Parton distributions for LHC applications

Pavel Nadolsky

CTEQ-TEA (Tung et al.) working group:

ANL/Shanghai University: J. Gao

University of Manchester: M. Guzzi

Michigan State University: J. Huston, J. Pumplin, D. Stump, C. Schmidt, J. Winter, C.-P. Yuan

Southern Methodist University: T.-J. Hou, P. Nadolsky, B. T. Wang, K. P. Xie

Xinjiang University: S. Dulat

Coordinated **T**heoretical **E**xperimental study of **Q**CD

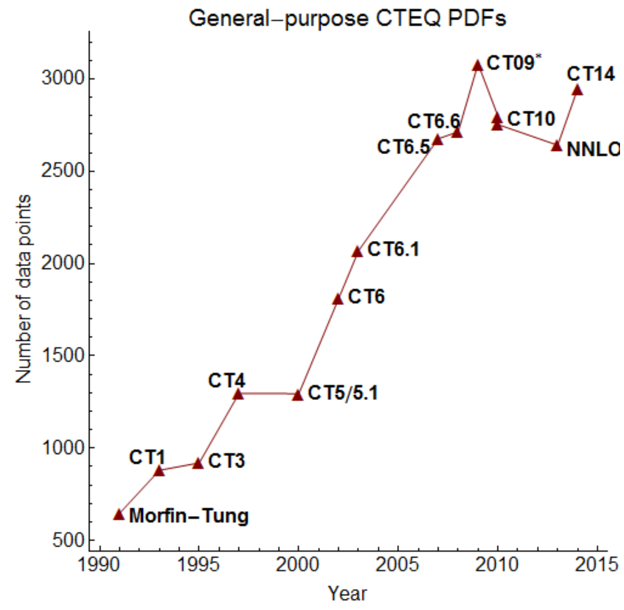
Initiated around 1990 to stimulate interactions between

- Experimentalists and theorists, especially at the newly built Tevatron
- High-energy physics and hadronic physics communities

This is achieved by various initiatives:

- **Global analysis** *(the term coined by J. Morfin and Wu-Ki Tung)* constrains PDFs or other nonperturbative functions with data from diverse hadronic experiments
- **Workshops and summer schools**
- **Annual Wu-Ki Tung award** for junior researchers working on intersections of experiment and theory

…



Similar in spirit to LHC-TI

Wu-Ki Tung Award for Early-Career Research on QCD

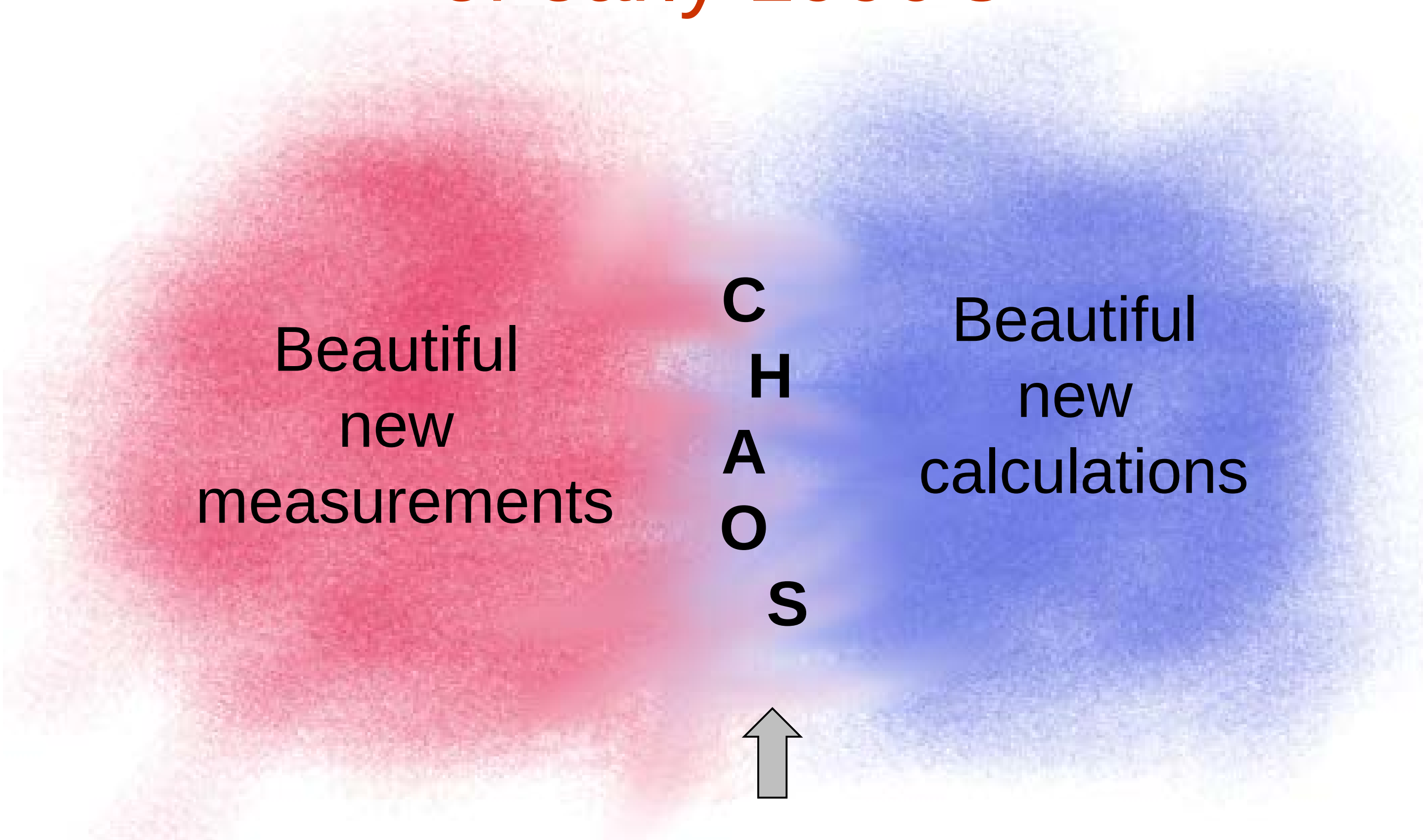
http://varelas.people.uic.edu/tung_award/

The Wu-Ki Tung award recognizes outstanding contributions made by early-career physicists on experimental or theoretical research in Quantum Chromodynamics
[including the interface of experiment and theory]

The annual application deadline is August 15.

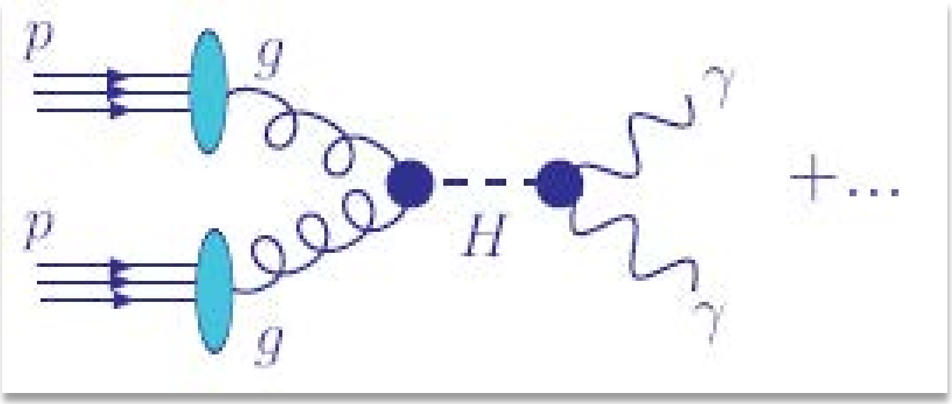
Past recipients include Stefan Hoeche, Mikko Voutilainen, Ciaran Williams

