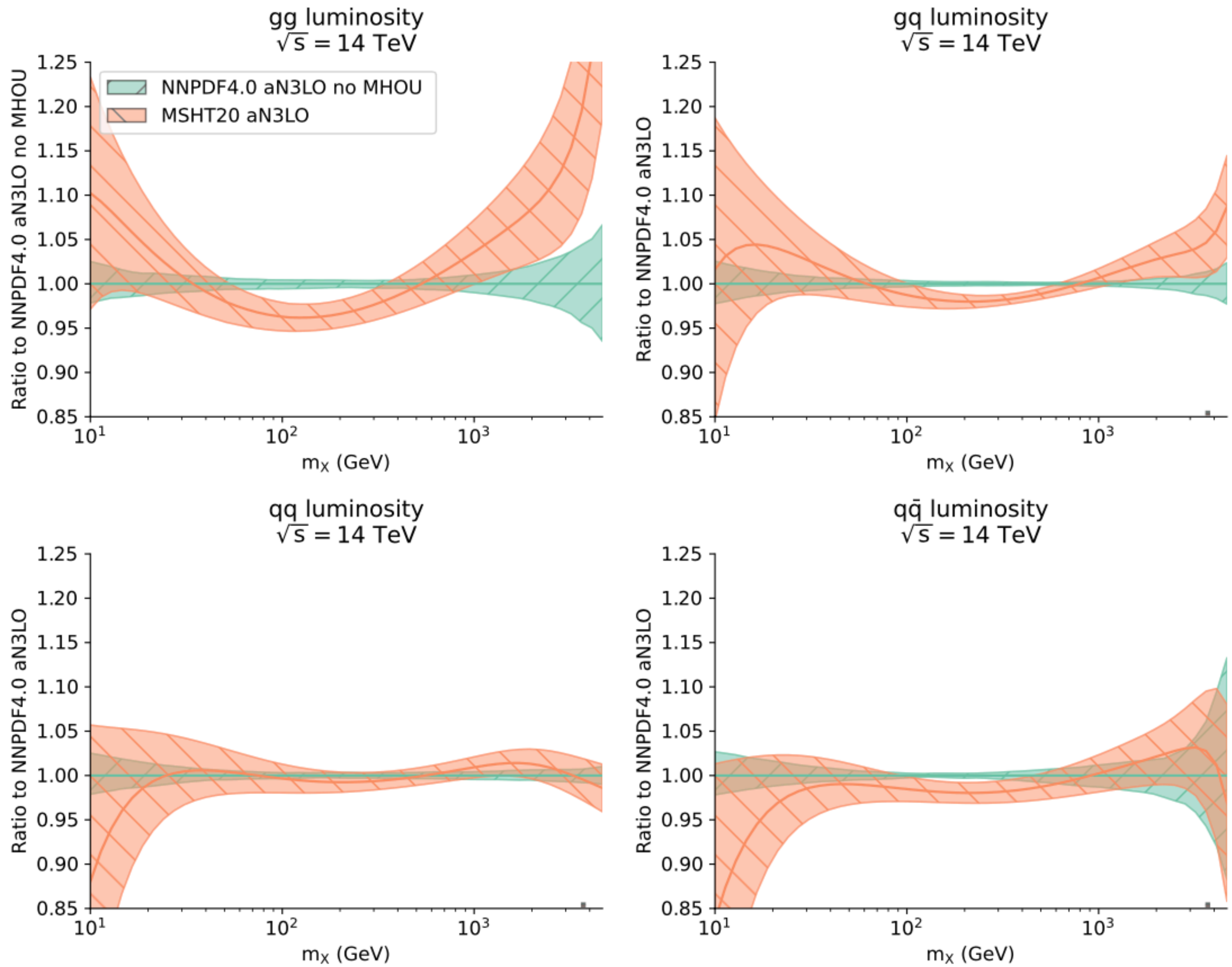
- **Good perturbative convergence**
- Impact of N^3LO corrections moderate, specially for the quark luminosities
- For the gluon-gluon luminosity, NNPDF4.0 finds a **small suppression** around Higgs mass (2% effect)

Results: impact of MHOUs at N³LO



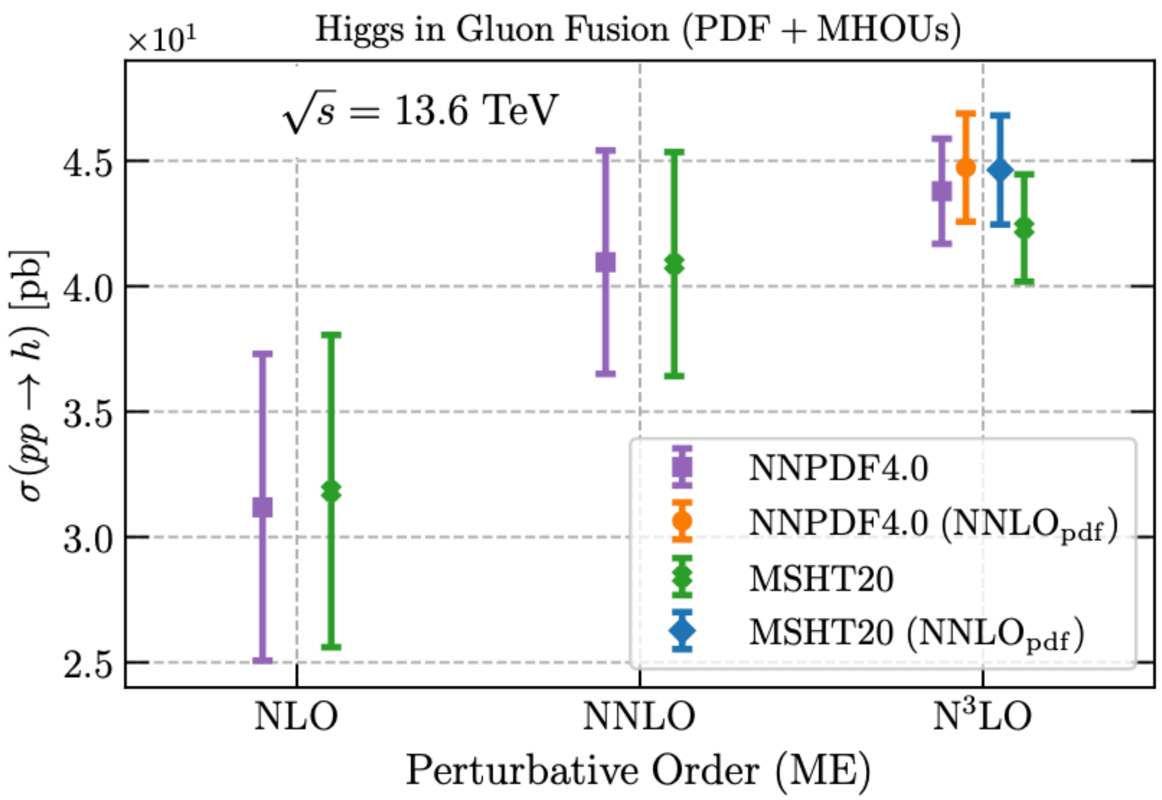
- Impact of **MHOUs is not negligible** even at N^3LO, both in terms of central values and uncertainties
- Motivates inclusion of **exact N^3LO calculations** for hadronic processes in the global PDF fit (*e.g.* Drell-Yan production, which is already available)
- Further highlights the relevance of MHOUs also for NNLO and NLO fits

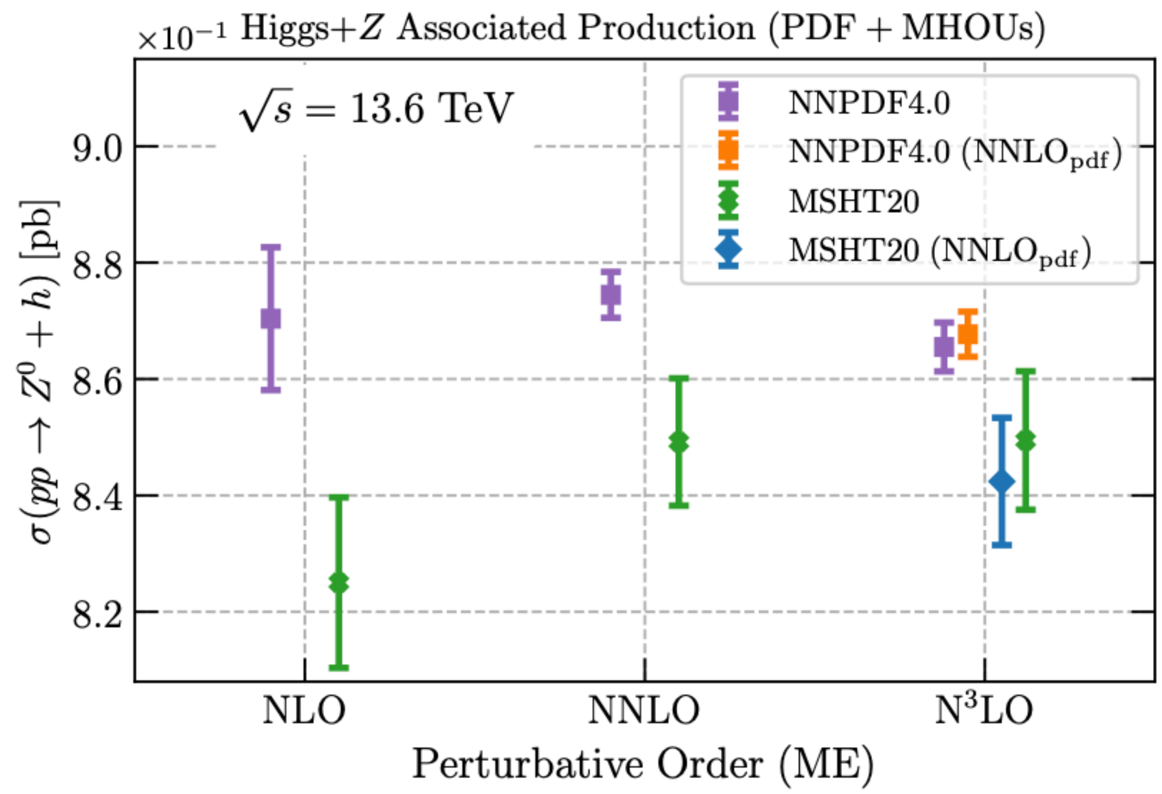
Results: comparison with MSHT20

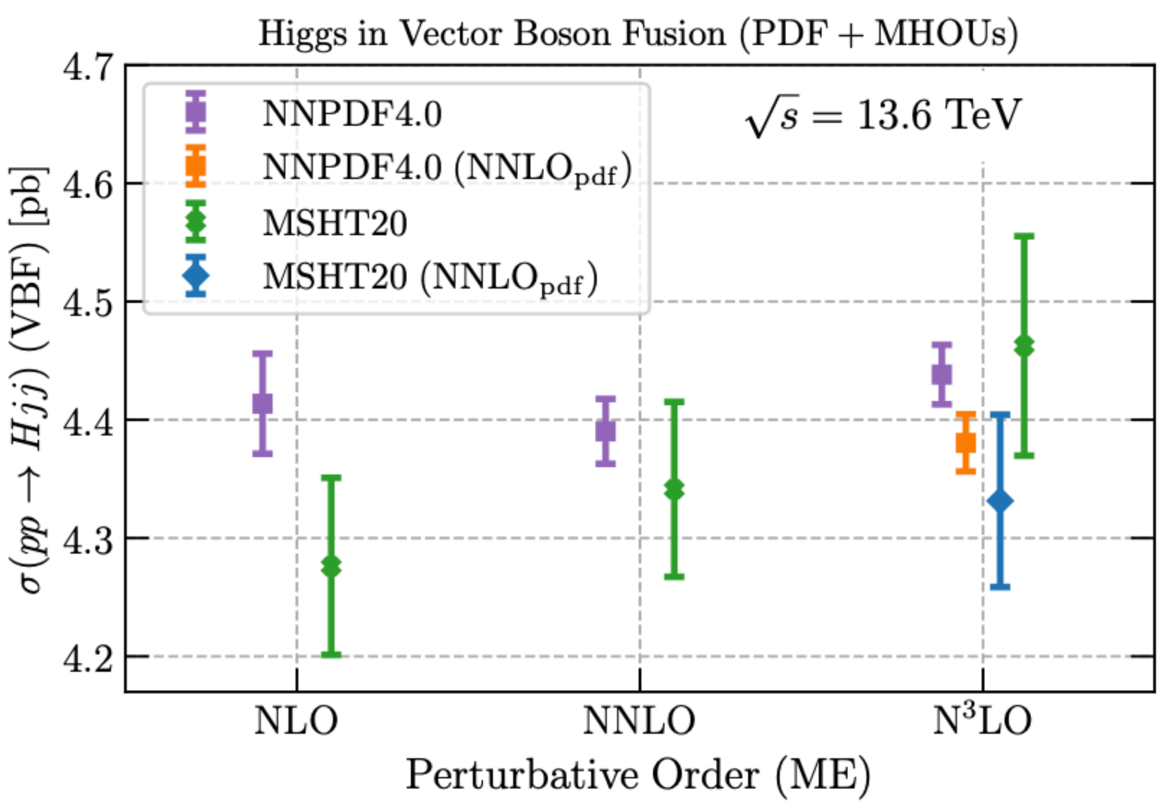


- **Good agreement** with MSHT20 for the quark luminosities
- Likewise for the gluon luminosities, except **around the Higgs mass** and for $m_X > 3$ **TeV**
- In general agreement between NNPDF4.0 and MSHT20 tends to **improve in the N³LO fits**

LHC phenomenology: Higgs production

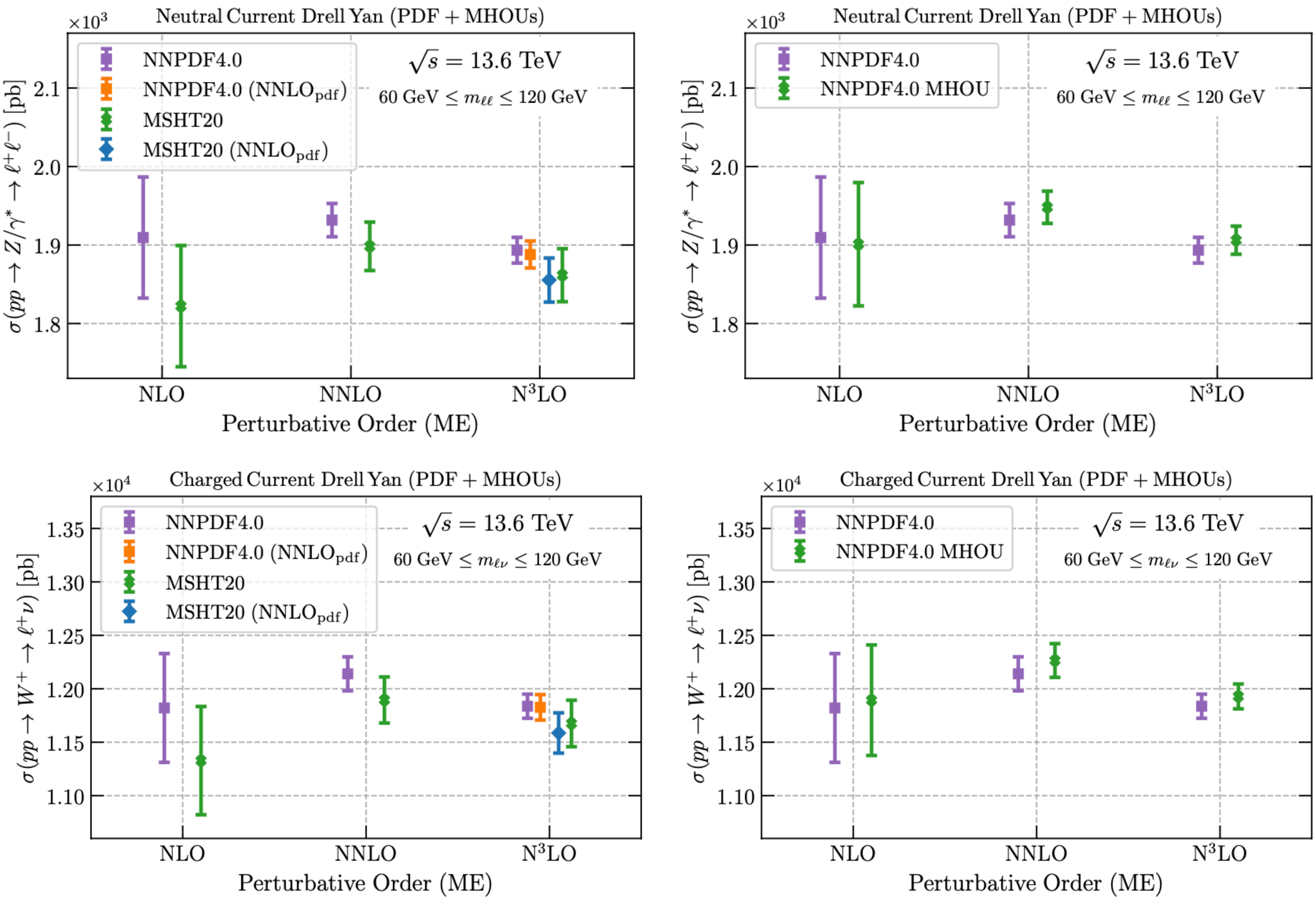






- N^{3}LO PDF corrections to **Higgs in gluon fusion small,** with a 1.5% suppression wrt NNLO PDFs
- N^{3}LO corrections improve agreement between NNPDF4.0 and MSHT20 for ***hZ***
- **Higgs VBF** also receives large corrections (in units of the very small N^{3}LO scale error)

