Recommendations for PDF usage in LHC predictions

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Introduction

Recent PDF4LHC recommendations for LHC Run II J.Phys.G 43, 023001 (2016)

→ significantly improved compared to recommendations of 2010 arXiv:1101.0538
→ addressing previous criticism for clarity of usage and the procedure

→ several potential dangerous shortcomings in the new proposed procedure
→ we aim at bringing them into discussions and propose alternative recommendations for the PDF usage

→ ideally, the next recommendations would include given observations and published as a one set from all PDF groups

Overview of Latest PDFs

ABM12, CT14, CJ15, JR14, NNPDF3.0, MMHT14, HERAPDF2.0

→ all are accurate at NNLO (CJ15 NLO) in QCD

Main sources of difference between different PDFs:

- → inclusion of different data
- → methods of determining 'best fit'
- → uncertainty treatment/sources
- → assumptions in procedure (parametrisation)
- → heavy flavour treatment
- → PDF and strong coupling constant α_s correlation

PDF sets	$\Delta\chi^2$ criterion	data sets used in analysis
ABM12 [2]	1	incl. DIS, DIS charm, DY
CJ15 [1]	100	incl. DIS, DY (incl. $p\bar{p} \to W^{\pm}X$), $p\bar{p}$ jets, γ+jet
CT14 [3]	100	incl. DIS, DIS charm, DY, $p\bar{p}$ jets, pp jets
HERAPDF2.0 [4]	1	incl. DIS, DIS charm, DIS jets
JR14 [5]	1	incl. DIS, DIS charm, DY, $p\bar{p}$ jets, DIS jets
MMHT14 [9]	2.3 . . . 42.3 (dynamical)	incl. DIS, DIS charm, DY, $p\bar{p}$ jets, pp jets, $t\bar{t}$
NNPDF3.0 [7]	1	incl. DIS, DIS charm, DY, $p\bar{p}$ jets, pp jets, $t\bar{t}$, $W +$ charm

...both theoretical and experimental inputs have direct impact on the obtained nonperturbative parameters, i.e. PDFs, α_s, quark masses

Heavy Flavour Schemes in PDFs

- **Fixed Flavour Number Scheme (FFNS)**

  only light flavours in the proton: i = 3 (4)
  c- (b-) quarks massive, produced in boson-gluon fusion,
  $Q^2 \gg m_{HQ}^2$: can be less precise, NLO coefficients contain terms $\sim ln(Q/m_{HQ})$

→ HQ at HERA: complete NLO Laenen, Riemersma, Smith, van Neerven '92
approx NNLO Bierenbaum, Blümlein, Klein '09;
Lo Presti, Kawamura, S.Moch., Vogt '12;
Behring, Bierenbaum, Blümlein, De Freitas, Klein, Wissbrock '14

- **Variable Flavour Number Scheme (VFNS)**

  - Zero Mass VFNS: all flavours massless. Breaks down at $Q^2 \sim m_{HQ}^2$
  - Generalized Mass VFNS: different implementations provided by PDF groups, smooth matching with FFNS for $Q^2 \rightarrow m_{HQ}^2$ must be assured

→ HQ at HERA: ACOT Aivazis, Collins, Olness, Tung '94, TR' Thorne, Roberts '98,
FONLL Forte, Laenen, Nason, Rojo'10, BMSN Buza,Matiounine, Smith,van Neerven '98

→ HQ masses defined in **pole** or **$\overline{\text{MS}}$** scheme (latter due to better perturbative stability is preferred)

Validation of Schemes with HERA Charm Data

Different schemes against HERA charm data

→ good agreement with FF and VFNS observed, approx NNLO generally yields better χ^2 for charm data