Today’s situation is reminiscent of early 1990’s



An interesting spot to be

Parton distributions describe long-distance dynamics in high-energy collisions



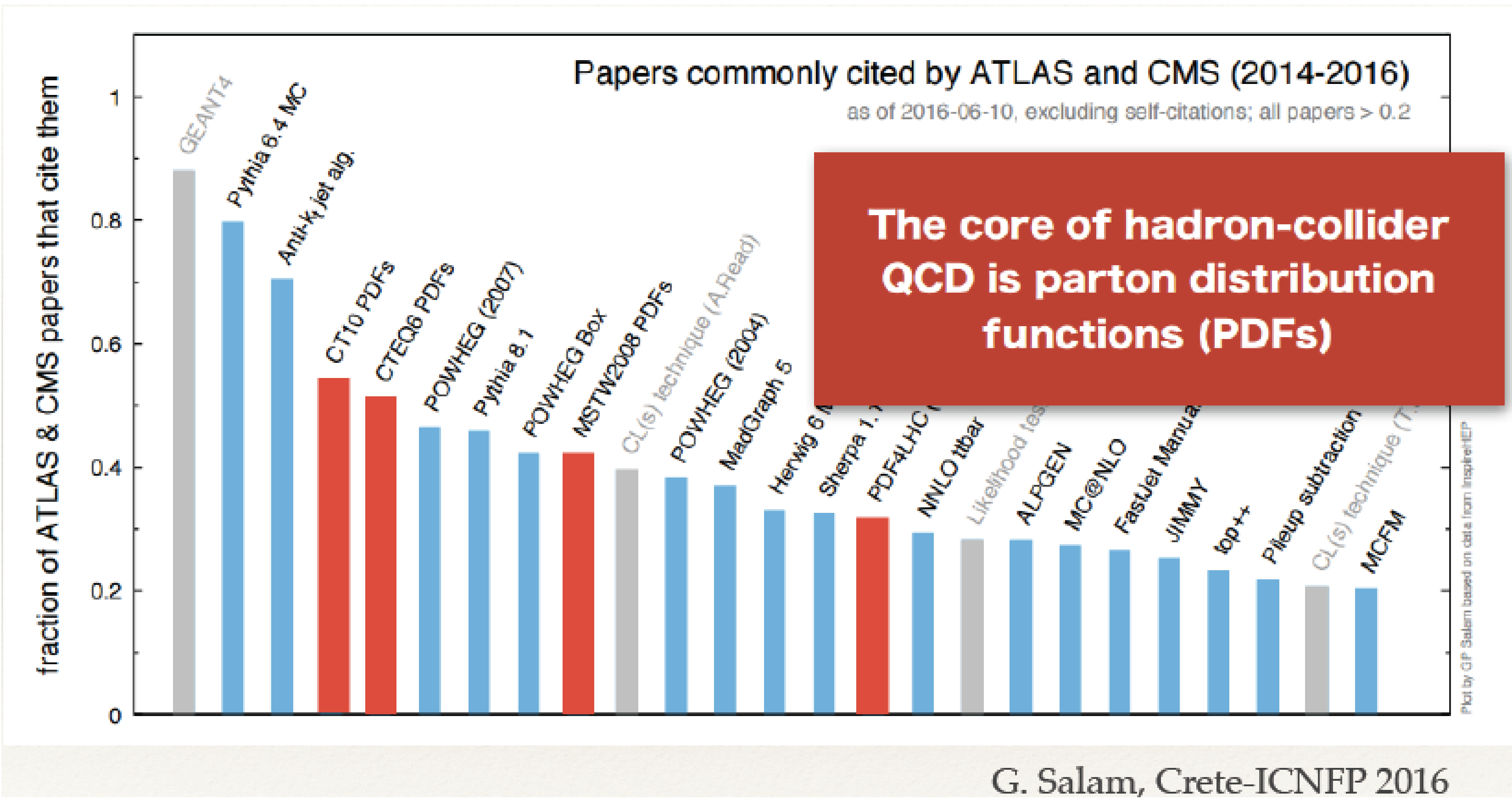
$$\sigma_{pp\to H\to\gamma\gamma X}(Q) = \sum_{a,b=g,q,\bar{q}} \int_0^1 d\xi_a \int_0^1 d\xi_b \hat{\sigma}_{ab\to H\to\gamma\gamma}\left(\frac{x_a}{\xi_a}, \frac{x_b}{\xi_b}, \frac{Q}{\mu_R}, \frac{Q}{\mu_F}; \alpha_s(\mu_R)\right)$$

$$\times f_a(\xi_a, \mu_F) f_b(\xi_b, \mu_F) + O\left(\frac{\Lambda_{QCD}^2}{Q^2}\right)$$

$\hat{\sigma}$ is the hard cross section

$f_a(x, \mu_F)$ is the distribution for parton a with momentum fraction x, at scale μ_F

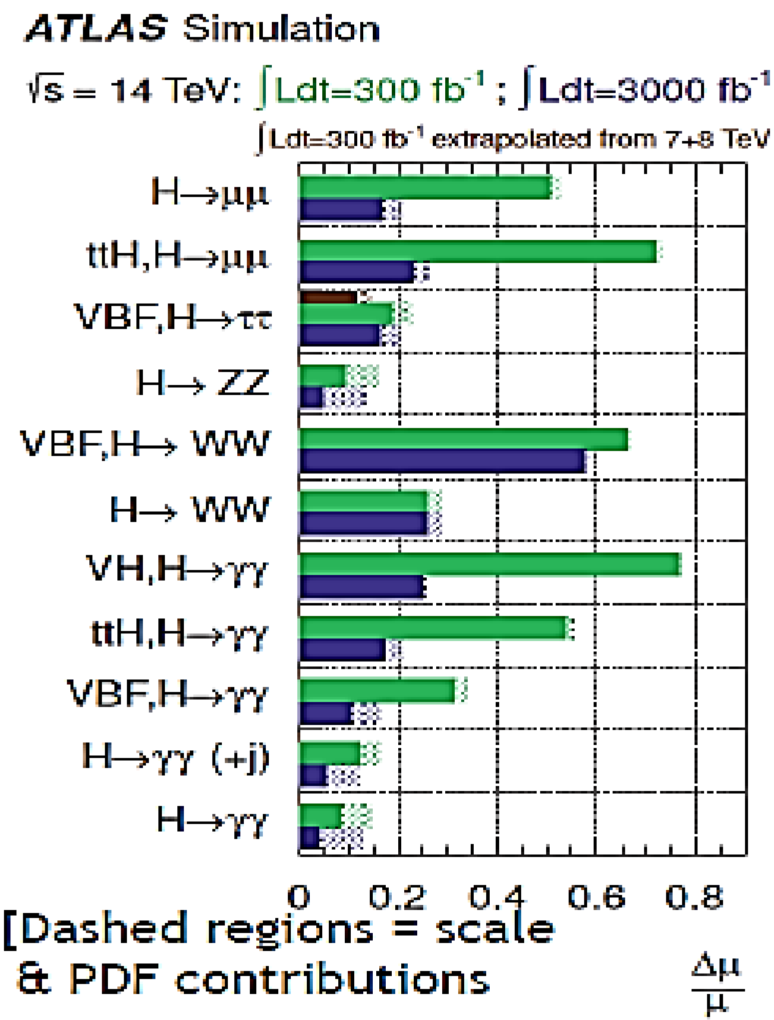
PDFs are important



QCD expectations for high-luminosity LHC

- Accuracy of PDFs must match accuracy of (N)NNLO calculations
- Measurements of Higgs cross sections/couplings become limited by PDFs in the HL-LHC era
- Searches for non-resonant production in TeV mass range will demand accurate predictions for **sea** PDFs at $x > 0.1$
- The target is to obtain PDFs that "achieve 1% accuracy for LHC predictions" within about a decade

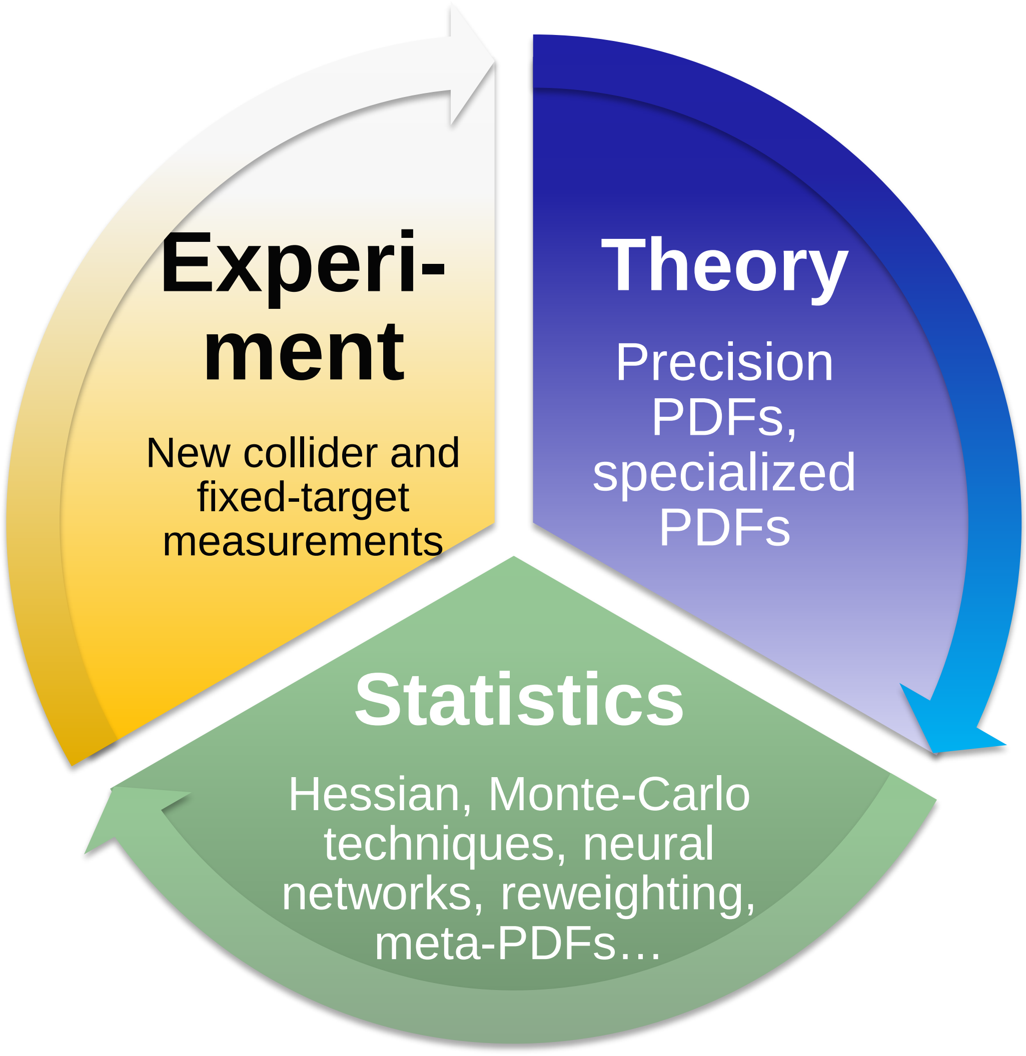
Projected Experimental Uncertainties



[Dashed regions = scale & PDF contributions

P. Newman, DIS'2016

Frontiers of the PDF analysis



Classes of PDFs

General-purpose

For (N)NLO calculations with $N_f \leq 5$ active quark flavors

From several groups:
ABM'16
HERA2.0
CT14
MMHT'14
NNPDF3.0
…

Specialized

For instance, for CT14:
CT14 LO
CT14 $N_f = 3$, 4, 6
CT14 HERA2
CT14 Intrinsic charm
CT14 QCD+QED

