Determination of PDFs at LO, NLO, NNLO with correlated uncertainties between orders using HERAFitter

arXiv:1404.4234

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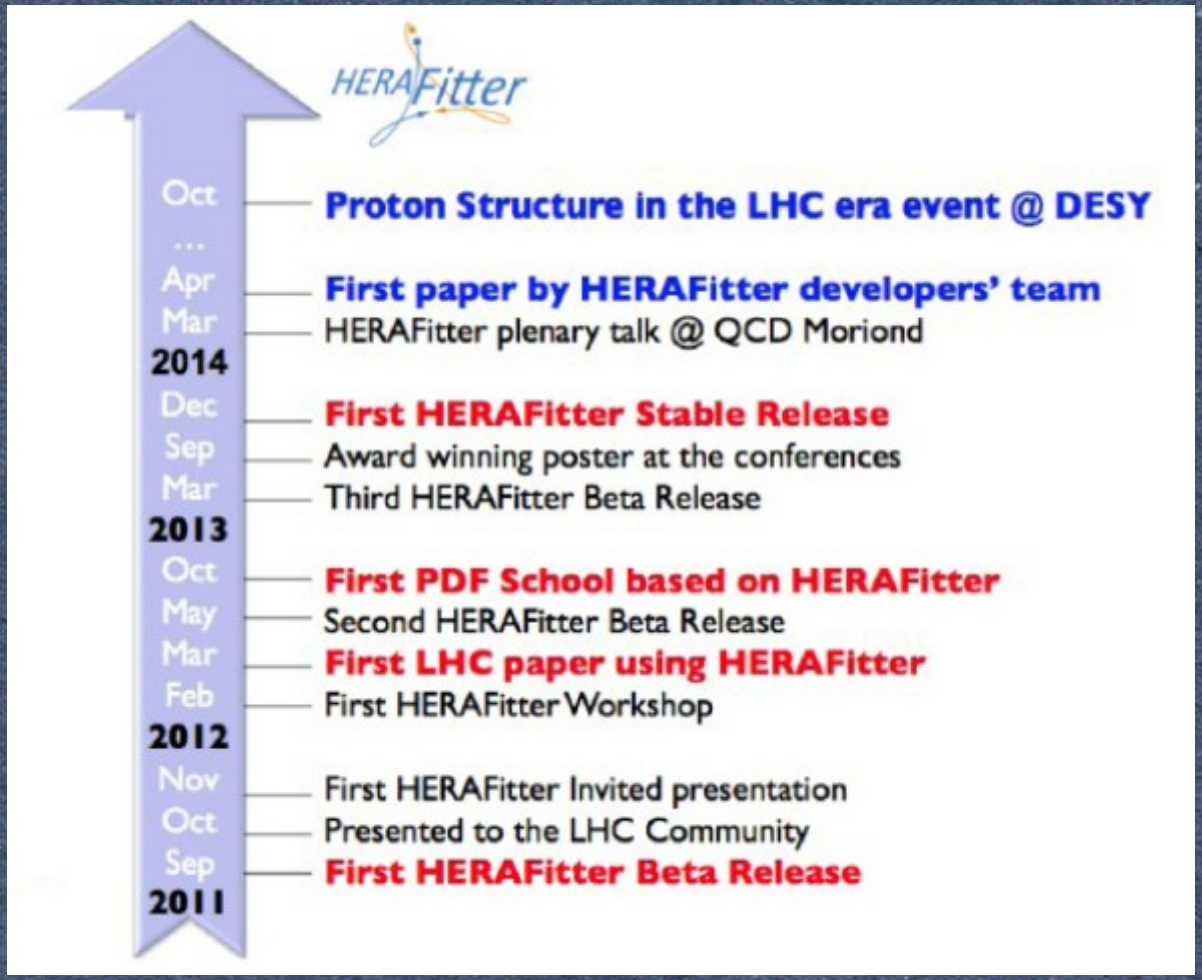
HERAFitter Project

HERAFitter project

www.herafitter.org

Different groups (CT, MSTW, NNPDF, HERAPDF, ABM, JR) use different data and methodology to extract PDFs → leads to differences in predicted cross sections



HERAFitter is an open source QCD fit platform, which provides a framework:

- for benchmarking and understanding such differences
- for studying impact of new data on PDFs

HERAFitter structure

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Modular structure of HERAFitter:

Initialization

Input Data

Data Type:
- collider ep
- collider pp, ppbar
- fixed target

Theory Predictions

Factorisation Theorem:
- PDF parametrisation
- QCD evalution
- cross section calculation

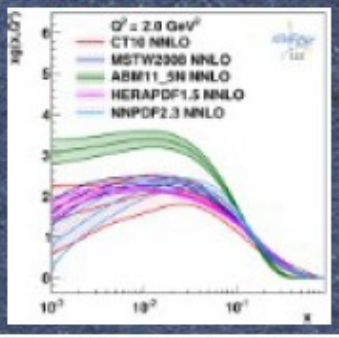
Minimisation

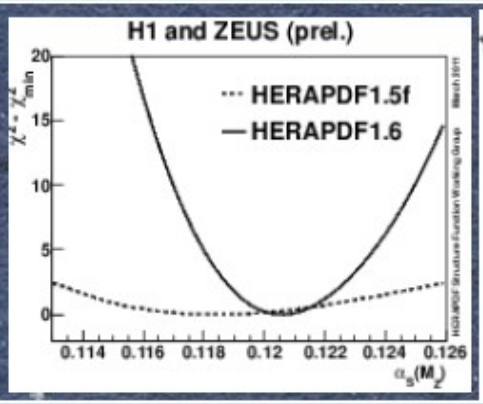
Treatment of uncertainties:
- Nuisance parameters
- Covariance matrix
- Monte Carlo method