→ PDF4LHC15 is presented for illustration purposes only

Note: different schemes sometimes use different definitions for the pert. order

PDF sets	m_c [GeV]	m_c renorm. scheme	theory method (F_2^c scheme)	theory accuracy for heavy quark DIS Wilson coeff.	χ^2/NDP for HERA data [148] with xFitter [149, 150] (with unc.)	(nominal)
ABM12 [2] [a]	$1.24^{+0.05}_{-0.03}$	$\overline{\text{MS}}$ $m_c(m_c)$	FFNS ($n_f = 3$)	NNLO$_{\text{approx}}$	65/52	66/52
CJ15 [1]	1.3	m_c^{pole}	SACOT [143]	NLO	117/52	117/52
CT14 [3] [b]						
(NLO)	1.3	m_c^{pole}	SACOT(χ) [144]	NLO	51/47	70/47
(NNLO)	1.3	m_c^{pole}	SACOT(χ) [144]	NLO	64/47	130/47
HERAPDF2.0 [4]						
(NLO)	1.47	m_c^{pole}	RT optimal [146]	NLO	67/52	67/52
(NNLO)	1.43	m_c^{pole}	RT optimal [146]	NLO	62/52	62/52
JR14 [5] [c]	1.3	$\overline{\text{MS}}$ $m_c(m_c)$	FFNS ($n_f = 3$)	NNLO$_{\text{approx}}$	62/52	62/52
MMHT14 [6]						
(NLO)	1.4	m_c^{pole}	RT optimal [146]	NLO	72/52	78/52
(NNLO)	1.4	m_c^{pole}	RT optimal [146]	NLO	71/52	83/52
NNPDF3.0 [7]						
(NLO)	1.275	m_c^{pole}	FONLL-B [145]	NLO	58/52	60/52
(NNLO)	1.275	m_c^{pole}	FONLL-C [145]	NLO	67/52	69/52
PDF4LHC15 [8] [d]	–	–	FONLL-B [145]	–	58/52	64/52
	–	–	RT optimal [146]	–	71/52	75/52
	–	–	SACOT(χ) [144]	–	51/47	76/47

[a] The value of m_c in ABM12 is determined from a fit to HERA data [148].
[b] The data comparision always applies the SACOT(χ) scheme at NLO as implemented in xFitter [149, 150]. The implementation of this scheme differs from the one used by CT14. Removing the Q^2-cut on the HERA data [148] one obtains χ^2/NDP = 158/52 (582/52) with PDF uncertainities and 258/52 (648/52) for the central fit at NLO (NNLO).
[c] The χ^2/NDP values are determined for the dynamical set JR14NNLO08VF.
[d] The data comparision uses the xFitter [149, 150] implementation of the schemes FONLL-B, RT optimal and SACOT(χ) with the set PDF4LHC_100 at NLO.

Strong Coupling Constant in PDF Fits

α_s is an important parameter in PDF fits → strong correlation with gluon PDF

→ in PDF fits α_s is fitted or fixed:

PDF sets	$\alpha_s(M_Z)$	method of determination
ABM12 Alekhin, Blümlein, S.M. '13	0.1132 ± 0.0011	fit at NNLO
CJ15 Accardi, Brady, Melnitchouk et al. '16	0.118 ± 0.002	fit at NLO
CT14 Dulat et al. '15	0.118	assumed at NNLO
HERAPDF2.0 H1+Zeus Coll.	$0.1183\ ^{+0.0040}_{-0.0034}$	fit at NLO
JR14 Jimenez-Delgado, Reya '14	0.1136 ± 0.0004	dynamical fit at NNLO
	0.1162 ± 0.0006	standard fit at NNLO
MMHT14 Martin, Motylinski, Harland-Lang, Thorne '14	0.118	assumed at NNLO
	0.1172 ± 0.0013	best fit at NNLO
NNPDF3.0 Ball et al. '14	0.118	assumed at NNLO
PDF4LHC15 Butterworth et al. '15	0.118	assumed at NLO
	0.118	assumed at NNLO

[a] In detail HERAPDF2.0 obtains at NLO $\alpha_s(M_Z) = 0.1183 \pm 0.0009(\text{exp}) \pm 0.0005(\text{model/parameterisation}) \pm 0.0012(\text{hadronisation})\ ^{+0.0037}_{-0.0030}(\text{scale})$, which have been added in quadrature in the table entry. The HERAPDF2.0 central variant uses a fixed value $\alpha_s(M_Z) = 0.118$.
[b] MMHT14 obtains $\alpha_s(M_Z) = 0.1172 \pm 0.0013$ at NNLO as a best fit.