Combined

PDF4LHC'15=CT14+MMHT'14+NNPDF3.0

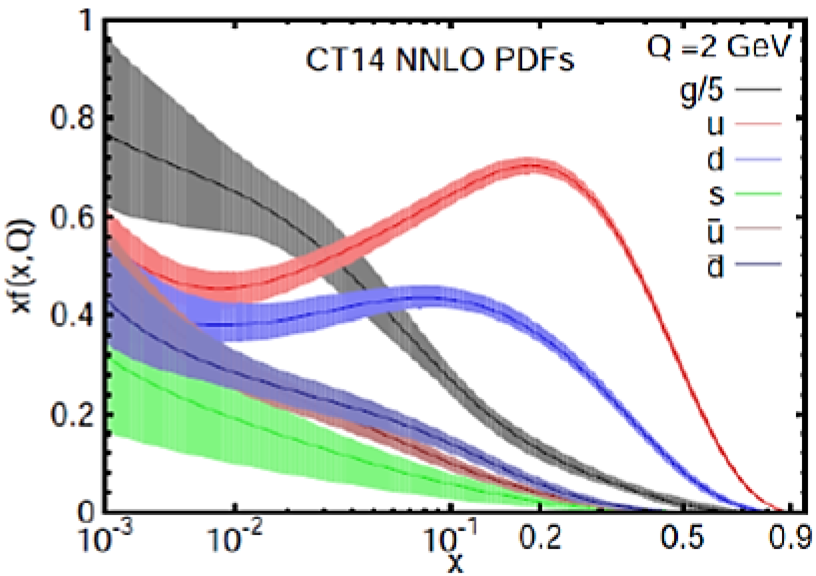
(S. Dulat et al., arXiv:1506.07443)

CT14 general-purpose PDFs…

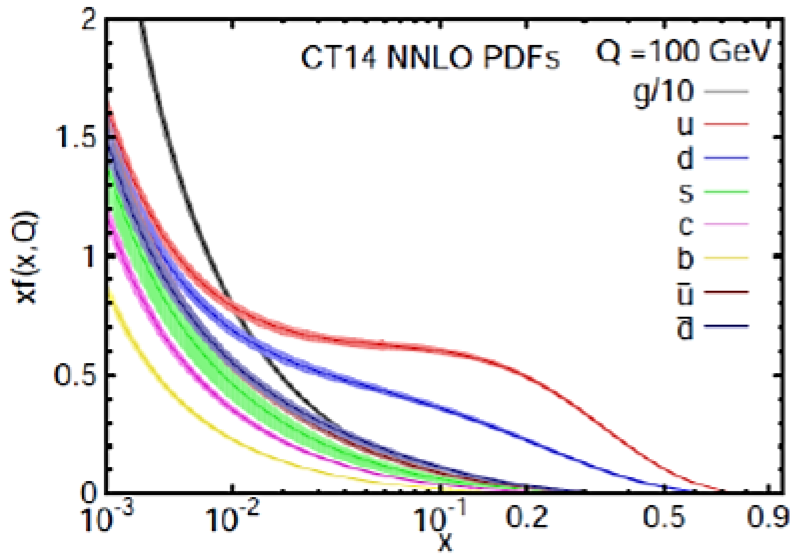
… include LHC Run 1 data and new Tevatron D0 Run 2 data on W-electron charge asymmetry

… use a more flexible parametrization for PDFs, compared to CT10

… are available at NNLO, NLO and LO, for $\alpha_s(M_Z) = 0.118 \pm 0.002$ at 90% c.l.; for 3, 4, 5, 6 active flavors



Q= 2 GeV



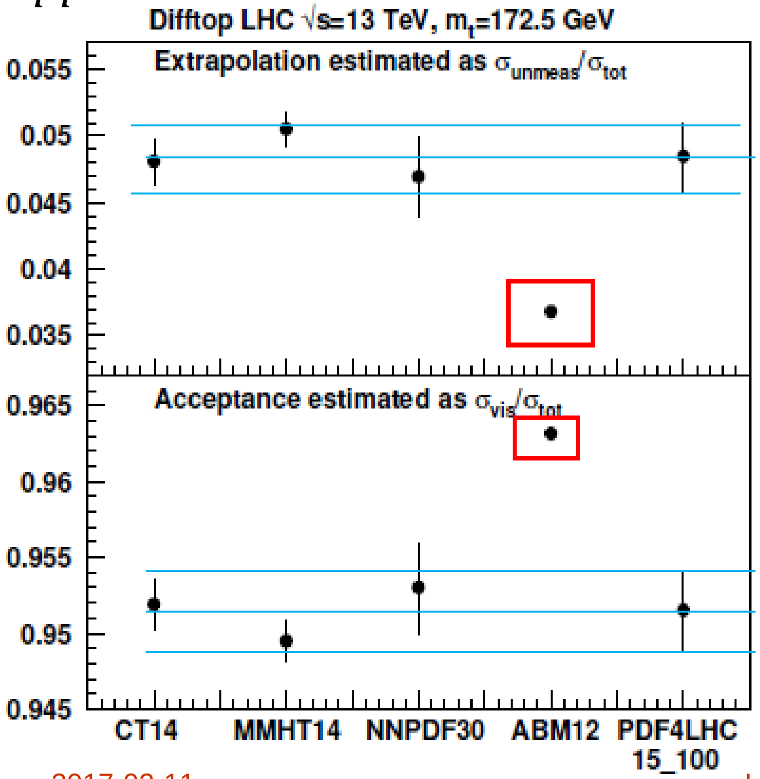
Q= 100 GeV

Some physics questions we examine

1. **CT17 (in progress):** how to extract useful information about PDFs from the LHC data? Dozens of new experiments, some disagreements between data, massive (N)NLO computations
2. **CT14 HERA2:** is DGLAP factorization consistent with DIS and LHC data? Yes *(arXiv:*1609.07968*)*
3. **CT14 QED** (*arXIv:1509.02905)* and **CT14 IC PDFs** *(T.-J. Hou et al., arXiv:1702.xxxxx)***:** allow for nonperturbative photon and charm distributions
4. **CT14 MC1 and MC2:** Monte Carlo replicas with asymmetric uncertainties and positivity *(T.-J. Hou et al., arXiv:1607.06066)*
   - Public program **mcgen** to generate such replicas on **metapdf.hepforge.org/mcgen**

Choosing the estimator for the PDF+α_s uncertainty

$pp \rightarrow t\bar{t}X$



⇒**PDF4LHC recommendations for LHC Run-II** (arXIV:1510.03865)

See also
A Critical Appraisal and Evaluation of Modern PDFs (arXIV:1603.08906)

Given numerous PDF sets, what is the PDF uncertainty in my analysis?

$pp \to t\bar{t}X$

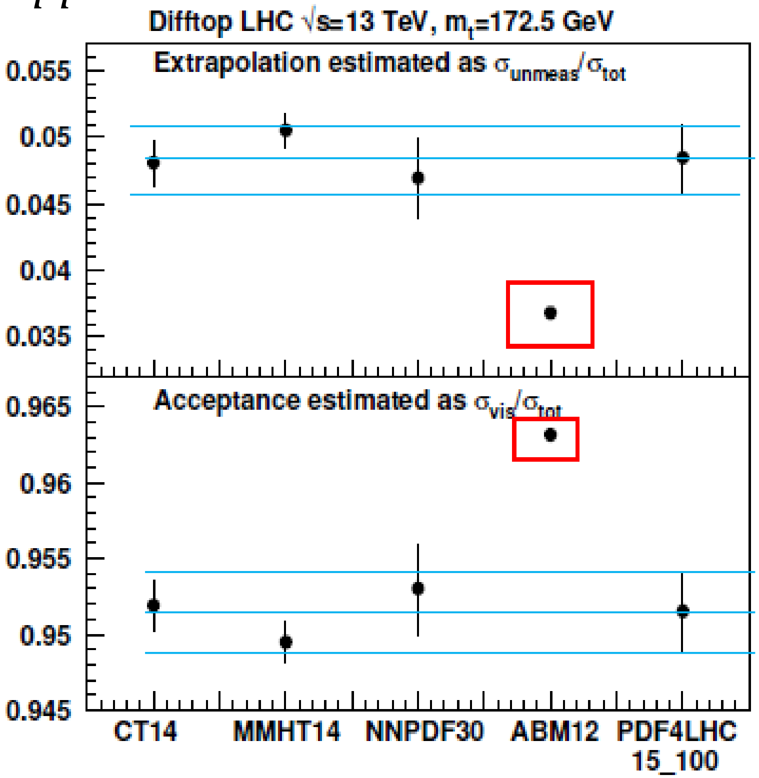


Figure: K. Lipka
1603.08906

The procedure for computing the PDF uncertainty must vary depending on the goals. The options may include

a) Using one individual set out of several similar ones (e.g., CT, MMHT, or NNPDF)

b) Using an envelope of all sets, including the outlier sets

c) 2015 recommendation by the PDF4LHC working group (arXiv:1510.03865)**:**

1. Several procedures spelled out for computation of PDF uncertainties, depending on the context
2. Estimation of PDF uncertainties is streamlined in many cases by using combined PDF4LHC15 sets based on CT14, MMHT14, and NNPDF3.0

Why PDF4LHC recommendation is necessary

Estimates of PDF uncertainties may vary drastically depending on the method.

An overly conservative estimate greatly reduces sensitivity to BSM physics.