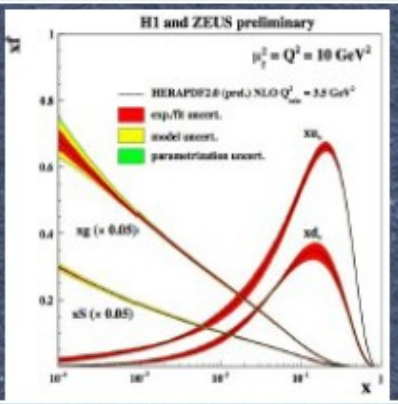
- Performance: 15min – 2h
- Fast tools needed to perform PDF fits: APPLGRID, FASTNLO

- LHAPDF grids
- alphas, mc, …
- data to theory comparison
- χ^2, shifts, pulls

Results







PDFs at LO, NLO, NNLO with Correlated Uncertainties: Motivation and Methodology

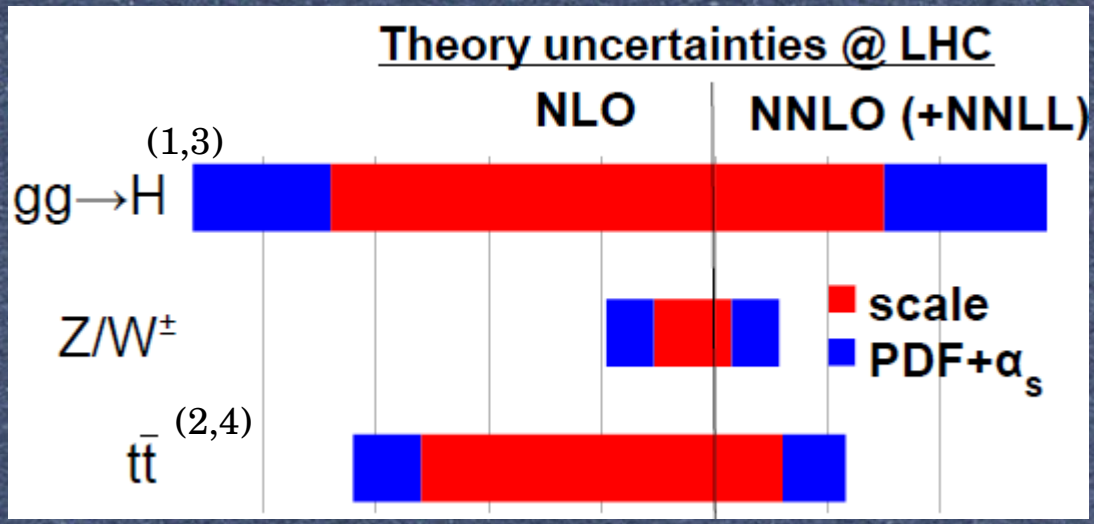
Introduction / Motivation

- Various processes at LHC are calculated at LO, NLO, NNLO accuracy in QCD. Cross sections are obtained by pairing PDF set with coefficient functions at the corresponding order.

- Theoretical uncertainties on predicted cross sections arise from PDFs themselves and from missing higher orders (determined by varying factorisation and renormalisation scales).

- NLO: scale variations often exceed PDF uncertainties.
- NNLO: sensitivity to scale is reduced and PDF uncertainties often exceed size of scale variations

* Plot by M. Lisovyi (talk at DIS 2014)



1) Anastasiou et al. 1202.3638, Ball et al. 1211.5142.
2) Cacciari et al. 1111.6859
3) Higgs XS working group
4) Czakan et al. 1303.6254

Introduction / Motivation

- To reduce theoretical (and experimental) uncertainties ratios of two processes cross sections can be used. Assume that for the first process both NLO and NNLO calculations exist, while for the second process only NLO. Theoretical predictions can be constructed in several ways:

$$\frac{\sigma_1^{NLO}(PDF^{NLO})}{\sigma_2^{NLO}(PDF^{NLO})}$$

- ✔ Cancelation of PDF unc.
- ✗ Large scale unc.

$$\frac{\sigma_1^{NNLO}(PDF^{NNLO})}{\sigma_2^{NLO}(PDF^{NLO})}$$

- ✗ PDF unc. do not cancel
- ✔ Scale unc. reduced

$$\frac{\sigma_1^{NNLO}(PDF^{NNLO})}{\sigma_2^{NLO}(PDF^{NNLO})}$$

- ✔ PDF unc. cancel
- ✔ Improved scale unc.
- ✗ Unclear definition in pQCD

$$\frac{\sigma_1^{NNLO}(PDF_{corr}^{NNLO})}{\sigma_2^{NLO}(PDF_{corr}^{NLO})}$$

- ✔ PDF unc. cancels
- ✔ Scale unc. reduced

Sets of PDFs with correlated uncertainties between different orders required

- Some Monte Carlo generators (Powheg, MC@NLO, aMC@NLO) use NLO matrix-element calculations which are matched to parton showers requiring LO PDFs for consistency → for a coherent determination of PDF uncertainties a set of PDFs correlated between LO and NLO is required

