

The PDF4LHC Recommendations for Run II

Based on J. Butterworth et al, arXiv:1510.03865 Journal of Physics G 43 (2016) 023001

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Higgs production cross-section in gluon fusion at the LHC is a crucial process to test the Higgs sector: the **higher the theory accuracy**, the more powerful our **discovery power for New Physics** is

Higgs couplings may indicate new physics: a few percent precision is a good target

Higgs Snowmass report (arXiv:1310.8361) Deviation from SM due to particles with M=1 TeV

Model	κ_V	κ_b	κ_γ
Singlet Mixing	$\sim 6\%$	$\sim 6\%$	$\sim 6\%$
2HDM	$\sim 1\%$	$\sim 10\%$	$\sim 1\%$
Decoupling MSSM	$\sim -0.0013\%$	$\sim 1.6\%$	$\sim4\%$
Composite	$\sim -3\%$	$\sim -(3-9)\%$	$\sim -9\%$
Top Partner	$\sim -2\%$	$\sim -2\%$	$\sim +1\%$

Future LHC data: measure H couplings at 2-8% level (cf 20-50% today), and to access rare decays such as $H \rightarrow \mu\mu$

Higgs production cross-section in gluon fusion at the LHC is a crucial process to test the Higgs sector: the **higher the theory accuracy**, the more powerful our **discovery power for New Physics** is



Find the progress in perturbative calculations! This process is known at N3LO, scale errors down $\delta\sigma \approx 3\%$!

Does this mean that we can probe BSM physics at this level of precision?

First will depend on the size of other theory uncertainties, first and foremost the **PDF and strong coupling uncertainties**

A well-defined PDF recommendation is mandatory for compare data with theory for Higgs physics



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Depending on how the **total PDF uncertainty on a given cross-section** is defined, results can differ by large amount, dramatically **degrading the BSM discovery potential of the LHC**



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A recommendation is required to establish a framework for the **consistent calculation of PDF uncertainties in different LHC processes** and **their correlation**, *i.e.*, in the case of Higgs production

Roadmap to PDF4LHC15



Input to the PDF4LHC15 combination

- 1. The PDF sets to be combined should be *based on a global dataset*, including a large number of datasets of diverse types (deep-inelastic scattering, vector boson and jet production, ...) from fixed-target and colliders experiments (HERA, LHC, Tevatron).
- 2. Theoretical hard cross sections for DIS and hadron collider processes should be evaluated up to two QCD loops in α_s , in a general-mass variable-flavor number scheme with up to $n_f^{\text{max}} = 5$ active quark flavors.¹ Evolution of α_s and PDFs should be performed up to three loops, using public codes such as HOPPET [105] or QCDNUM [106], or a code benchmarked to these.
- 3. The central value of $\alpha_s(m_Z^2)$ should be fixed at an agreed common value, consistent with the PDG world-average [107]. This value is currently chosen to be $\alpha_s(m_Z^2) = 0.118$ at both NLO and NNLO.² For the computation of α_s uncertainties, two additional PDF members corresponding to agreed upper and lower values of $\alpha_s(m_Z^2)$ should also be provided. This uncertainty on $\alpha_s(m_Z^2)$ is currently assumed to be $\delta \alpha_s = 0.0015$, again the same at NLO and NNLO.

The input values of m_c and m_b should be compatible with their world-average values; either pole or $\overline{\text{MS}}$ masses are accepted.

4. All known experimental and procedural sources of uncertainty should be properly accounted for. Specifically, it is now recognized that the PDF uncertainty receives several contributions of comparable importance: the measurement uncertainty propagated from

FFN vs GM-VFN

Thorne, arXiv:1402.3536



- The use of FFN heavy quark scheme as opposed to GM-VFN leads to a suppression (enhancement) of the large-x (small-x) gluon, which is made more prominent if a DIS-only dataset is used
- ♀ The fit quality to the **high-Q2 inclusive HERA data** is worse in the FFN than in the GM-VFN. Explained by the slow perturbative convergence of the FFN scheme in certain *x* regimes (*ie* intermediate *x*)
- The spread between FFN and GM-VFN fits is not a genuine theoretical uncertainty
- Similar results obtained by NNPDF, *arXiv:1303.1189*

Monte Carlo combination

First of all, select the **PDF sets that enter the combination**. Must be reasonably consistent among them for a meaningful combination. The 2015 combination is based on **CT14**, **MMHT14** and **NNPDF3.0**

Transform the Hessian PDF sets into their Monte Carlo representation:

$$F^{k} = F(q_{0}) + \frac{1}{2} \sum_{j=1}^{N_{\text{eig}}} \left[F(q_{j}^{+}) - F(q_{j}^{-}) \right] R_{j}^{k}, \quad k = 1, \dots, N_{\text{rep}},$$