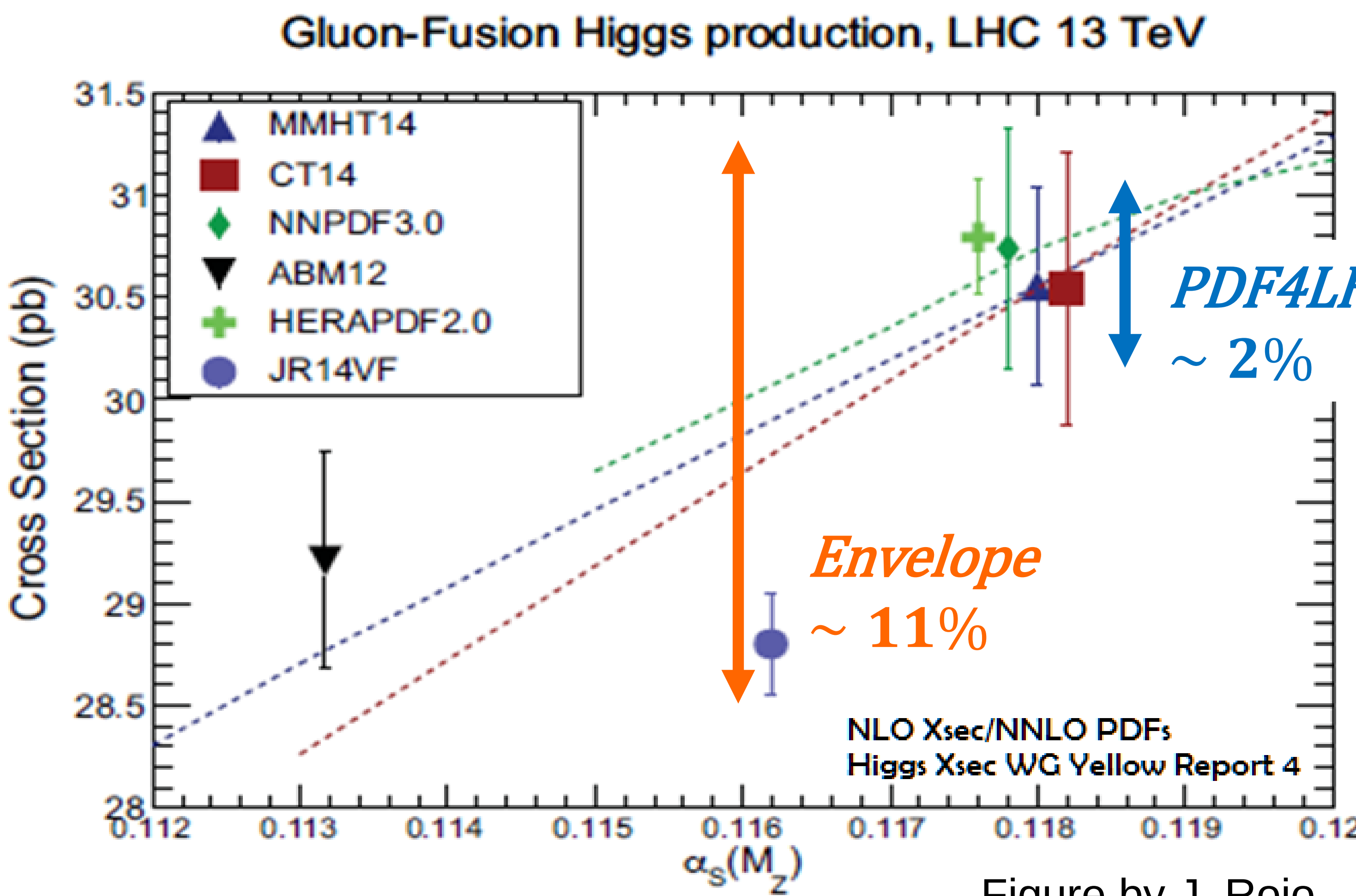


Figure by J. Rojo

Why PDF4LHC recommendation is needed

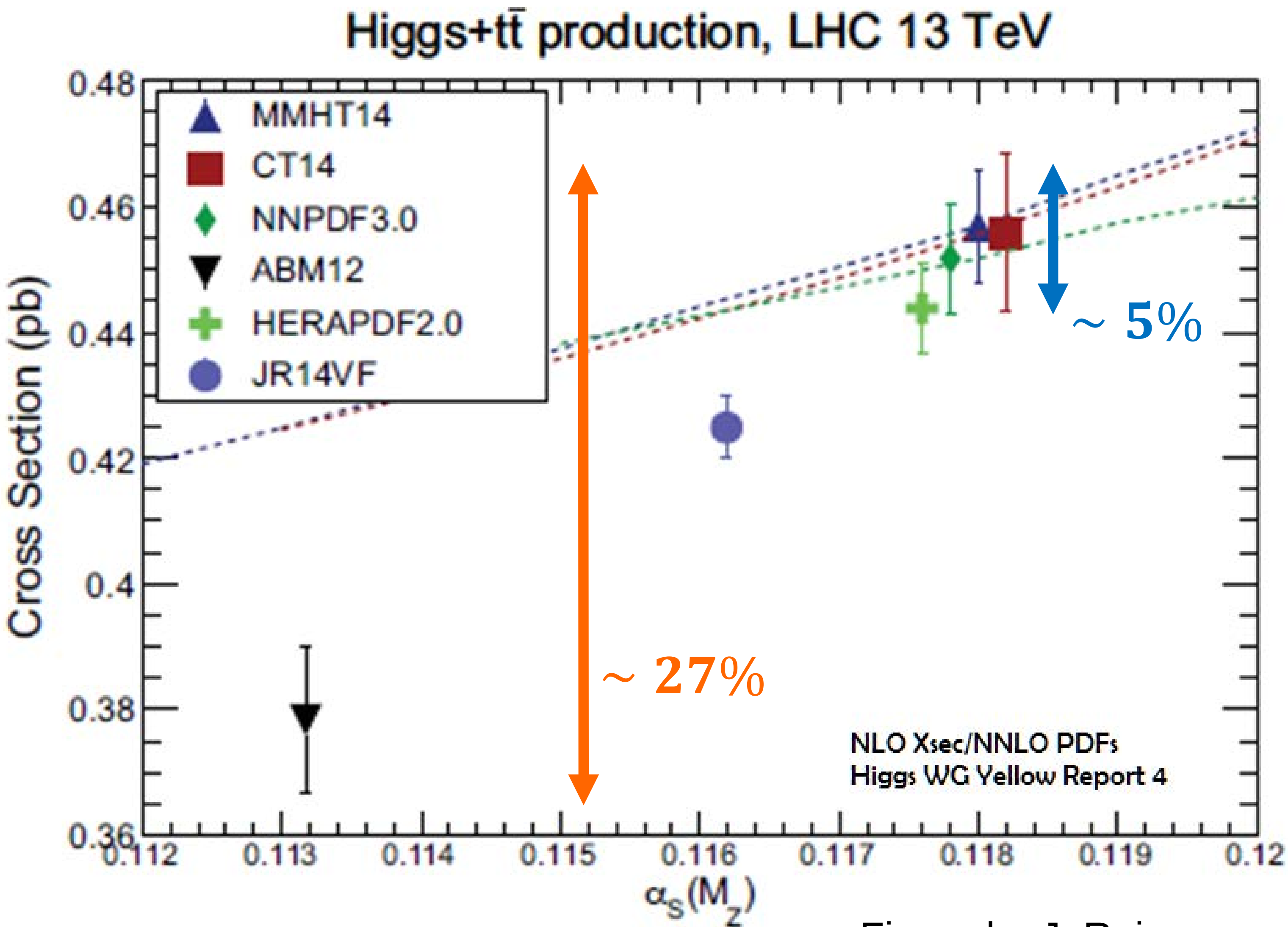


Figure by J. Rojo

OUTP-15-17P
SMU-HEP-15-12
TIF-UNIMI-2015-14
LCTS/2015-27

PDF4LHC recommendations for LHC Run II

Jon Butterworth[1], Stefano Carrazza[2], Amanda Cooper-Sarkar[3], Albert De Roeck[4,5], Joël Feltesse[6], Stefano Forte[2], Jun Gao[7], Sasha Glazov[8], Joey Huston[9], Zahari Kassabov[2,10], Ronan McNulty[11], Andreas Morsch[4], Pavel Nadolsky[12], Voica Radescu[13], Juan Rojo[14] and Robert Thorne[1].

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A major revision of the previous PDF4LHC recommendation in arxiv:1101.0538, arXiv:1211.5142

Before the PDF4LHC recommendations

Everyone proceeds at their own volition

After the PDF4LHC'15 recommendation

- Most traffic follows "the standard direction"
- Contraflow is tolerated in a few circumstances specified in the recommendation report

PDF4LHC publication, topics

1. **Review of updates on PDFs from various groups**

NNLO Global PDF sets: CT14, MMHT'14, NNPDF3

PDFs using other methodologies: ABM'12, CJ15, HERAPDF2.0

→

2. Average PDF sets by PDF4LHC group: PDF4LHC15_30, _100, _MC

Criteria for combination

$\alpha_s(M_Z) = 0.1180 \pm 0.0015$ at 68% c.l.