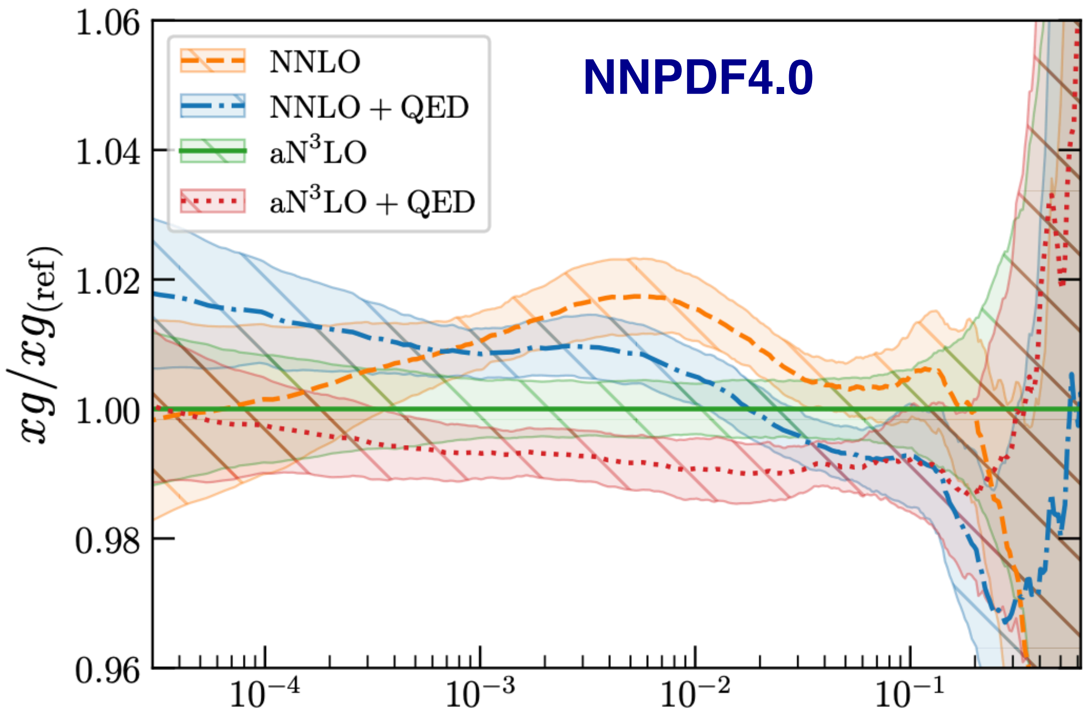
LHC phenomenology: Drell-Yan

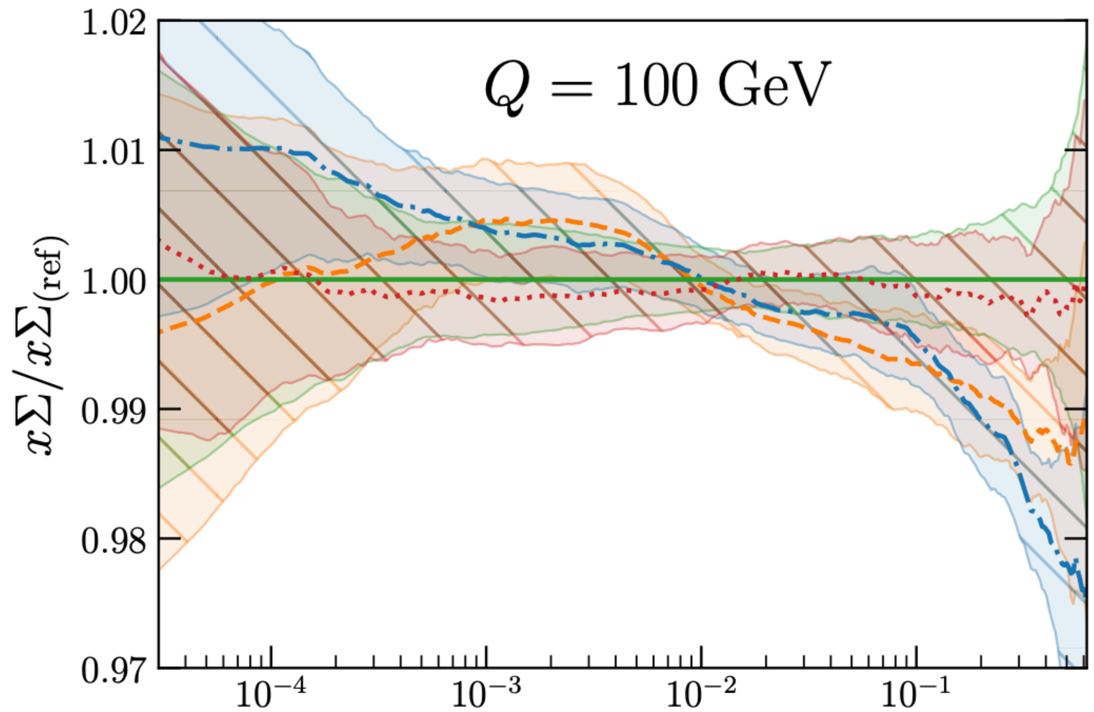


Good perturbative convergence at N^3LO also for **quark-initiated processes**

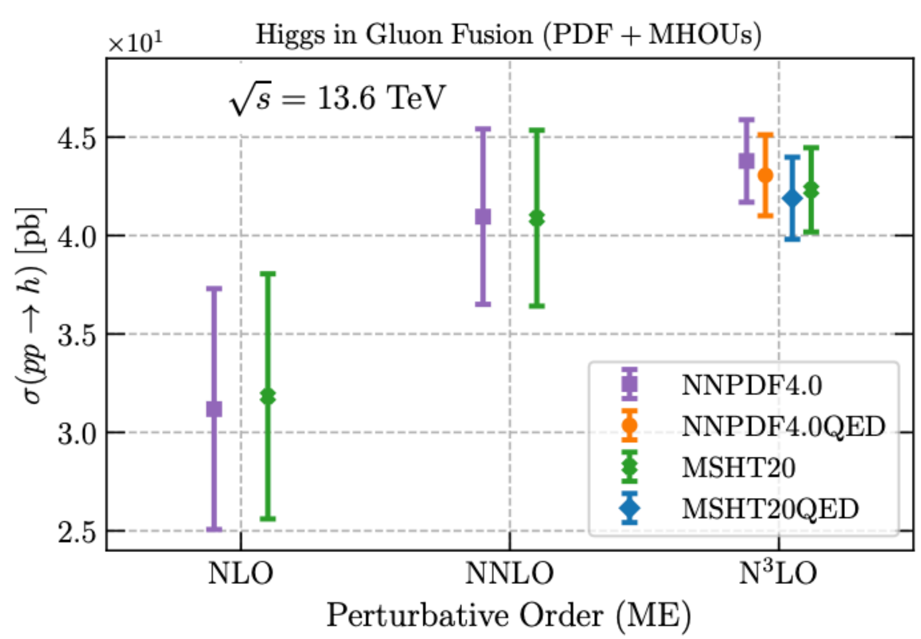
NNPDF4.0 aN3LO + QED

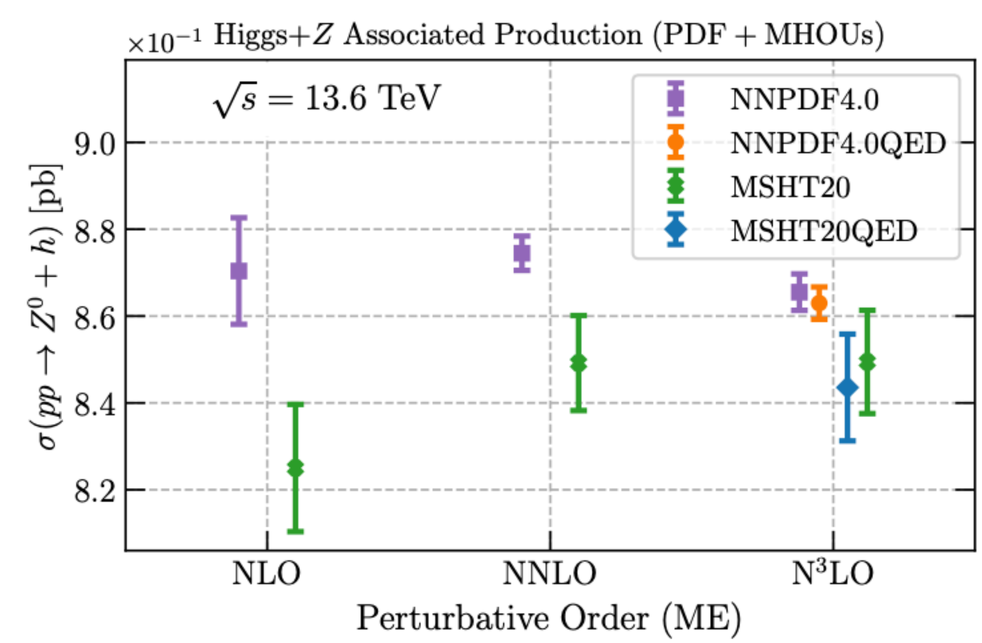
- PDFs with **QED corrections** and **photon PDF** key for accurate LHC phenomenology
- Multiple processes receive sizable photon-initiated contributions
- QED effects **suppress the gluon by up to 1%** due to photon PDF ``eating up” proton momentum





Somehow, relevance of adopting **QED PDFs as baseline for LHC calculations** not widely perceived ….

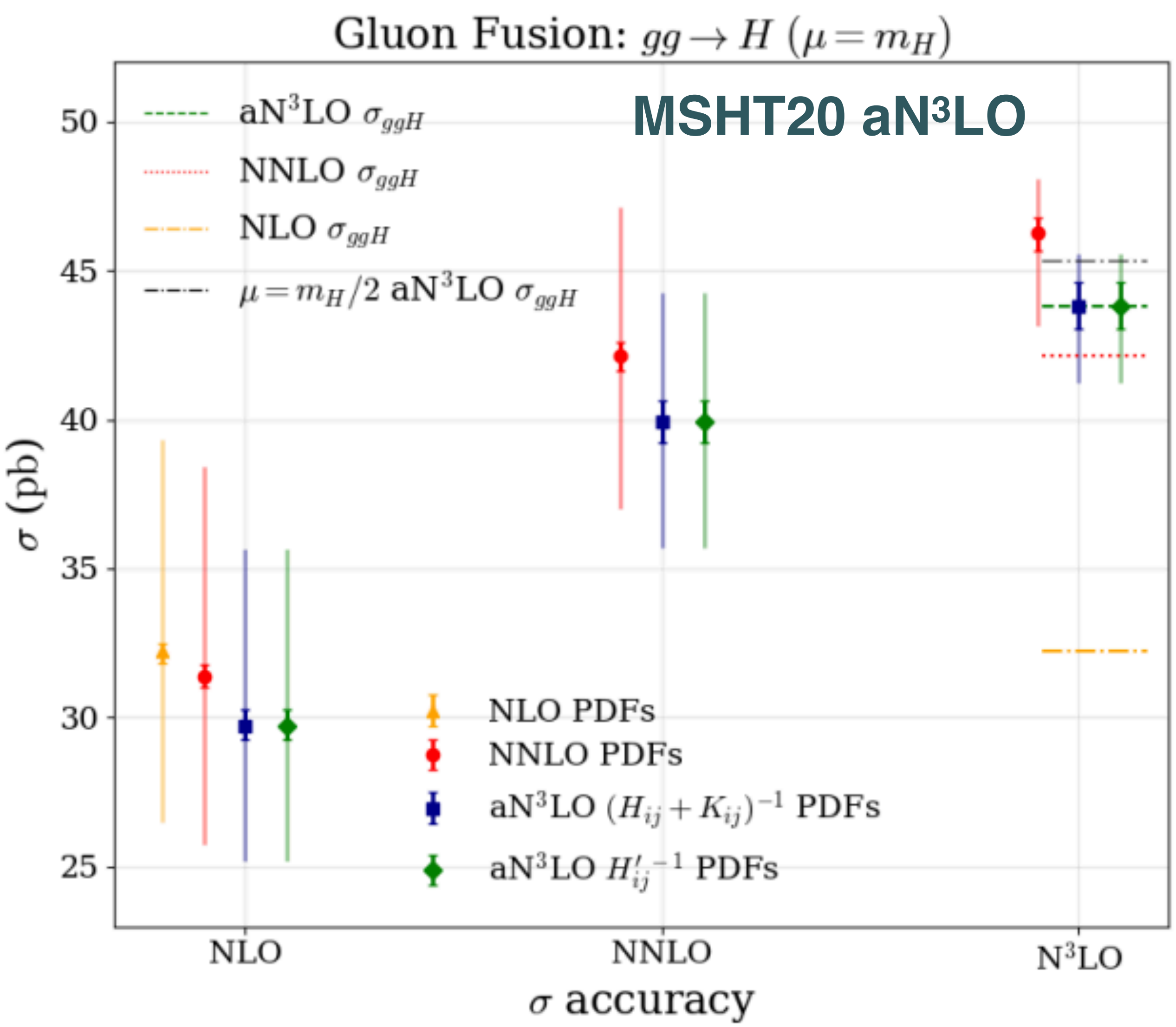


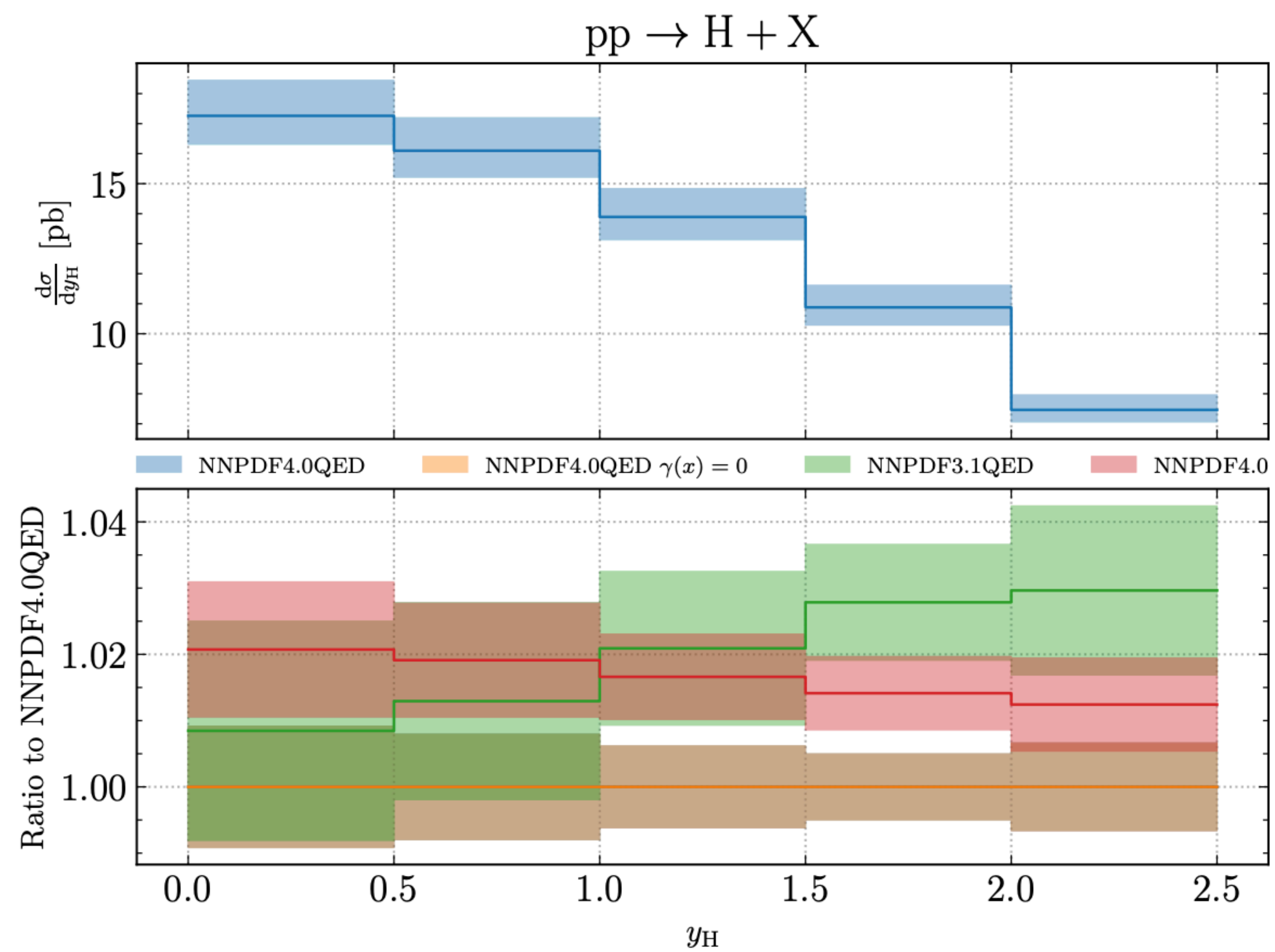


Combination of aN^{3}LO (& QED) PDFs for Higgs production

Motivation

- **aN³LO corrections to the PDFs** lead to sizeable changes in Higgs cross-sections
- Qualitatively similar trend observed in **MSHT20 and NNPDF4.0**
- **QED effects** on the PDFs must also be accounted in LHC phenomenology





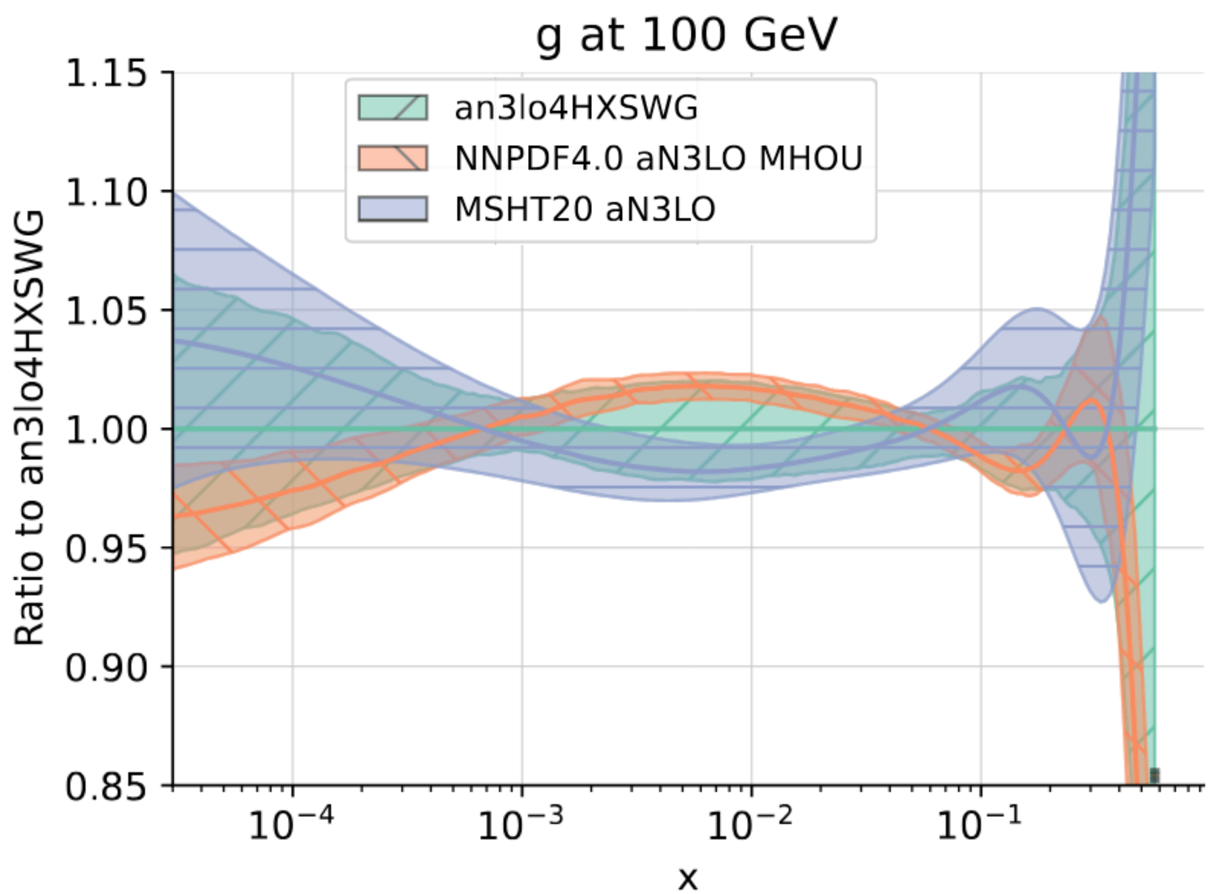
The availability of aN³LO+QED PDFs represent the **most accurate option** for the deployment of N³LO calculations for Higgs predictions