→ range of fitted α_s varies from 0.1132 to 0.1183 (NNLO)

PDG: α_s = 0.1181 ±0.0013 (NNLO)

→ differences in α_s are from different physics models and analysis procedures (higher twist, correlation of errors, etc.)

Cross Section Predictions at LHC: Higgs

PDF uncertainties in Higgs productions at LHC are significant

→ similarly to top quarks, Higgs cross section is strongly gluon and α_s dependent

Exact N^3LO QCD corrections available Anastasiou, Duhr, Dulat, Herzog, Mistlberger ‘15

Cross section at NNLO for m_H = 125.0 GeV, √s = 13 TeV, $\mu_R=\mu_F=m_H$

ABM12 Alekhin, Blümlein, S.M. ‘13	39.80 ± 0.84 pb
CJ15 (NLO) Accardi, Brady, Melnitchouk et al. ‘16	$45.45\,^{+\,0.17}_{-\,0.11}$ pb
CT14 Dulat et al. ‘15	$42.33\,^{+\,1.43}_{-\,1.68}$ pb
HERAPDF2.0 H1+Zeus Coll.	$42.62\,^{+\,0.35}_{-\,0.43}$ pb
JR14 (dyn) Jimenez-Delgado, Reya ‘14	38.01 ± 0.34 pb
MMHT14 Martin, Motylinski, Harland-Lang, Thorne ‘14	$42.36\,^{+\,0.56}_{-\,0.78}$ pb
NNPDF3.0 Ball et al. ‘14	42.59 ± 0.80 pb
PDF4LHC15 Butterworth et al. ‘15	42.42 ± 0.78 pb

→ large spread in predictions amounts to ~11% differences (larger than available theory uncertainty)

→ (similar) correlation of Higgs cross sections on the charm mass value observed

Cross Section Predictions at LHC: Higgs

Higgs cross section predictions at NNLO with MMHT and NNPDFs

MMHT14 (values in brackets correspond to χ^2 and σ(H) obtained with fixed α_s)

m_c^{pole} [GeV]	$\alpha_s(M_Z)$ (best fit)	χ^2/NDP (HERA data [148])	$\sigma(H)^{NNLO}$ [pb] best fit $\alpha_s(M_Z)$	$\sigma(H)^{NNLO}$ [pb] $\alpha_s(M_Z) = 0.118$
1.15	0.1164	78/52 (71/52)	40.48	(42.05)
1.2	0.1166	76/52 (70/52)	40.74	(42.11)
1.25	0.1167	75/52 (76/52)	40.89	(42.17)
1.3	0.1169	76/52 (77/52)	41.16	(42.25)
1.35	0.1171	78/52 (79/52)	41.41	(42.30)
1.4	0.1172	82/52 (83/52)	41.56	(42.36)
1.45	0.1173	88/52 (89/52)	41.75	(42.45)
1.5	0.1173	96/52 (96/52)	41.81	(42.51)
1.55	0.1175	105/52 (106/52)	42.08	(42.58)

→ best χ^2 is observed at lower charm mass compared to one used in the nominal fit

NNPDF (χ^2 values obtained with FONLL-C scheme)