3. Recommendation on selecting PDF sets for various LHC applications

A. New physics searches

B. Precision tests of SM and PDFs

C. Monte-Carlo simulations

D. Acceptance estimates

Average PDF sets **can** be used **for bulk of applications** in A, C, D

Averaging of PDF ensembles

Combination workflow:

1. Generate 900 MC replicas from all input Hessian and MC ensembles (currently CT14, MMHT14, NNPDF3.0) using Thorne-Watt procedure

   Other PDF sets can be added in the future if they satisfy the recommendations' criteria

2. Reduce the number of final replicas from 900 to 100 or 30 by keeping most relevant PDF combinations, and by minimizing information loss

Three replica reduction techniques

1. Compressed Monte Carlo PDFs

PDF4LHC15_nnlo(nlo)_mc; *Carrazza et al., arXiv:1504.06469*

100 PDF error sets; keeps some information about asymmetric errors

2. META Hessian PDFs

PDF4LHC15_nnlo(nlo)_30; *Gao, Nadolsky, arXiv:1401.0013*

30 PDF error sets using METAPDF technique; Gaussian errors for now; better reproduces uncertainties using a limited number (30) of error PDFs

3. MCH Hessian PDFs

PDF4lhc15_nnlo(nlo)_100; *Carrazza et al., arXiv:1505.06736*

100 PDF error sets using MCH technique; better reproduces the uncertainties of the 900 MC set prior

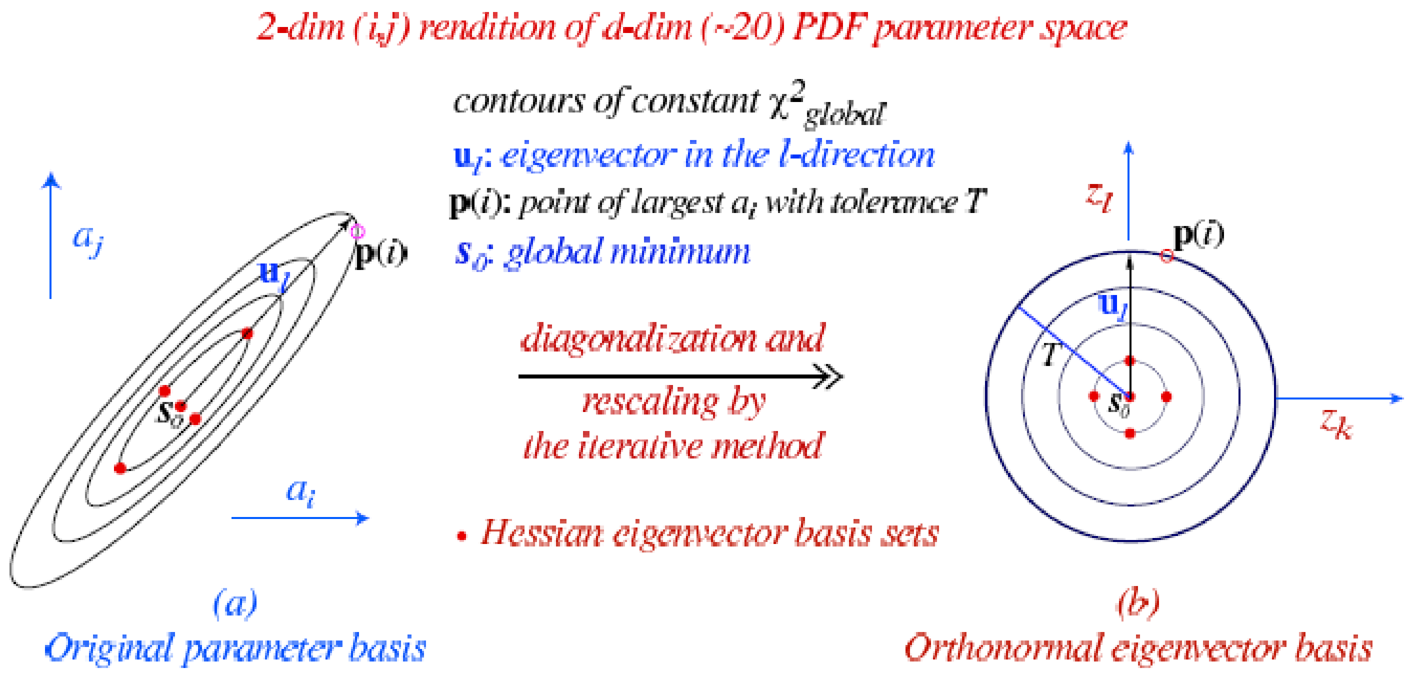
Averaging of PDFs, the meta-PDF method

Gao, Nadolsky, arXiv:1401.0013

1. Select the input PDF ensembles (CT, MSTW, NNPDF…)
2. Generate 900 Monte-Carlo replicas from both Hessian and Monte-Carlo ensembles (subtleties!)
3. Fit each PDF error set in the input ensembles by a common functional form with D~150 parameters ("**meta-parametrizations**")
4. Approximate the d-dimensional probability distribution of meta-parameters by a d'-dimensional distribution ($d' \ll d$) using the principal component analysis or another reduction method. Construct a small number of final Hessian PDFs from the d'-dim. manifold

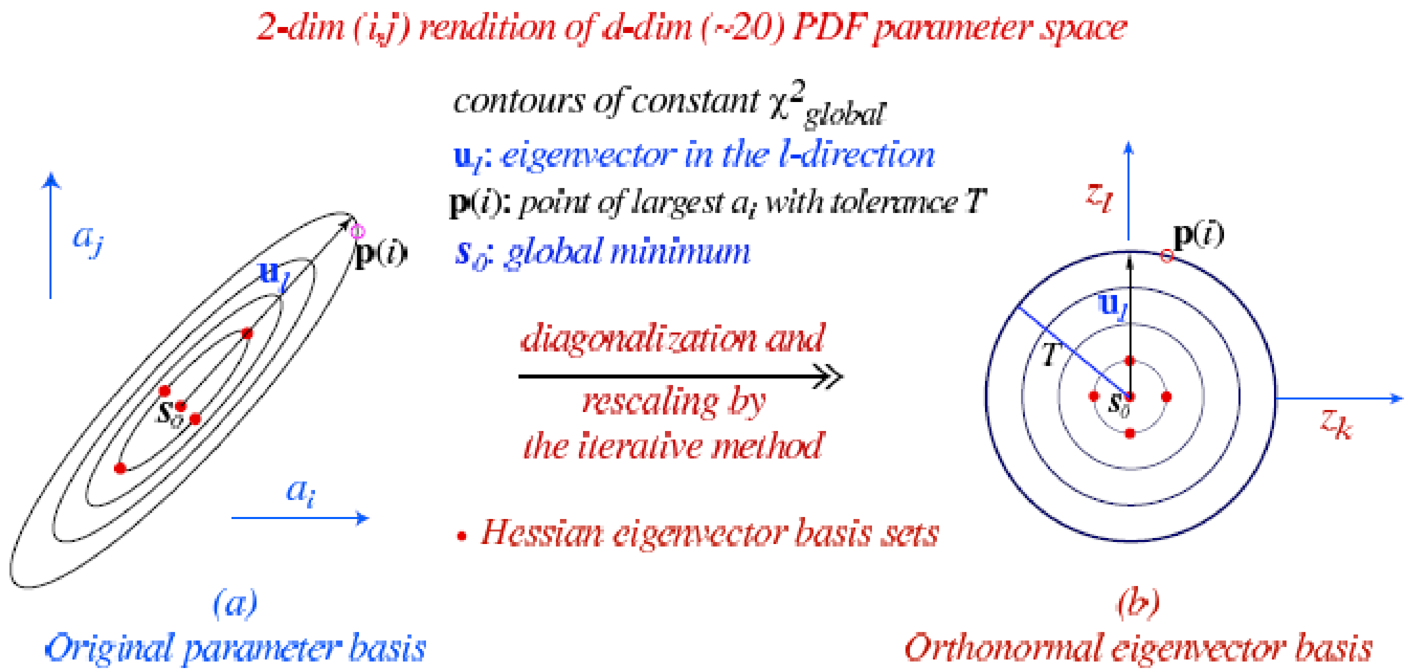
Only in the META set

Hessian PDFs



- PDF parameters approximately follow a Gaussian distribution
- The ellipsoidal boundary of a d-dim. confidence region can be delineated by $2d$ independent "eigenvector" PDFs

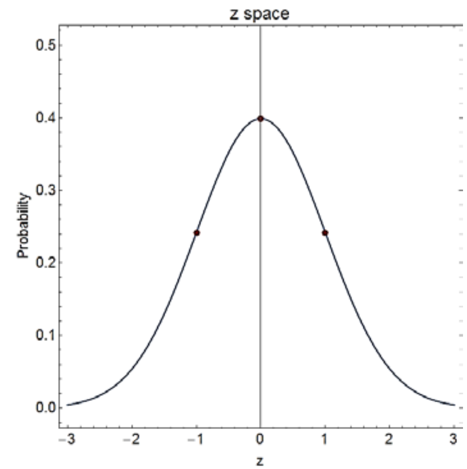
Hessian PDFs

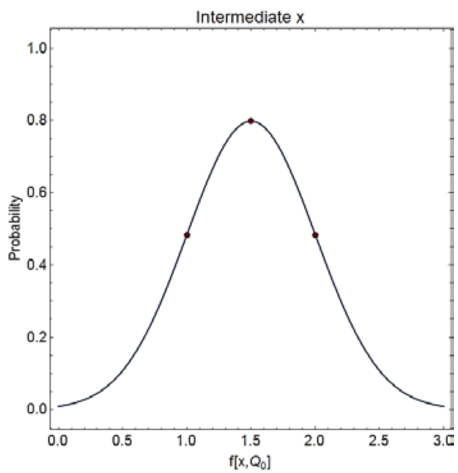


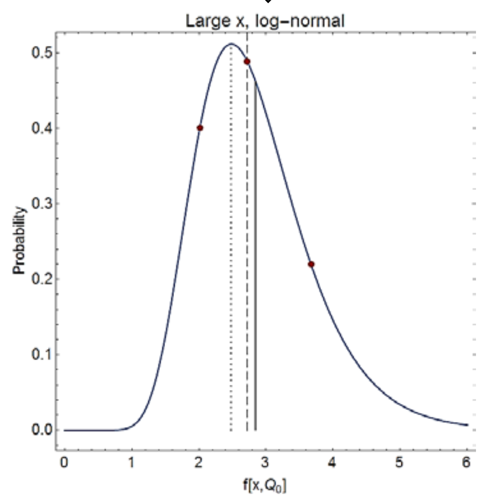
Along any direction z_i:

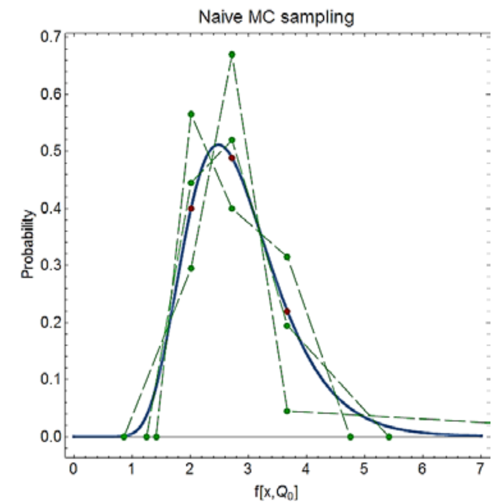
- the best-fit set corresponds to cumulative probability $P = 0.5$
- two 68% extreme sets $z_i^{\pm}$ correspond to $P = 0.16$ and 0.84

The x-space probability can be non-Gaussian





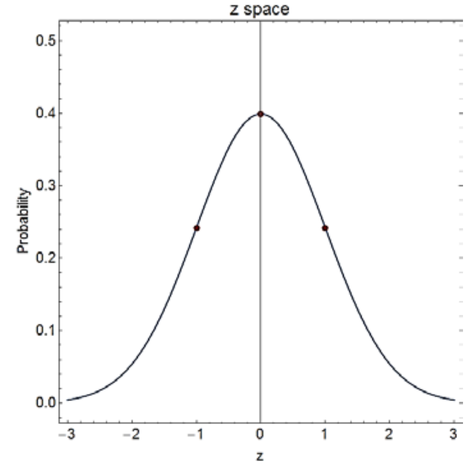


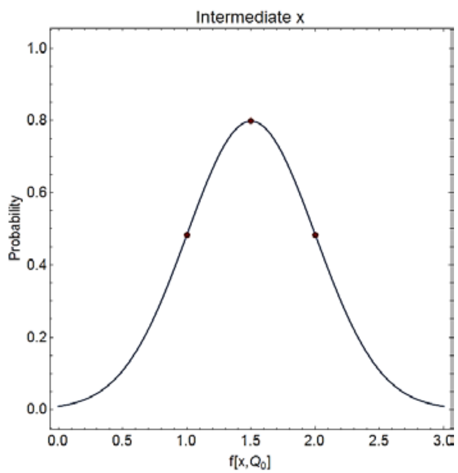


Well-constrained
x regions

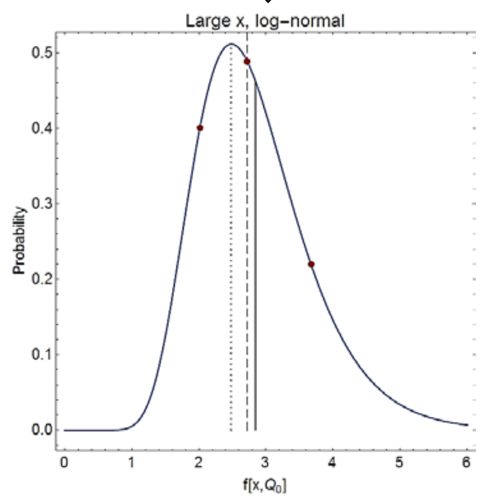
Large x
$f(x) \sim (1-x)^a$

The x-space probability can be non-Gaussian





Well-constrained
x regions



Large x
$f(x) \sim (1-x)^a$

The **mcgen** code converts Hessian replicas into the MC ones according to the normal (CT14 MC1) or log-normal (CT14 MC2) distributions

CT14 Monte-Carlo replica ensembles (MC1 and MC2) with asymmetric errors and positivity

arXiv:1607.06066

N_{rep} Monte-Carlo replicas are constructed from predictions $X_{\pm i}$ for Hessian eigenvector sets as

NEW

$$X^{(k)} = X(\{0\}) + \delta X^{(k)} - \Delta$$

$$\delta X^{(k)} \equiv \sum_{i=1}^{D} \frac{X_{+i} - X_{-i}}{2} R_i^{(k)} + \frac{1}{2} \sum_{i,j=1}^{D} (X_{+i} + X_{-i} - 2X_0) \left(R_i^{(k)}\right)^2$$

Random real values $R_i^{(k)}$ are sampled from the standard normal distribution

CT14 MC1 replicas are constructed from $X = f_a(x, Q_0)$, can be negative
CT14 MC2 replicas are constructed from $X = log\ [f_a/f_{a0}]$, where $f_{a0}(x, Q_0)$ is the central Hessian PDF; **each replica PDF is non-negative**

The uncertainties are given by **asymmetric** standard deviations,

NEW

$$\delta_{68}^{MC,>} X = \sqrt{\langle (X - \langle X \rangle)^2 \rangle_{X > \langle X \rangle}}$$

$$\delta_{68}^{MC,<} X = \sqrt{\langle (X - \langle X \rangle)^2 \rangle_{X < \langle X \rangle}}$$

f_a/f_{a0} values for individual replicas

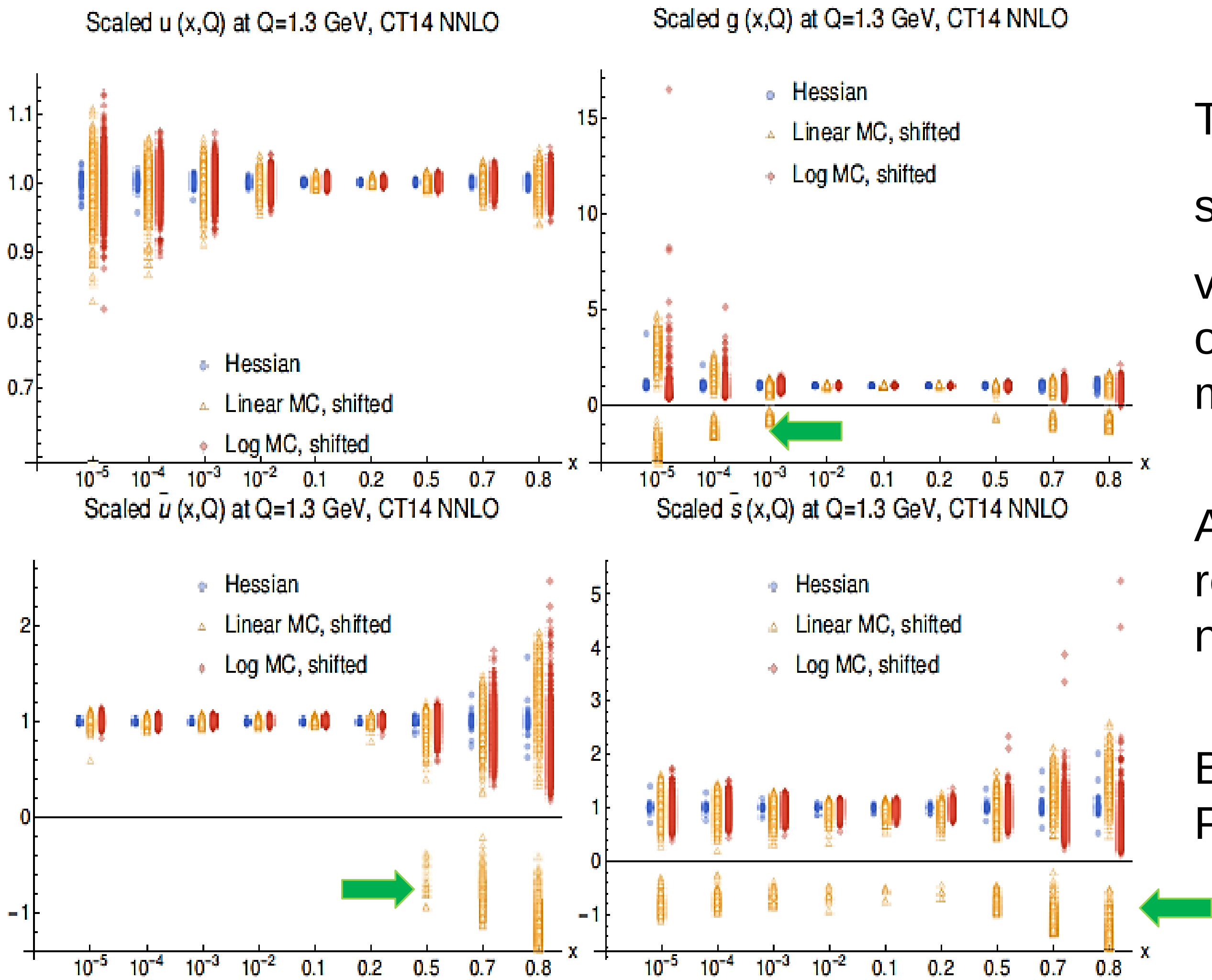


FIG. 2: Distributions of individual replicas for MC1 (linear MC, shifted) and MC2 (log MC, shifted) ensembles.

The vertical axes have scale $\left|\frac{f}{f_{a0}}\right|^{0.2} sign(f)$ to visualize relative variations of $\pm$ signs in an extended magnitude range

A fraction of 1000 MC1 replica PDFs can be negative (**green arrows**).