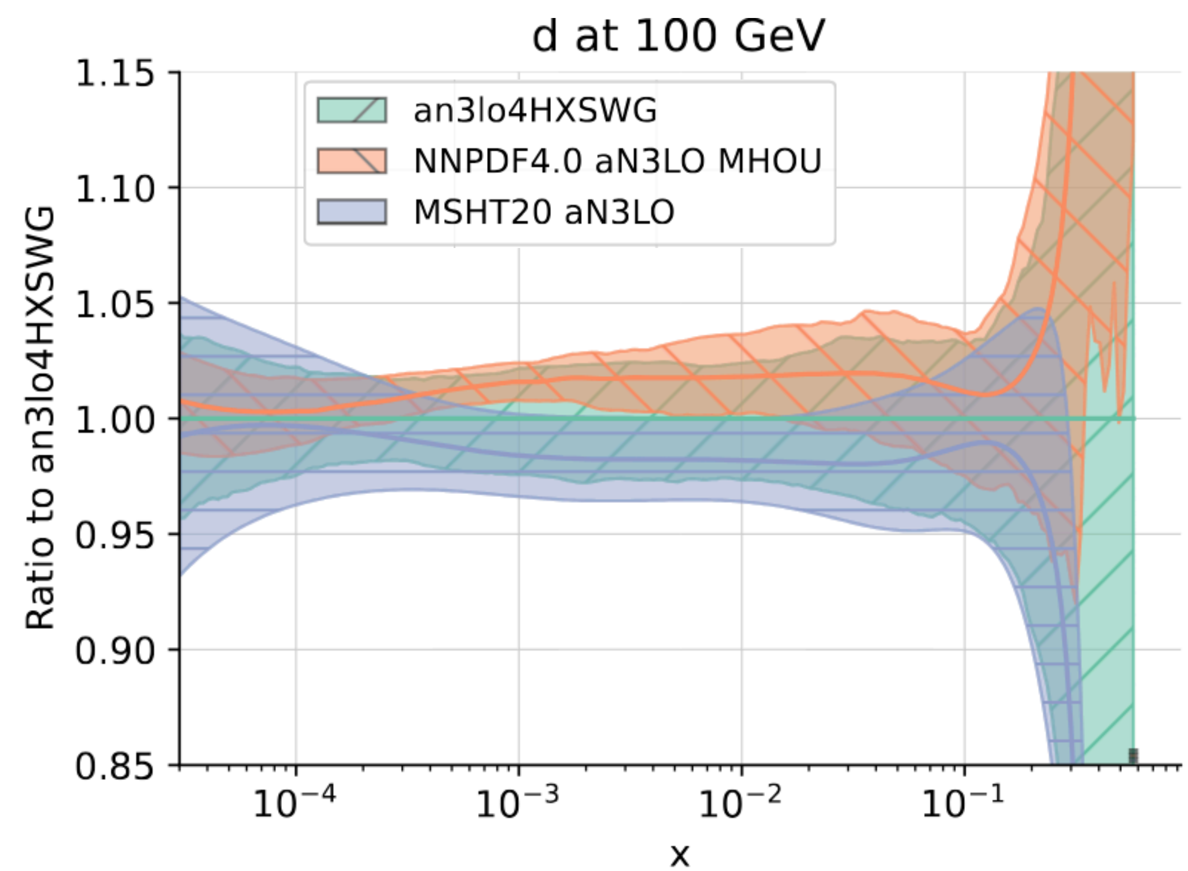
Methodology

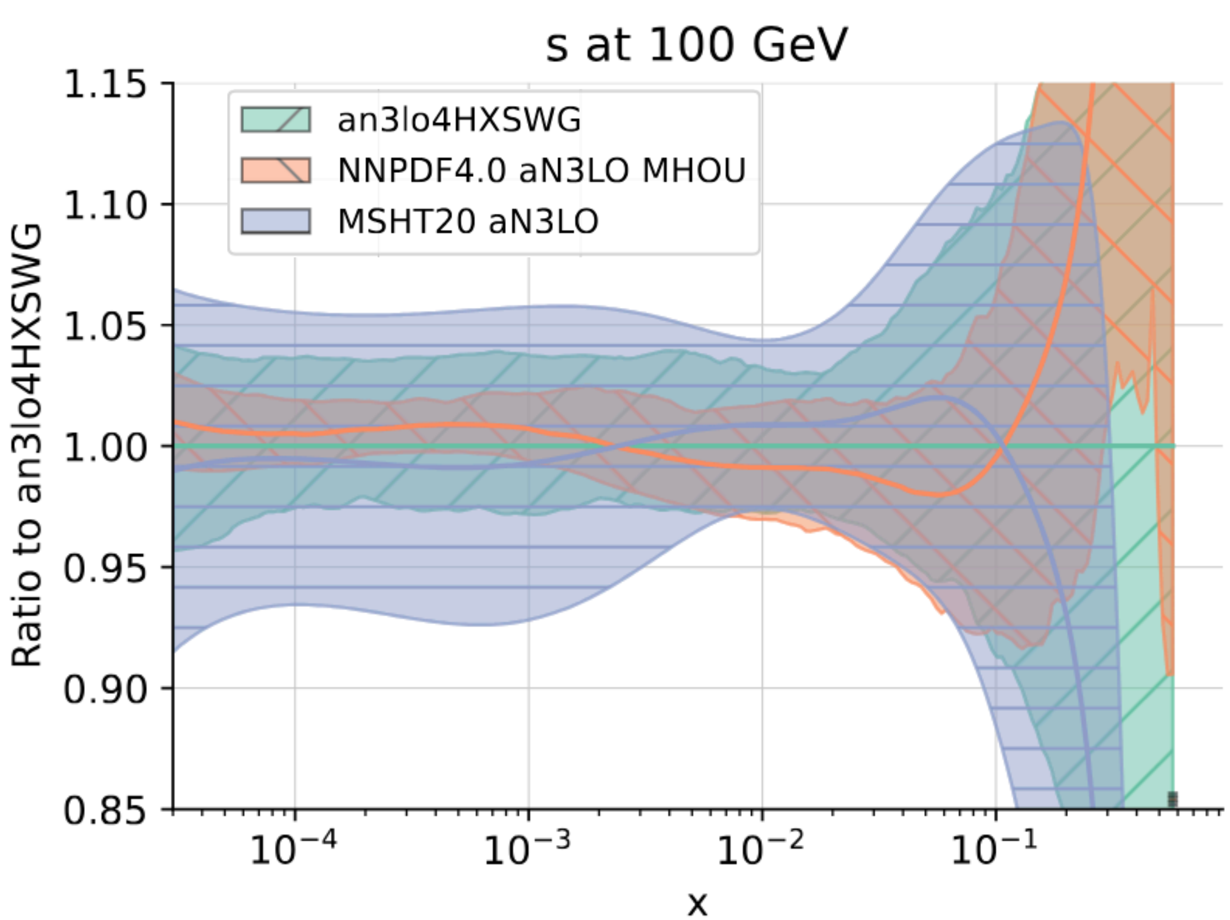
- Same approach as for **PDF4LHC15/21 combinations**: $N_{\rm rep} = 100$ replicas of MSHT20 (from native Hessian) combined with $N_{\rm rep} = 100$ replicas of NNPDF4.0
- Both for **aN³LO and aN³LO+QED variants**, together with NNLO and NNLO+QED as baseline
- Can be extended should other aN³LO PDF determination become available

	PDF set	pert. order (PDF)
reference	PDF4LHC21_mc	$\mathrm{NNLO_{QCD}}$
new combined sets	MSHT20xNNPDF40_nnlo	$\mathrm{NNLO_{QCD}}$
	MSHT20xNNPDF40_nnlo_qed	$\mathrm{NNLO_{QCD}} \otimes \mathrm{NLO_{QED}}$
	MSHT20xNNPDF40_an3lo	$\mathrm{aN^3LO_{QCD}}$
	MSHT20xNNPDF40_an3lo_qed	$\mathrm{aN^3LO_{QCD}} \otimes \mathrm{NLO_{QED}}$
inputs	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	$\mathrm{aN^3LO_{QCD}} \otimes \mathrm{NLO_{QED}}$

Results: PDFs



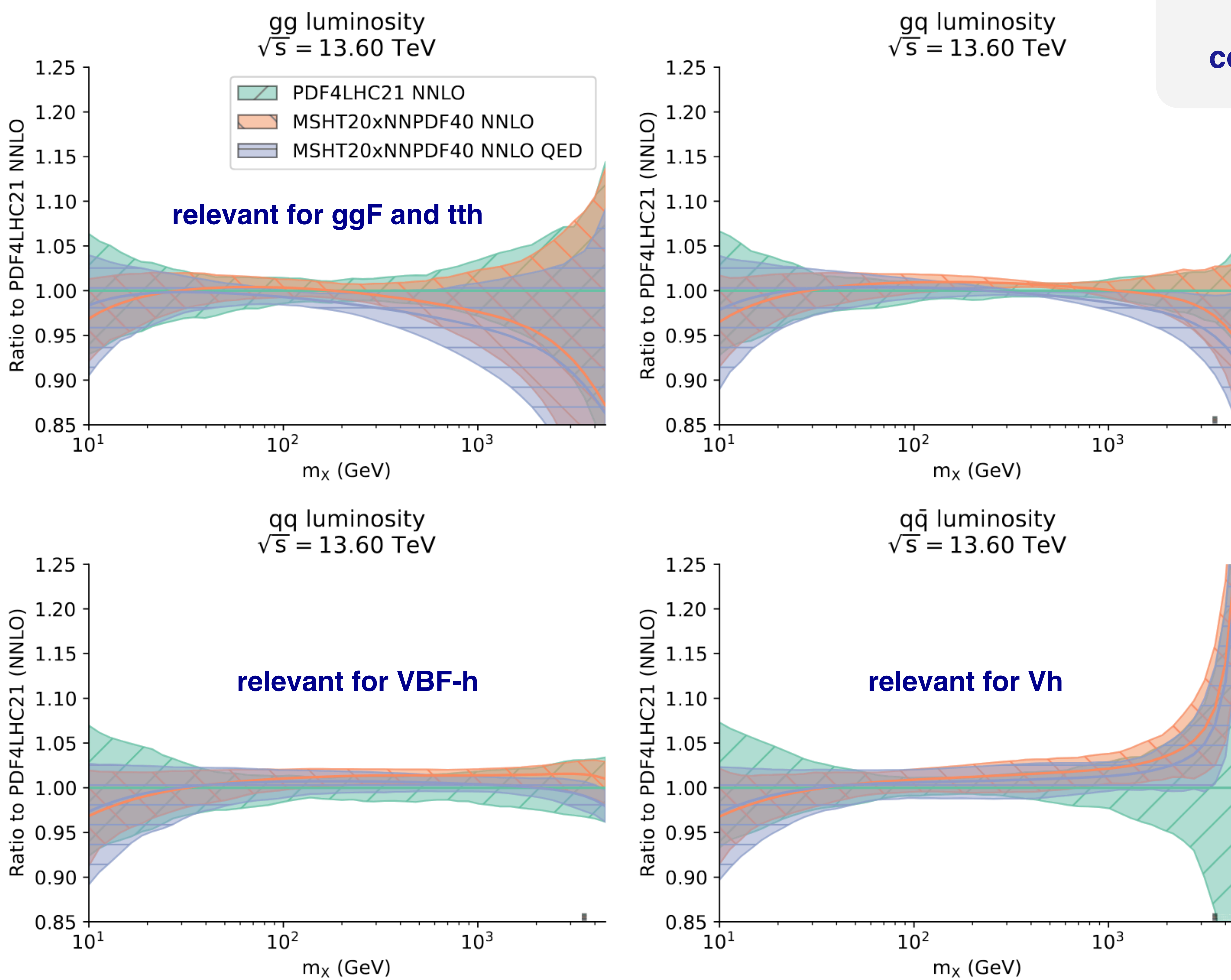




- Unweighted combination *a la* PDG
- PDFs **combined at face value**, no attempt to minimise differences among them
- Bulk of differences between MSHT20 and NNPDF4.0 **already present at NNLO**
- Exception being the gluon PDF, for which **MSHT favours a stronger suppression**