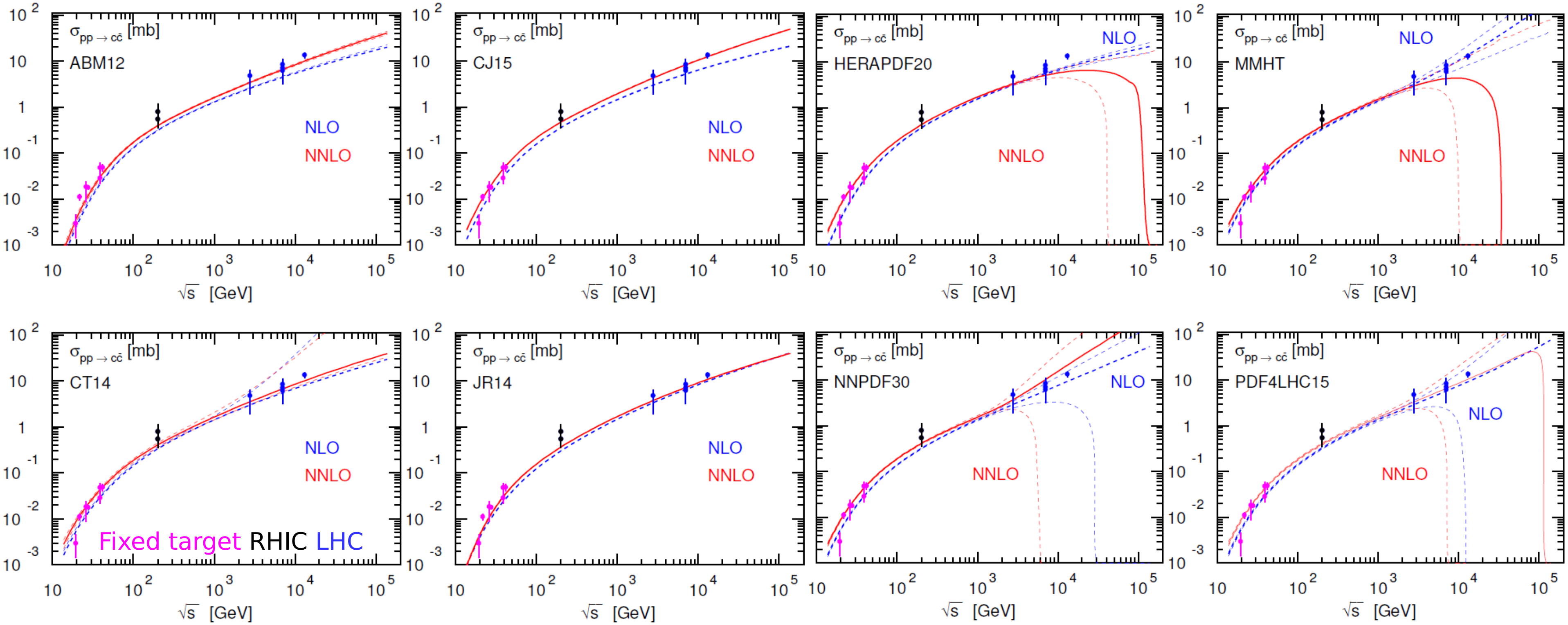
PDF sets	m_c^{pole} [GeV]	$\alpha_s(M_Z)$ (fixed)	χ^2/NDP (HERA data [148])	$\sigma(H)^{NNLO}$ [pb] fixed $\alpha_s(M_Z)$
NNPDF2.1 [152]	$\sqrt{2}$	0.119	65/52	44.18 ± 0.49
	1.5	0.119	78/52	44.54 ± 0.51
	1.6	0.119	92/52	44.74 ± 0.50
	1.7	0.119	110/52	44.95 ± 0.51
NNPDF2.3 [225]	$\sqrt{2}$	0.118	71/52	43.77 ± 0.41
NNPDF3.0 [7]	1.275	0.118	67/52	42.59 ± 0.80

→ linear rise of Higgs cross sections with the increase of the charm mass

Cross Section Predictions at LHC: Heavy Quarks

Benchmarking PDFs with heavy quark hadro-production at LHC

Cross section for $pp \rightarrow \overline{cc}$ as a function of √s at NLO and NNLO