But, all Hessian and MC2 PDFs are positive

Parameter distributions in the META method

When expressed as the meta – parametrizations, PDF functions can be combined by averaging their meta-parameter values

Standard error propagation is feasible, e.g., to treat the meta-parameters as discrete data in the linear (Gaussian) approximation for small variations

The effective number of error PDFs is reduced by PCA (diagonalization of the covariance matrix), while keeping the most reliable information about the PDFs

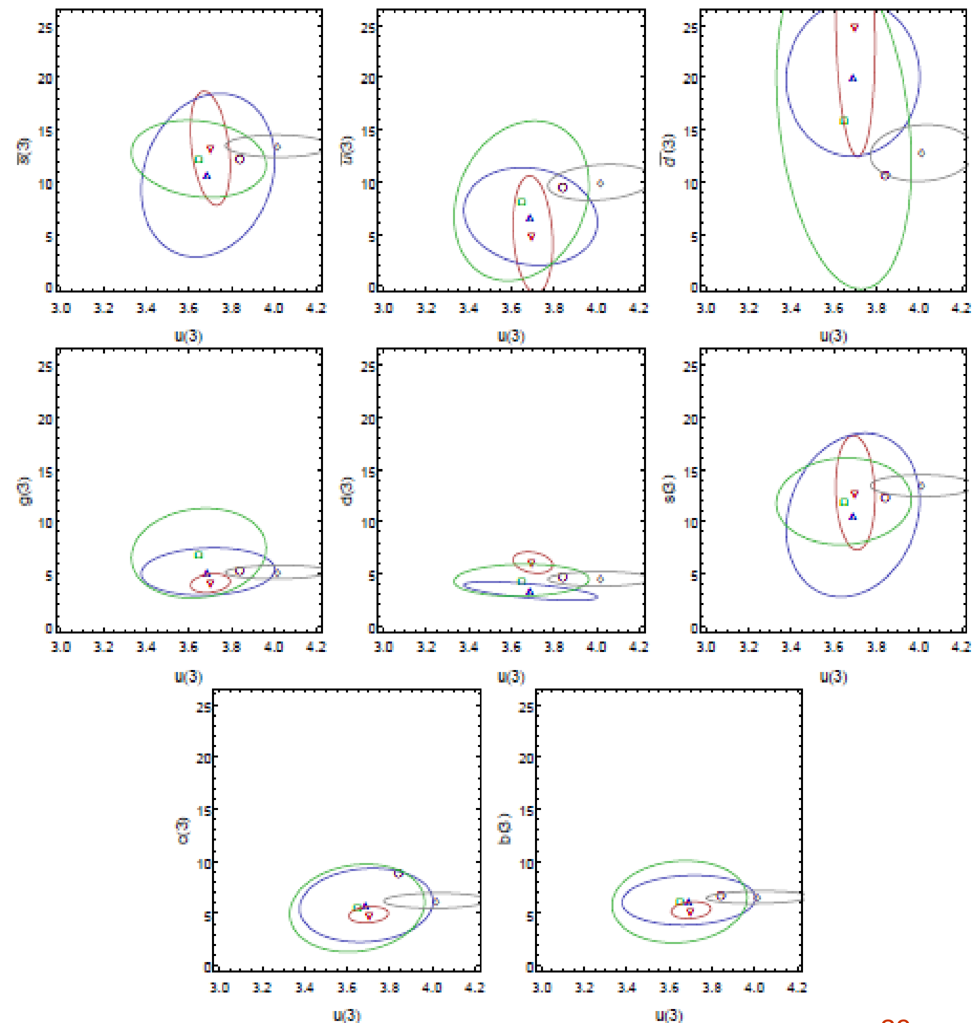
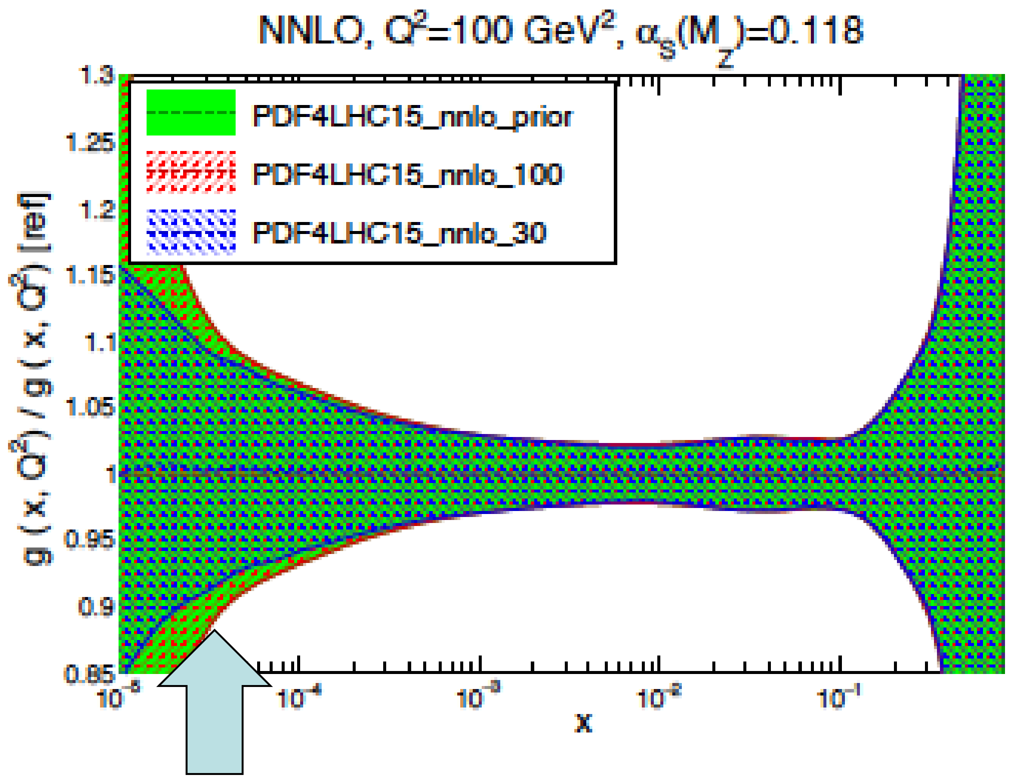


Figure 10: Fitted PDF parameters and 90% c.l. ellipses for CT10 (blue up triangle), MSTW08 (red down triangle), NNPDF2.3 (green square), HERAPDF1.5 (gray diamond) and ABM11 (magenta circle).

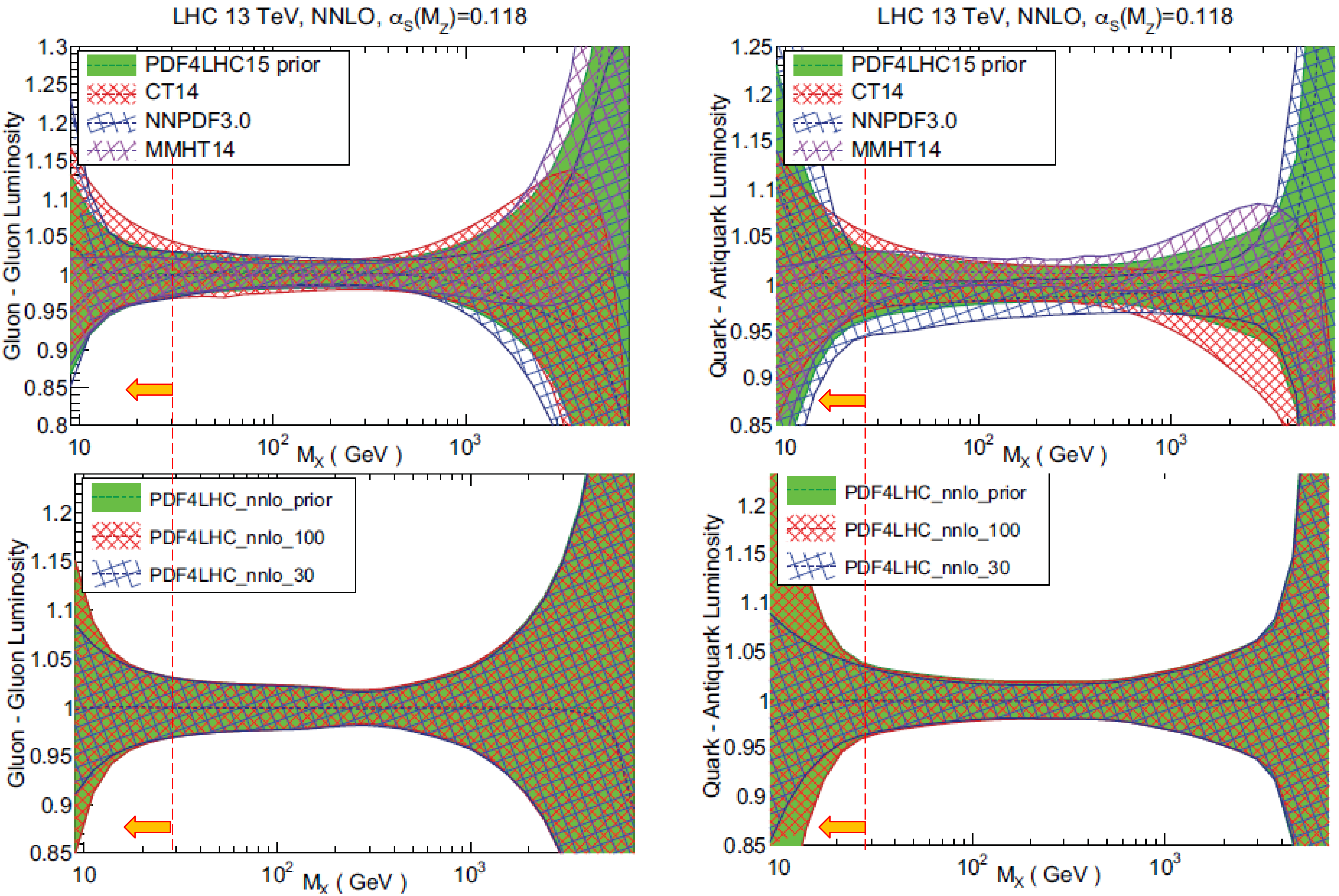
Comparisons of PDF4LHC ensembles with 900, 100, 30 replicas



Three PDF4LHC sets reproduce well the 900-replica prior. Keep in mind that the uncertainty of the prior has an uncertainty of its own. By their construction, the lowest Hessian eigenvector sets are known the best, the highest sets are known with less confidence.

