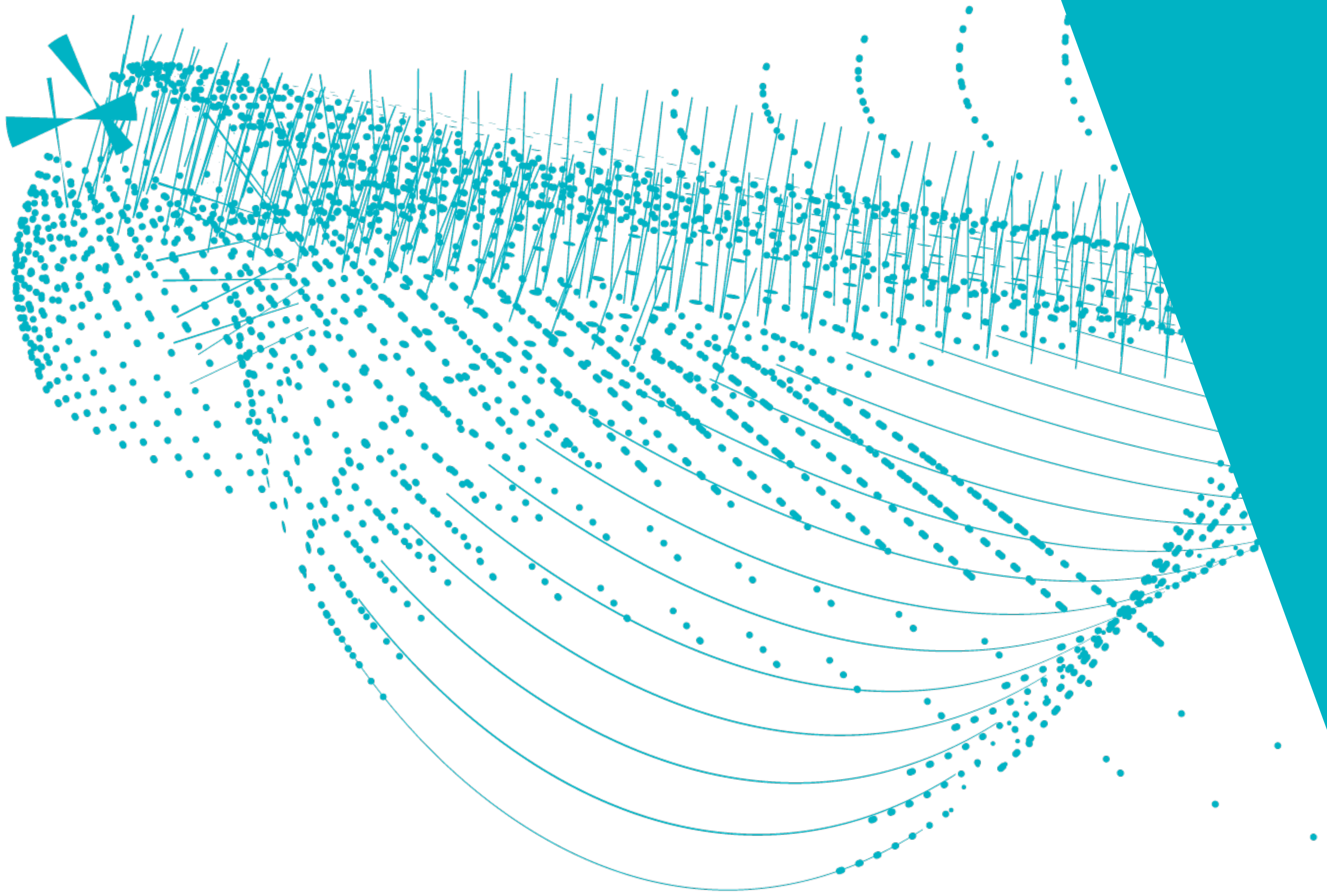
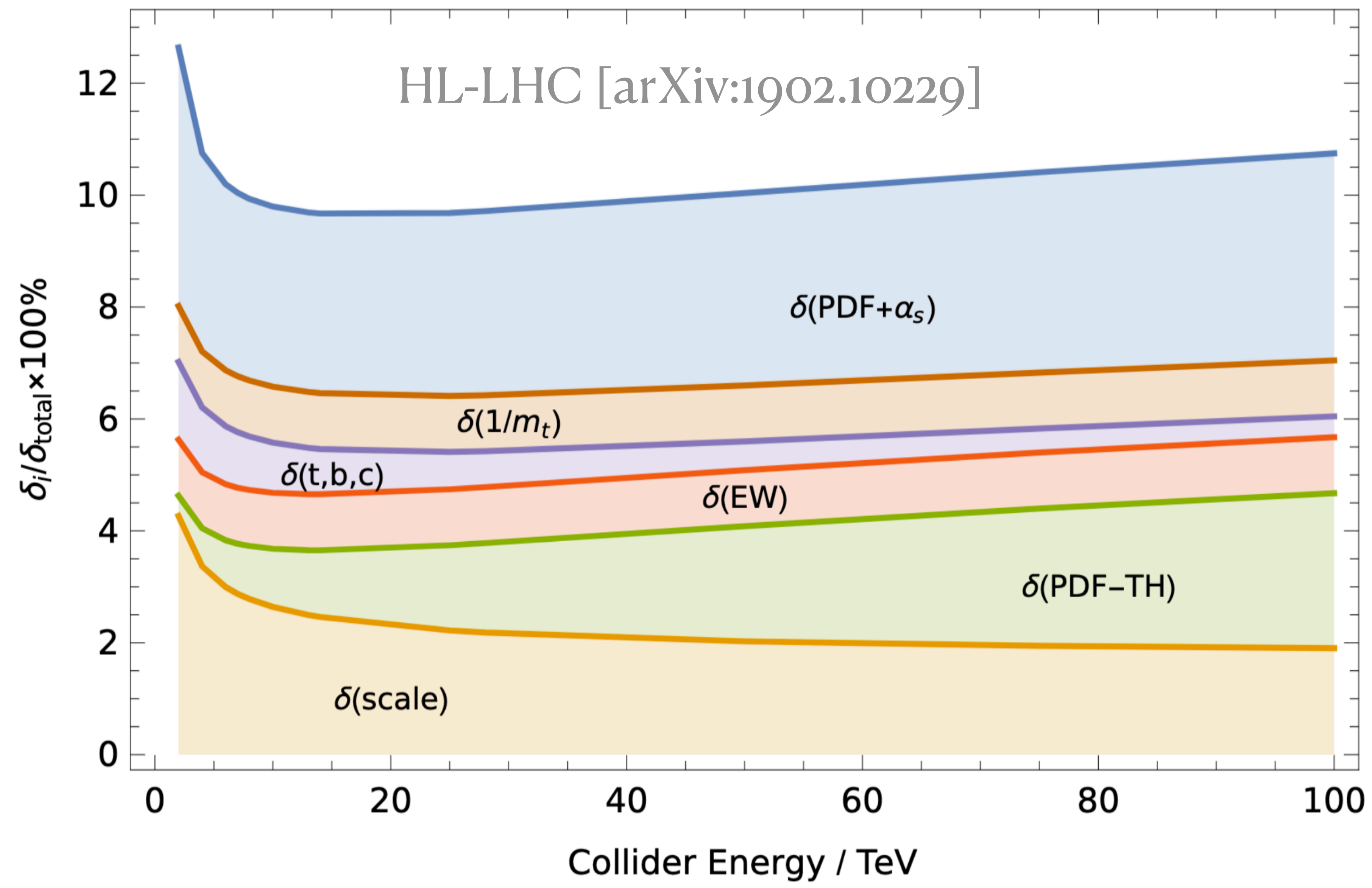
NNPDF updates and the path towards NNPDF4.1: Data, theory, and Methodology

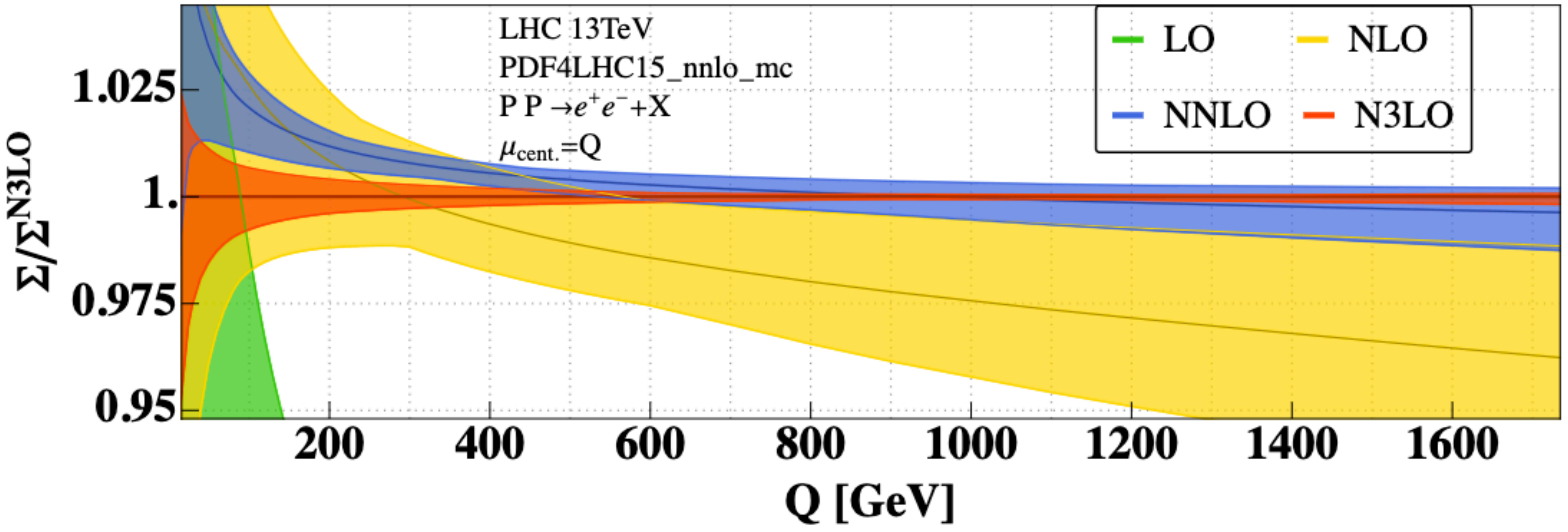


Tanjona R. Rabemananjara on behalf of the NNPDF collaboration
DIS 2025, March 25th 2025
Cape Town, South Africa

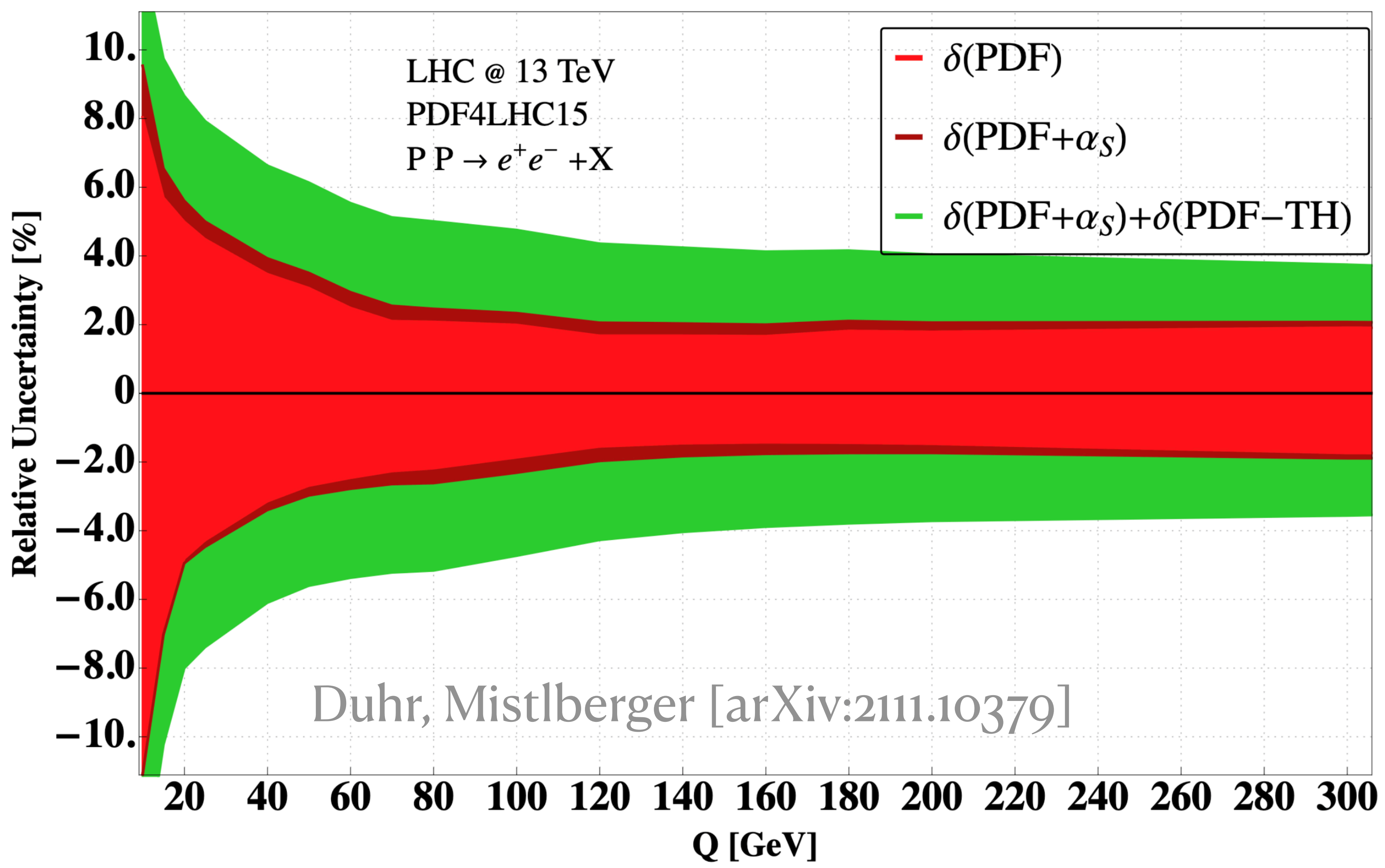
Motivation: Why do we still care about PDFs?