Watt and Thorne, arXiv:1205.4024 Forte, arXiv:1011.5247 Forte and Watt, arXiv:1301.6754

Assume equal likelihood for all input sets: combine the **same number of replicas**

The resulting Monte Carlo ensemble has a **robust statistical interpretation**. Similar results compared to the **original PDF4LHC envelope**, but now with the statistically correct treatment of outliers



Monte Carlo reduction: CMC-PDFs

Compress the MC900 prior down to a **smaller number of replicas**, in a way that all the relevant estimators (mean, variances, correlations, higher moments) for the PDFs are fully reproduced



$$\begin{aligned} \text{ERF} &= \sum_{k} \frac{1}{N_{k}} \sum_{i} \left(\frac{C_{i}^{(k)} - O_{i}^{(k)}}{O_{i}^{(k)}} \right)^{2}, \\ \text{ERF}_{CV} &= \frac{1}{N_{CV}} \sum_{i=-n_{f}}^{n_{f}} \sum_{j=1}^{N_{x}} \left(\frac{f_{i}^{\text{CV}}(x_{j},Q) - g_{i}^{\text{CV}}(x_{j},Q)}{g_{i}^{\text{CV}}(x_{j},Q)} \right)^{2} \\ f_{i}^{\text{CV}}(x_{j},Q) &= \frac{1}{N_{\text{rep}}} \sum_{r=1}^{N_{\text{rep}}} f_{i}^{r}(x_{j},Q) \end{aligned}$$

Similar for **variances**, **correlations**, **skewness**, **kurtosis** and the **Kolmogorov** distance

Minimise **distance between prior and compressed sets** using Genetic Algorithms applied to an **Error Function**, which ensures the reproduction of all statistical properties of the prior

Carrazza, Latorre, J. R., Watt, arXiv:1504.06459

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Non-Gaussian features in LHC cross-sections

CMC100 reproduces correctly **non-Gaussian features in MC900**, such as **double-hump distribution**



Motivation for Hessian reduction strategies

- In regions where **MC900** is approximately Gaussian, a **Hessian representation** is by definition more efficient than **CMC-PDFs**, since it needs to reproduce **only central values and covariances**
- Moreover, a Hessian representation has several advantages, such as the use of PDF uncertainties as nuisance parameters, the applicability of Hessian profiling, or the possibility of further reductions when applied to specific processes
- Two Hessian reduction methods have been developed. Essentially common idea, differ in the choice of linear expansion basis



Comparison of reduction algorithms



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Comparison of reduction algorithms

- The three reduction methods **successfully reproduce the variances** (PDF uncertainties) of the prior PDF4LHC15 combination
- The **highest accuracy** is achieved for the **PDF4LHC15_100**, with then similar performance of PDF4LHC_30 and PDF4LHC_mc



Usage of the PDF4LHC15 sets

1. Comparisons between data and theory for Standard Model measurements

Recommendations: Use *individual PDF sets*, and, in particular, as many of the modern PDF sets [5–11] as possible.

2. Searches for Beyond the Standard Model phenomena

Recommendations: Use the PDF4LHC15_mc sets.

Rationale: BSM searches, in particular for *new massive particles in the TeV scale*, often require the knowledge of PDFs in regions where available experimental constraints are limited, notably close to the hadronic threshold where $x \rightarrow 1$ [127]. In these extreme kinematical regions the PDF uncertainties are large, the *Monte Carlo combination of PDF sets is likely to be non-Gaussian. c.f.* Figs. 10 and 11.

3. Calculation of PDF uncertainties in situations when computational speed is needed, or a more limited number of error PDFs may be desirable

Recommendations: Use the PDF4LHC15_30 sets.

4. Calculation of PDF uncertainties in precision observables

Recommendation: Use the PDF4LHC15_100 sets.

Rationale: For several LHC phenomenological applications, the highest accuracy is sought for, with, in some cases, the need to *control PDF uncertainties to the percent level*, as currently allowed by the development of high-order computational techniques in the QCD and electroweak sectors of the Standard Model.