QCD fit

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- Sets of PDFs with correlated uncertainties at LO, NLO and NNLO are determined using HERAFitter preserving correlations between uncertainties in different orders.
- Combined HERA I inclusive DIS measurements are used as an input data, taking into account correlated systematic uncertainties originating from 114 different sources.
- To stay in kinematic region where QCD is applicable data is required to satisfy $Q^2_{min} > 7.5\ GeV^2$ condition.
- PDFs at the starting scale of $Q^2_0 = 1.7\ GeV^2$ are parametrised using 13 free parameters:

$$xg(x) = A_g \cdot x^{B_g} \cdot (1-x)^{C_g} - A_g' \cdot x^{B_g'} \cdot (1-x)^{C_g'}$$
$$xu_v(x) = A_{u_v} \cdot x^{B_{u_v}} \cdot (1-x)^{C_{u_v}} \cdot (1+E_{u_v} x^2)$$
$$xd_v(x) = A_{d_v} \cdot x^{B_{d_v}} \cdot (1-x)^{C_{d_v}}$$
$$x\bar{U}(x) = A_{\bar{U}} \cdot x^{B_{\bar{U}}} \cdot (1-x)^{C_{\bar{U}}}$$
$$x\bar{D}(x) = A_{\bar{D}} \cdot x^{B_{\bar{D}}} \cdot (1-x)^{C_{\bar{D}}}$$

* Here: $x\bar{U} = x\bar{u}$, $x\bar{D} = x\bar{d} + x\bar{s}$, $xs = x\bar{s}$, $x\bar{s} = r_s\, x\bar{d}$
* QCD sum rules constrain normalisation parameters: A_{u_v}, A_{d_v}, A_g
* Condition that $x\bar{u} \to x\bar{d}$ as $x \to 0$ constrains $B_{\bar{U}} = B_{\bar{D}}$ and $A_{\bar{U}} = A_{\bar{D}}/(1+r_s)$
* To suppress negative gluon at high x C_g' is set to 25

- Parametrisation uncertainty is estimated by adding one free parameter at a time and constructing an envelope of largest deviations (following HERAPDF prescription).

QCD model

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- The following settings are used in the fits:

Settings	LO	NLO	NNLO	Variation
HF scheme	RT Opt	RT Opt	RT Opt	--
$r_s = \bar{s}/\bar{d}$	1.0	1.0	1.0	± 0.3
M_c [GeV]	1.38	1.38	1.32*	± 0.06
M_b [GeV]	4.75	4.75	4.75	+ 0.25 / - 045
M_t [GeV]**	14317.82	14317.82	14317.82	--
α_s	0.13***	0.1184	0.1184	± 0.002
Q^2_0 [GeV^2]	1.7	1.7	1.7	- 0.2
Q^2_{min} [GeV^2]	7.5	7.5	7.5	± 2.5

- Variation of the choices above shown in the last column are included in model uncertainties of the fit.
- Model and parametrisation uncertainties are treated correlated between orders.

** M_c scan at NNLO was performed using HERA DIS and charm data*

*** Top mass is chosen as large as possible in QCDNUM, in order to stay in 5 flavor regime at high Q^2 values*

**** Motivated by HERAPDF1.5LO*

Extraction of correlated PDFs

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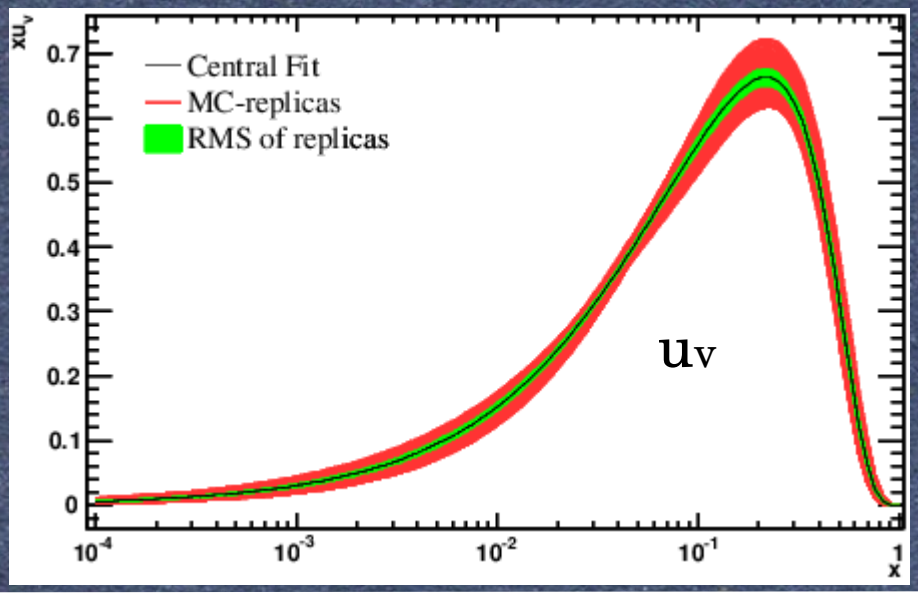
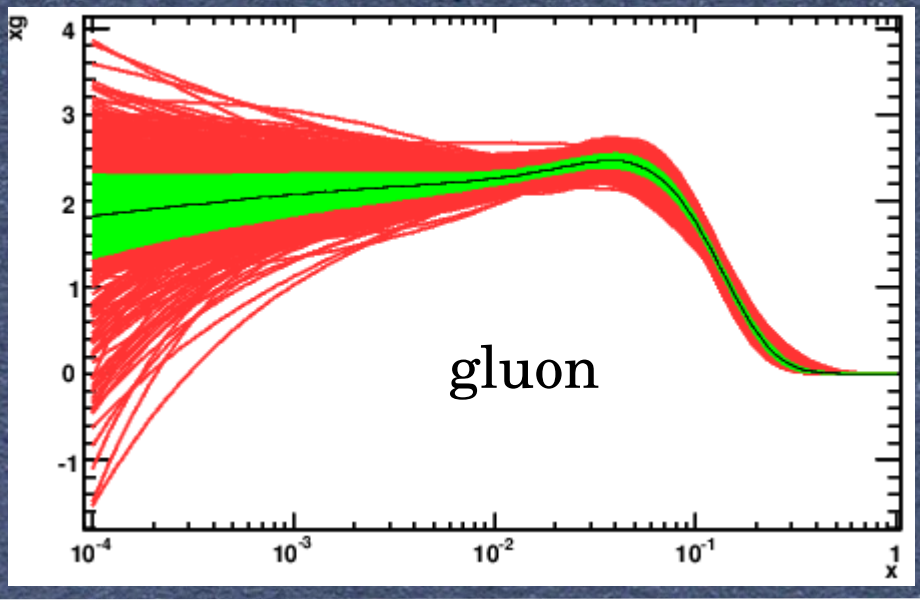
In order to determine experimental PDF uncertainties preserving correlation between LO, NLO, NNLO Monte Carlo replica method is used:

- 1337 MC replicas are prepared by randomly fluctuating measured cross sections within their uncertainties,
- a QCD fit to each replica is performed consistently at different orders,
- synchronization of the fit between orders is done by using the same seed, when constructing MC replicas,
- central set of PDFs is obtained by taking the average of the replicas,
- experimental uncertainties are determined by taking RMS of the replicas.





Extraction of correlated PDFs

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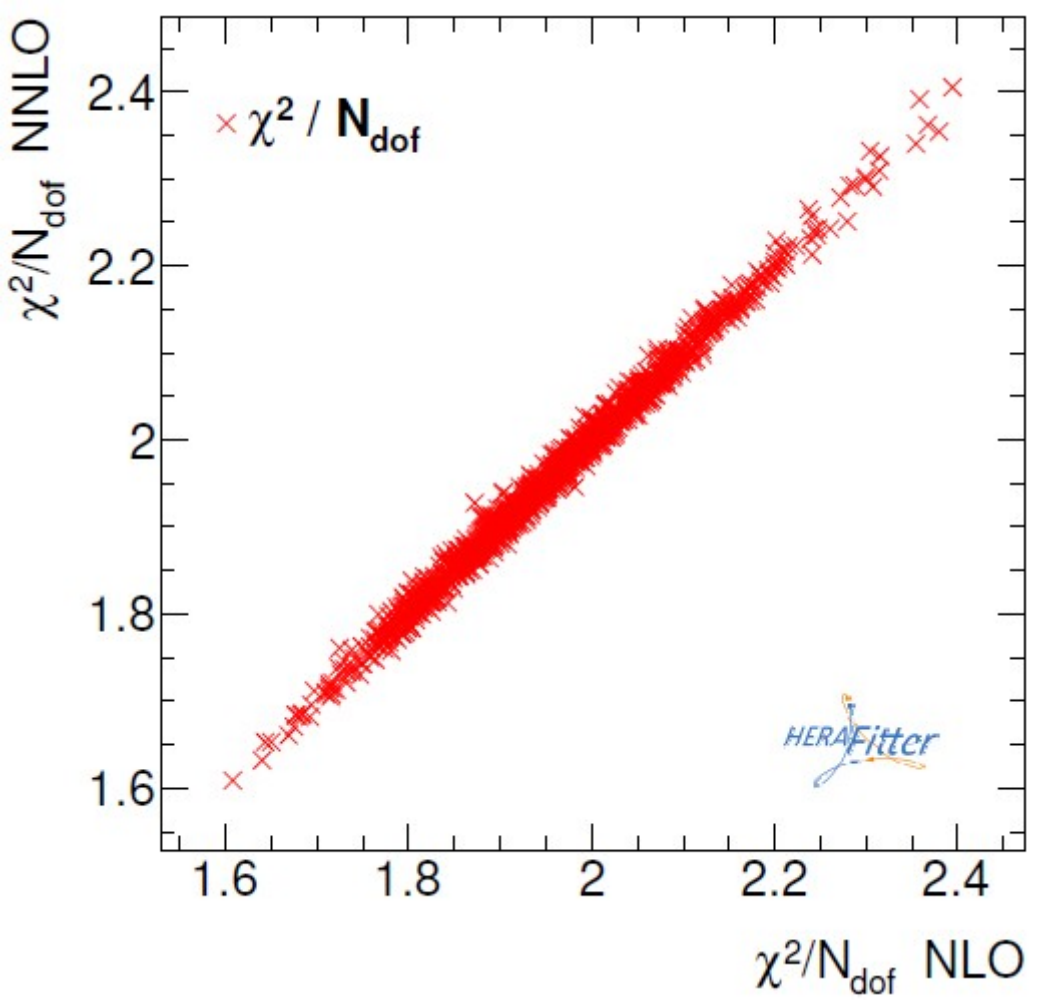

- χ^2 / Ndof correlation between NLO and NNLO.
- High degree of correlation is observed between all three orders.