- **PDFs are becoming a bottleneck for LHC precision calculations** with the largest uncertainties along with the incomplete knowledge of $\alpha_s \Longleftrightarrow$ New Physics
- **Progress on N3LO calculations** for Higgs (ggF, VBF, VH) & NC/CC DY processes requires **N3LO PDFs**
- **QED effects in PDFs** are **no longer negligible** as experimental measurements become more precise and determination of parton densities more accurate
- **Theoretical uncertainties** on PDFs are crucial to assess accuracy/uncertainties on MHOUs & IHOUs

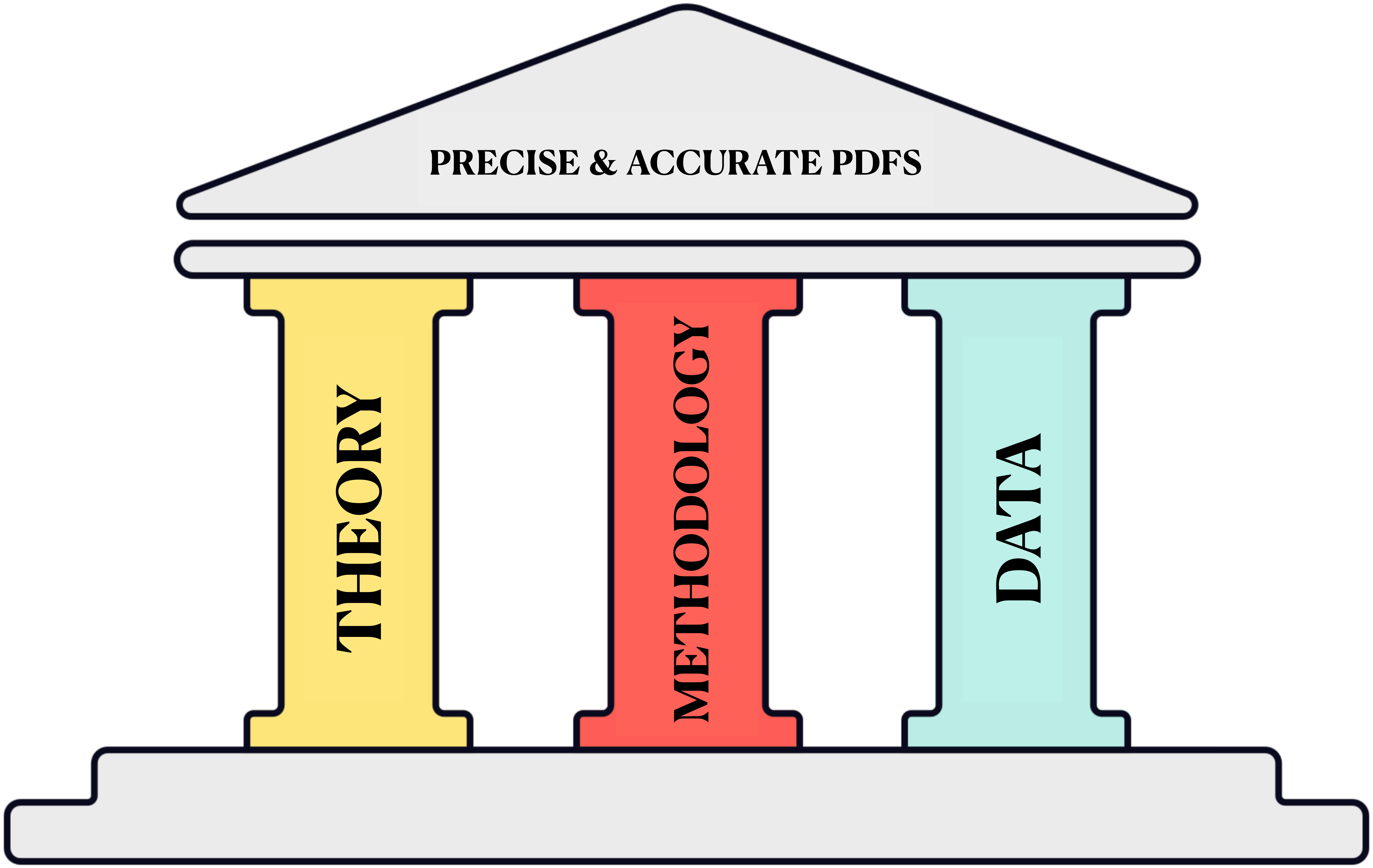




Duhr, Mistlberger [arXiv:2111.10379]



Outline of the Talk



NNPDF Timeline

2Q 2026	NNPDF4.1	[WIP]
3Q 2025	PDFs with Higher-Twist corrections	[WIP]
2Q 2025	Closure test with inconsistencies	[WIP]
2Q 2025	alpha_s determination with aN3LO⊗QED⊗MHOU	[WIP] (see RS's talk this afternoon)
03/2025	NNPDFpol2.0 - helicity dependent PDFs	[arXiv:2503.11814] (presented in WG5)
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Part I: Theory

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Missing Higher Order Uncertainties (MHOUs) @ (a)N{2,3}LO

For a given observable $\mathcal{O}$, **MHOUs** are commonly estimated by **varying the unphysical scales** in the **parton evolutions** and in the **partonic cross-sections**:

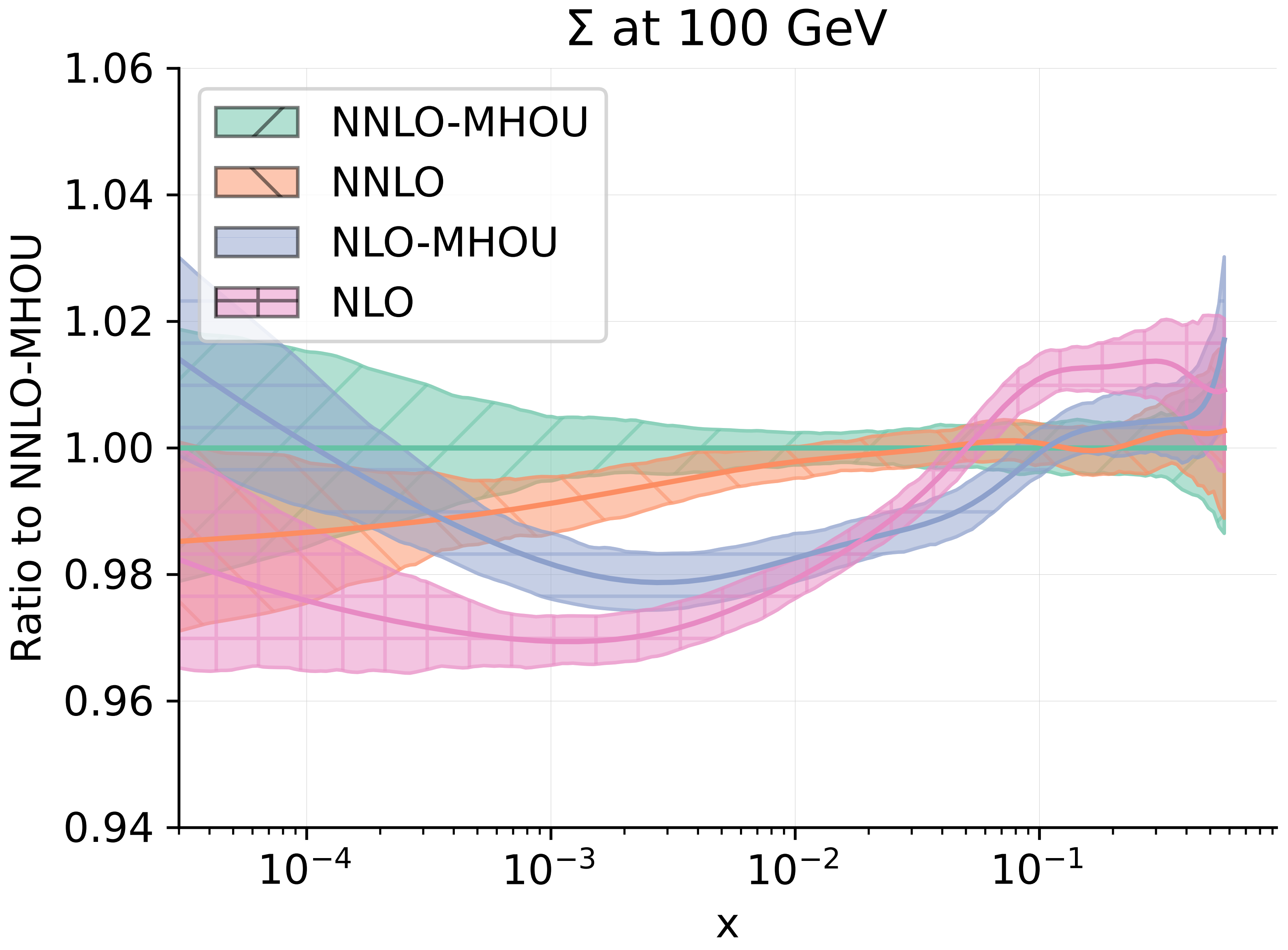
$$\mathcal{O}\left(\alpha_s\left(\mu^2\right), \frac{Q^2}{\mu_F^2}, \frac{Q^2}{\mu_R^2}\right) = \mathcal{L}\left(\alpha_s\left(\mu_F^2\right), \frac{Q^2}{\mu_F^2}\right) \mathcal{O}\left(\alpha_s\left(\mu_R^2\right), \frac{Q^2}{\mu_R^2}\right)$$

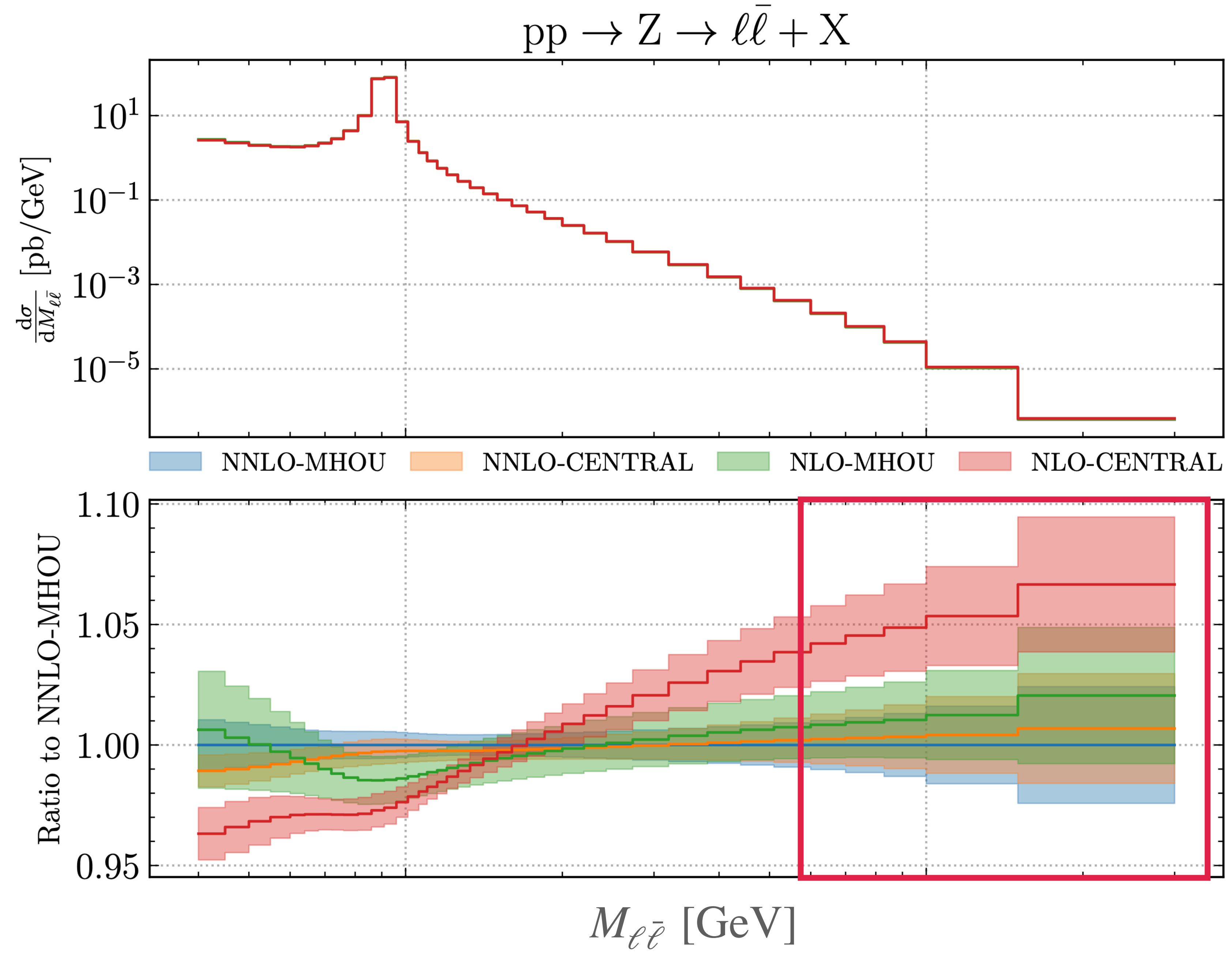
Variation of **Factorisation Scale** $\kappa_F = Q^2/\mu_R^2$ estimates MHOUs from Anomalous Dimensions in the evolution while variation of **Renormalisation Scale** $\kappa_R = Q^2/\mu_R^2$ estimates MHOUs from partonic cross-sections.