Results: Luminosities

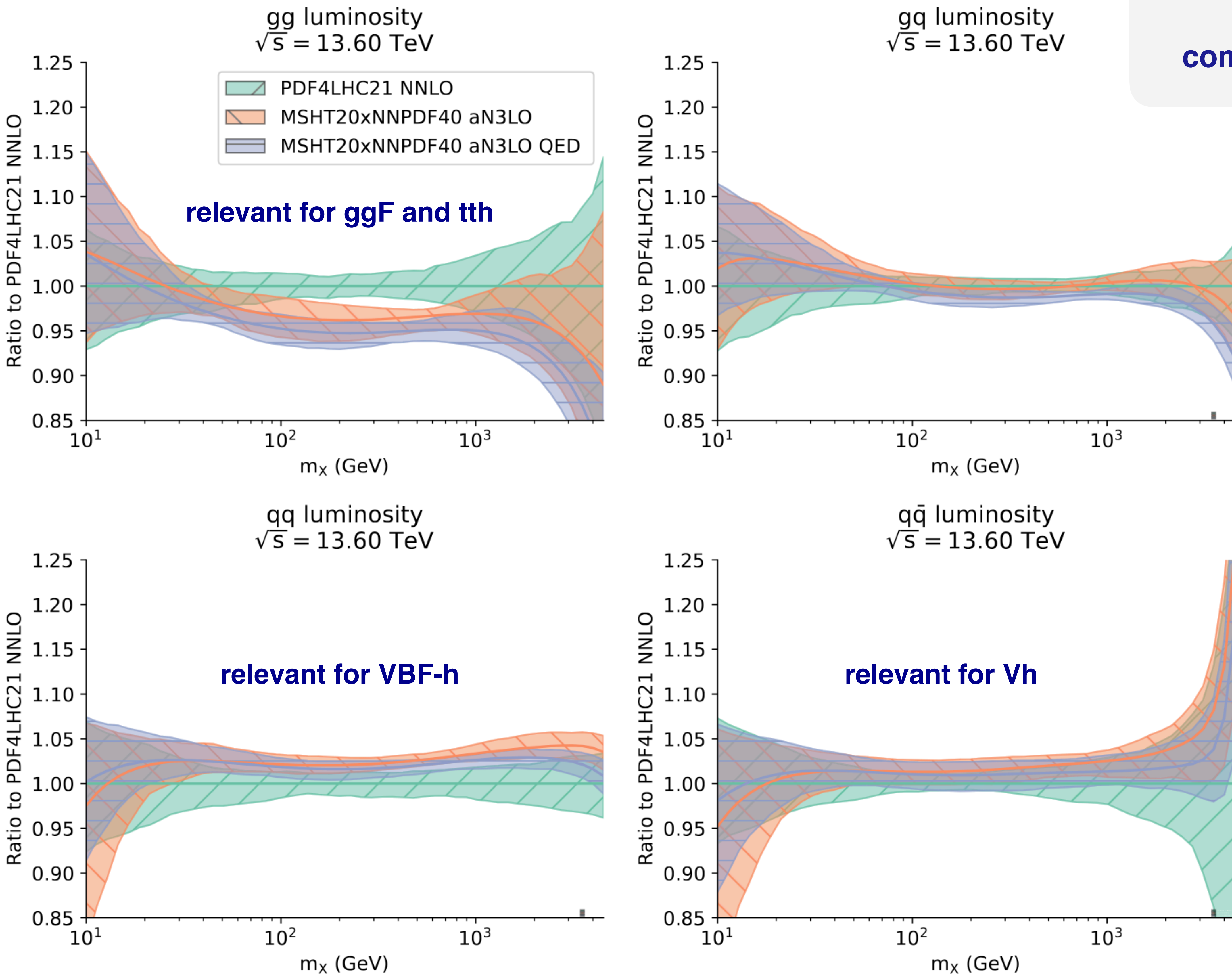
NNLO combination



Baseline is PDF4LHC21 NNLO: **current choice of HXSWG**

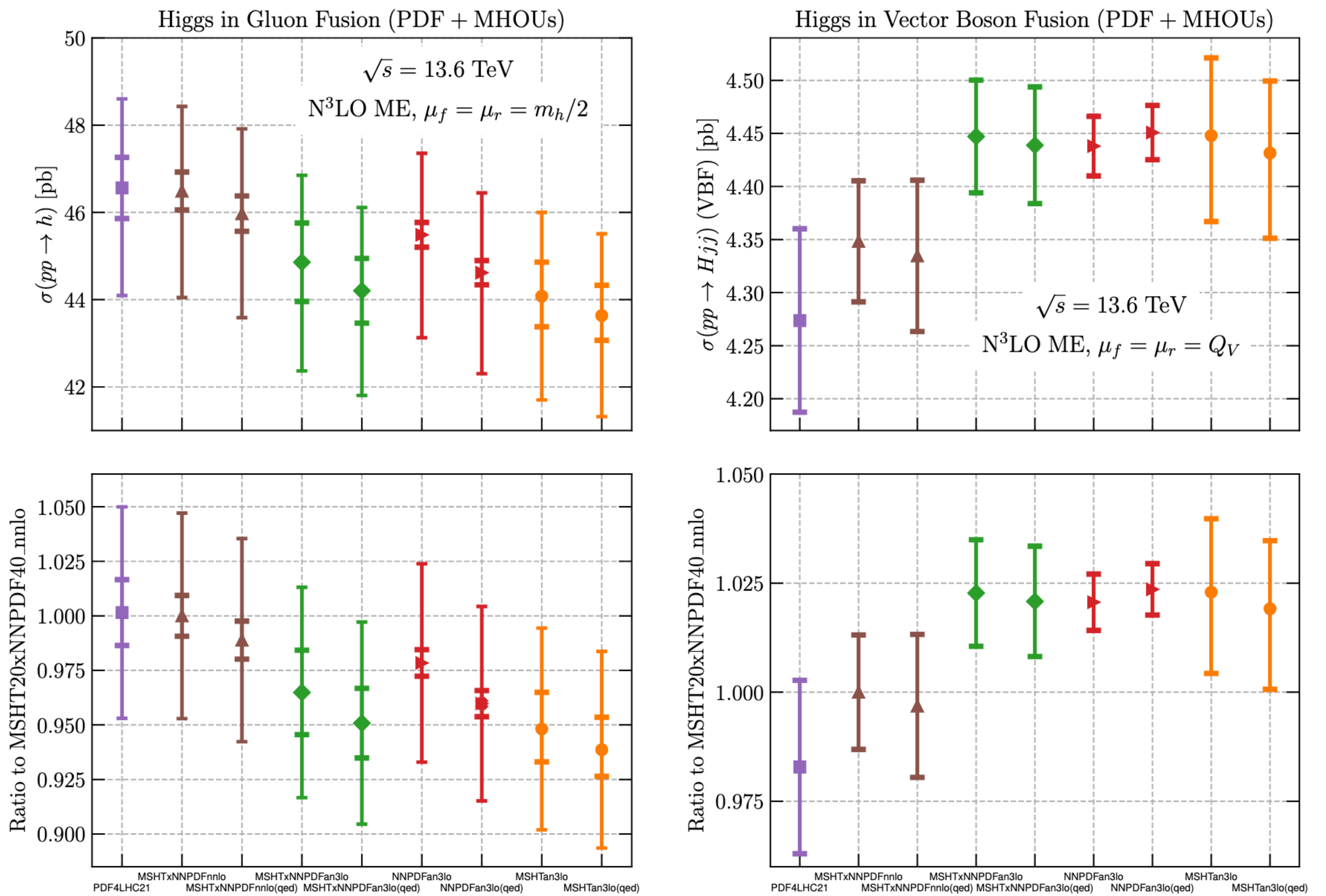
Results: Luminosities

N^3LO combination



Baseline is PDF4LHC21 NNLO: **current choice of HXSWG**

Results: cross-sections



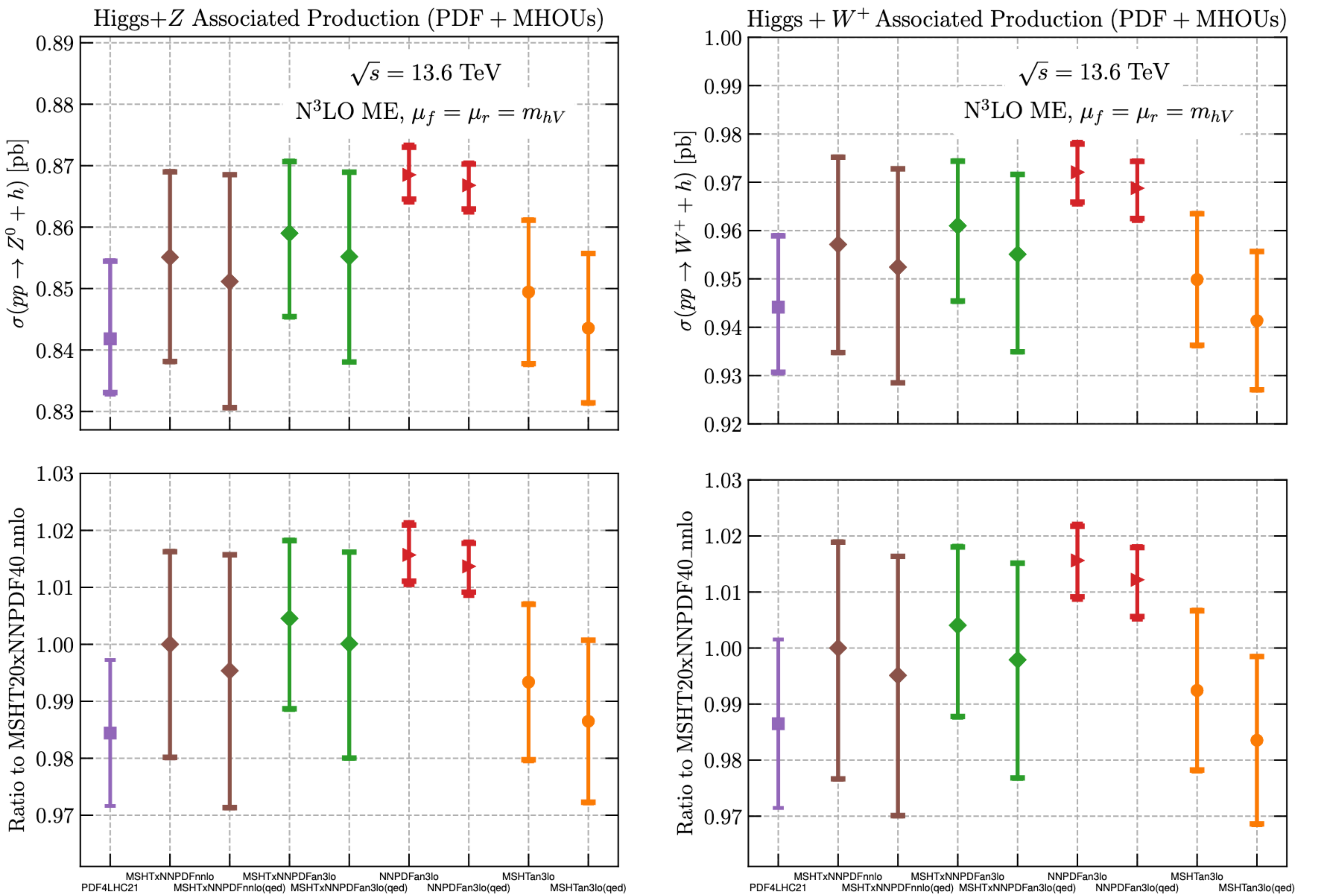
aN³LO (+QED) PDF corrections: **-3.5% (-5%)**

PDF4LHC21 very close to aN³LO combination

aN³LO (+QED) PDF corrections: **+2.5% (+2.5%)**

aN³LO combination: +1.8% higher than PDF4LHC21

Results: cross-sections



Impact of aN^{3}LO & QED PDF corrections at the **few-permille level** for hV

Impact of different NNLO PDF combination: **up to +1.5%**

Predicting higher orders

Compare **actual NNLO to aN^{3}LO shift** in the PDFs to the HXSWG approximation based on the **NLO to NNLO shift**

$$\Delta^{\rm exact}_{\rm NNLO} \equiv \left| \frac{\sigma^{\rm N^3LO}_{\rm N^3LO-PDF} - \sigma^{\rm N^3LO}_{\rm NNLO-PDF}}{\sigma^{\rm N^3LO}_{\rm N^3LO-PDF}} \right| . \qquad \Delta^{\rm app}_{\rm NNLO} \equiv \frac{1}{2} \left| \frac{\sigma^{\rm NNLO}_{\rm NNLO-PDF} - \sigma^{\rm NNLO}_{\rm NLO-PDF}}{\sigma^{\rm NNLO}_{\rm NNLO-PDF}} \right|$$

	ggF	**VBF-h**
$\Delta^{\rm exact}_{\rm NNLO}$ (NNPDF4.0)	2.2%	1.3%
$\Delta^{\rm exact}_{\rm NNLO}$ (MSHT20)	5.3%	2.3%
$\Delta^{\rm exact}_{\rm NNLO}$ (combination)	3.3%	2.3%
$\Delta^{\rm app}_{\rm NNLO}$ (NNPDF4.0)	0.2%	0.2%
$\Delta^{\rm app}_{\rm NNLO}$ (MSHT20)	1.4%	1.3%
$\Delta^{\rm app}_{\rm NNLO}$ (combination)	0.9%	0.5%

Previous HXSWG estimates of aN^{3}LO PDF effects **severely undershoot true shift**

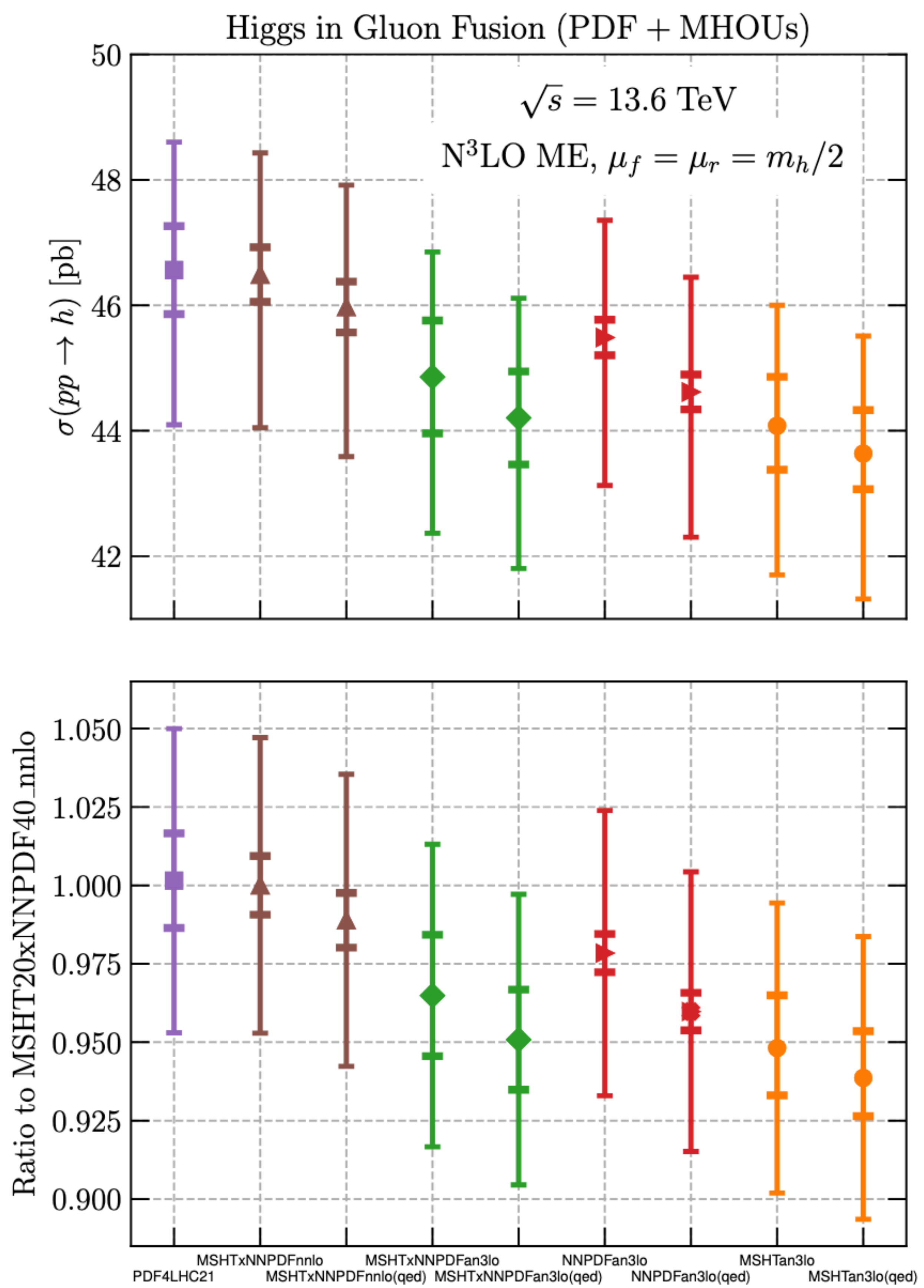
Towards Yellow Report 5

LHCHXSWG must choose baseline PDFs to be used for **Yellow Report 5**

- Use new aN³LO combination for **central values**?
- Keep PDF4LHC21 NNLO, use new aN³LO combination to estimate **theory error**?
- **QED or no QED** effects in the PDFs?

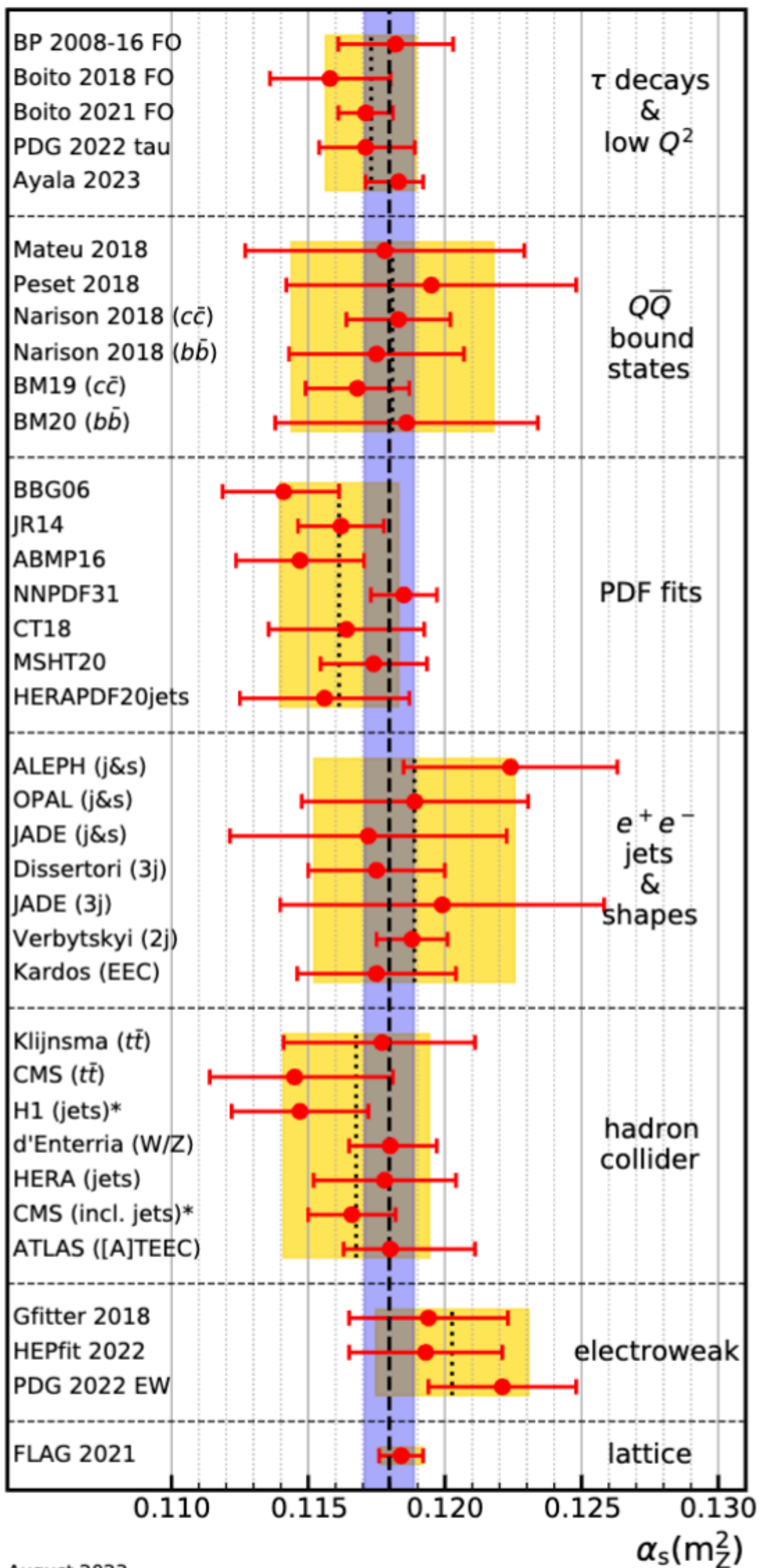
Not just cosmetics, potentially **large modifications to** the YR5 cross-sections.

Needs executive decision!