Eigenvector representation

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Eigenvector representation typically requires fewer PDF sets to describe the PDF uncertainties → more convenient than the MC representation for many applications.

- a procedure suggested for extraction of META PDFs is used *[arXiv:1401.0013]*,
- full covariance matrix of PDFs at the starting scale on the QCDNUM x-grid is extracted,
- covariance matrix is then diagonalized and leading eigenvalues are kept,
- central set and eigenvectors are than evaluated to larger scales using QCDNUM.
- For NLO – NNLO 39 eigenvectors are already in a very good agreement with MC representation.

Eigenvector representation

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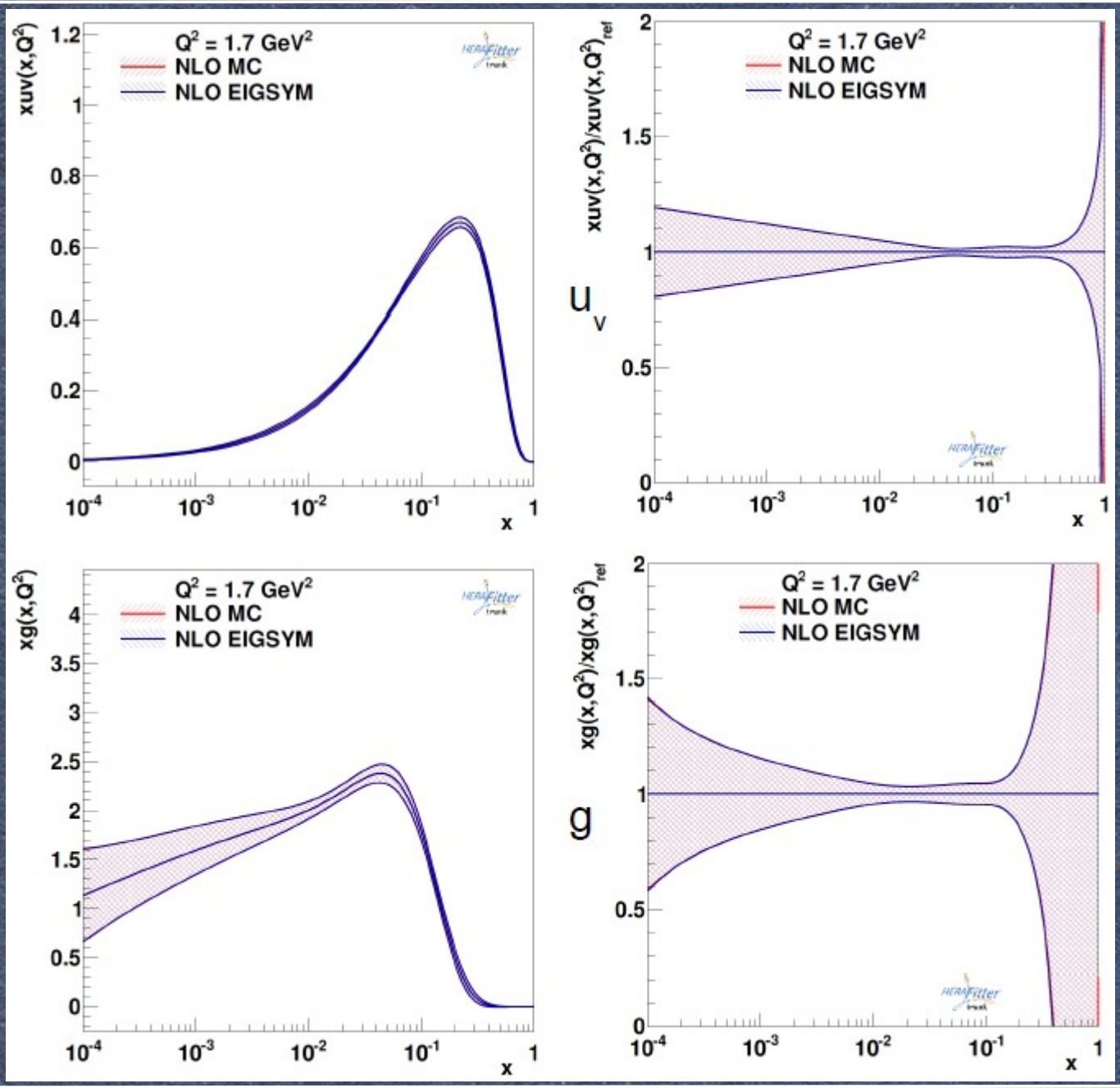

- Example of u_v and gluon distributions with uncertainties from eigenvectors and replicas (at NLO starting scale).
- A good agreement between eigenvectors and original MC replicas is observed.