Towards HXSWG Yellow Report IV

The **PDF4LHC15 combined sets** are being used to produce the benchmark cross-sections of **Yellow Report 4** of the **Higgs Cross-Section Working Group**

NNLL+NLO Higgs p_T



The task of the report is to provide the theory predictions for Higgs analysis at the LHC Run II

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An alternative proposal

A recent paper suggests alternative procedures for PDF usage at the LHC:

Recommendations for PDF usage in LHC predictions

arXiv:1603.08906, see also Ringaile's talk

 A. Accardi^{a,b}, S. Alekhin^{c,d}, J. Blümlein^e, M.V. Garzelli^c, K. Lipka^f,
 W. Melnitchouk^b, S. Moch^c, R. Plačakytė^f, J.F. Owens^g, E. Reya^h, N. Sato^b, A. Vogtⁱ and O. Zenaiev^f

(i) Precision theory predictions

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 .

Do we have any reason to **disregard experimental data**, including LHC constraints on PDFs?

- Should we mix state-of-the art PDF sets with PDFs obtained several years ago?
- Solution Is it justified to believe that the **PDG average of** $\alpha_{s}(M_{z})$ is not correct?

This would tend to **redundant calculations with many PDF sets** and to **blow up PDF uncertainties in precision physics and BSM searches**

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Is the charm mass a tuning parameter?

compatible with the world average of the PDG [39]. Thus, in some PDF fits, the numerical value of the charm-quark mass effectively takes over the role of a "tuning" parameter for the Higgs cross section.

- Are global PDF fits really so sensitive to the value of the charm mass?
- When m_c is varied in a wide range, changes in NNPDF, MMHT and CT Higgs cross-sections are within their PDF uncertainties
- The GM-VFN schemes used by the three groups extensively benchmarked up to NNLO





 σ_{tot} for $m_c(m_c) = 1 - 1.36$ GeV and matching parameter λ varied independently, $Q_0 = 1$ GeV. Black boxes are for $m_c(m_c) = 1.28$ GeV (close to world average), for the explored λ . The error ellipse is for nominal 90% C.L. @ $Q_0 = 1.3$ GeV.

The PDF4LHC15 recommendations

- The extensive discussions within the PDF4LHC working group during the last two years have led to the 2015 recommendations for PDF usage at Run II
- These are based on a set of tools to **combine PDF sets** and reduce the resulting number of eigenvectors/replicas in order to **streamline the usage of PDF sets** by the LHC experiments
- While there is room for further optimisation, the **general strategy is robust and flexible enough** to accommodate any future PDF4LHC combination
- The PDF4LHC15 recommendations are intended for many backbone LHC analyses at Run II, including the exciting exploration of the Higgs sector



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Additional Material

SM-PDFs

- PDF sets specialised to a particular set of processes might be useful to reduce the CPU burden of theory calculations, and facilitate the treatment of PDF uncertainties and PDF-induced correlations
- One clear example are Higgs analysis in the HXS WG, but similar Specialized Minimal PDFs (SM-PDFs) can be useful in the TOP4LHC WG (if restricted to top physics) and for the W mass measurement (if restricted to W, Z production)
- We have developed SM-PDFs that basically achieve the same result as the MC2H PDFs but restricted to a particular subset of LHC cross-sections
- Same method as MC2H, but different **choice of matrix** *X* used to construct the PDF covariance matrix, restricted to **values of** *x* **and PDF flavours relevant** for a given set of processes
- SM-PDFs can be recombined among them -> Adiabatically, the full MC2H set is recovered

Process	MC900		NNPDF3.0		MMHT14	
	$T_R = 5\%$	$T_R = 10\%$	$T_R = 5\%$	$T_R = 10\%$	$T_R = 5\%$	$T_R = 10\%$
h	15	11	13	8	8	7
$t\bar{t}$	4	4	5	4	3	3
W, Z	14	11	13	8	10	9
H+tt+Z+W	17	14	18	11	10	10

Number of Neig in the SM-PDF sets forr various processes for a given Tolerance T

General strategy

Select which **cross-sections** are relevant for some specific application, generate **APPLgrids** for these, determine the region where the **correlations between PDFs and these observables is large**, and perform the **MC2H transformation** only for these, for some choice of **tolerance**



General strategy

Identify, for each input cross-section, the PDF flavours and region of Bjorken-x with high correlation



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SM-PDFs for Higgs physics

First exercise: construct **Specialised Minimal PDFs for Higgs physics**:

Input cross-sections for SM-PDFs for Higgs ph					
process	distribution	grid name	$N_{ m bins}$	range	
gg ightarrow h	incl xsec	ggh_13tev	1	-	
	$d\sigma/dp_t^h$	ggh_pt_13tev	10	[0,200] GeV	
	$d\sigma/dy^h$	ggh_y_13tev	10	[-2.5, 2.5]	
VBF hjj	incl xsec	vbfh_13tev	1	-	
	$d\sigma/dp_t^h$	vbfh_pt_13tev	5	[0,200] GeV	
	$d\sigma/dy^h$	vbfh_y_13tev	5	[-2.5, 2.5]	
hW	incl xsec	hw_13tev	1	-	
	$d\sigma/dp_t^h$	hw_pt_13tev	10	[0,200] GeV	
	$d\sigma/dy^h$	hw_y_13tev	10	[-2.5, 2.5]	
hZ	incl xsec	hz_13tev	1	-	
	$d\sigma/dp_t^h$	hz_pt_13tev	10	[0,200] GeV	
	$d\sigma/dy^h$	hz_y_13tev	10	[-2.5.2.5]	
$htar{t}$	incl xsec	httbar_13tev	1	1.03	
	$d\sigma/dp_t^h$	httbar_pt_13tev	10		
	$d\sigma/dy^h$	httbar_y_13tev 10 1.02		1.02	

- Use the MC900 prior as input
- We check that with 10 (symmetric)
 eigenvectors we can reproduce all
 Higgs cross-sections and differential
 distributions
- This means that of the starting 100
 eigenvectors, 90 are not required for
 Higgs physics



SM-PDFs for Top physics

- Then construct Specialised Minimal PDFs for Top quark physics. Specific request from TOPLHC WG.
- Included the following set of distributions computed with aMC@NLO and aMCfast

SM-PDFs for W mass determination

- Then construct Specialised Minimal PDFs for W mass determination studies quark physics. Should be useful for ongoing ATLAS and CMS analysis
- **Included the following set of distributions:**

Process	APPLgrid	\sqrt{s} (TeV)	$N_{ m bins}$	Range	Cuts
Z	z_13tev	13	1	-	$p_T(l) \ge 10 \text{ GeV}, \ \eta^l \le 2.5$
	z_lmpt_13tev	13	10	$[0,200] \mathrm{GeV}$	$p_T(l) \ge 10 \text{ GeV}, \eta^l \le 2.5$
	z_lmy_13tev	13	10	[-2.5, 2.5]	$p_T(l) \ge 10 \text{ GeV}, \ \eta^l \le 2.5$
	z_lppt_13tev	13	10	$[0,200] \mathrm{GeV}$	$p_T(l) \ge 10 \text{ GeV}, \ \eta^l \le 2.5$
	z_lpy_13tev	13	10	[-2.5, 2.5]	$p_T(l) \ge 10 \text{ GeV}, \ \eta^l \le 2.5$
	z_zpt_13tev	13	10	$[0,200]~{ m GeV}$	$p_T(l) \ge 10 \text{ GeV}, \ \eta^l \le 2.5$
	z_zy_13tev	13	5	[-4,4]	$p_T(l) \ge 10 \text{ GeV}, \eta^l \le 2.5$
	z_lplminvmass_13tev	13	10	$[50, 130] { m GeV}$	$p_T(l) \ge 10 \text{ GeV}, \eta^l \le 2.5$
	z_lplmpt_13tev	13	10	$[0,200]~{ m GeV}$	$p_T(l) \ge 10 \text{ GeV}, \ \eta^l \le 2.5$

Process	APPLgrid	\sqrt{s} (TeV)	$N_{ m bins}$	Range	Cuts
W	w_13tev	13	1	-	$p_T(l) \ge 10 \text{ GeV}, \ \eta^l \le 2.5$
	w_cphi_13tev	13	10	[-1,1]	$p_T(l) \ge 10 \text{ GeV}, \ \eta^l \le 2.5$
	w_etmiss_13tev	13	10	[0,200] GeV	$p_T(l) \ge 10 \text{ GeV}, \ \eta^l \le 2.5$
	w_lpt_13tev	13	10	[0,200] GeV	$p_T(l) \ge 10 \text{ GeV}, \ \eta^l \le 2.5$
	w_ly_13tev	13	10	[-2.5, 2.5]	$p_T(l) \ge 10 \text{ GeV}, \ \eta^l \le 2.5$
	w_mt_13tev	13	10	$[0,200]~{ m GeV}$	$p_T(l) \ge 10 \text{ GeV}, \ \eta^l \le 2.5$
	w_wpt_13tev	13	10	$[0,200]~{ m GeV}$	$p_T(l) \ge 10 \text{ GeV}, \ \eta^l \le 2.5$
	w_wy_13tev	13	10	[-4, 4]	$p_T(l) \ge 10 \text{ GeV}, \ \eta^l \le 2.5$

SM-PDFs for W mass determination

- Then construct Specialised Minimal PDFs for W mass determination studies. Should be useful for ongoing ATLAS and CMS analysis
- A somewhat **larger number of eigenvectors selected** here, since W,Z production involve all PDF flavours in a wide range of x),
- Even in this case with only 8 to 14 eigenvectors we can reproduce the original MC900 result