The strong coupling from a aN^{3}LO PDF fit

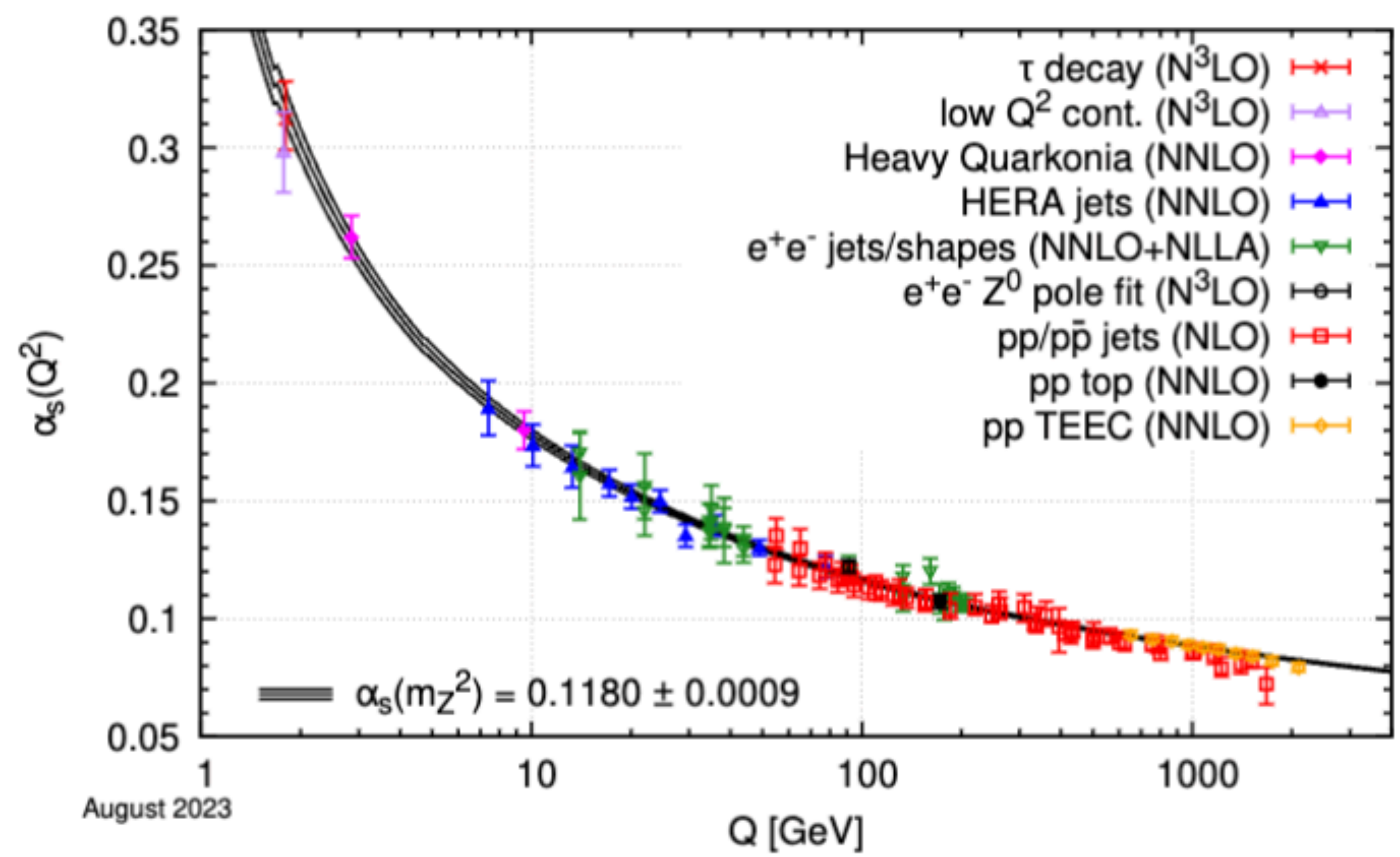
Motivation I



- Determination of $\alpha_s(Q)$ and its running is a prime goal of particle physics
- Average from **PDF fits is the lowest value of all groups of processes**, leading to some (moderate) tension with lattice result

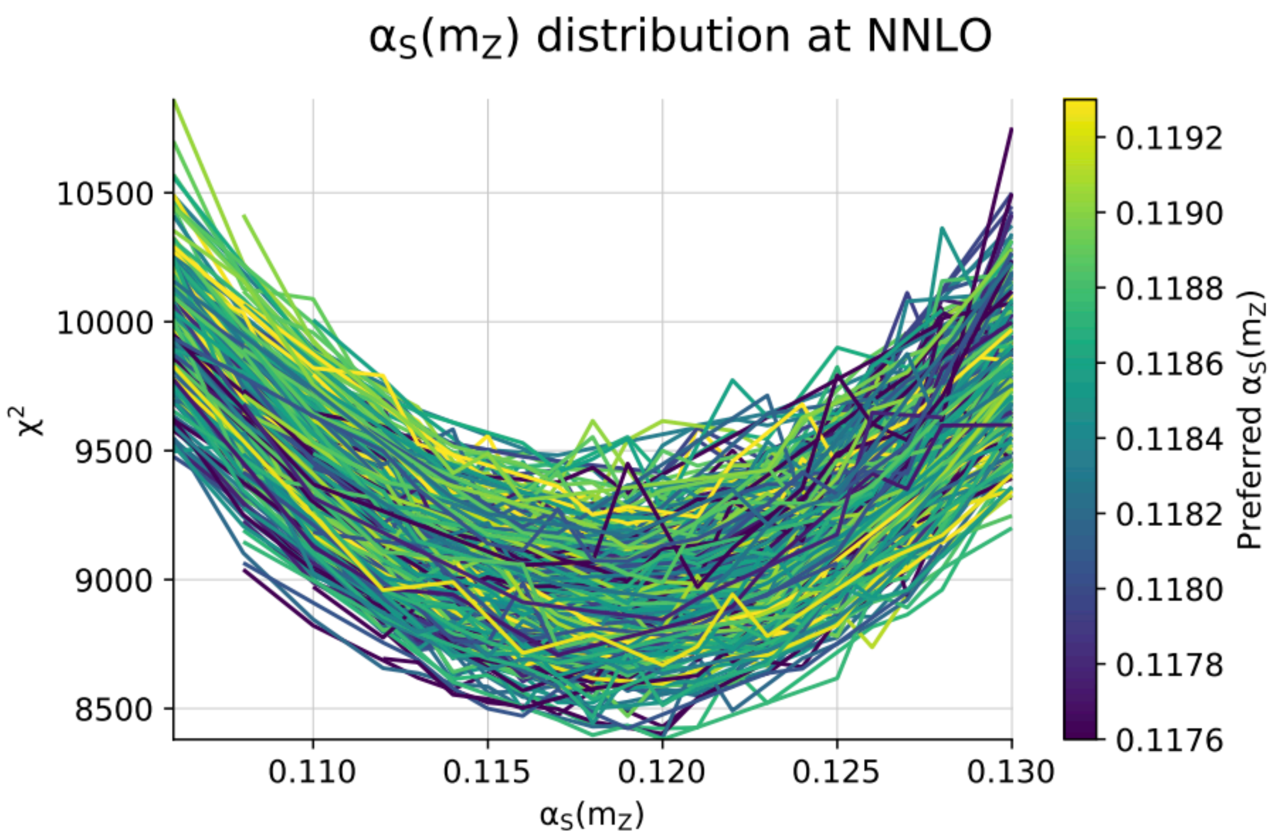
$$\alpha_s(m_Z^2) = 0.1175 \pm 0.0010 \qquad \text{(PDG 2023 without lattice)}\,.$$

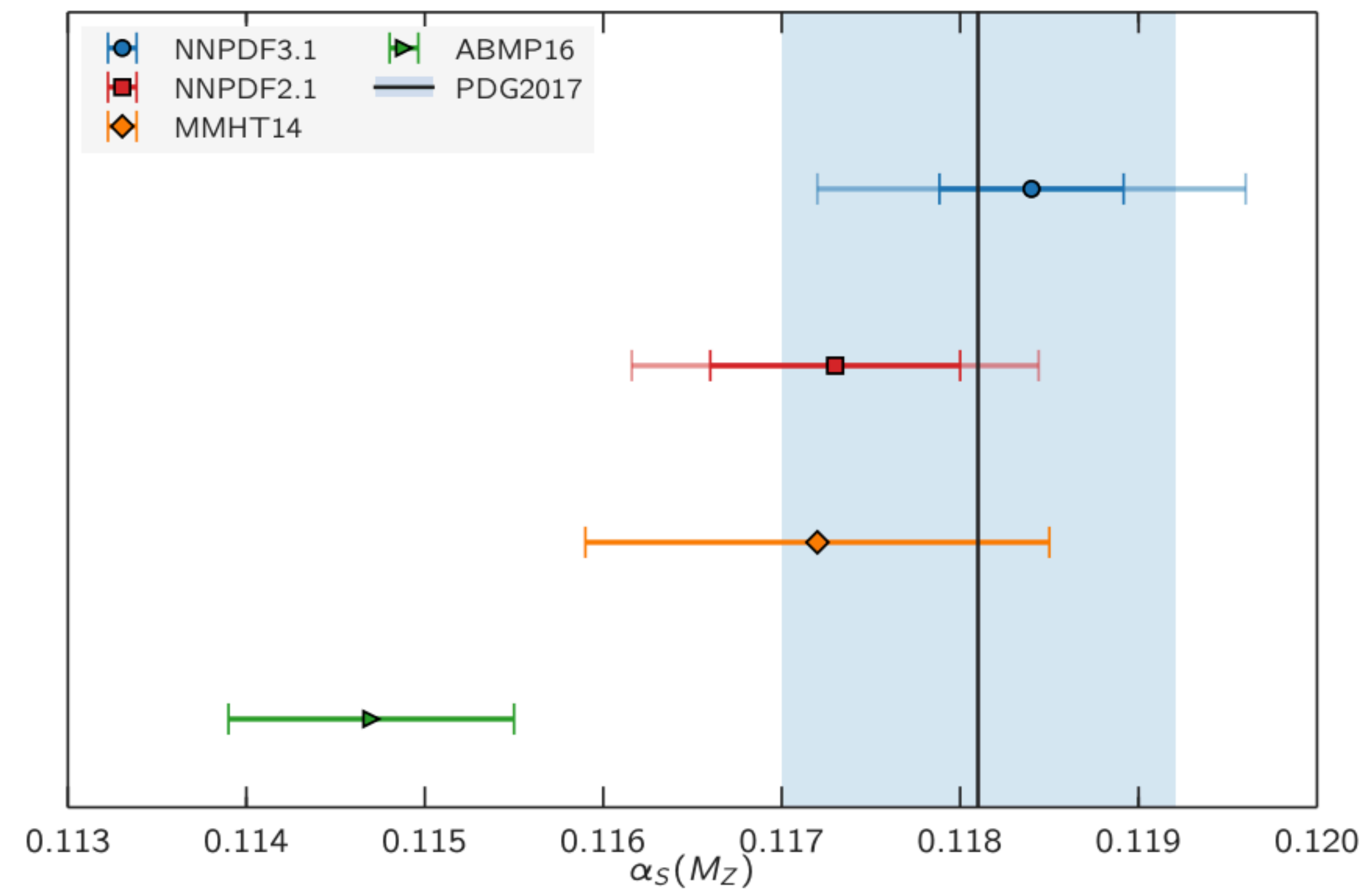
$$\alpha_s(m_Z^2) = 0.1184 \pm 0.0008 \qquad \text{(FLAG 2021 estimate)}$$

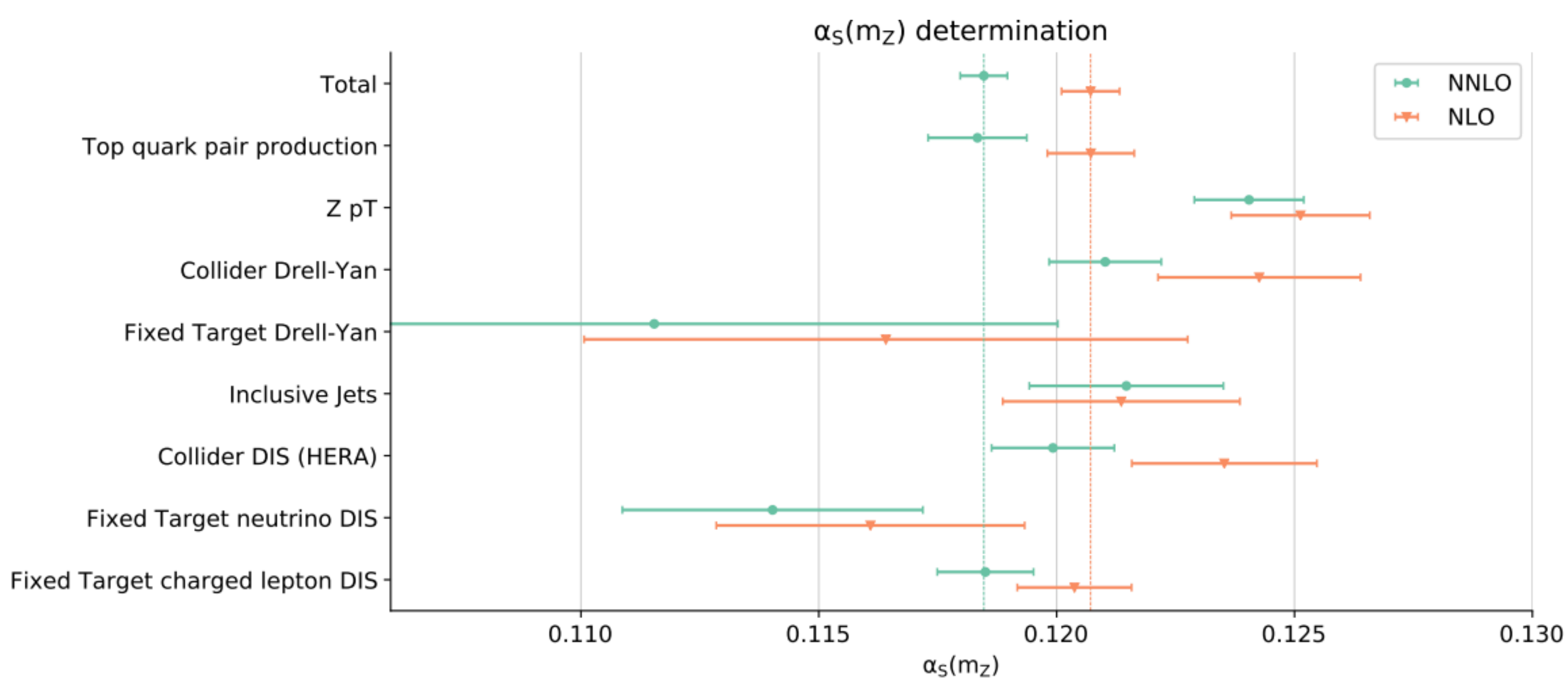


Motivation II

$$\alpha_s^{\rm NNLO}(m_Z) = 0.1185 \pm 0.0005^{\rm exp} \pm 0.0001^{\rm meth} \pm 0.0011^{\rm th}$$





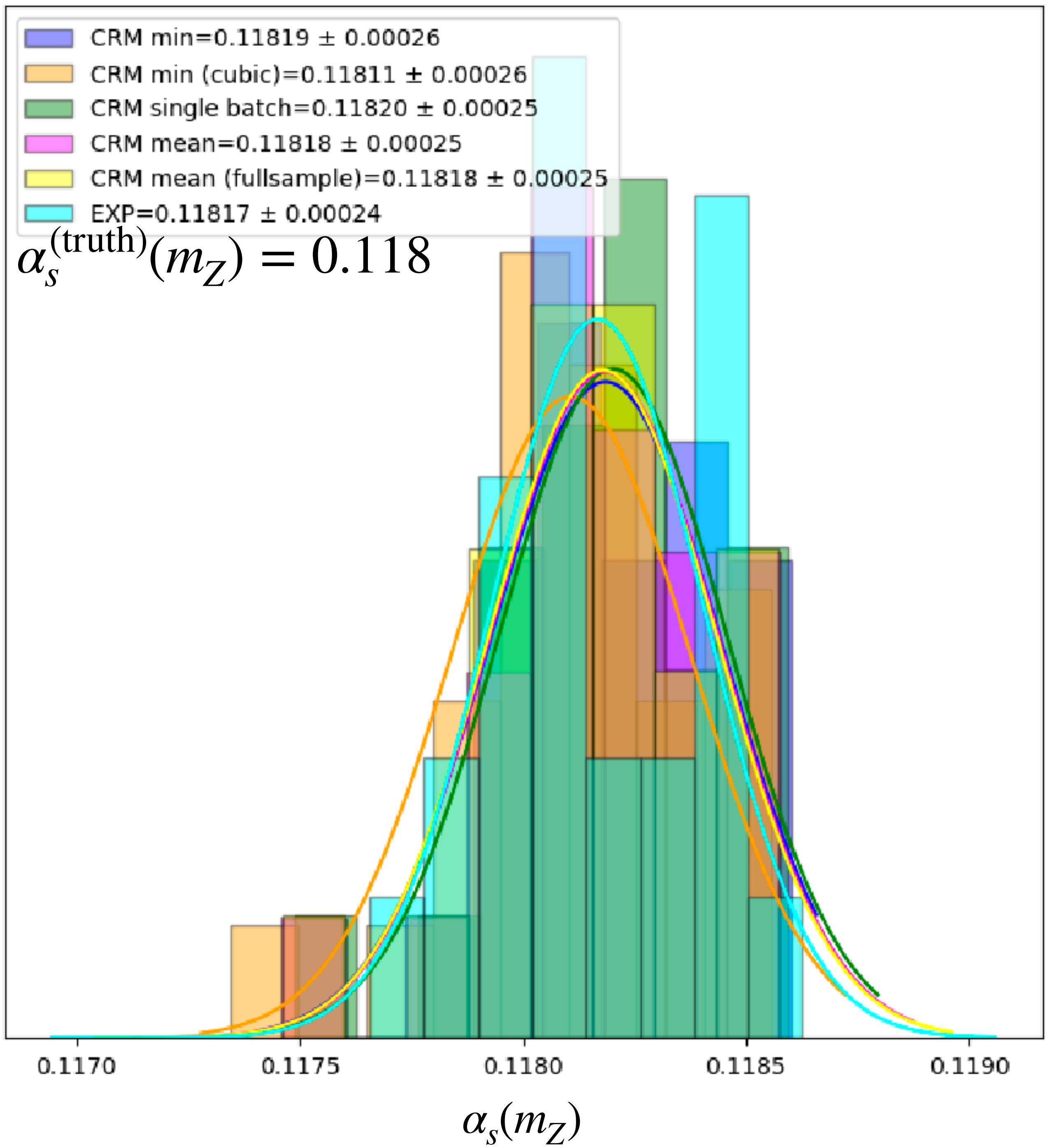


- Previous NNPDF-based determination was limited to **NNLO, no MHOU estimate**, most LHC data from Run I