PDF correlations between different orders

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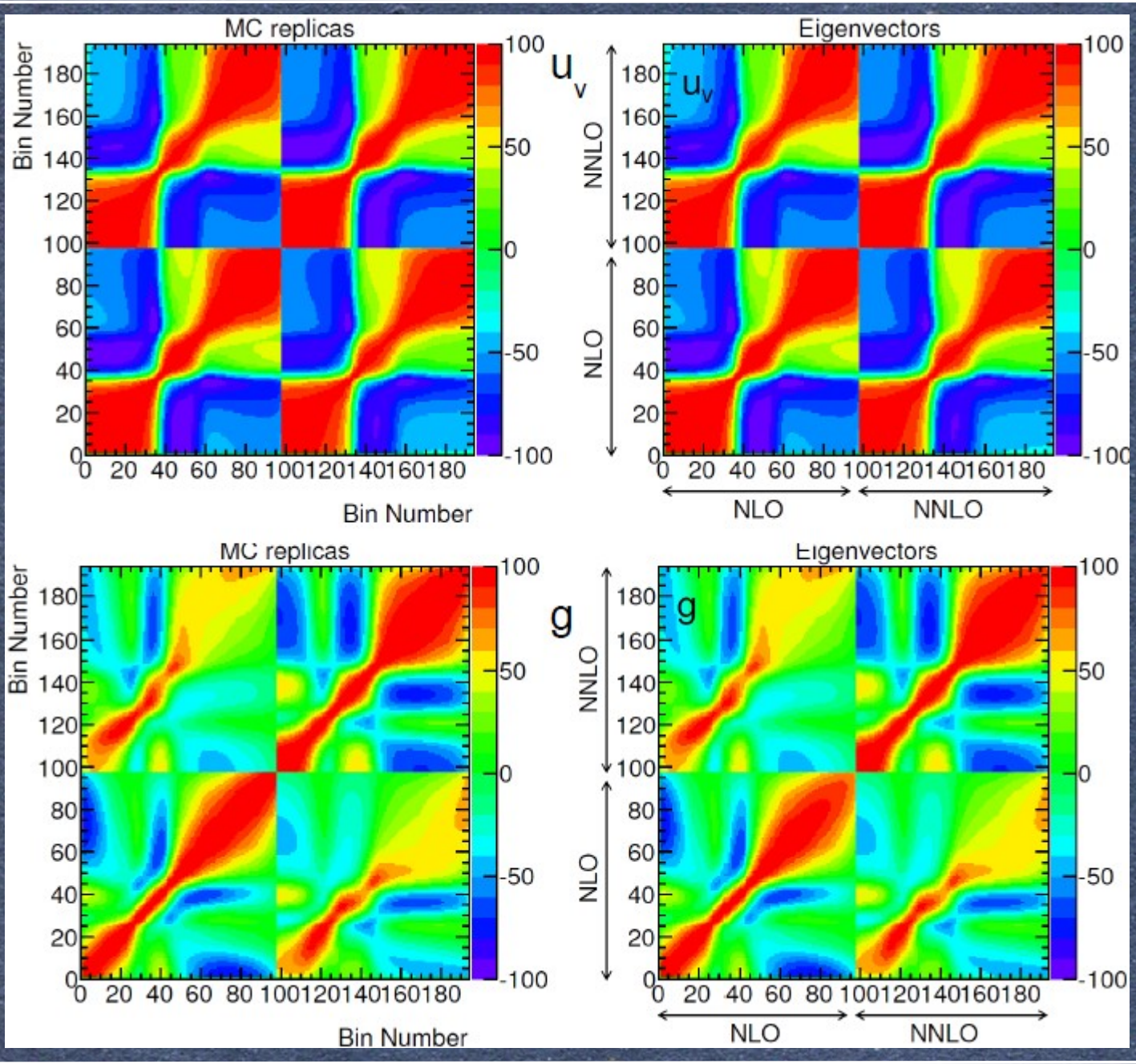

- Correlation coefficients as a function of the x-grid point for the NLO (bins 1 - 97) and NNLO (bins 98 - 194) PDFs.
- All PDFs show high degree of correlation between similar x values.
- Strong correlation between NLO and NNLO PDFs (a bit less for high-x gluon).
- Eigenvectors well reproduce all correlations (small variations at high x).

Methodology summary

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- Fit using HERA data only
- Synchronize QCD fit settings for fits at LO, NLO, NNLO (functional form, starting scale, data cuts).
- Use MC method for uncertainties, synchronize seeds for fits at different orders
- Produce a set of PDFs with correlated uncertainties between different orders.

Usage Example

WW / Z correlations

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- WW diboson and Z boson production are expected to have similar PDF dependencies → WW / Z cross section ratio cancels part of theoretical (also experimental) uncertainties.
- Correlated PDFs are used to make optimal predictions for WW / Z ratio.
- WW cross section is calculated at NLO using MCFM v6.6 and Z cross section is calculated at NLO and NNLO using FEWZ.
- Uncertainties due to missing higher-order corrections are estimated by varying renormalisation and factorisation scales up and down and constructing an envelope of maximal positive and negative deviations.
- Predictions are then compared to recent measurement by CMS *[E.P.J. C73 (2013) 2610]*.