MHOUs can be added as a nuisance parameter to the Covariance Matrix **[arXiv:1906.10698; arXiv:2105.05114]**

$$\mathrm{cov}_{i,j} = \mathrm{cov}_{i,j}^{\mathrm{exp}} + \mathrm{cov}_{i,j}^{\mathrm{MHOU}}, \quad \mathrm{cov}_{i,j}^{\mathrm{MHOU}} = \frac{1}{N_{\mathrm{var}} - 1} \sum_{k=1}^{N_{\mathrm{var}}} \left(S_{i,k} - \bar{S}_i\right)\left(S_{j,k} - \bar{S}_j\right)$$

7-point scale variation prescription is used. Points belonging to the same process are CORRELATED by κ_R-variation while κ_F correlates all the points.





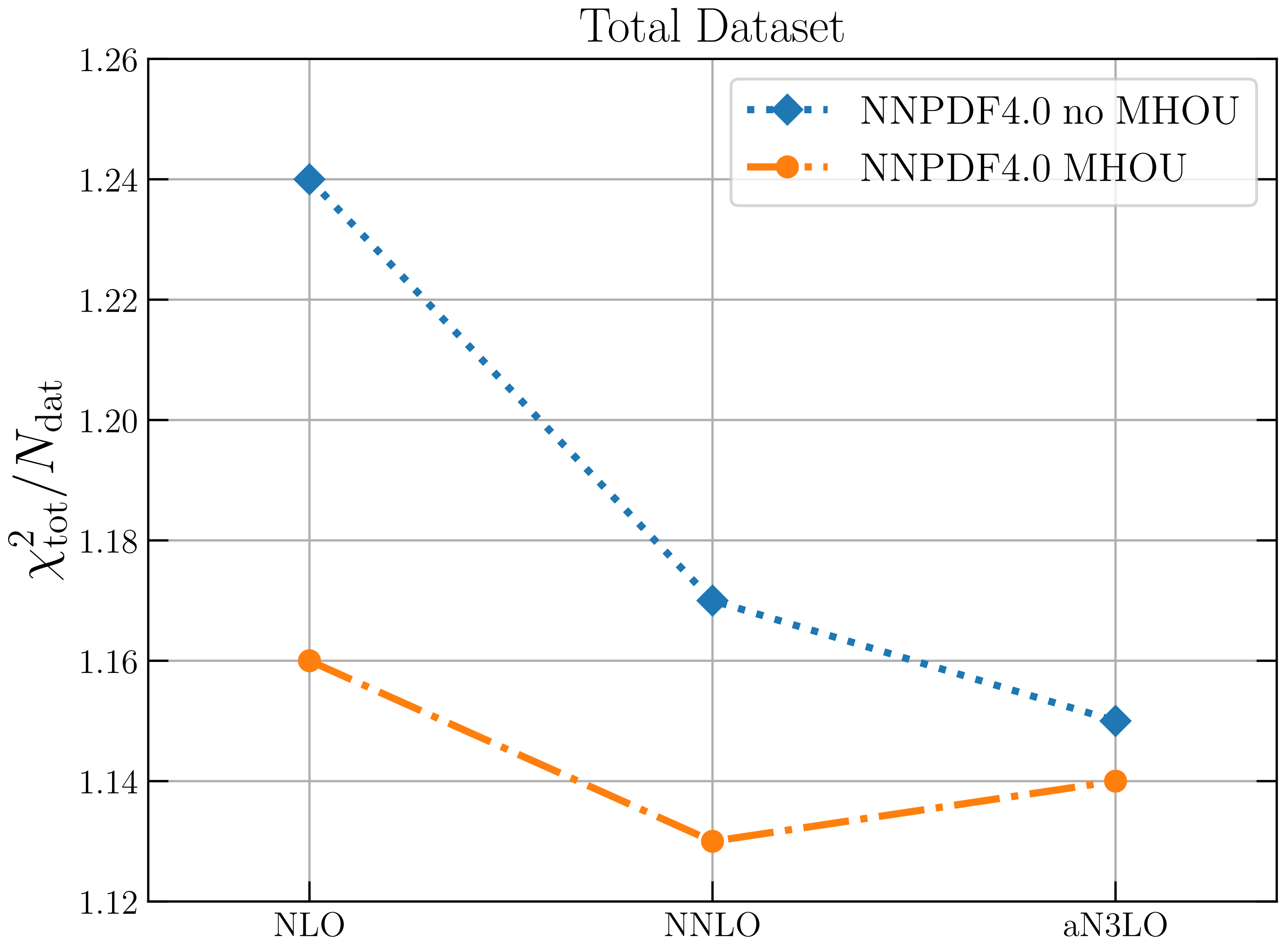
Approximate N3LO (aN3LO) determination

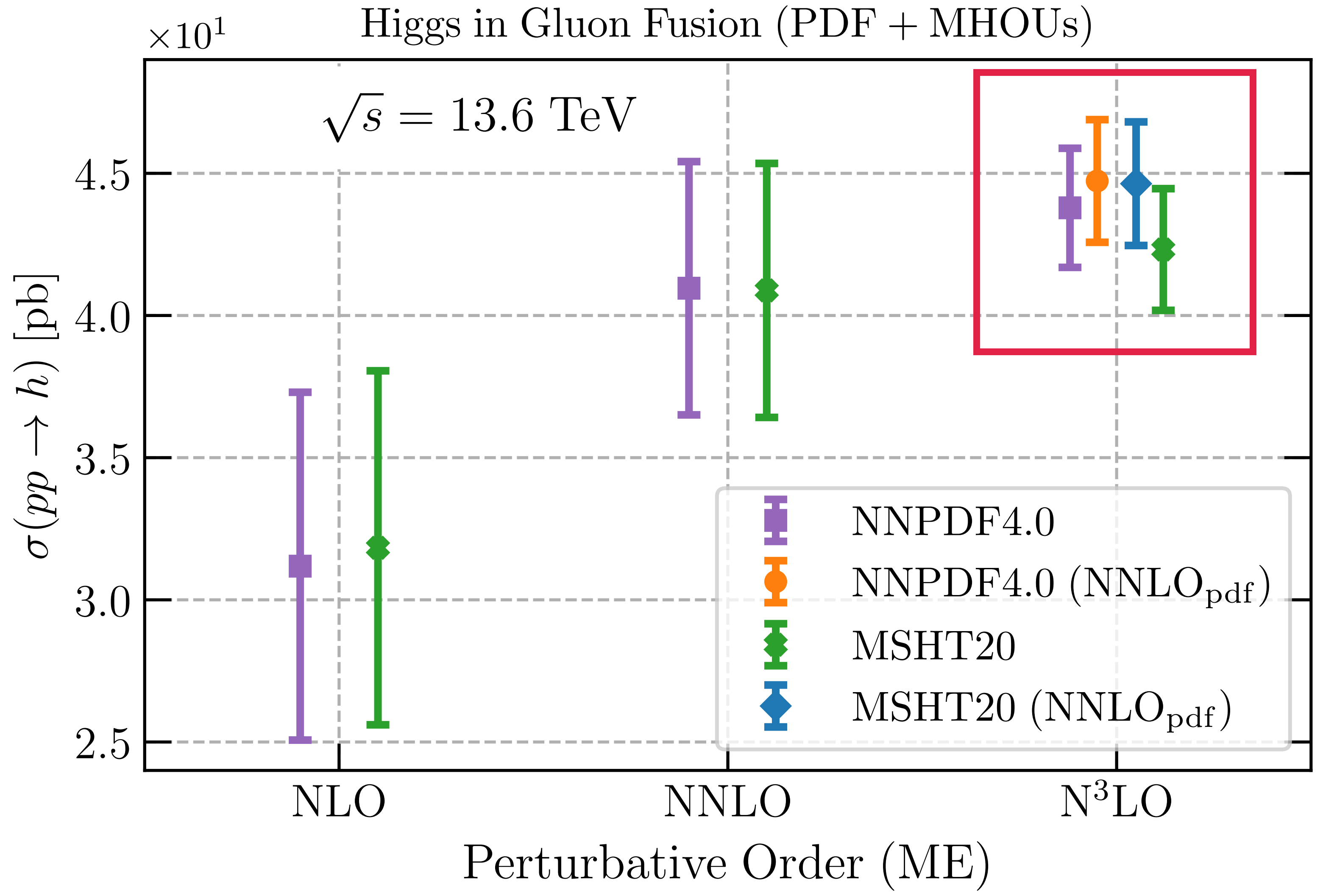
NNPDF4.0 determination of aN3LO PDFs:

- **DGLAP Evolution**: accurate numerical approximations splitting functions (10 lowest moments, large-x and small-x limits)
- **Matching conditions**: all relevant terms are known (all exact, $a_{Hg}^{(3)}$ parametrised)
- **DIS Coefficients Functions**: massless coefficients (both NC and CC) are known. Massive NC can be approximated
- **Hadronic coefficients**: some DY coefficients are known, but not yet available in a format suitable for PDFs fits, corrections to Jets and processes are still unknown

New N3LO terms that will be part of NNPDF4.1:

- Higher splitting function moments: $P_{gg}^{(3)}, P_{gq}^{(3)}$ [arXiv:2404.09701; arXiv:2410.08089]
- Improved parametrisation for $a_{H,g}^{(3)}$ **matching conditions** [arXiv:2403.00513]





~1.5% suppression w.r.t. NNLO PDFs

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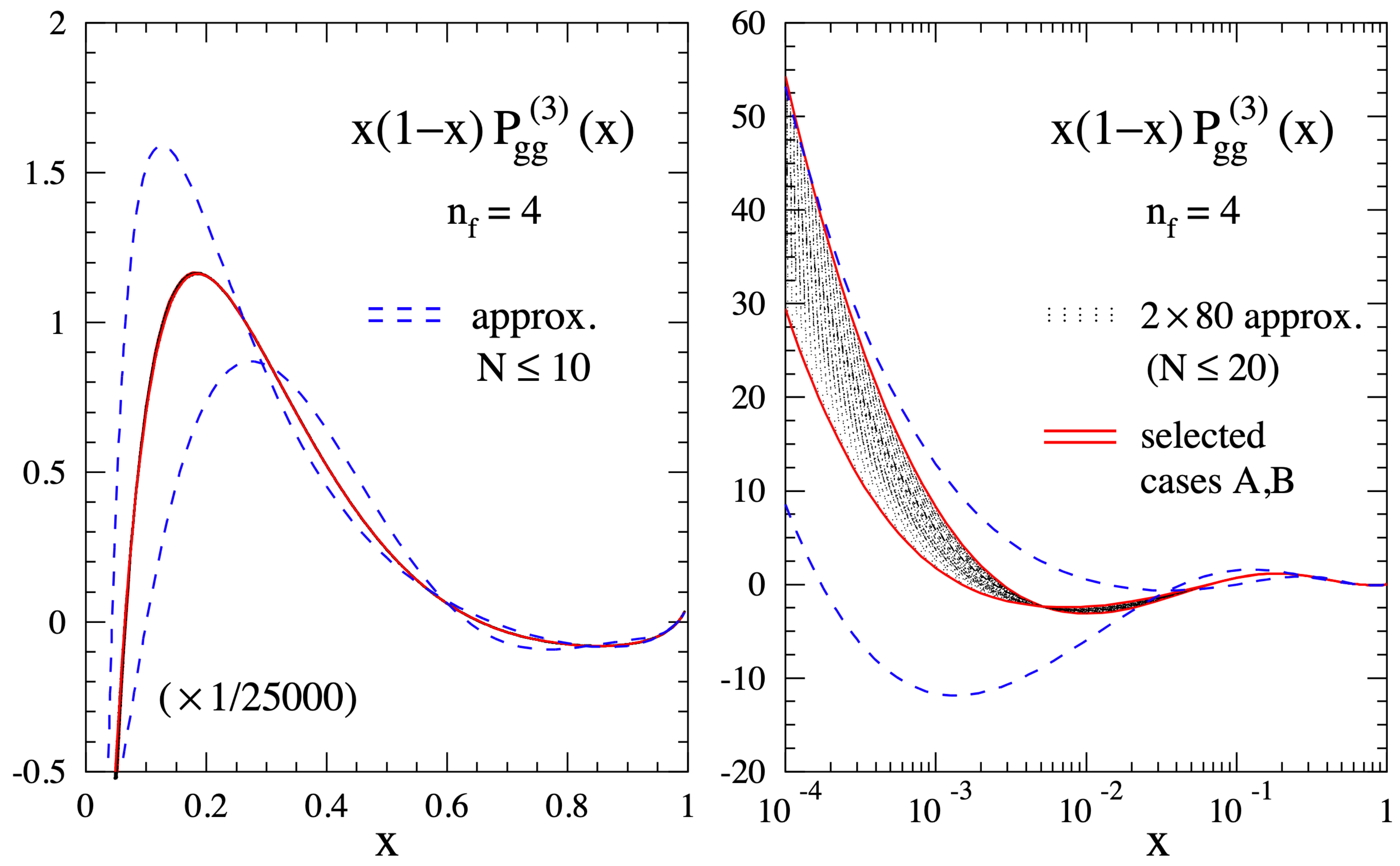
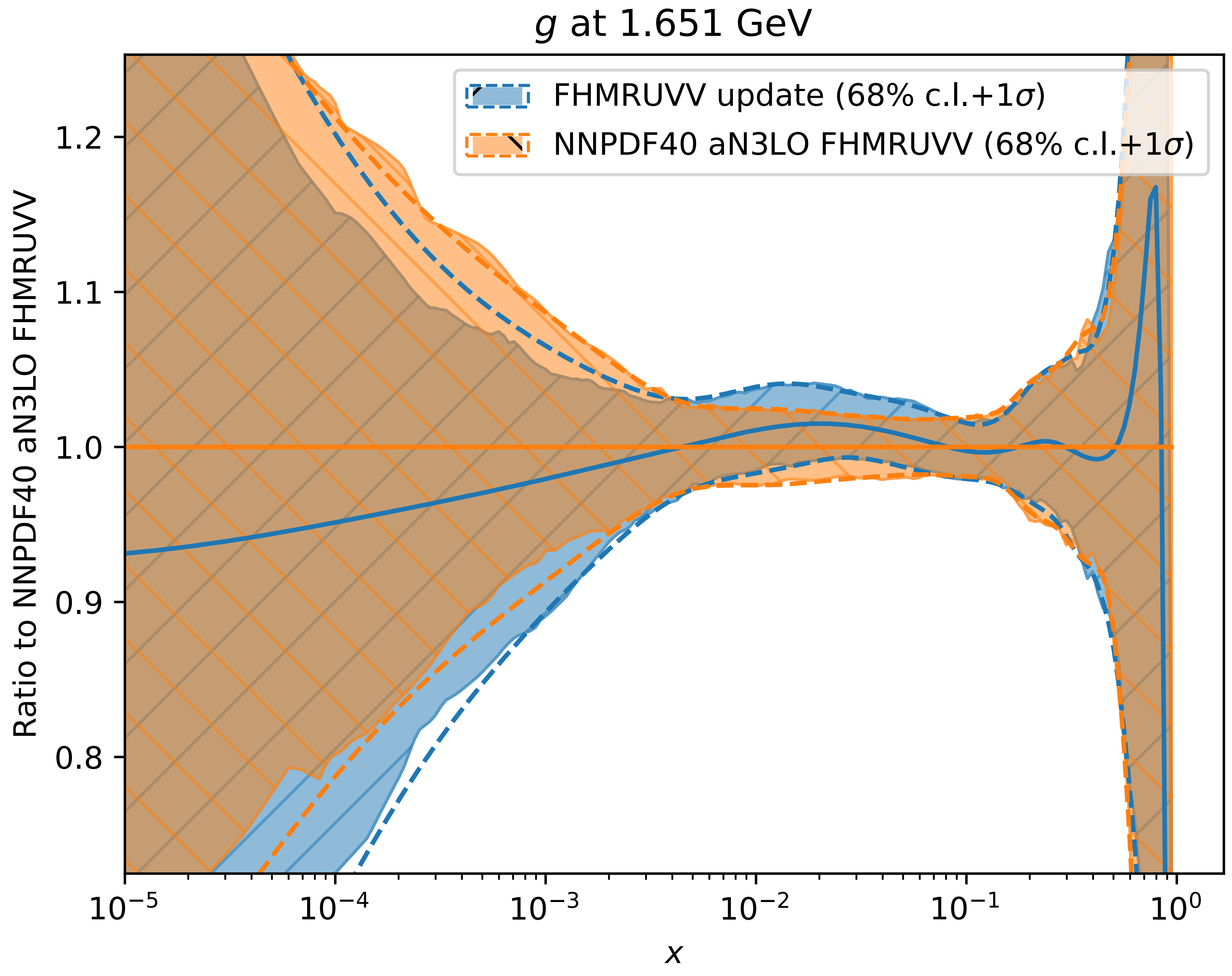