- Goal is to update to the NNPDF4.0 dataset & methodology using aN^{3}LO theory

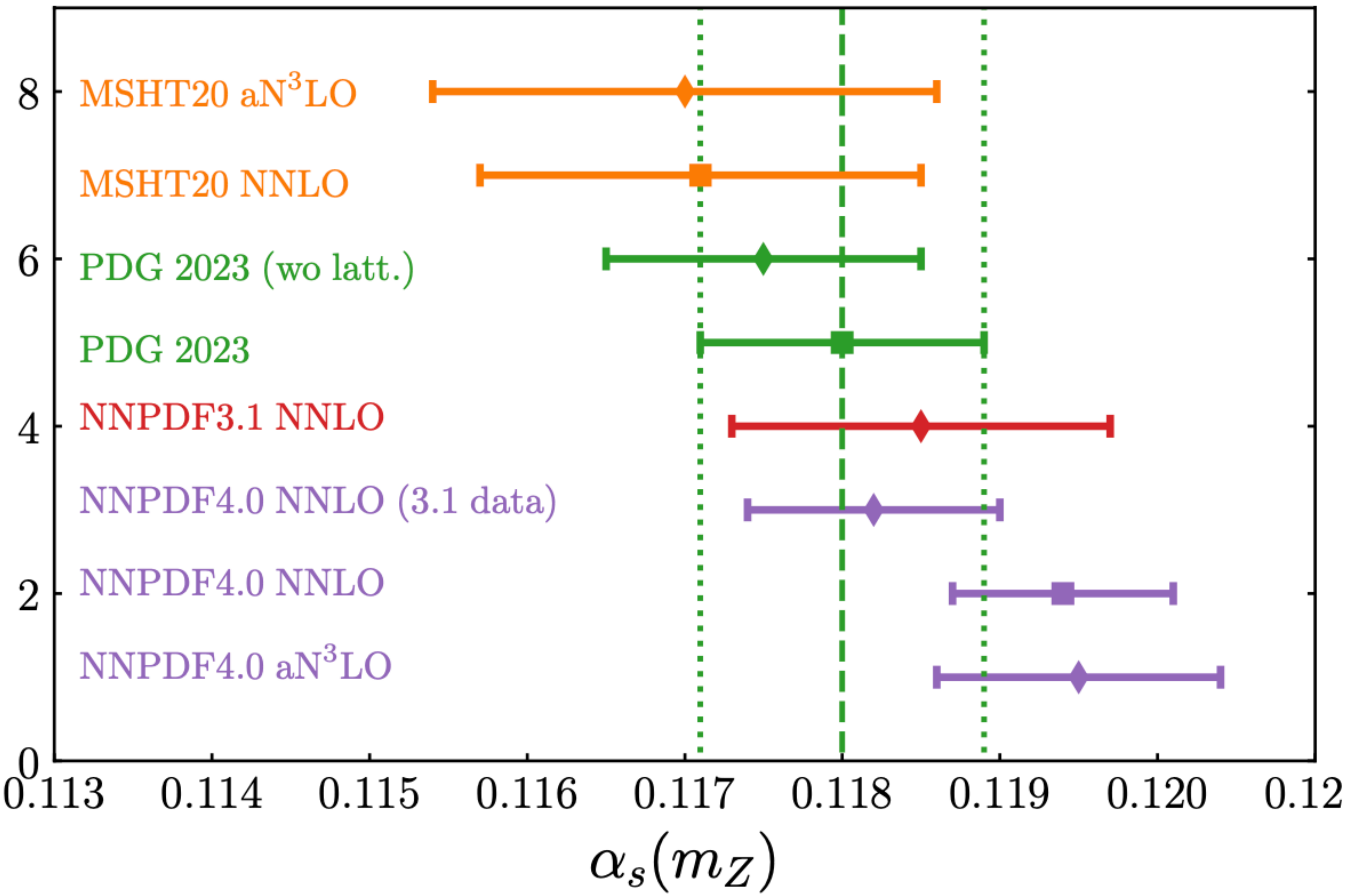
Closure Tests

- Generate data based on a given value of $\alpha_s(m_Z)$
- Verify it is reproduced by the fit using **three independent fitting methodologies**



- Discovered many ``plausible" methodologies that **fail the closure test.** For example, varying the value of $\alpha_s(m_Z)$ in the t_0 covariance matrix **does not reproduce** the input value! (D'Agostini bias)

Results

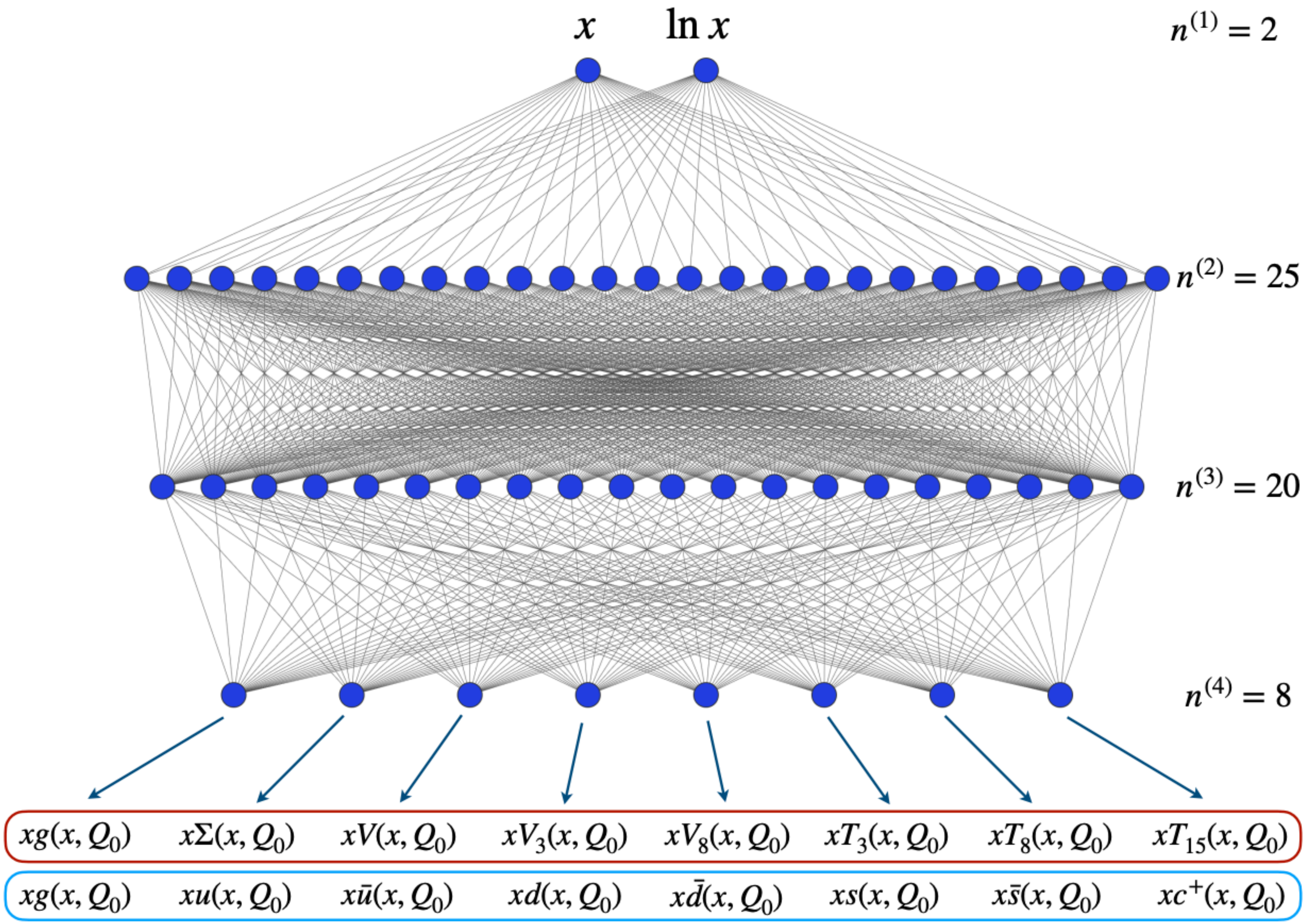


MHOUs included via the theory covariance matrix formalism

- **Stability of results** with respect to inclusion of N^3LO correction
- Consistency with previous NNPDF3.1 extraction for a common dataset
- Agreement with PDG average, will push ``PDF-fit average'' **towards PDG mean**
- WIP: impact of QED corrections and the **photon PDF** in the fit

Ensemble-based hyperoptimization in ML

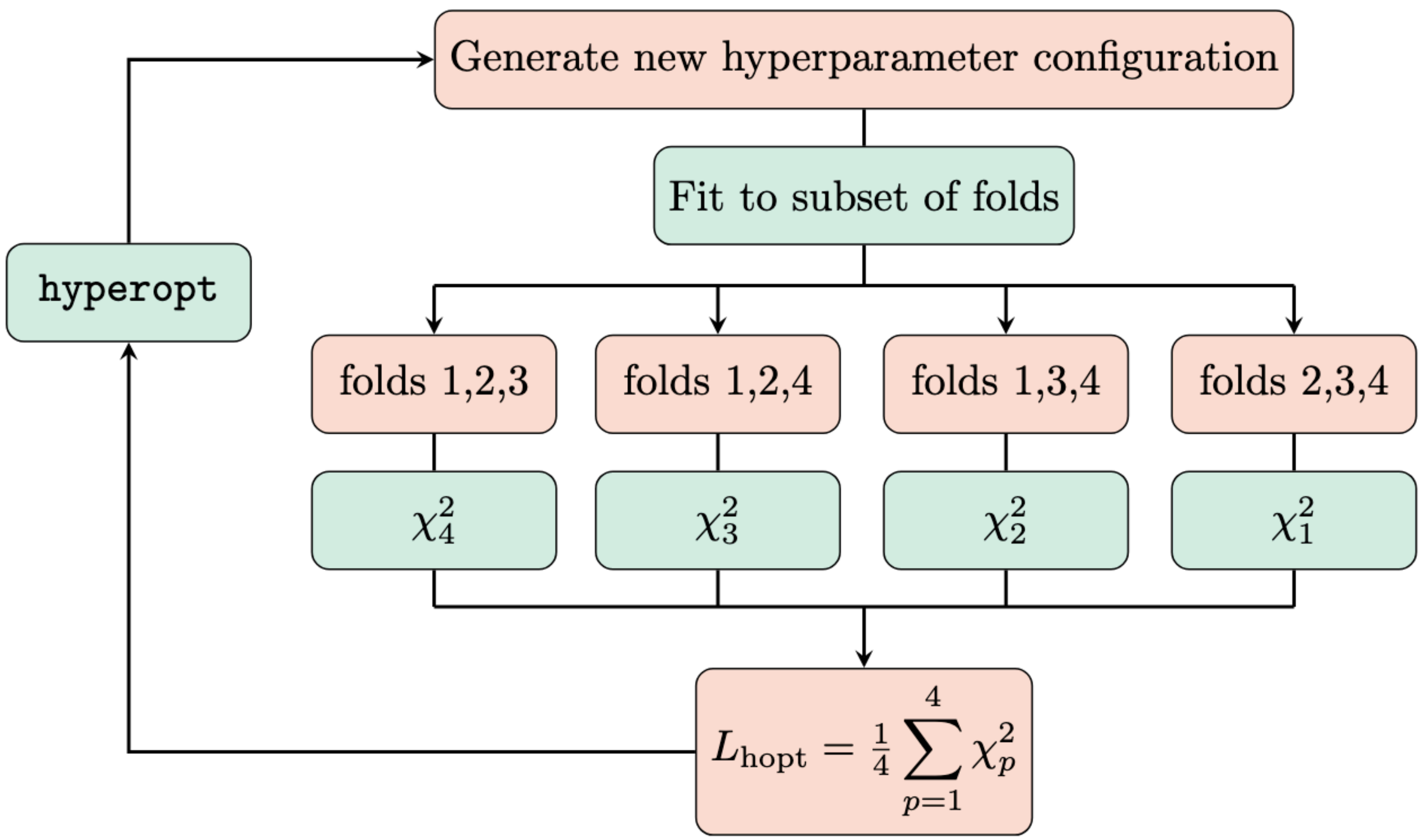
Hyperoptimisation in Machine Learning



- ML applications rely on a **large number of hyperparameters** which are not fixed by the training algorithm: architecture, optimiser, initialisation, stopping, activation functions …
- Choosing hyperparameters is a challenge in many cases. **Bias-free optimisation** is crucial!

Hyperoptimisation in Machine Learning

NNPDF4.0



- Partition global dataset into ***n*** **folds**
- Exclude one fold at a time, perform *n* fits
- Select hyperparameters leading to **best** χ^2 **to the non-fitted data**

This work

$$\varphi^2_{\chi^2} \equiv \left\langle \chi^2\left[T, D^{(0)}\right]\right\rangle_{\rm rep} - \chi^2\left[\langle T\rangle_{\rm rep}, D^{(0)}\right]$$

$$\varphi^2_{\chi^2} = \frac{1}{n_{\rm dat}}\sum_{i,j=1}^{n_{\rm dat}} ({\rm cov})^{-1}_{ij}\, T_{ji}$$

$$L_{\rm hopt}^{(\varphi^2)}\left(\hat{\boldsymbol{\theta}}\right) \equiv \left(\frac{1}{n_{\rm fold}}\sum_{p=1}^{n_{\rm fold}} \varphi^2_{\chi^2_p}\left(\hat{\boldsymbol{\theta}}\right)\right)^{-1}$$

- Select hyperparameters leading to **best** χ^2 & **largest PDF errors in non-fitted data**
- **e.g.** models with the **best generalisation power** are selected

Requires major restructure of NNPDF code to be able to train multiple ML models in parallel!

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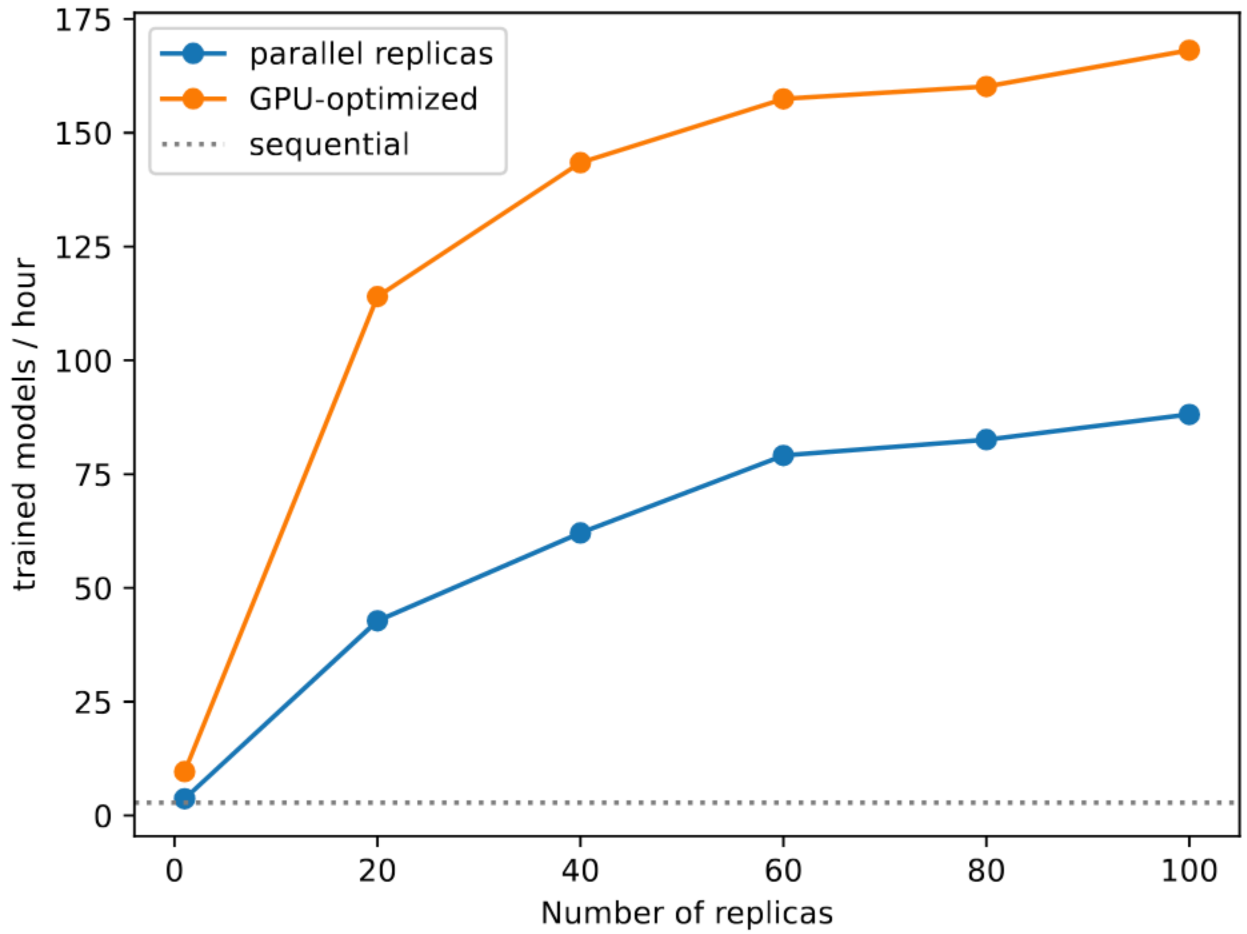
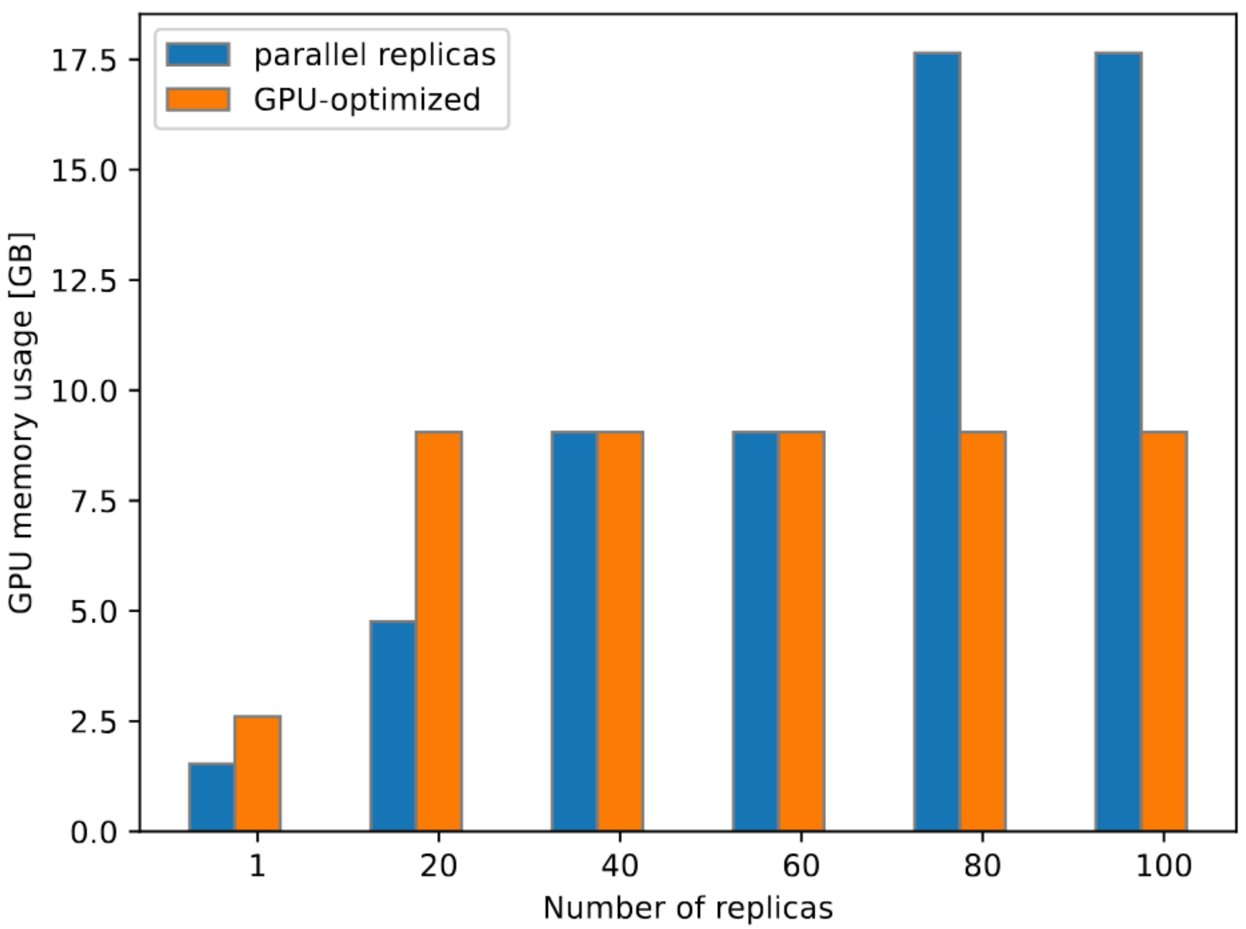
GPU-optimised NNPDF fits