WW / Z correlations

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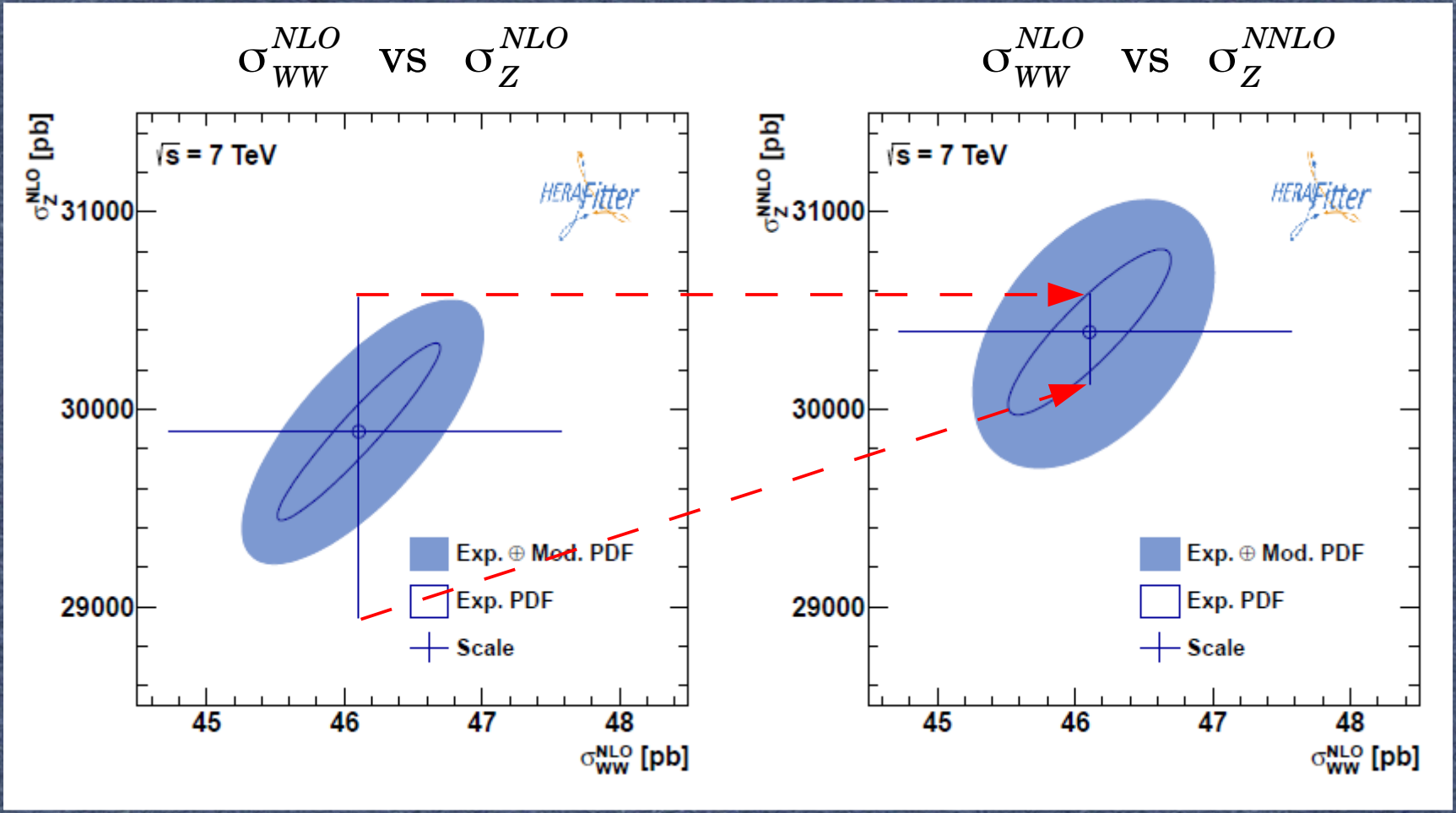

- Similar PDF dependence leads to high correlation of PDF uncertainties. Correlation is reduced when using NNLO calculation for Z production.
- Scale uncertainty is reduced when using NNLO calculation for Z production.

Model and parametrisation uncertainties

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Variation	$\sigma_{WW}^{\mathrm{NLO}}$ %	$\sigma_{Z}^{\mathrm{NLO}}$ %	$\sigma_{Z}^{\mathrm{NNLO}}$ %
$r_s(-0.3)$	1.00	-0.29	-0.33
$r_s(+0.3)$	-0.81	0.39	0.42
$M_c(-0.06\ \mathrm{GeV})$	-0.81	-0.89	-0.76
$M_c(+0.06\ \mathrm{GeV})$	0.55	0.66	0.61
$M_b(-0.45\ \mathrm{GeV})$	0.13	0.11	-0.02
$M_b(+0.25\ \mathrm{GeV})$	-0.07	-0.07	0.00
$\alpha_S(M_Z)(-0.002)$	-0.54	-1.27	-1.17
$\alpha_S(M_Z)(+0.002)$	0.52	1.23	1.17
$Q^2_{\mathrm{min}}(-2.5\ \mathrm{GeV}^2)$	-0.25	-0.35	0.23
$Q^2_{\mathrm{min}}(+2.5\ \mathrm{GeV}^2)$	0.75	0.73	-1.06
$Q^2_0(-0.2\ \mathrm{GeV}^2)$	-0.21	-0.19	-0.14
$+D_{u_v}$	-0.03	-0.32	0.97
$+D_{\bar{U}}$	-0.04	-0.02	-0.01
$+E_{\bar{U}}$	0.01	0.00	0.00