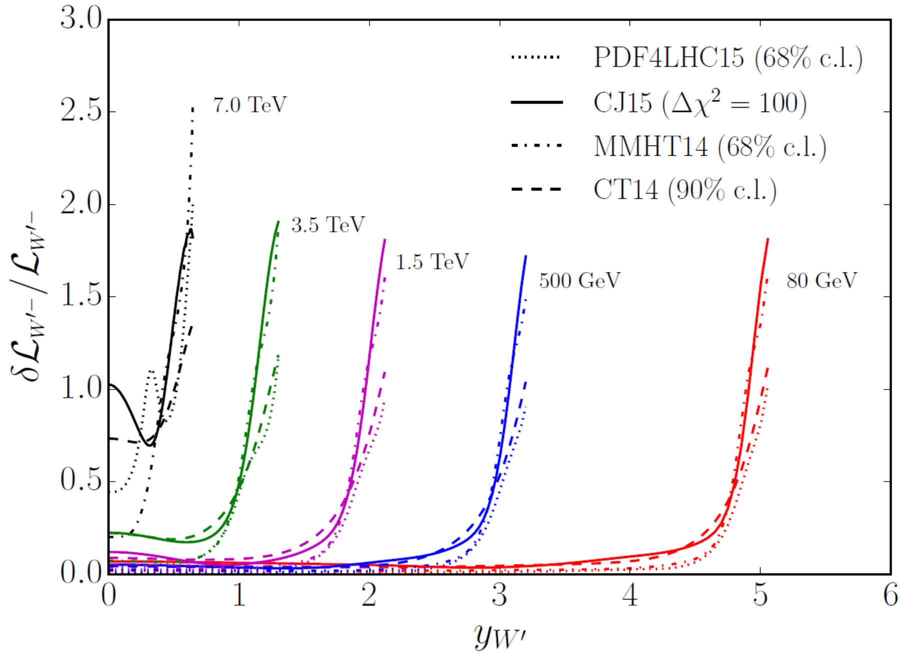


→ negative cross sections observed with HERA, MMHT and PDF4LHC15 PDFs
(most likely due to negative gluon in given PDFs, PDF4LHC15 due to averaging?)

Cross Section Predictions at LHC: W'

Searches for new heavy particles at LHC rely on large-x PDFs
→ large PDF uncertainties due to limited data availability in the large-x region

Example: (uncertainty on) parton luminosity for W' production for various PDFs



→ with increase of mass or rapidity ($y_{W'}$), increases and mom. fraction, $x_{1,2} = (M_{W'}/\sqrt{s})\,e^{\pm y_{W'}}$
i.e. $\mathcal{L}^- \sim \bar{u}(x_2)d(x_1)$

→ PDF uncertainties start to increase drastically for x $\gtrsim$ 0.65, i.e. region with little data constraining d-quark and theoretical assumptions are important (at large $M_{W'}$, uncertainties rise due to poor constraints on ubar)

PDFs often use different methodology for PDF uncertainties
- → care should be taken when utilizing PDF uncertainty bands
- → results from combined sets like PDF4LHC15 should be cross checked with individual PDF sets

Recommendations for PDF usage

Two distinct cases are considered:

I. Precision theory predictions, a class of predictions, either within or beyond SM

Recommendation: Use the individual PDF sets ABM12, CJ15, CT14, JR14, HERA-PDF2.0, MMHT14 and NNPDF3.0 (or as many as possible), together with the respective uncertainties for the chosen PDF set, the strong coupling $\alpha_s(M_Z)$ and the heavy quark masses m_c, m_b and m_t.

II. Other theory predictions

Recommendation: Use any one of the PDF sets listed in `LHAPDF(v6)`.