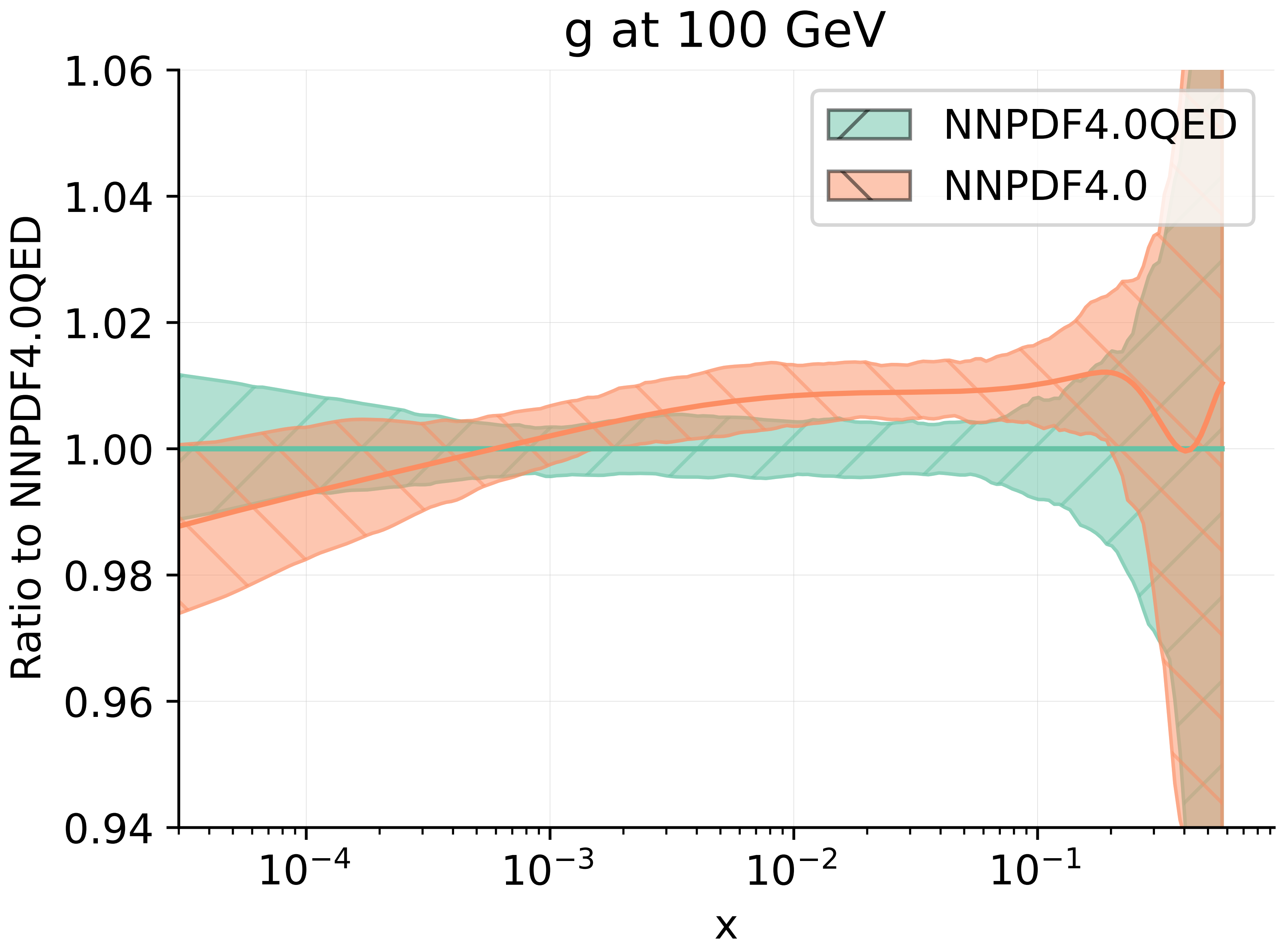
QED corrections & Photon PDF

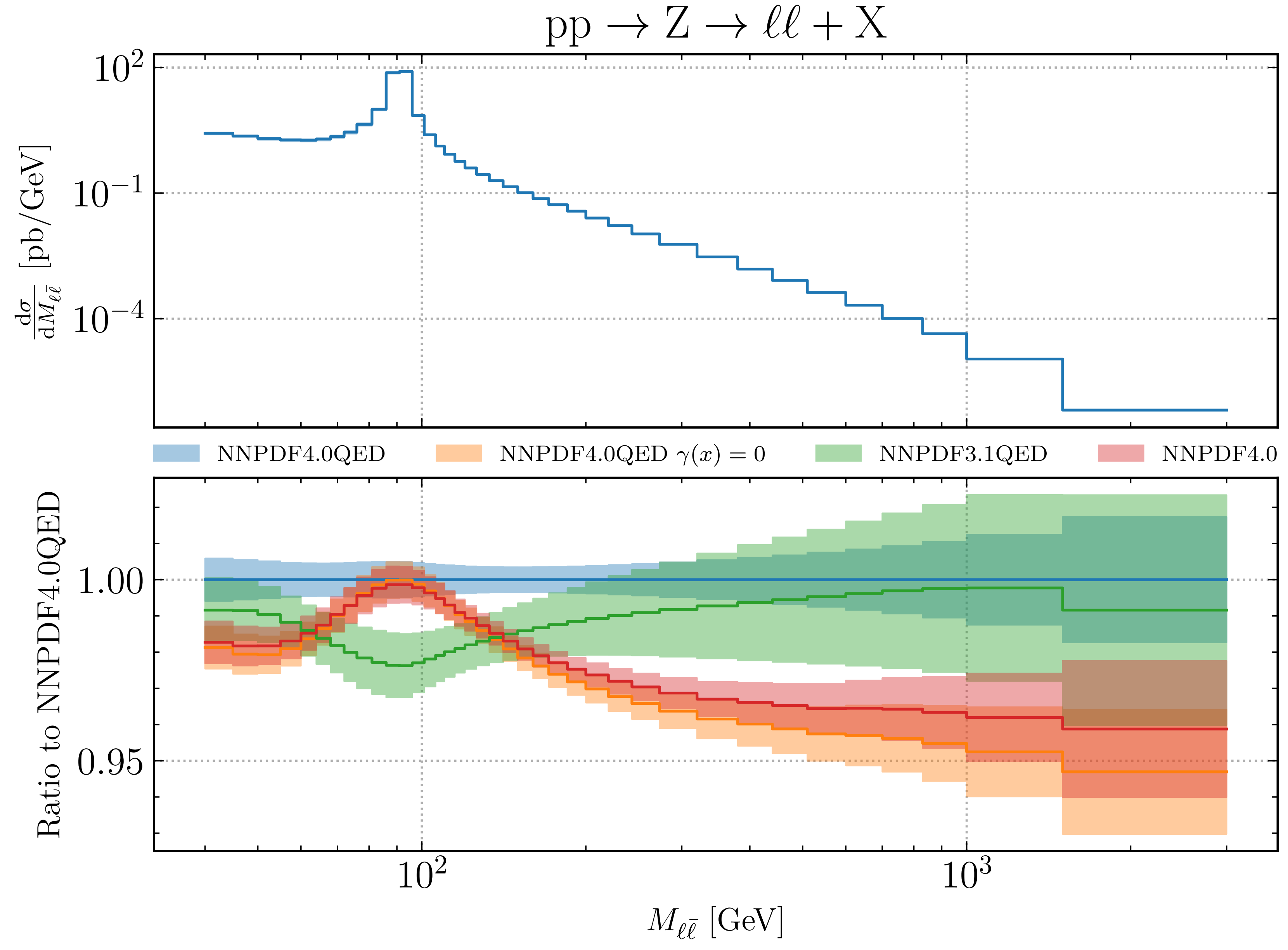
γ-PDFs are computed from **DIS structure functions** [arXiv:1607.04266]:

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

- Depending on the kinematic region the structure functions are computed form: **Elastic DIS**, **Resonance**, **Shallow Inelastic**, **DIS**
- $\gamma(x,Q^2)$ is computed iteratively during the fit
- Mixed QED⊗QCD DGLAP evolution: **more difficult to diagonalise due to how γ couples differently to up-like and down-like quarks** $\Longrightarrow$ **Unified Evolution Basis**
- While $\gamma(x,Q^2)$ depends on the PDFs through the structure functions, it affects their determination during the iterative procedure.
- Additional **mixed QED⊗QCD Momentum Sum rules**:

$$\int_0^1 dx\left(x\Sigma + xg + x\gamma\right)(x,Q^2) = 1$$





State-of-the-Art: "aN3LO⊗QED⊗MHOU"

QED corrections & γ-PDF are key for LHC phenomenology:

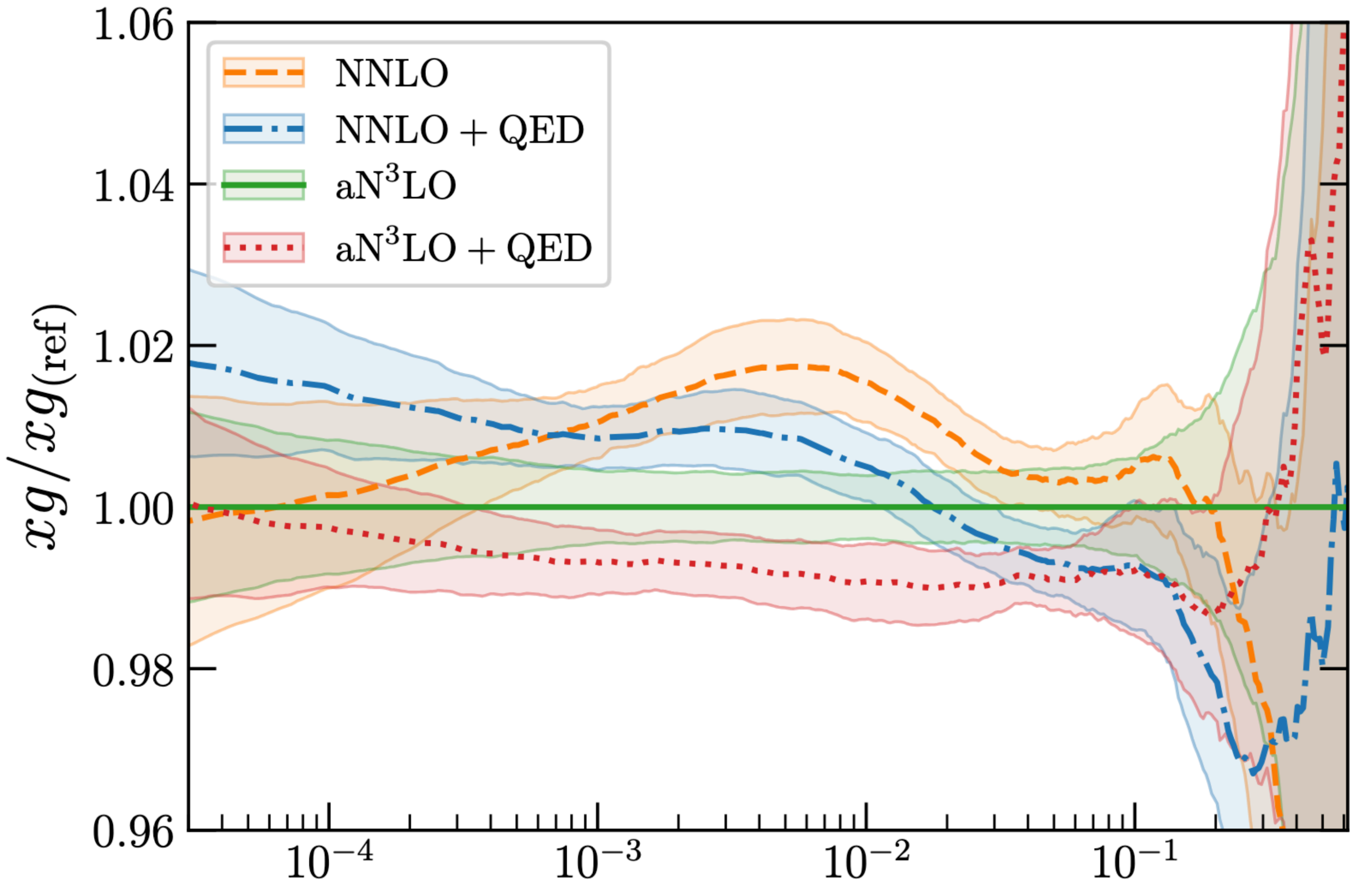
❖ QED effects are of the same size as aN3LO