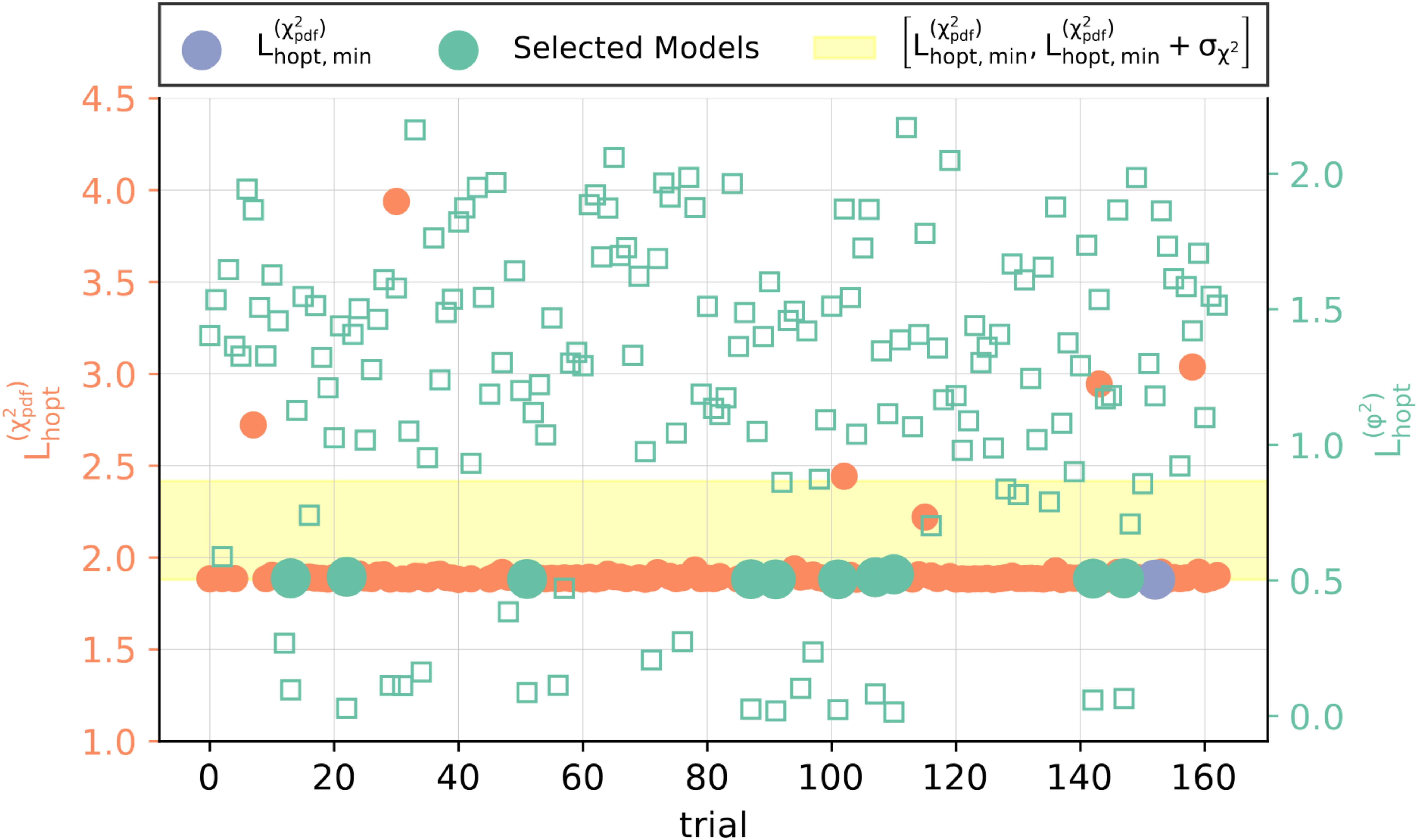




Replicas	10	50	100
Energy reduction	78%	87%	91%
Cost reduction	-45%	47%	55%

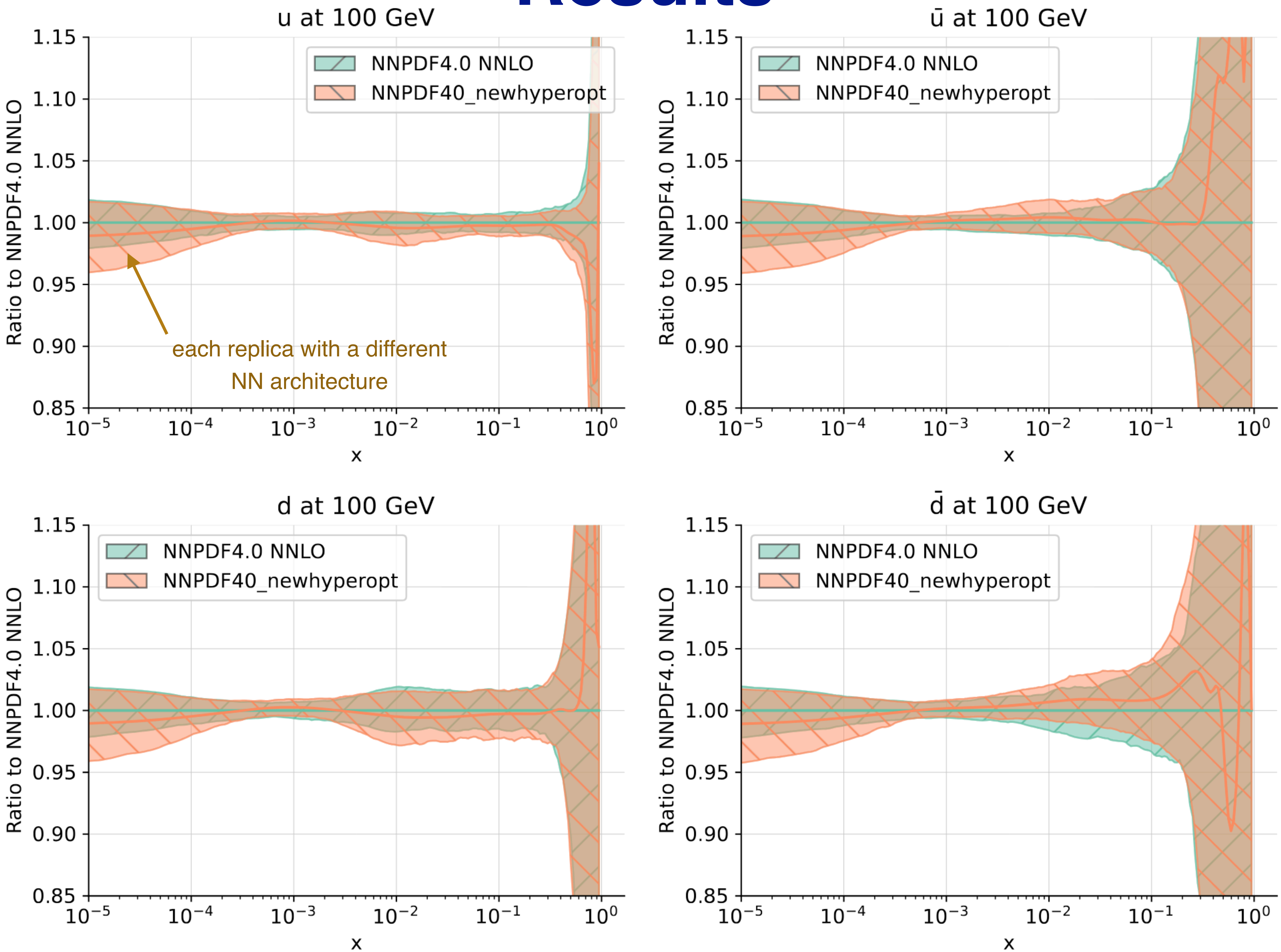
- **Speed up by a factor 200** from new GPU-optimise NNPDF code
- Memory usage kept under control, independent of number of models trained in parallel
- Up to 90% energy reduction: **faster, more affordable, and more sustainable** ML model training!

Results



Select not the best single set of hyperparameters but **instead randomly sample over the complete population of acceptable hyperparameters** displaying comparable performance

Results



Despite radical change in hyperparameter determination methodology, **excellent consistency with NNPDF4.0 & moderate increase of PDF errors**: non-trivial validation of NNDF robustness

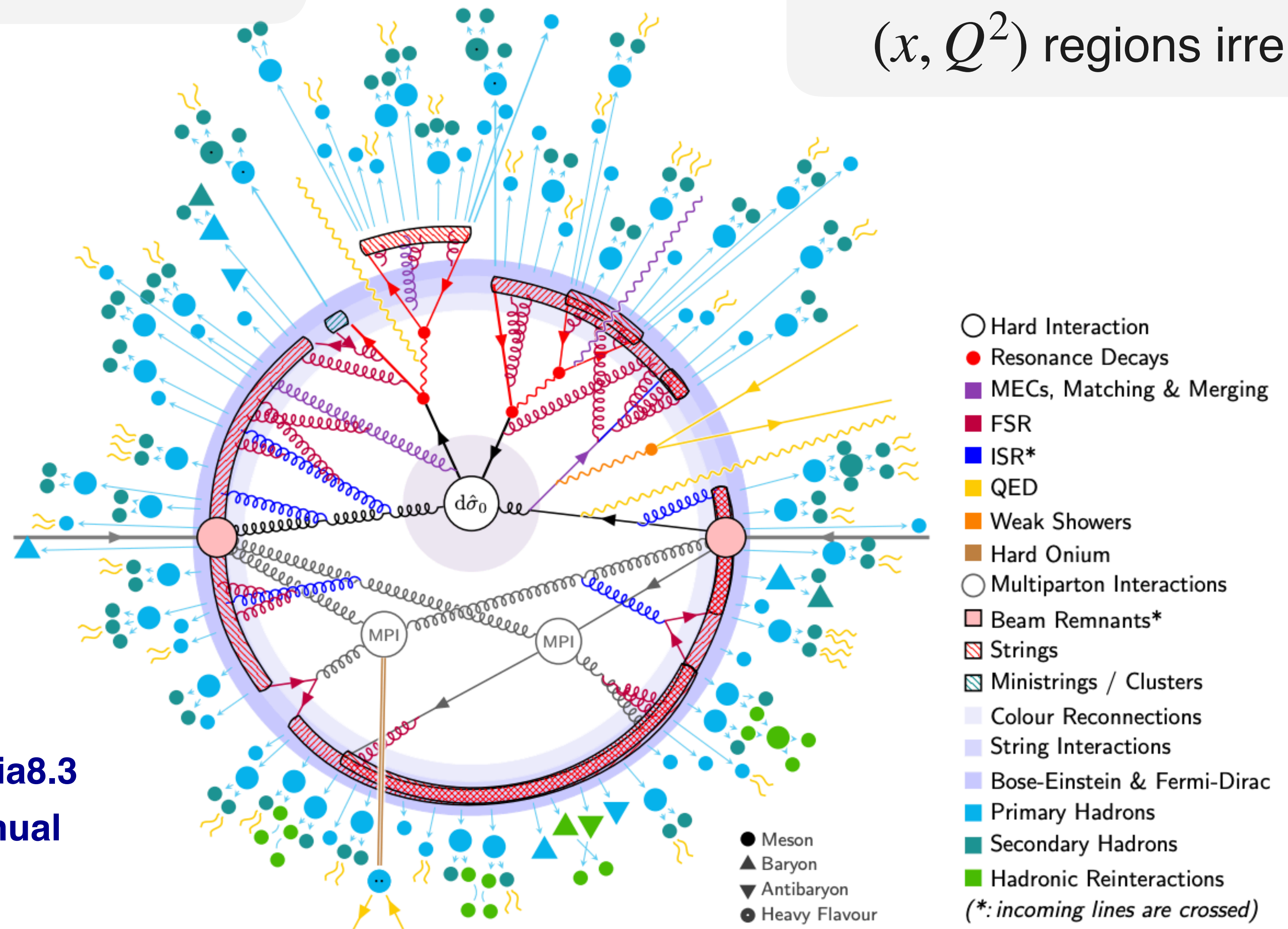
PDFs for (N)NLO Monte Carlo Generators

PDFs & Event Generators

Why ``**regular" PDF sets** are sometimes sub-optimal when used within event generators?

ISR showers require positive-definite PDFs down to $Q \sim 1$ GeV

MC integration & sampling requires smooth, numerically stable PDFs even in (x, Q^2) regions irrelevant for pheno



Pythia8.3 manual

Modelling of UE & MPI demand smooth extrapolation to very small-x & gluon PDF raising sufficiently fast

Simulation of **QED showers & photon-initiated processes** demands fits with QED effects included

PDFs & Event Generators

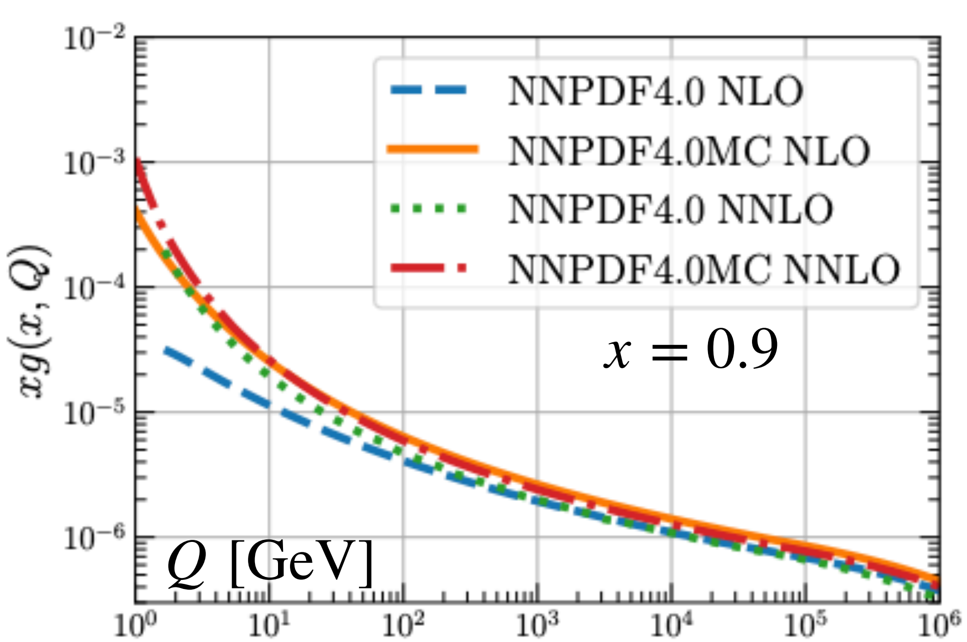
The NNPDF4.0MC PDFs satisfy these requirements not only a LO but also at **NLO and NNLO**

How? Answer is quite technical, let me focus on the **results** but feel free to ask me for details

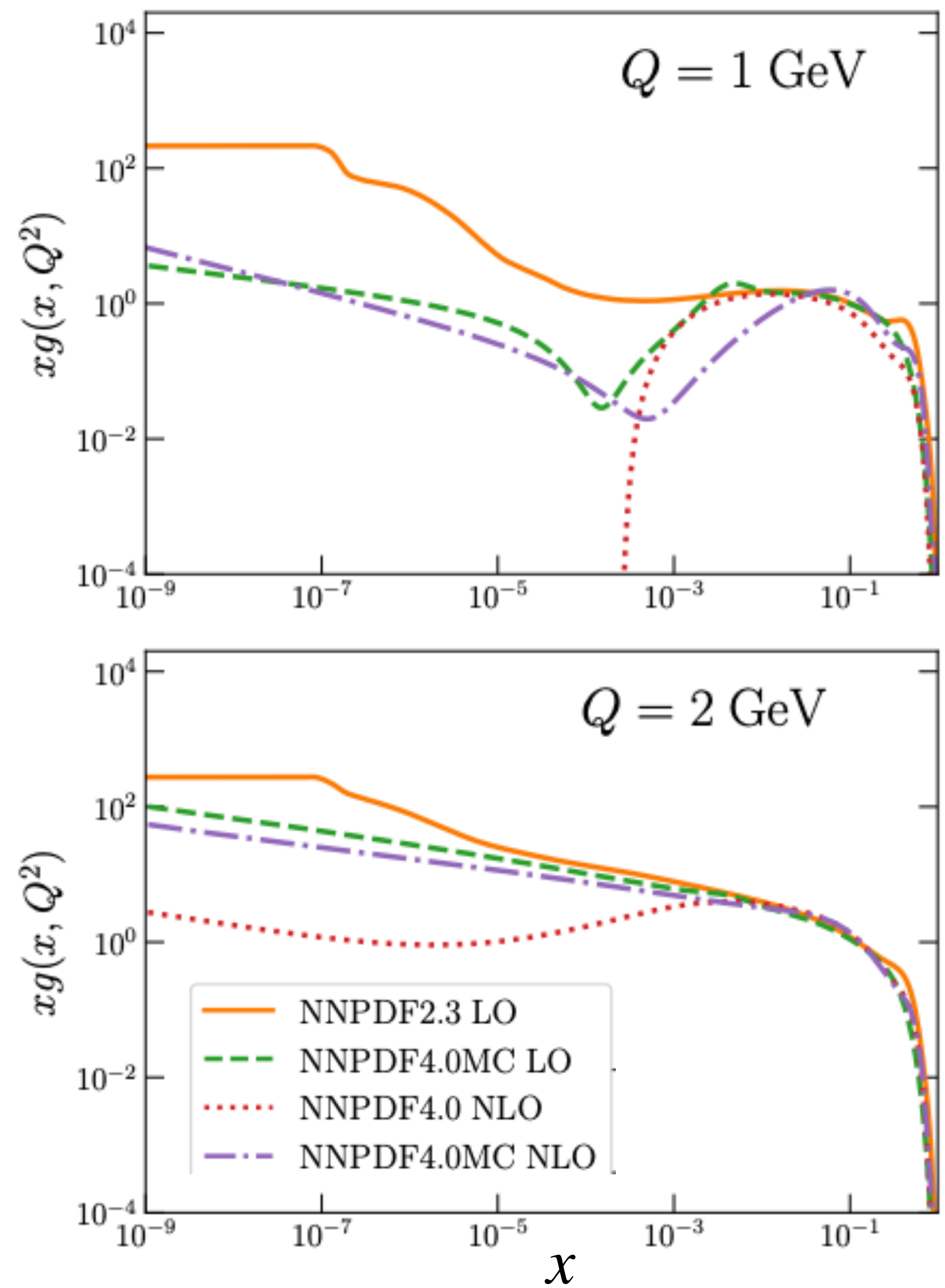
Satisfactory **NNLO** χ^2, only small worsening wrt baseline PDFs