Note: the recent developments in modern tools often allow to include different PDFs in the theory calculations via *reweighting* methodology (i.e. weights from different PDFs stored on event basis)

→ allows to evaluate effects from different PDFs in efficient way

Summary

The Parton Distribution Functions of the proton are generally rather well known (thanks to very precise experimental data and theoretical improvements)

→ various processed have been benchmarked and the importance of the choices for parameters like quark masses and α_s have been illustrated

→ illustrates several potential shortcomings in the PDF4LHC proposed recommendations

→ an alternative (simplified) recommendations for PDF usage at LHC proposed

We are open to constructive comments and discussions

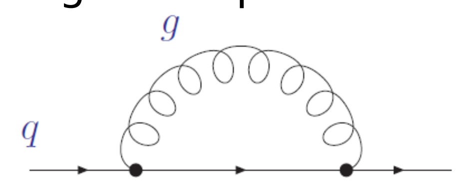
Back-Up Slides

Heavy Quark Masses

Pole mass

→ Based on (unphysical) concept of heavy-quark being a free parton

$$\not{p} - m_q - \Sigma(p, m_q)\Big|_{p^2=m_q^2}$$



→ heavy-quark self-energy $\Sigma(p,m_q)$ receives contributions from regions of all loop momenta – also from momenta of $O(\Lambda_{QCD})$

→ Renormalon ambiguity in definition of pole mass of $O(\Lambda_{QCD})$

Bigi, Shifman, Uraltsev, Vainshtein '94; Beneke, Braun '94; Smith, Willenbrock '97

$\overline{\text{MS}}$ mass

→ Free of infrared renormalon ambiguity

→ Conversion between m_{pole} and MS mass $m(\mu_R)$ in perturbation theory known to four loops in QCD Marquard, Smirnov, Smirnov, Steinhauser '15

PDG: charm: $m_c(m_c) = 1.27^{+0.07}_{-0.11}$ GeV, bottom: $m_b(m_b) = 4.20^{+0.17}_{-0.07}$ GeV

→ heavy quark masses used in some PDF fits are not always compatible with quoted numbers in PDG

Cross Section Predictions at LHC: Heavy Quarks

Top-quark pair production at LHC: acceptance (with Difftop, JHEP 01 2015 082)