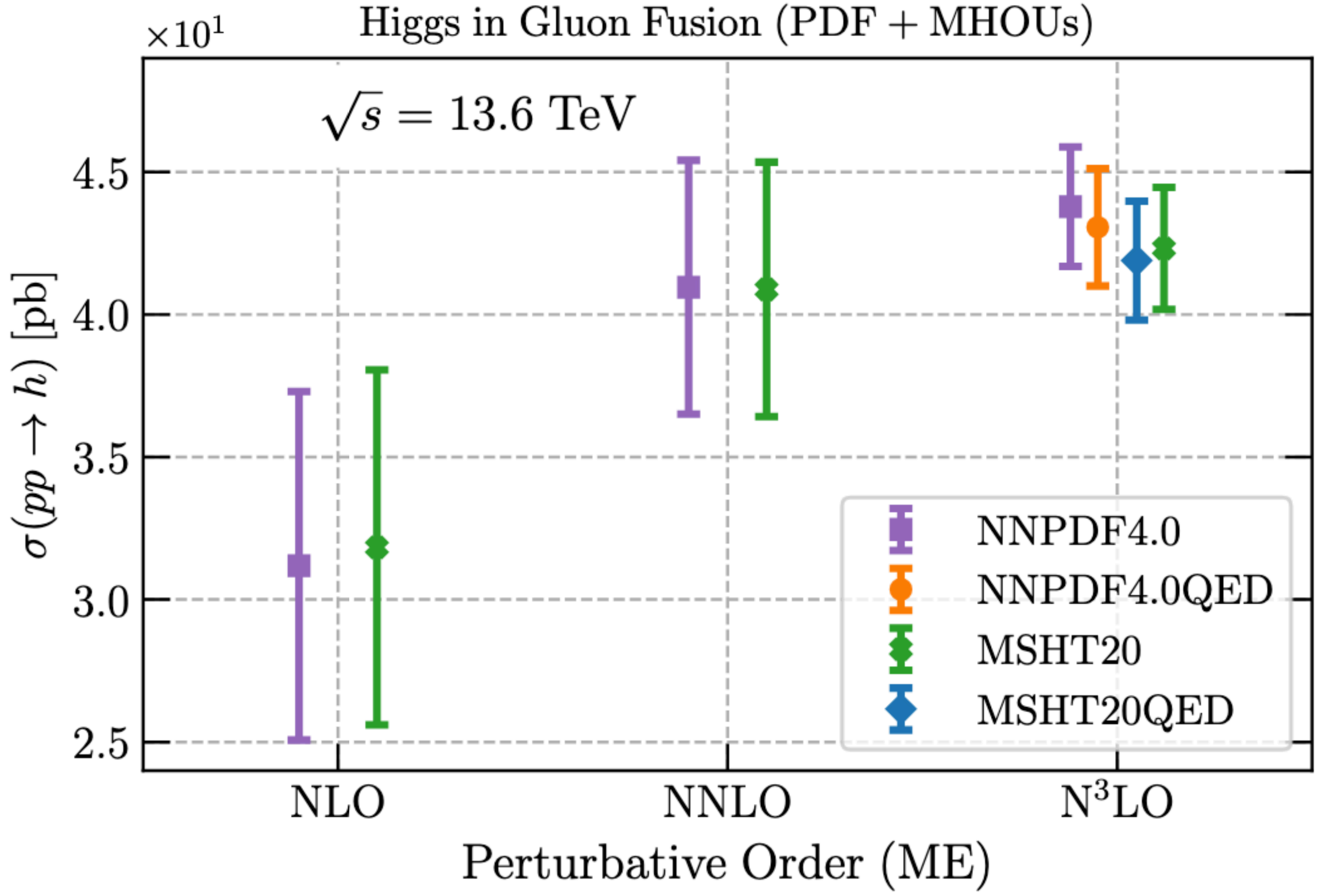
❖ Photon suppresses gluon momentum by up to 1%

Various LHC processes receive seizable γ-initiated contributions:

❖ aN3LO⊗QED result in a few percent suppression for ggH

❖ Difference between NNLO & N3LO predictions are reduced when using the appropriate PDFs at each order





Part II: Methodology

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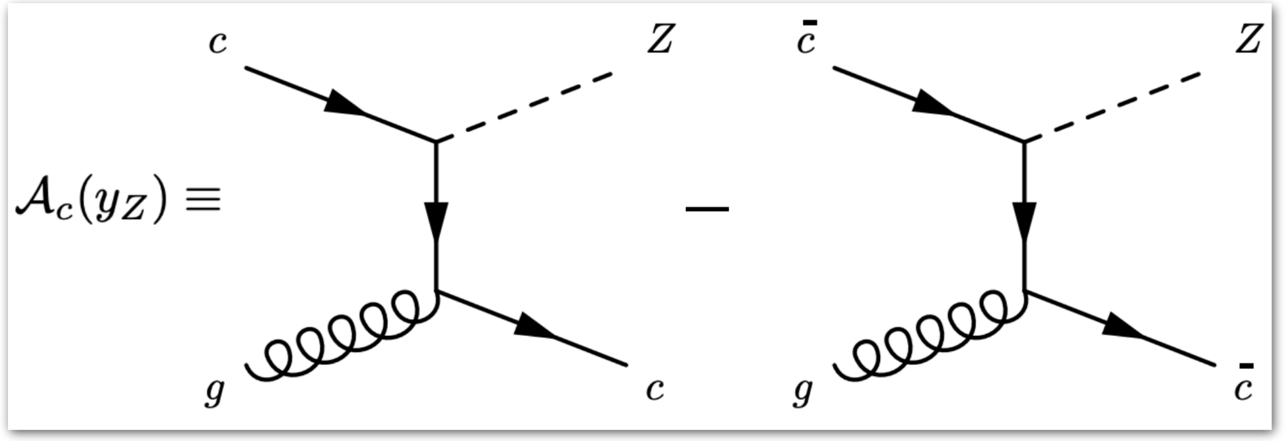
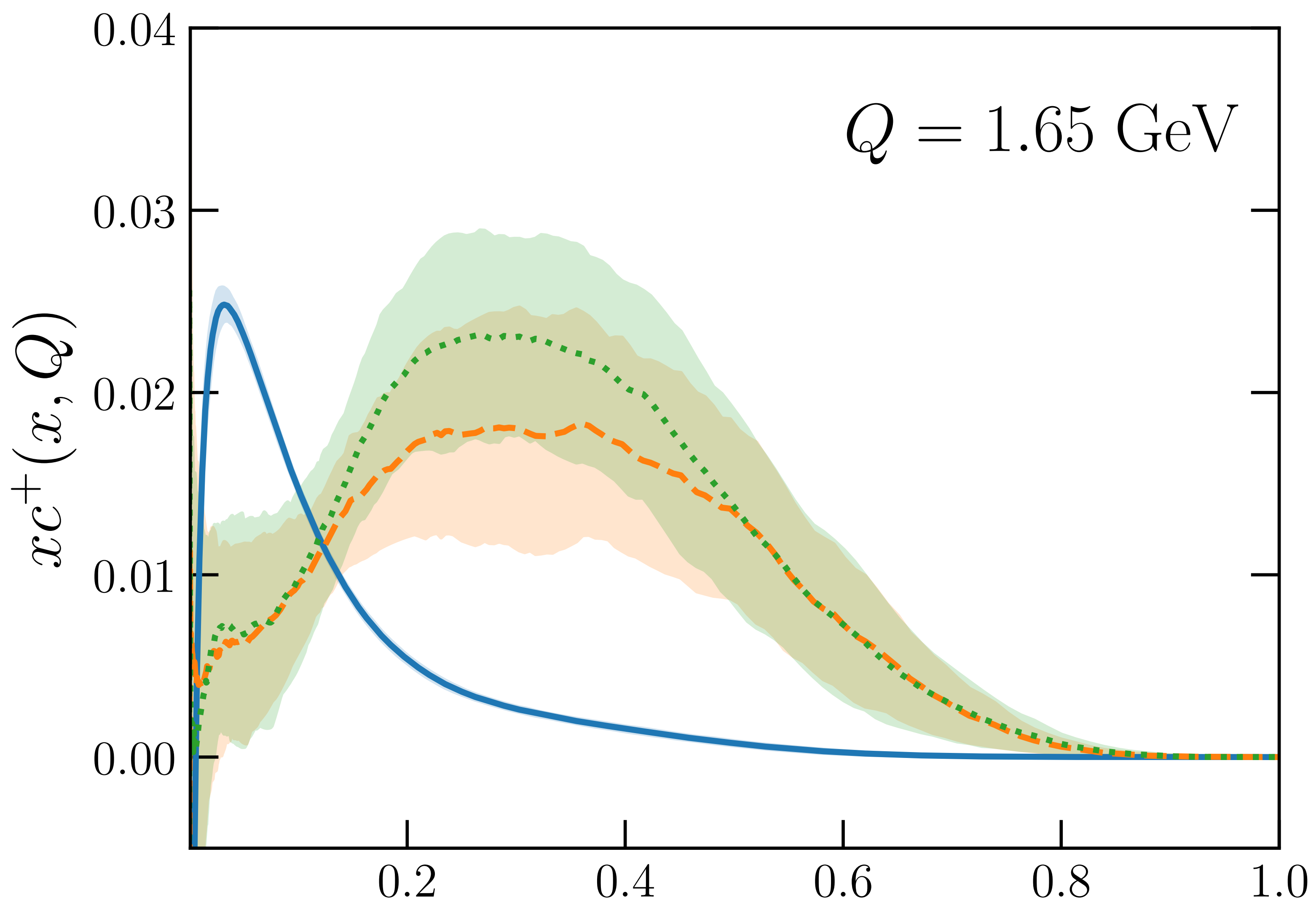
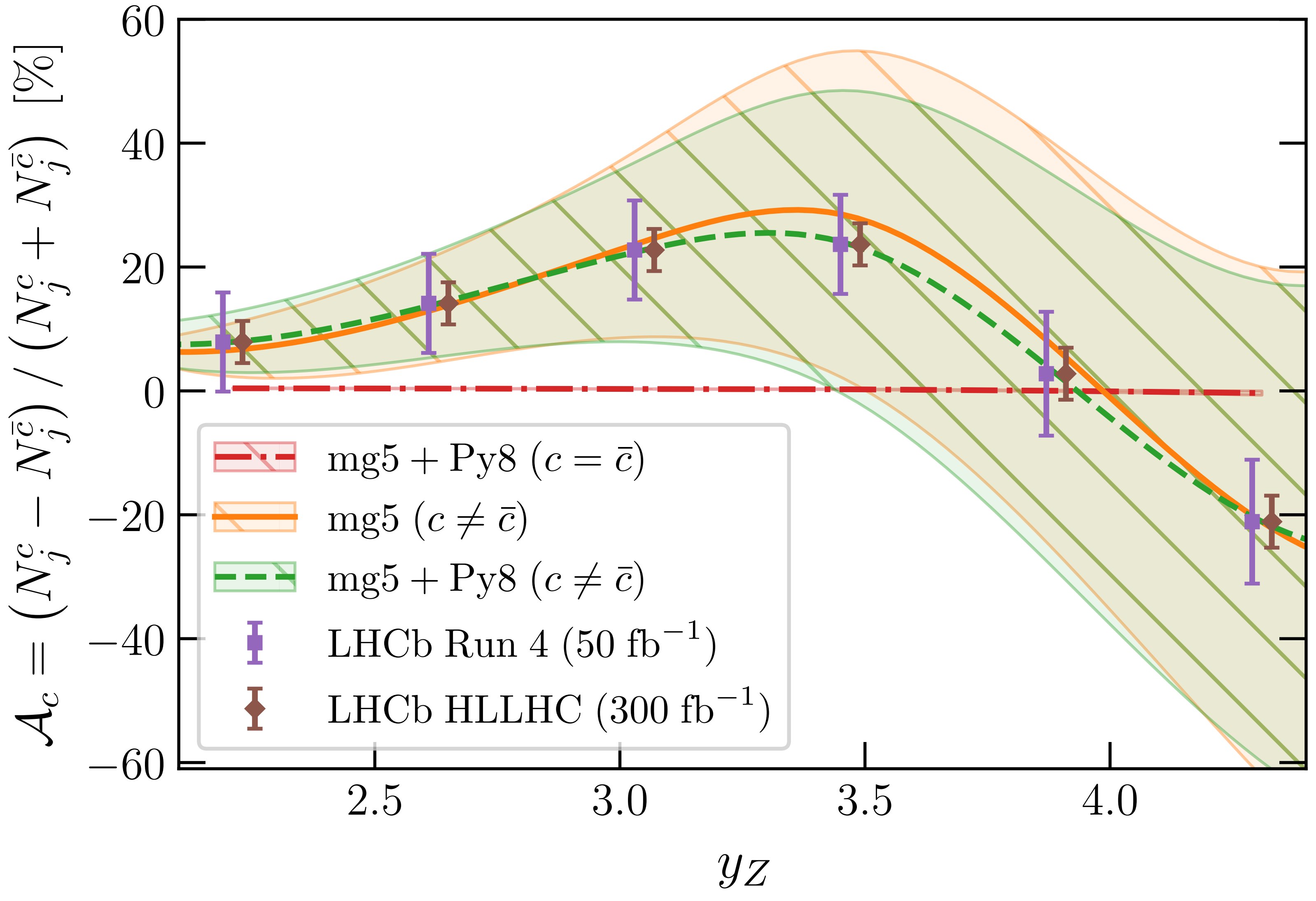
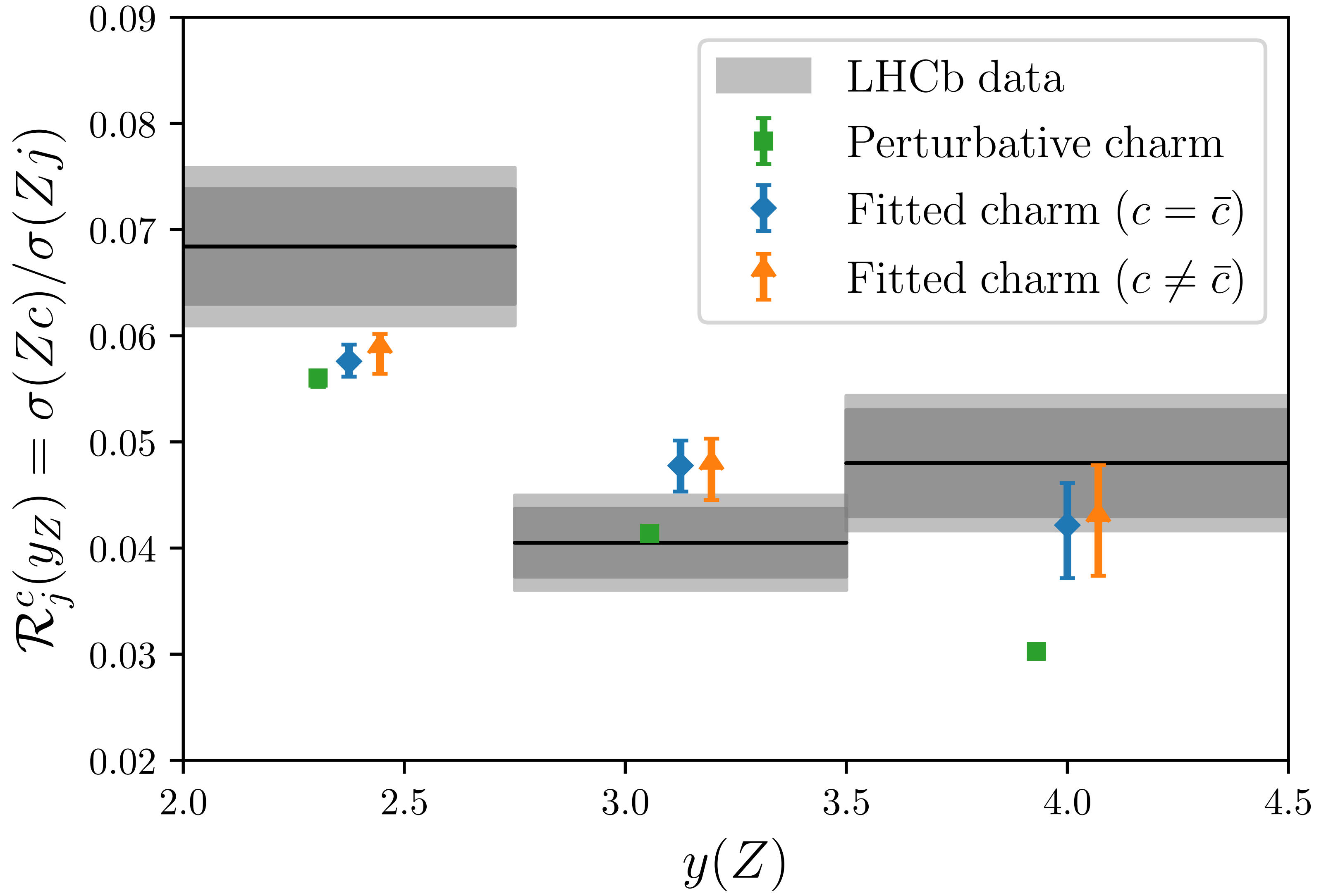