Dataset by process group	NLO n_{dat}	NLO QCD BL	NLO QCD MC	NLO QCD+QED BL	NLO QCD+QED MC	NNLO n_{dat}	NNLO QCD BL	NNLO QCD MC	NNLO QCD+QED BL	NNLO QCD+QED MC
DIS NC	1953	1.35	1.37	1.38	1.54	2110	1.22	1.30	1.22	1.29
DIS CC	988	0.91	0.92	0.94	0.95	989	0.90	0.89	0.90	0.89
DY NC	669	1.58	1.84	1.67	2.04	736	1.20	1.30	1.22	1.33
DY CC	197	1.38	1.56	1.40	1.61	157	1.45	1.55	1.47	1.57
Top pairs	66	2.40	2.14	2.51	2.47	64	1.27	1.16	1.31	1.27
Single-inclusive jets	356	0.82	0.88	0.83	0.93	356	0.94	1.01	0.93	1.00
Dijets	144	1.51	1.55	1.56	1.62	144	2.01	2.01	1.94	1.93
Photon	53	0.57	0.60	0.64	0.74	53	0.76	0.67	0.74	0.68
Single top	17	0.36	0.36	0.38	0.36	17	0.37	0.38	0.39	0.40
Total	4443	1.28	1.30	1.30	1.44	4626	1.16	1.22	1.17	1.22

Numerically stable in **deep extrapolation regions**

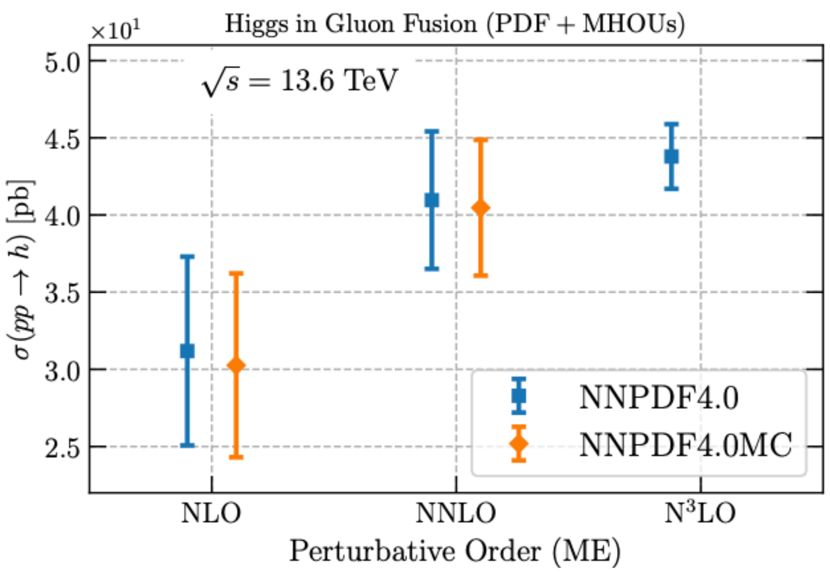


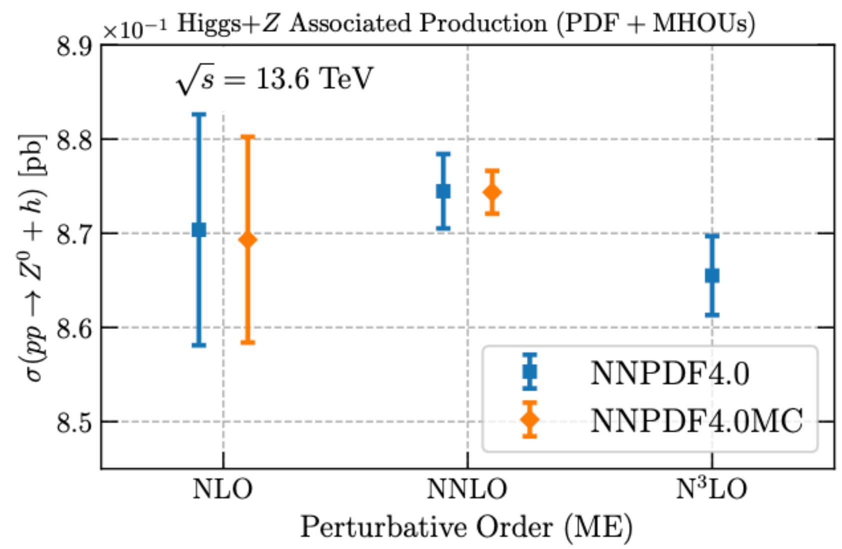
Positive, steeply rising **small-*x* gluon**

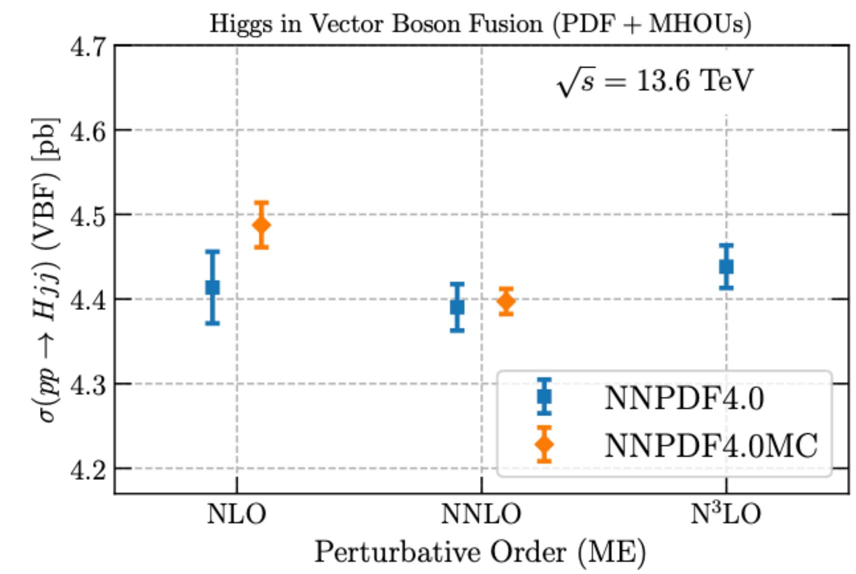


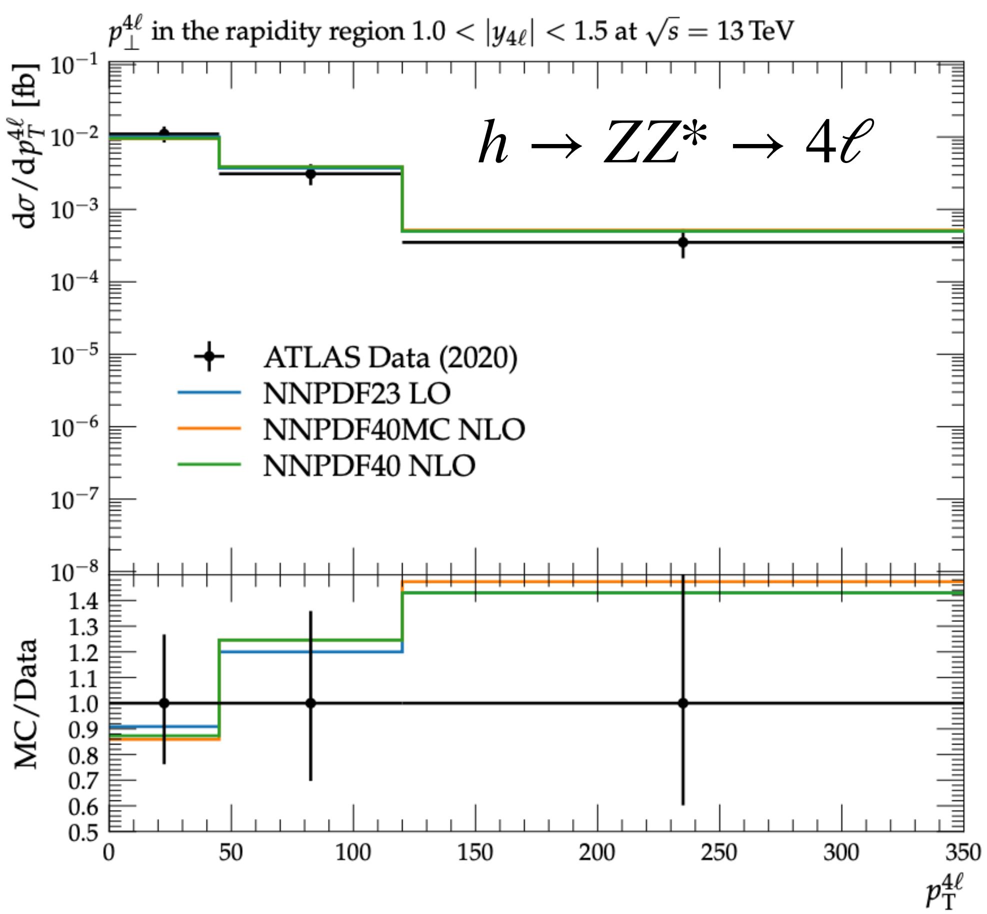
PDFs & Event Generators

The NNPDF4.0MC PDFs **successfully tested by various MC developers** (PanScales, SHERPA, …), ready to be used for event generation at the LHC









- For **high-p_T cross-sections**, MC variants are very close to the regular NNPDF4.0 NLO and NLO PDFs

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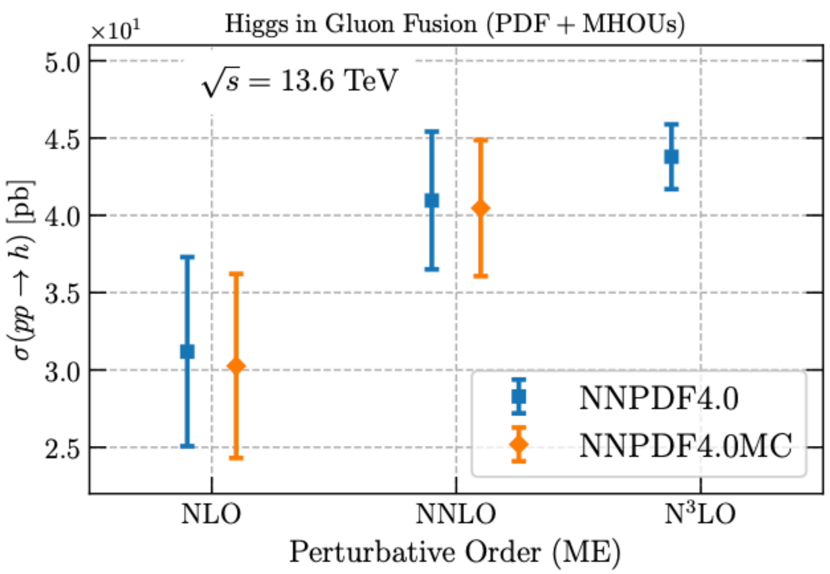

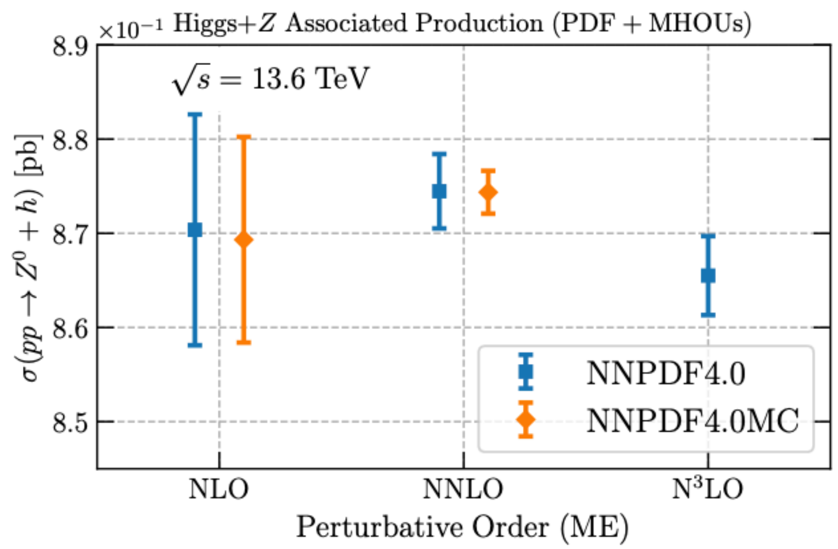

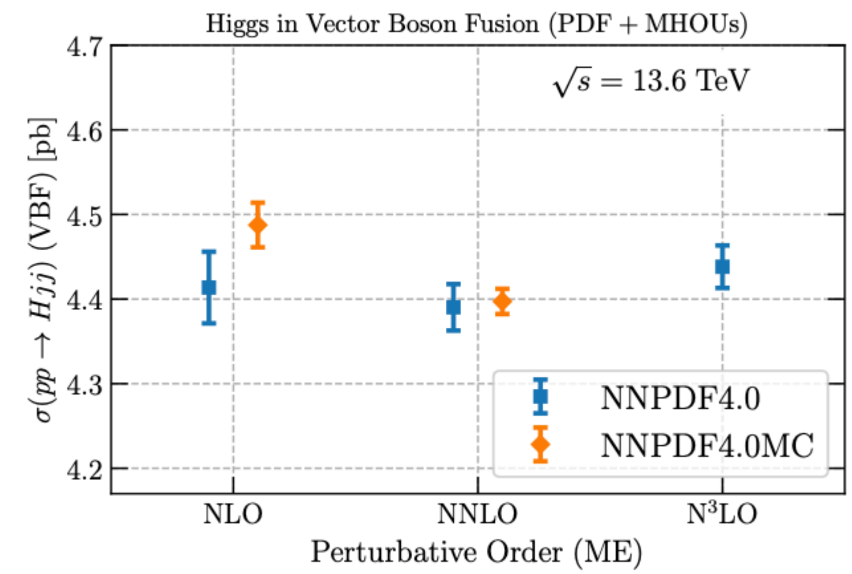

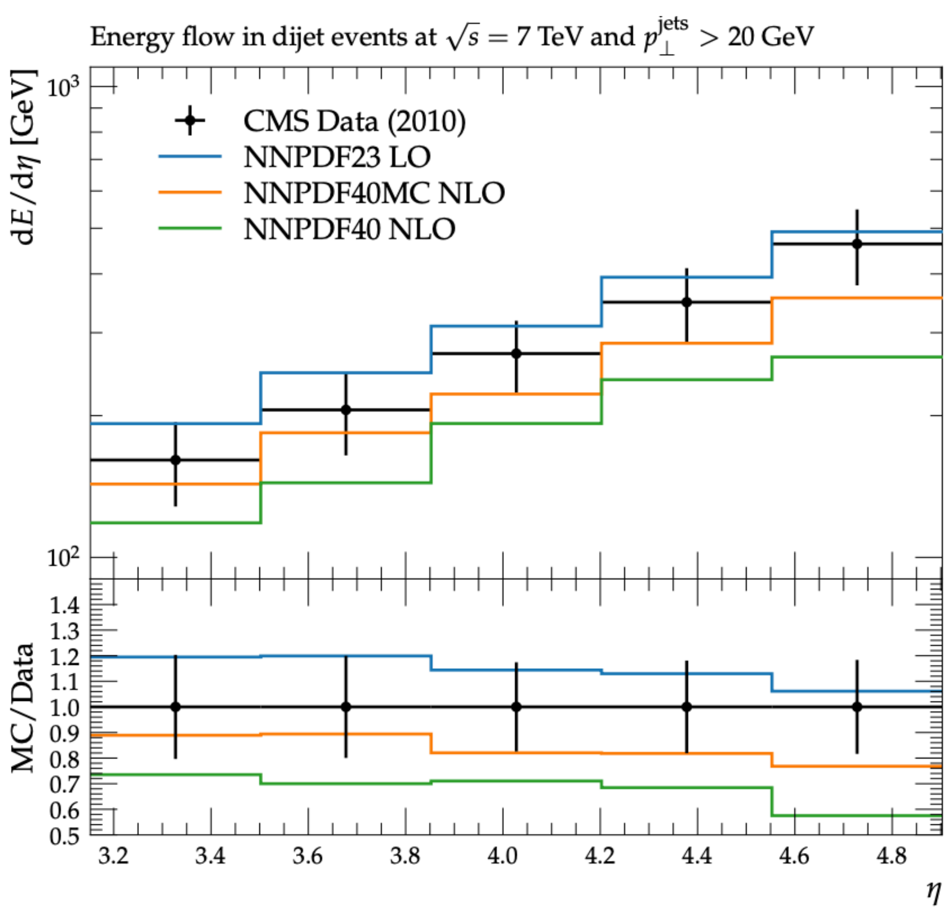

- For **high-p$_T$ cross-sections**, MC variants are very close to the regular NNPDF4.0 NLO and NLO PDFs
- For **soft-QCD processes** (UE, MPI, energy flow, multiplicities) a dedicated MC tune based on these new NNPD4.0MC sets is required

Potentially, NNPDF4.0MC enables an excellent simultaneous description of **both hard and soft QCD process**!

Summary and outlook

- ☑ A key ingredient to **LHC phenomenology at 1% precision** are N^{3}LO PDFs which account for all sources of theory uncertainties

- ☑ The new NNPDF4.0 aN^{3}LO determination enables **consistent N^{3}LO calculations** of LHC cross-sections, and also accounts for QED corrections and the photon PDFs

- ☑ Combination of MSHT20 and NNPDF4.0 aN^{3}LO PDFs indicates **large effects** for Higgs production in gluon-fusion and vector-boson fusion: how to account for these in YR5?

- ☑ A precision determination of the strong coupling based on aN^{3}LO calculations **agrees with the PDG average** and pulls the PDF-fit average towards the lattice QCD average

- ☑ **Technical developments in ML training** essential to enable many of the NNPDF physics goals

- ☑ PDFs tailored for **NLO and NNLO Monte Carlo generations available**, tuning of non-perturbative QCD physics is progress

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Thanks for your attention