Variation	$\sigma_{WW}^{\mathrm{NLO}} / \sigma_{Z}^{\mathrm{NLO}}$ $\times 10^{-3}$	$\sigma_{WW}^{\mathrm{NLO}} / \sigma_{Z}^{\mathrm{NNLO}}$ $\times 10^{-3}$
$r_s(-0.3)$	0.020	0.020
$r_s(+0.3)$	-0.018	-0.019
$M_c(-0.06\ \mathrm{GeV})$	0.001	-0.001
$M_c(+0.06\ \mathrm{GeV})$	-0.002	-0.001
$M_b(-0.45\ \mathrm{GeV})$	0.000	0.002
$M_b(+0.25\ \mathrm{GeV})$	0.000	-0.001
$\alpha_S(M_Z)(-0.002)$	0.011	0.010
$\alpha_S(M_Z)(+0.002)$	-0.011	-0.010
$Q^2_{\mathrm{min}}(-2.5\ \mathrm{GeV}^2)$	0.002	-0.007
$Q^2_{\mathrm{min}}(+2.5\ \mathrm{GeV}^2)$	0.000	0.028
$Q^2_0(-0.2\ \mathrm{GeV}^2)$	0.000	-0.001
$+D_{u_v}$	0.005	-0.015
$+D_{\bar{U}}$	0.000	-0.001
$+E_{\bar{U}}$	0.000	0.000

- r_s is anti-correlated between Z and WW.
- M_c, M_b, α_s and Q^2_0 variations are correlated between NLO and NNLO and mostly cancel in the ratio.
- The variation of Q^2_{min} cut on data have anti-correlated effect on Z at NLO and at NNLO

Prediction vs data

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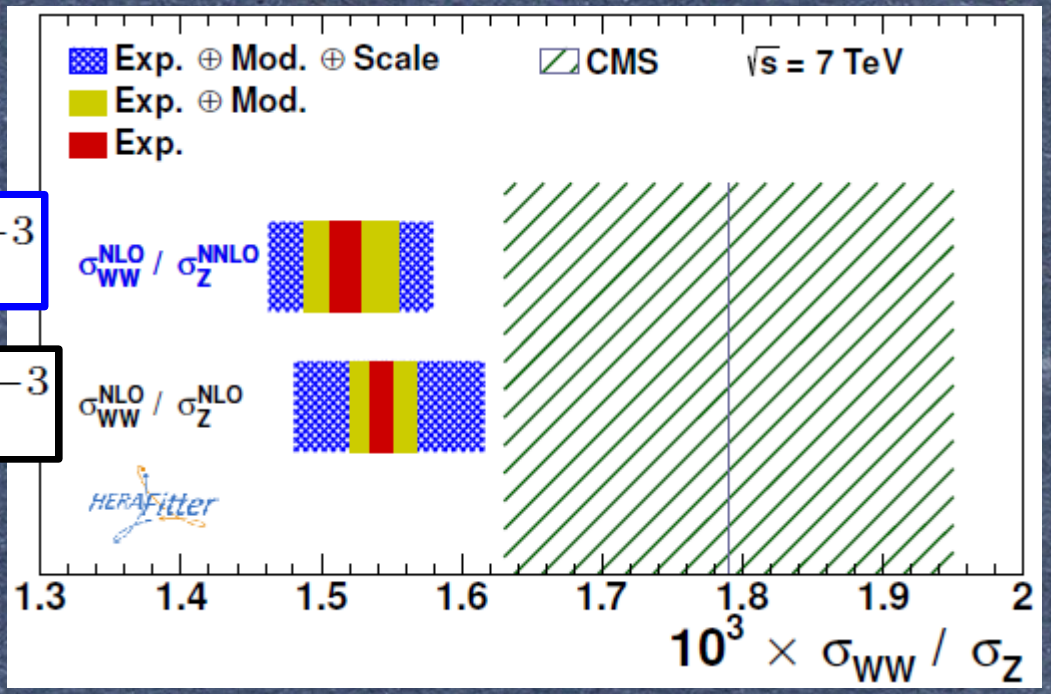
Ratio	Value $\times 10^{-3}$	Exp. PDF $\times 10^{-3}$	Mod. PDF $\times 10^{-3}$	Scale $\times 10^{-3}$
$\frac{\sigma_{WW}^{\mathrm{NLO}}}{\sigma_{Z}^{\mathrm{NLO}}}$	1.543	± 0.008	$^{+0.023}_{-0.021}$	$^{+0.069}_{-0.058}$
$\frac{\sigma_{WW}^{\mathrm{NLO}}}{\sigma_{Z}^{\mathrm{NNLO}}}$	1.517	± 0.010	$^{+0.036}_{-0.027}$	$^{+0.050}_{-0.046}$

$$\sigma_{WW}^{\mathrm{NLO}}/\sigma_{Z}^{\mathrm{NNLO}} = [1.517^{+0.051}_{-0.047}] \times 10^{-3}$$

$$\sigma_{WW}^{\mathrm{NLO}}/\sigma_{Z}^{\mathrm{NLO}} = [1.543^{+0.073}_{-0.062}] \times 10^{-3}$$



- Predictions of the ratio WW to Z production cross sections are compared to the CMS measurement *[E.P.J. C73 (2013) 2610]*.
- The usage of the mixed-order NLO – NNLO predictions, allows to reduce the total uncertainty due to the reduction of the scale uncertainty for Z production prediction.

Summary

- Sets of LO, NLO and NNLO PDFs correlated at different orders were extracted using HERAFitter.
- A high degree of correlation was observed for PDFs at different orders and similar x.
- The correlated NLO and NNLO PDFs were used to calculate WW/Z ratio. Significant correlation of the PDF uncertainties was observed.
- The total theoretical uncertainty is reduced for the mixed-order calculation by 30-40% due to reduced scale uncertainties.
- PDFs will be released in LHAPDF v6 soon: HF14cor*.