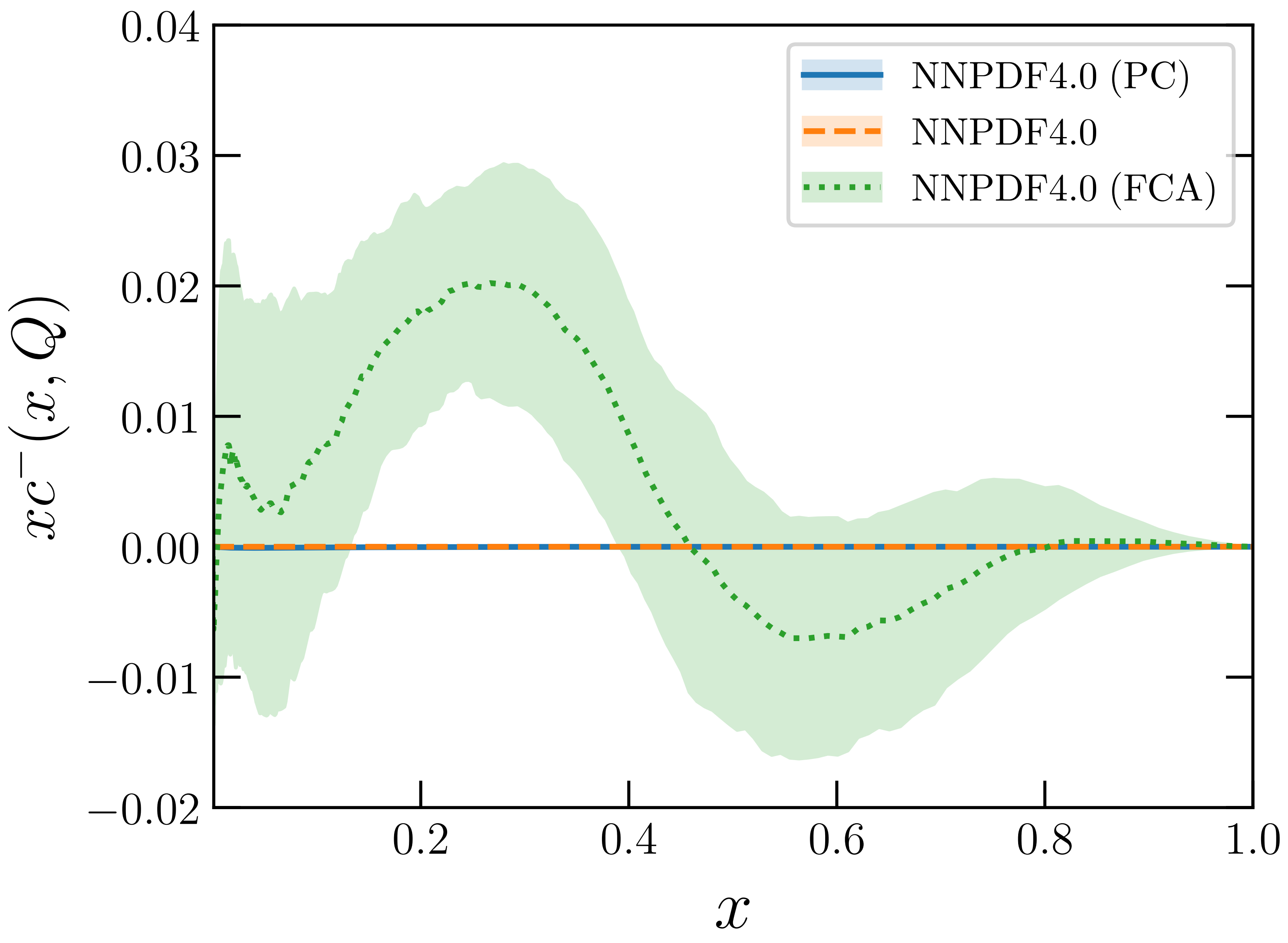
Separate determination of $c/\bar{c}$ PDFs

- There is no reason why intrinsic charm valence should vanish
- Projections for $Z + c$-jet at the LHCb favours non-vanishing valence charm
- Future LHC data will verify or falsify a non-zero charm valence.
- NNPDF4.1 will be based on a determination of a separate charm and anti-charm PDFs









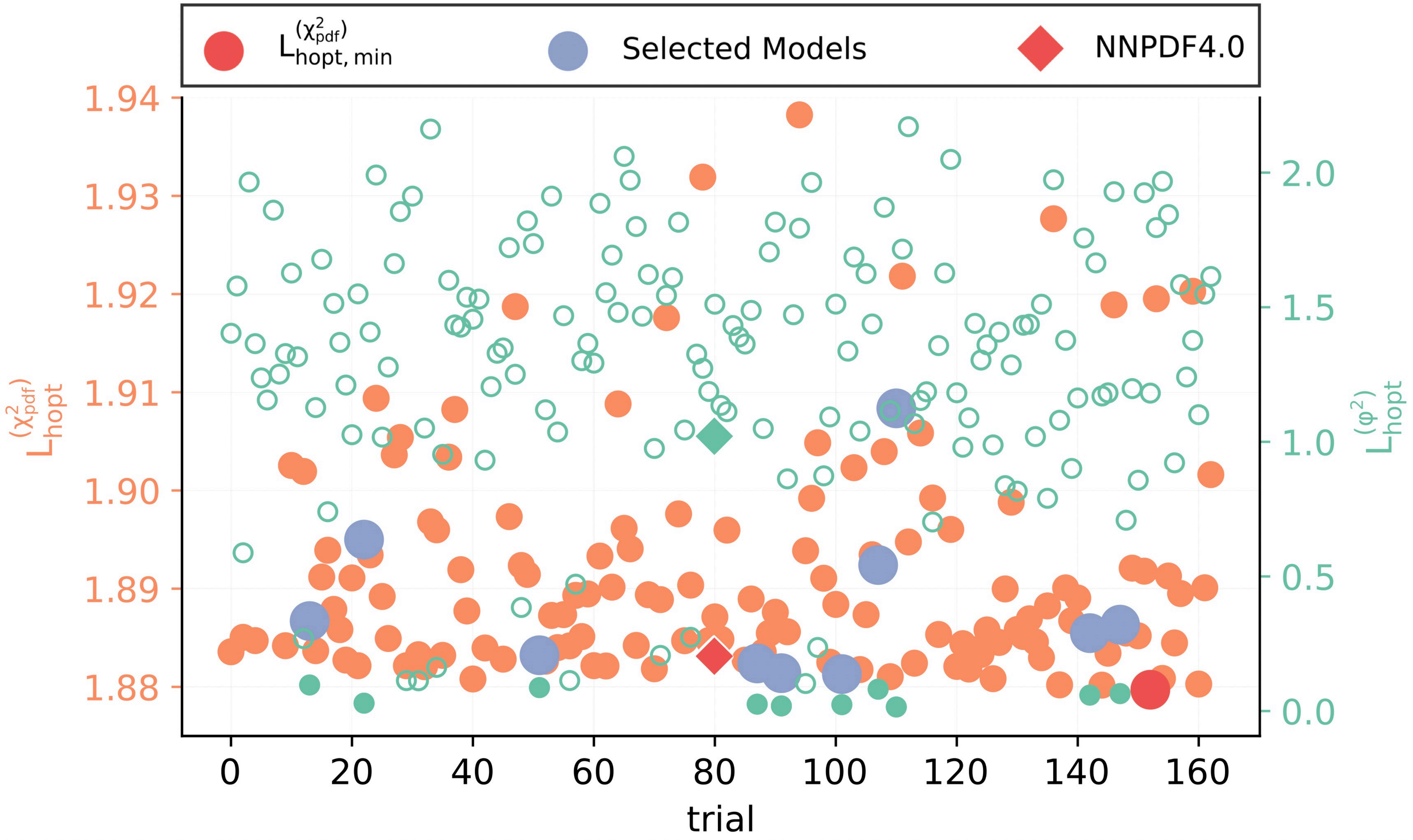
Ensemble-based Hyperparameter Optimisation

- ML applications rely on a **large number of hyper-parameters** with each combination defining a particular model
- Selection of the set of hyperparameters is crucial for a model to describe best the data & able to generalise $\Longleftrightarrow$ **Uncertainty quantifications**
- In NNPDF4.1, hyperparameter optimisation will be done **accounting for the full PDF distribution**
- The methodology still relies on the k-fold procedure but using a different $L_{\text{hopt}}^{(\chi^2)}$ definition:

$$L_{\text{hopt}}^{\left(\chi^2_{\text{pdf}}\right)}(\hat{\boldsymbol{\theta}}) = \frac{1}{n_{\text{fold}}} \sum_{p=1}^{n_{\text{fold}}} \overset{*}{\min_{\boldsymbol{\theta}\in\Theta}} \left(\left\langle \chi^2_{\text{PDF},p}(\boldsymbol{\theta}, \hat{\boldsymbol{\theta}}) \right\rangle_{\text{rep}} \right)$$

- With an additional selection metric that maximises the generalisation power of the models:

$$\varphi^2_{\chi^2} = \frac{1}{n_{\text{dat}}} \sum_{i,j=1}^{n_{\text{dat}}} (\text{cov})^{-1}_{ij} T_{ji}, \quad L_{\text{hopt}}^{(\varphi^2)}(\hat{\boldsymbol{\theta}}) \equiv \left(\frac{1}{n_{\text{K}}} \sum_{p=1}^{n_{\text{K}}} \varphi^2_{\chi^2_p}(\hat{\boldsymbol{\theta}}) \right)^{-1}$$