Climbing up the ladder

- The number of eigenvectors required increases monotonically as more and more input cross-sections are included in the procedure
- In the limit where all possible cross-sections are included, the **original MC2H set is reproduced**

LHC Phenomenology

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MC2H LHC phenomenology

CMC-PDFs

Reasonable agreement as well for the correlations between different PDF flavours

In this contour plot, the differences in the correlation coefficients of MC900 and CMC100 between different PDF flavours are represented

Correlation coefficients are computed at Q = 8 GeV, and in the range of x of [10⁻⁵,0.9] logarithmically spaced

MC2H(PCA)

Define a matrix for the deviations wrt central value of all replicas of MC900

$$X_{lk}(Q) = f_{\alpha}^{(k)}(x_i, Q) - f_{\alpha}^{(0)}(x_i, Q), \quad l \equiv N_x(\alpha - 1) + i$$

where **i** runs over a grid of **Nx** points in **x**, **alpha** is the PDF flavour, and **k** runs over the **Nrep** replicas The covariance matrix of **MC900** is then defined as

$$\operatorname{cov}_{ll'}(Q) = \frac{1}{N_{\operatorname{rep}} - 1} \sum_{k}^{N_{\operatorname{rep}}} X_{lk} X_{kl'}^t \qquad \operatorname{cov}(Q) = \frac{1}{N_{\operatorname{rep}} - 1} X X^t$$

It is now possible to construct a representation of this covariance matrix as a linear combination of MC replicas, using Singular Value Decomposition

MC2H(PCA)

- ✤ It can then be shown that the matrix Z=XV contains the Hessian parameters which yield a representation of the PDF covariance matrix as linear combination of MC replicas
- First construction is **purely analytical**, without any numerical approximation involved
- Thus MC2H(PCA) achieves an exact representation of the PDF covariance matrix: by construction, this is a perfect Hessian representation
- Number of eigenvectors very large, N_{eig}=N_{pdf} N_x, but with SVD methods possible to optimise the way information is stored by reducing N_{eig} while minimising information loss, ordering eigenvectors.
- Use Principal Value Decomposition to reduce N_{eig} in a perfectly controlled manner (select coeff with largest singular values) so that results are stable within some fixed tolerance
- \Rightarrow Optimal number (without compromising the accuracy of the method) is around N_{eig} = 100
- Basic assumption: reproduce the entire PDF covariance matrix, even in regions where the underlying probability distribution is non-Gaussian

Correlation matrix

Since the method is essentially exact, one expects that the **PDF correlation matrix** is **perfectly reproduced** (modulo the eigenvector reduction step)

Correlation matrix

Since the method is essentially exact, one expects that the **PDF correlation matrix** is **perfectly reproduced** (modulo the eigenvector reduction step)

Tiny residual differences at the level of few perfect of the correlation coefficient at most, irrelevant for LHC phenomenology

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PDFs in BSM searches

CJ PDFs include more DIS
 data at large-x, but restricted to
 NLO in the ZM-VFN scheme.
 Also, treatment of dynamical
 higher twists depends strongly
 on fit methodology, and
 missing correlated systematics
 in many experiments.

Useful for specific cross-checks, but many caveats needed

Moreover, CJ12 results
 consistent with the
 PDF4LHC15 uncertainties, for
 instance well within the
 NNPDF3.0 error band for d/u

40

MC2H

Also verified that we can produce a Hessian representation of a native Hessian set, MMH14, via an intermediate Monte Carlo representation

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PDF4LHC mandate and activities

The PDF4LHC Working Group has been tasked with:

- 1. performing benchmark studies of PDFs and of predictions at the LHC, and
- 2. making recommendations for a standard method of estimating PDF and PDF+ $\alpha_s(m_Z^2)$ uncertainties at the LHC through a combination of the results from different individual groups.

This mandate has led to several benchmarking papers [12, 13] and to the 2010 PDF4LHC recommendation [14] which has undergone several intermediate updates, with the last version available (along with a summary of PDF4LHC activities) from the PDF4LHC Working Group website:

http://www.hep.ucl.ac.uk/pdf4lhc/.

- Created in 2010 by the CERN directorate
- **Regular PDF4LHC meetings**, discussions between PDF fitters and experimentalists
- Several benchmarking studies produced: genuine improved understanding of differences/similarities between PDF fits, with subsequent improved agreement

The PDF4LHC report on PDFs and LHC data: Results from Run I and preparation for Run II

arxiv:1507.0056

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CMC-PDFs

Good agreement between MC900 and CMC from a number of compressed replicas $N_{rep} > 50$