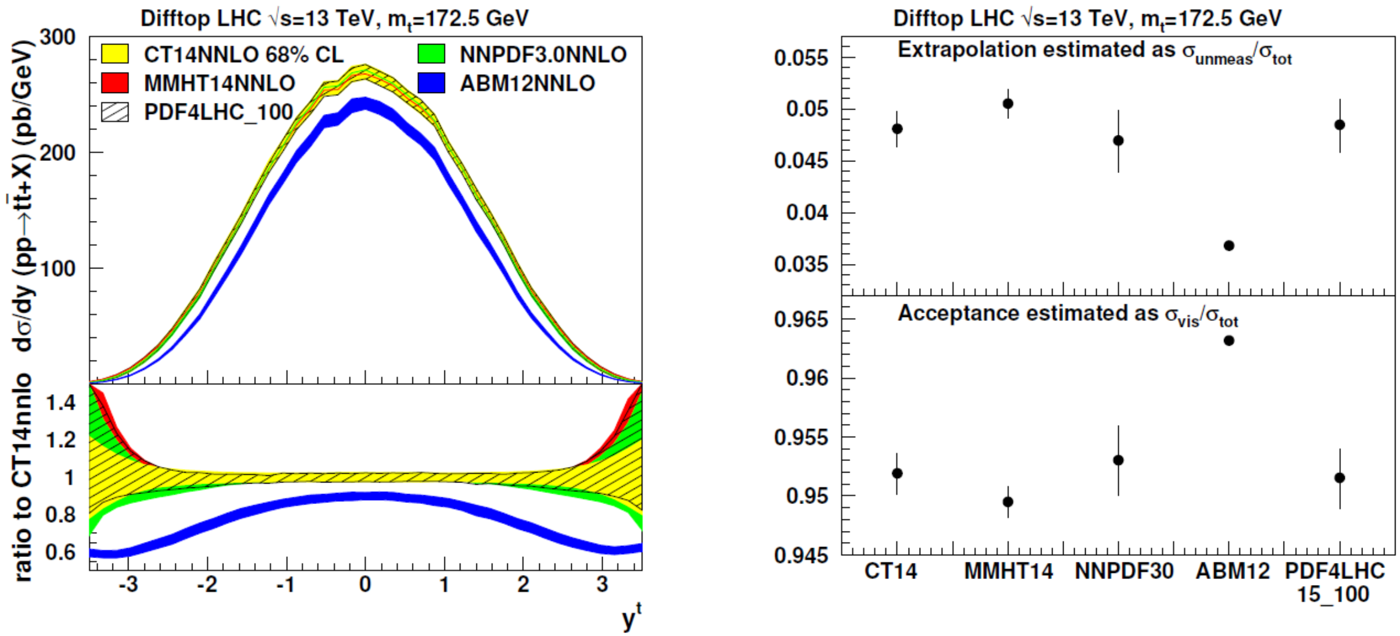


FIG. 15: (Left panel) Predictions for top-quark pair production cross sections at approximate NNLO as a function of the top-quark rapidity using different PDFs at NNLO with the respective PDF uncertainty (depicted by bands of different style). (Right panel) The acceptance and extrapolation estimators with the respective PDF uncertainties, obtained by using different PDF sets.

→ significant differences observed with respect to e.g. ABM PDFs

→ PDF4LHC15_100 set is not fully covering PDF uncertainties of PDFs used in combination

Note: acceptance estimators are given for illustration purposes and not expected to describe precisely true experimental efficiency

Cross Section Predictions at LHC: Higgs

Higgs cross section predictions at NNLO with MSTW2008

MSTW2008 (values in brackets correspond to σ(H) obtained with fixed α_s)

m_c^{pole} [GeV]	$\alpha_s(M_Z)$ (best fit)	χ^2/NDP (HERA data [148])	$\sigma(H)^{NNLO}$ [pb] best fit $\alpha_s(M_Z)$	$\sigma(H)^{NNLO}$ [pb] $\alpha_s(M_Z) = 0.118$
1.05	0.1157	73/52	40.65	(41.63)
1.1	0.1159	69/52	40.85	(41.70)
1.15	0.1160	66/52	41.04	(41.78)
1.2	0.1162	64/52	41.25	(41.85)
1.25	0.1164	64/52	41.47	(41.93)
1.3	0.1166	63/52	41.69	(42.00)
1.35	0.1168	63/52	41.93	(42.09)
1.4	0.1171	65/52	42.16	(42.16)
1.45	0.1173	68/52	42.42	(42.24)
1.5	0.1175	73/52	42.64	(42.31)
1.55	0.1177	80/52	42.88	(42.38)
1.6	0.1180	88/52	43.16	(42.46)
1.65	0.1182	99/52	43.34	(42.51)
1.7	0.1184	112/52	43.59	(42.58)
1.75	0.1186	127/52	43.81	(42.63)

TABLE 9: The values of the charm-quark mass (on-shell scheme m^{pole}) and the strong coupling $\alpha_s(M_Z)$ in the MSTW analysis [153] using the set `MSTW2008nnlo_mcrange` together with the value for χ^2/NDP for the HERA data [148] and the Higgs cross section at NNLO in QCD (computed in the effective theory) at $\sqrt{s} = 13$ TeV for $m_H = 125.0$ GeV at the nominal scale $\mu_r = \mu_f = m_H$. The numbers in parentheses are obtained using the PDF set `MSTW2008nnlo_mcrange_fixasmz` with the value of $\alpha_s(M_Z)$ fixed to $\alpha_s(M_Z) = 0.118$.

→ best χ^2 is observed at lower charm mass compared to one used in the nominal fit

→ linear rise of Higgs cross sections with the increase of the charm mass