The outcome **is not a single Model**

Randomly sample over the complete population of acceptable hyperparameters displaying comparable performance

Ensemble-based Hyperparameter Optimisation: Results

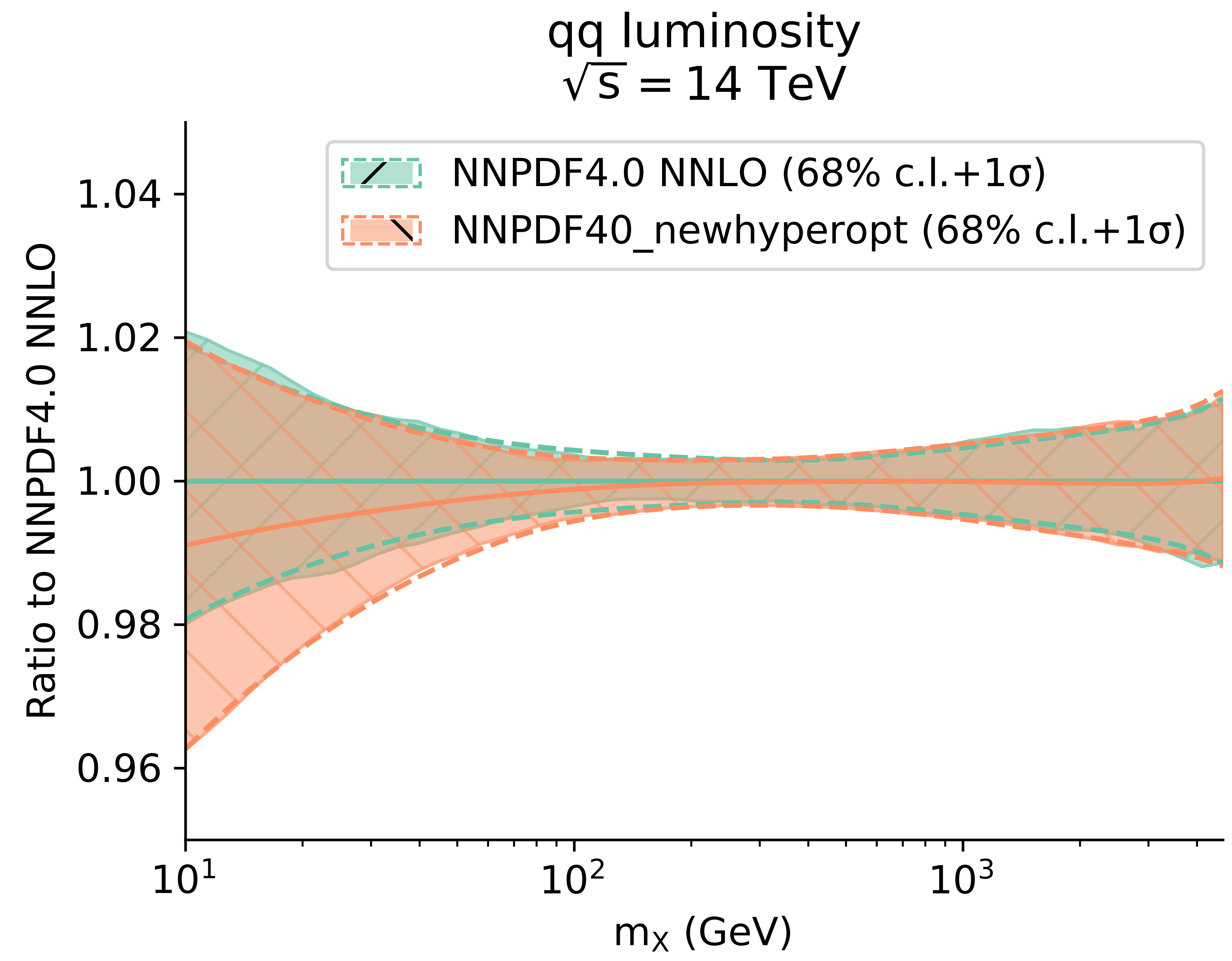
Ensemble-based hyperparameter optimisation is only possible with **hardware acceleration (GPUs)** and that provide various technical advantages:

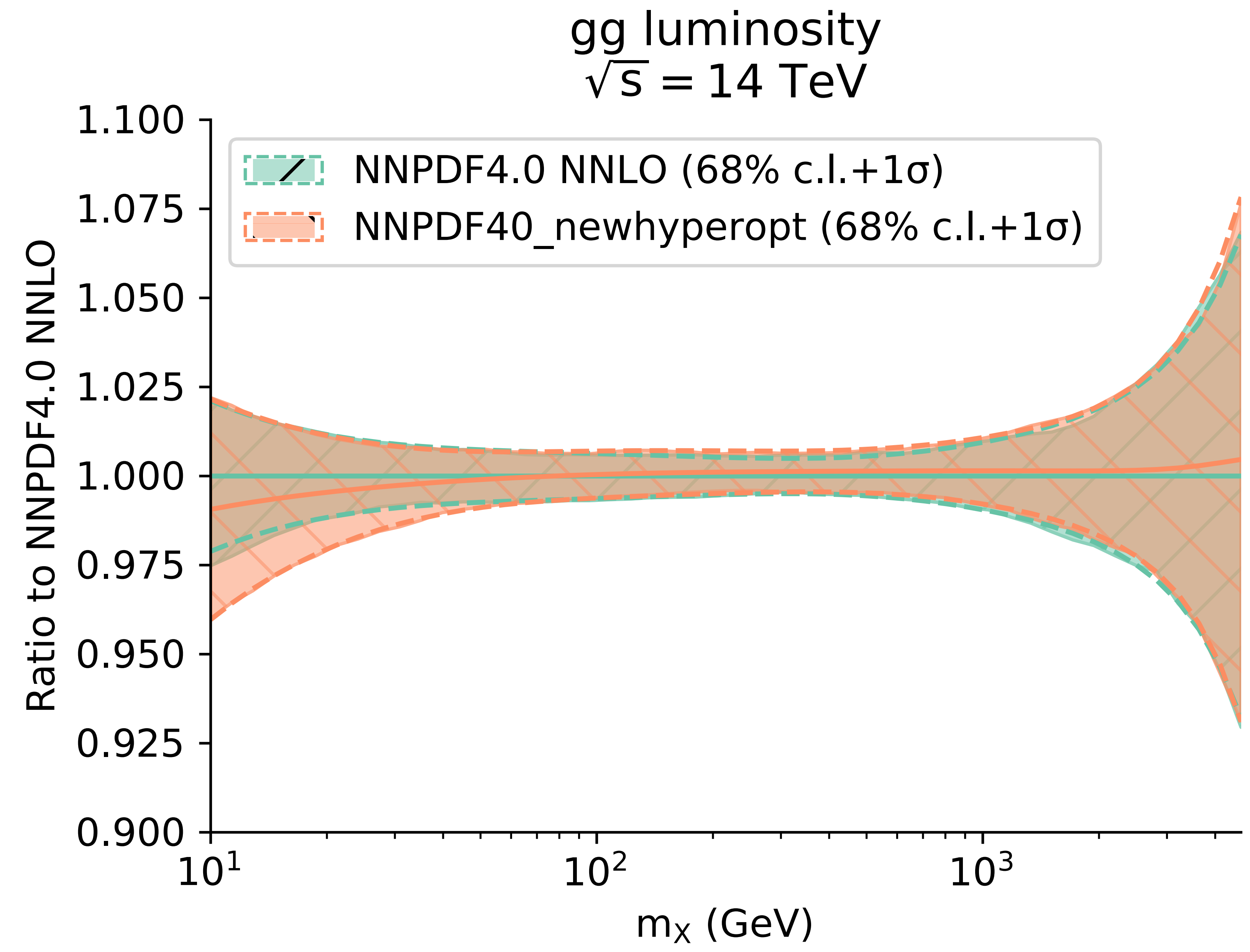
# Replicas	10	50	100
Energy reduction	78%	87%	91%
Cost reduction	−45%	47%	55%

❖ Speed scales with the number of replicas (up to a factor of ~200)

❖ No significant increase of memory with the number of replicas

❖ Up to 90% energy reduction $\Longleftrightarrow$ More sustainable ML training





At the PDF level:

❖ **Excellent consistency with NNPDF4.0** with a moderate increase of the uncertainties in the extrapolation regions

❖ Non-trivial validation of the NNPDF methodology

Part III: Data

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How well do PDFs accommodate new data?

- Test PDF sets against new precise measurements from Run I/II using NNLO theories (w/o K-factors)
- Aim to assess how well PDF sets describe unseen data and whether these data will have effects on fits
- Agreement between data and theoretical predictions are quantified using the χ^2 definition:

$$\chi^2 = \frac{1}{n_{\rm dat}} \sum_{i,j=1}^{n_{\rm dat}} \left(T_i^{(0)} - D_i\right) \left(\mathrm{cov}^{-1}\right)_{ij} \left(T_j^{(0)} - D_j\right)$$

- Contributions to the covariance matrix include all sources of theoretical uncertainties:

$$\mathrm{cov}_{ij} = \left(\mathrm{cov}_{\rm exp}\right)_{ij} + \left(\mathrm{cov}_{\rm th}\right)_{ij}$$

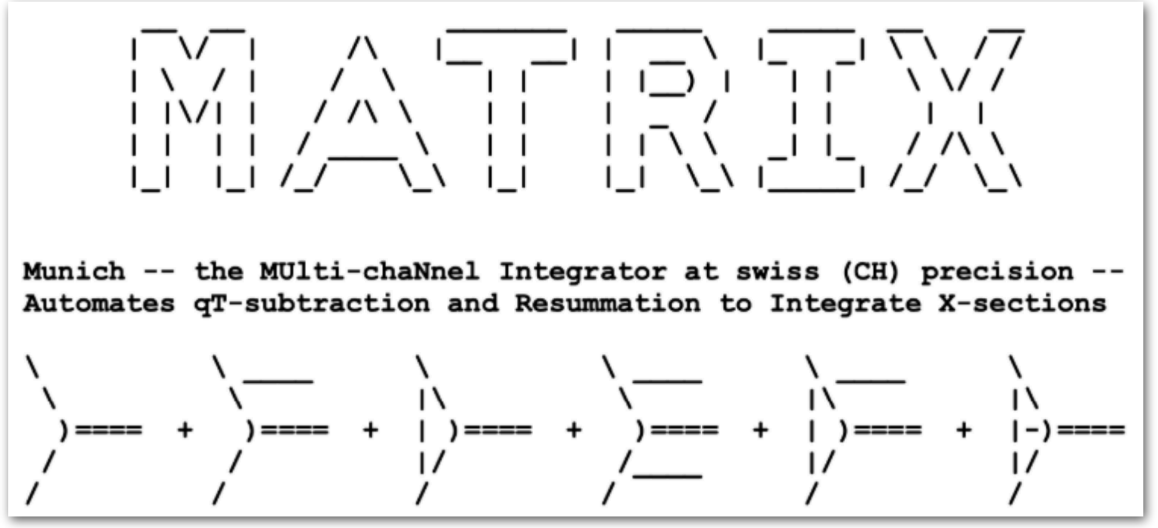
$$\left(\mathrm{cov}_{\rm th}\right)_{ij} = \left(\mathrm{cov}_{\rm mho}\right)_{ij} + \left(\mathrm{cov}_{\rm pdf}\right)_{ij} + \left(\mathrm{cov}_{\rm as}\right)_{ij}$$

$$\left(\mathrm{cov}^{\rm HES}_{\rm pdf}\right)_{ij} = \sum_{k=1}^{n_{\rm eig}} \left(T_i^{(k)} - T_i^{(0)}\right)\left(T_j^{(k)} - T_j^{(0)}\right)$$

$$\left(\mathrm{cov}^{\rm MC}_{\rm pdf}\right)_{ij} = \frac{1}{n_{\rm rep}} \sum_{k=1}^{n_{\rm rep}} \left(T_i^{(k)} - \langle T_i\rangle_{\rm rep}\right)\left(T_j^{(k)} - \langle T_j\rangle_{\rm rep}\right)$$

PineAPPL

https://github.com/NNPDF/pineappl



https://matrix.hepforge.org/

https://ploughshare.web.cern.ch/ploughshare/

$$\left(\mathrm{cov}_{\rm mho}\right)_{ij} = \frac{1}{3}\left\{\Delta_i^{+0}\Delta_j^{+0} + \Delta_i^{-0}\Delta_j^{-0} + \Delta_i^{0+}\Delta_j^{0+} + \Delta_i^{0-}\Delta_j^{0-} + \Delta_i^{++}\Delta_j^{++} + \Delta_i^{--}\Delta_j^{--}\right\}$$

$$\Delta_i\left(\kappa_R, \kappa_F\right) = T_i\left(\mu_R = \kappa_R \mu_R^{(0)}, \mu_F = \kappa_R \mu_F^{(0)}\right) - T_i\left(\mu_R^{(0)}, \mu_F^{(0)}\right)$$

$$\Delta_i^{+0} = \Delta_i(2,1), \quad \Delta_i^{-0} = \Delta_i(1/2,1), \quad \Delta_i^{0+} = \Delta_i(1,1/2)$$
$$\Delta_i^{0-} = \Delta_i(1,1/2), \quad \Delta_i^{++} = \Delta_i(2,2), \quad \Delta_i^{--} = \Delta_i(1/2,1/2)$$

$$\left(\mathrm{cov}_{\rm as}\right)_{ij} = \frac{1}{2}\left\{\Delta^+_{i,\alpha_s}\Delta^+_{j,\alpha_s} + \Delta^-_{i,\alpha_s}\Delta^-_{j,\alpha_s}\right\}$$

$$\Delta^+_{i,\alpha_s} \equiv T_i\left(\alpha_s = 0.119\right) - T_i\left(\alpha_s = 0.118\right)$$
$$\Delta^-_{i,\alpha_s} \equiv T_i\left(\alpha_s = 0.118\right) - T_i\left(\alpha_s = 0.117\right)$$

Experimental Data included in the study

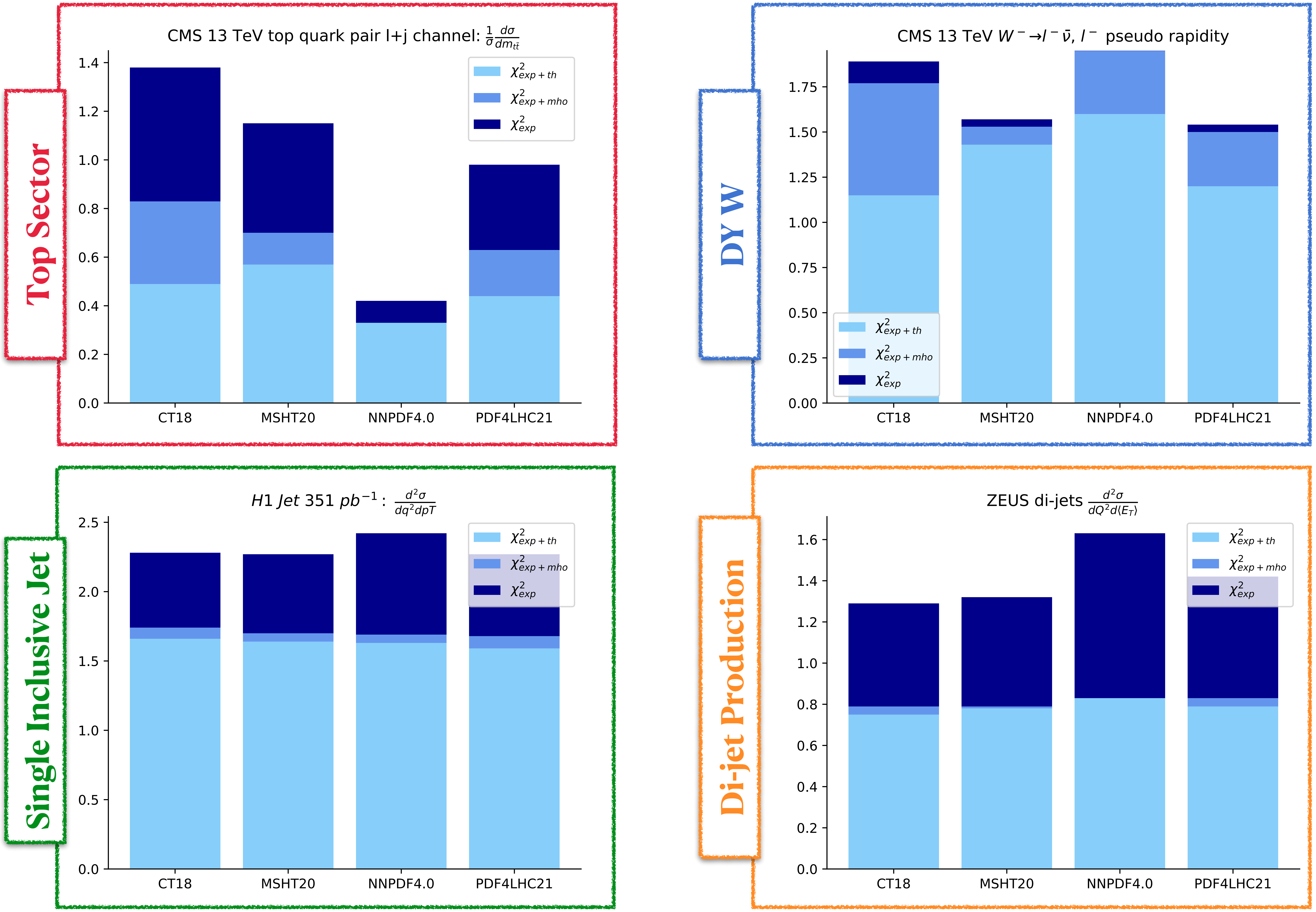
Process	Experiment	Final State	Observable	$\sqrt{s}$ (TeV)	$\mathcal{L}$ (fb^{-1})	$n_{\rm dat}$
LHC W, Z	ATLAS	Z p_T spectrum	$\left(\frac{1}{\sigma}\right)\frac{d\sigma}{dp_T^{\ell\ell}}$	13	36.1	38
	CMS	W incl. prod.	$\frac{d\sigma}{d\|\eta\|}$	13	35.9	36
	LHCb	Z incl. forward prod.	$\frac{d\sigma}{dy^Z}$	13	5.1	17
	ATLAS	Z incl. prod.	$\frac{d\sigma}{d\|y\|}$	8	20.2	7
top-pair	ATLAS	all-hadronic	$\left(\frac{1}{\sigma}\right)\frac{d\sigma}{dm_{t\bar{t}}}$	13	36.1	9
			$\left(\frac{1}{\sigma}\right)\frac{d\sigma}{d\|y_{t\bar{t}}\|}$	13	36.1	12
			$\left(\frac{1}{\sigma}\right)\frac{d^2\sigma}{d\|y_{t\bar{t}}\|dm_{t\bar{t}}}$	13	36.1	11
	ATLAS	ℓ+jets	$\left(\frac{1}{\sigma}\right)\frac{d\sigma}{dm_{t\bar{t}}}$	13	36.1	9
			$\left(\frac{1}{\sigma}\right)\frac{d\sigma}{dp_T^t}$	13	36.1	8
			$\left(\frac{1}{\sigma}\right)\frac{d\sigma}{d\|y_t\|}$	13	36.1	5
			$\left(\frac{1}{\sigma}\right)\frac{d\sigma}{d\|y_{t\bar{t}}\|}$	13	36.1	7
	CMS	ℓ+jets	$\left(\frac{1}{\sigma}\right)\frac{d\sigma}{dm_{t\bar{t}}}$	13	137	15
			$\left(\frac{1}{\sigma}\right)\frac{d\sigma}{dp_T^t}$	13	137	16
			$\left(\frac{1}{\sigma}\right)\frac{d\sigma}{d\|y_{t\bar{t}}\|}$	13	137	10
			$\left(\frac{1}{\sigma}\right)\frac{d\sigma}{d\|y_t\|}$	13	137	11
			$\left(\frac{1}{\sigma}\right)\frac{d^2\sigma}{d\|y_{t\bar{t}}\|dm_{t\bar{t}}}$	13	137	35

LHC jets	ATLAS	incl. jet $R = 0.6$	$\frac{d^2\sigma}{dp_T d\|y\|}$	13	3.2	177
	CMS	incl. jets $R = 0.4$ (0.7)	$\frac{d^2\sigma}{dp_T d\|y\|}$	13	36.3 (33.5)	78
	ATLAS	di-jets $R = 0.6$	$\frac{d^2\sigma}{dm_{jj} d\|y^*\|}$	13	3.2	136
HERA jets	H1	incl. jet (low Q^2)	$\frac{d^2\sigma}{dQ^2 dp_T}$	0.319	0.29	48
	H1	incl. jet (high Q^2)	$\frac{d^2\sigma}{dQ^2 dp_T}$	0.319	0.351	24
	ZEUS	incl. jet	$\frac{d^2\sigma}{dQ^2 dE_T}$	0.300	0.038	30
	ZEUS	incl. jet	$\frac{d^2\sigma}{dQ^2 dE_T}$	0.319	0.082	30
	H1	di-jets (low Q^2)	$\frac{d^2\sigma}{dQ^2 d\langle p_T\rangle}$	0.319	0.29	48
	H1	di-jets (high Q^2)	$\frac{d^2\sigma}{dQ^2 d\langle p_T\rangle}$	0.319	0.351	24
	ZEUS	di-jets	$\frac{d^2\sigma}{dQ^2 d\langle E_T\rangle}$	0.319	0.374	22

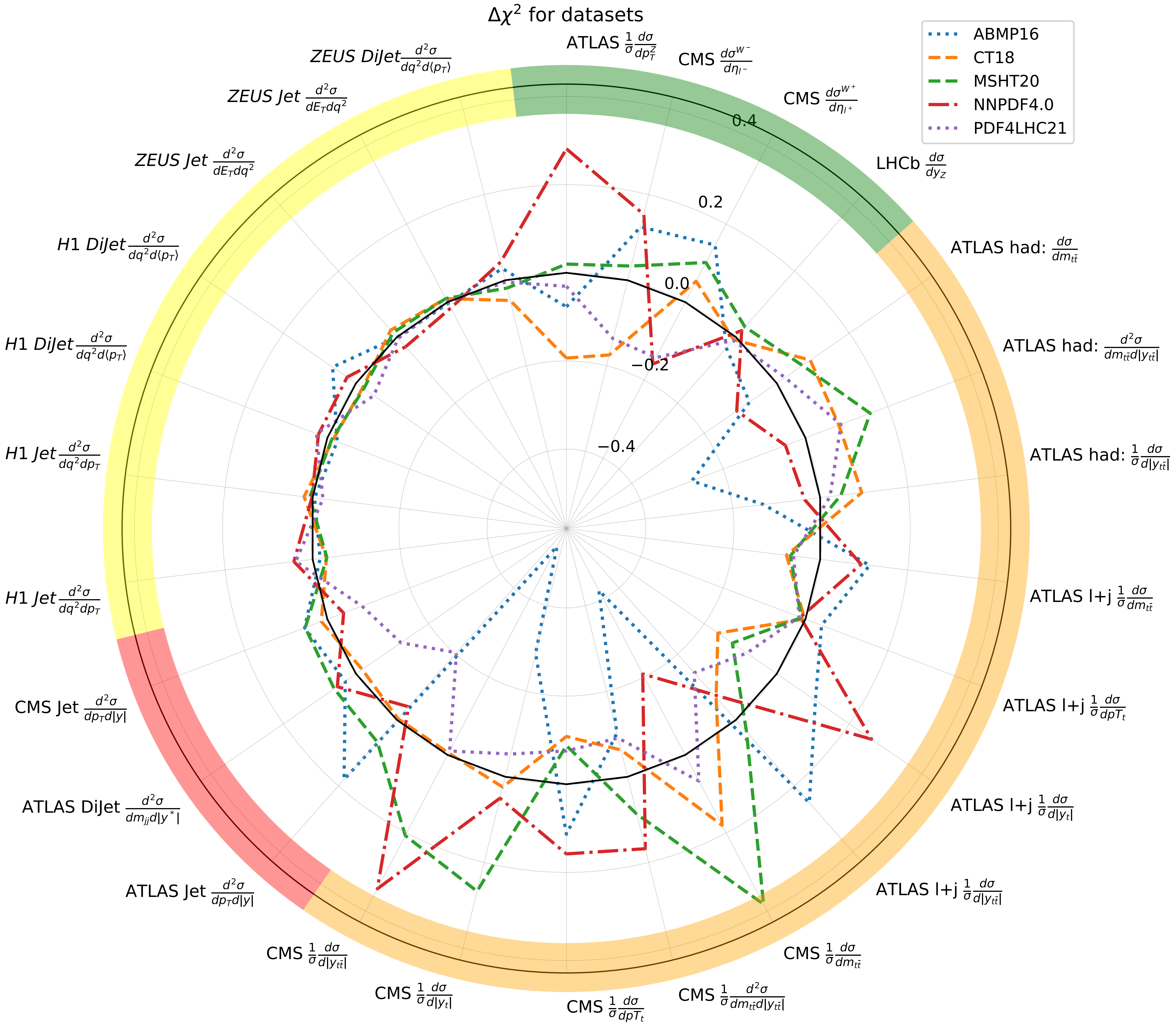
Dataset selection criteria:

- Not included in NNPDF4.0 except for ALTAS Z @ 8 TeV
- Publicly available on HepData
- Provide info on PDFs of # partons & computable @ NNLO interfaced to PineAPPL fast interpolation grids

χ^2 comparisons for various PDFs



- ❖ All PDF sets have similar predictive power
- ❖ The inclusion of MHO uncertainties can have significant impact on the description of data
- ❖ By taking into account all possible sources of uncertainties (MHO, PDF, α_s), the differences at the cross section level dissipate
- ❖ LHC measurements do not strongly discriminate among PDF



$\Delta\chi^2$ Results

❖ Relative change in the total χ^2 due to a change in the input PDF

$$\Delta\chi^{2(i)} = \frac{\chi^{2(i)}_{\text{exp+th}} - \left\langle \chi^2_{\text{exp+th}} \right\rangle_{\text{pdfs}}}{\left\langle \chi^2_{\text{exp+th}} \right\rangle_{\text{pdfs}}}$$

where

$$\left\langle \chi^2_{\text{exp+th}} \right\rangle_{\text{pdfs}} = \frac{1}{n_{\text{pdfs}}} \sum_{i=1}^{n_{\text{pdfs}}} \chi^{2(i)}_{\text{exp+th}}$$

❖ **No systematic outlier** seen in the data description despite noticeable differences at the level of PDF

❖ As anticipated, PDF4LHC21 represents the **average** (with $\Delta\chi^2 \sim 0$)

Conclusions & Outlook

- The precision era at the LHC requires precise & accurate PDFs and advancements are needed for the **"three pillars"**: theory, methodology, and data

- Significant progress in the NNPDF global analysis for a state-of-the-art determination at aN3LO⊗QED⊗MHOUs

- Significant improvements in the Hyperparameter Optimisation using ensemble-based methodology ⟺ **demonstrates the robustness of the NNPDF uncertainty estimate**

- A quantitative appraisal of PDF fits using precision LHC measurements show that **all PDF sets have similar predictive power** despite significant differences at the PDF level

- NNPDF4.1 will be based on the best theory (at the very least with pure NNLO hadronic predictions) and fitting methodology, as well as more precision LHC measurements

THANKS FOR YOUR ATTENTION

"Wanderer above the Sea of Fog" by Caspar David Friedrich