The 30-member ensemble keeps the lowest, best known sets and thus provides a lower estimate for the _900 prior uncertainty, known with higher confidence. When this estimate is not sufficient, or non-Gaussianities are important, use the 100 and MC sets

Ranges with differences between input PDFs, prior, and reduced sets



Choosing the right PDF set for an LHC application

6.1 Delivery and guidelines

The PDF4LHC15 combined PDFs are based on an underlying Monte Carlo combination of CT14, MMHT14 and NNPDF3.0, denoted by MC900, which is made publicly available in three different reduced delivery forms:

- **PDF4LHC15_mc**: a *Monte Carlo PDF set* with $N_{rep} = 100$ replicas.
- **PDF4LHC15_30**: a *symmetric Hessian PDF set* with $N_{eig} = 30$ eigenvectors.
- **PDF4LHC15_100**: a *symmetric Hessian PDF set* with $N_{eig} = 100$ eigenvectors.

In the three cases, combined sets are available at NLO and at NNLO, for the central value of $\alpha_s(m_Z^2) = 0.118$. In addition, we provide additional sets which contain the central values for $\alpha_s(m_Z^2) = 0.1165$ and $\alpha_s(m_Z^2) = 0.1195$, and that can be used for the computation of the combined PDF+α_s uncertainties, as explained in Sect. 6.2. Finally, for ease of usage, the combined sets for $\alpha_s(m_Z^2) = 0.118$ are also presented bundled with the α_s-varying sets in dedicated grid files. The specifications of each of the combined NNLO PDF4LHC15 sets that are available from LHAPDF6 are summarized in Table 5; note that the corresponding NLO sets are also available.

Usage of the PDF4LHC15 sets. As illustrated in Sect. 5, the three delivery options provide a reasonably accurate representation of the original prior combination. However, each of these methods has its own advantages and disadvantages, which make them more suited in different specific contexts. We now attempt to provide some general guidance about which of the three PDF4LHC15 combined sets should be used in specific phenomenological applications.

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.

   Rationale: Measurements such as jet production, vector-boson single and pair production, or top-quark pair production, have the power to constrain PDFs, and this is best utilized and illustrated by comparing with many individual sets.

   As a rule of thumb, *any measurement that potentially can be included in PDF fits* falls in this category.

   The same recommendation applies to the *extraction of precision SM parameters*, such as the strong coupling $\alpha_s(m_Z^2)$ [75, 124], the W mass M_W [125], and the top quark mass m_t [126] which are directly correlated to the PDFs used in the extraction.

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 $x \to 1$ [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.

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The PDF4LHC document contains detailed guidelines to help decide which individual or combined PDFs to use depending on the circumstances

To assist in choosing the best PDF(s), demonstrative comparisons were generated of typical LHC cross sections for recent PDFs

1. **MC2H gallery of LHC cross sections:** ApplGrid, typical experimental cuts

www.hep.ucl.ac.uk/pdf4lhc/mc2h-gallery/

2. SMU gallery of LHC cross sections: ApplGrid or full calculations, minimal cuts

www.physics.smu.edu/botingw/2016_pdf4lhc/

www.physics.smu.edu/botingw/2016_pdf4lhc/

Predictions for LHC observables based on PDF4LHC15 PDFs

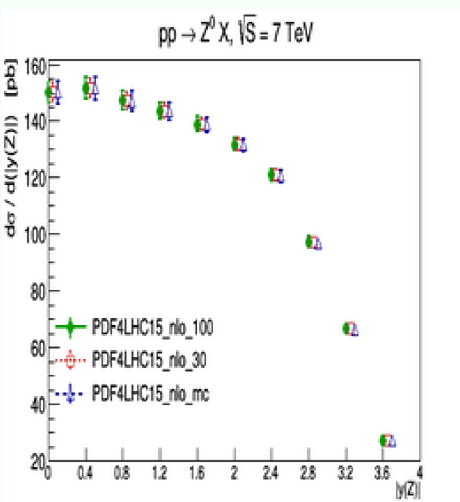
1. $p + p \rightarrow Z + X$
   - PDF4LHC15 PDFs (NLO)
   - PDF4LHC15 PDFs (NNLO)
   - PDF4LHC15_nnlo_100, HERA, ABM PDFs
   - PDF4LHC15_nnlo_100, CT14, MMTH14, NNPDF3.0 PDFs
2. $p + p \rightarrow W^+ + X$
   - PDF4LHC15 PDFs (NLO)
   - PDF4LHC15 PDFs (NNLO)
   - PDF4LHC15_nnlo_100, HERA, ABM PDFs
   - PDF4LHC15_nnlo_100, CT14, MMTH14, NNPDF3.0 PDFs

SMU gallery for basic processes at 7, 8, 13 TeV

Developed by Bo Ting Wang and Keping Xie

$p + p \rightarrow Z + X$

PDF4LHC15 PDFs (NLO)



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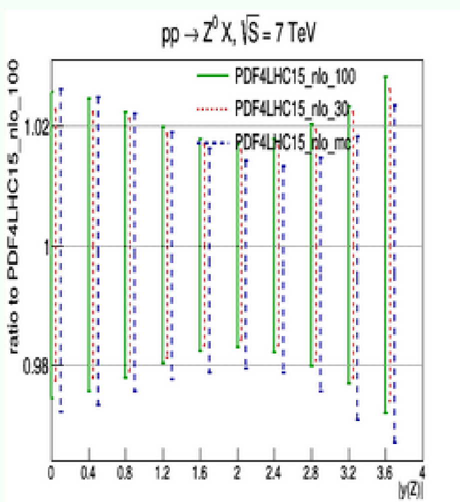

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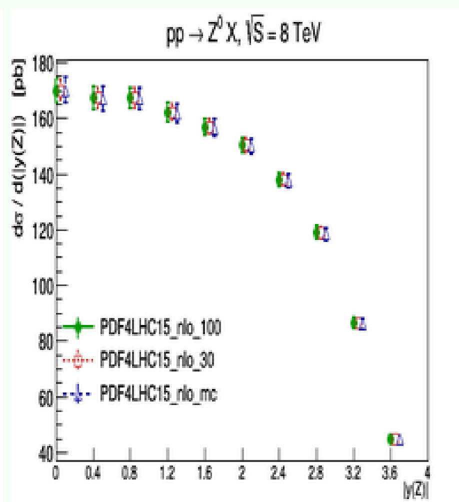

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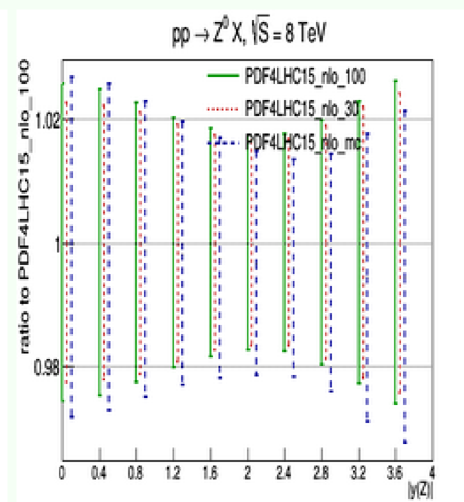


[pdf]

Gallery of phenomenological comparisons for LHC

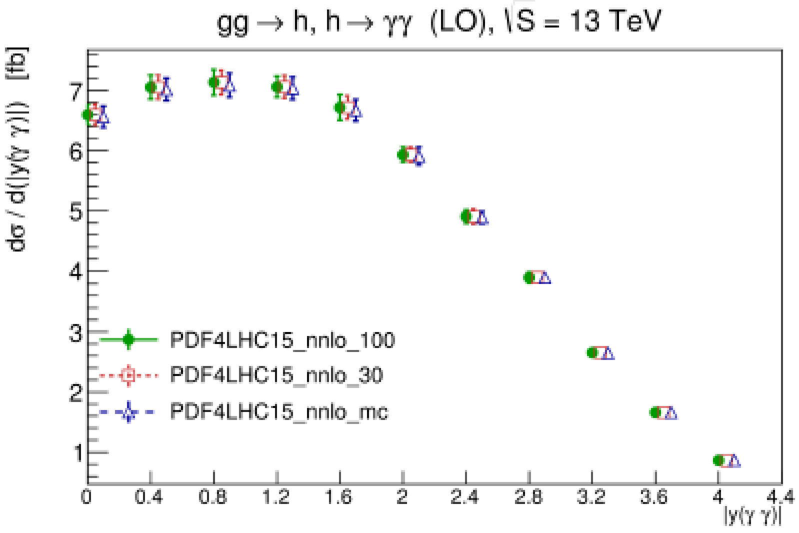
Process	Order	Type of calculation
•p + p → Z + X	NLO	aMCFast/APPLgrid
•p + p → W^+ + X	NLO	aMCFast/APPLgrid
•p + p → W^- + X	NLO	aMCFast/APPLgrid
•p + p → $t\bar{t}$ + X	NLO	aMCFast/APPLgrid
•p + p → $t\bar{t}$ + X	NLO	aMCFast/APPLgrid
•p + p → $t\bar{t}\gamma\gamma$+X	NLO	aMCFast/APPLgrid
•ATLAS inclusive jets	NLO	NLOJET++/APPLgrid
•ATLAS inclusive dijets	NLO	NLOJET++/APPLgrid
•P + p → W^+ c + X	NLO	aMCFast/APPLgrid
•P + p → W^- c + X	NLO	aMCFast/APPLgrid
•P + p → H + X	LO,NLO	MCFM
•P + p → H+ jet + X	LO, NLO	MCFM

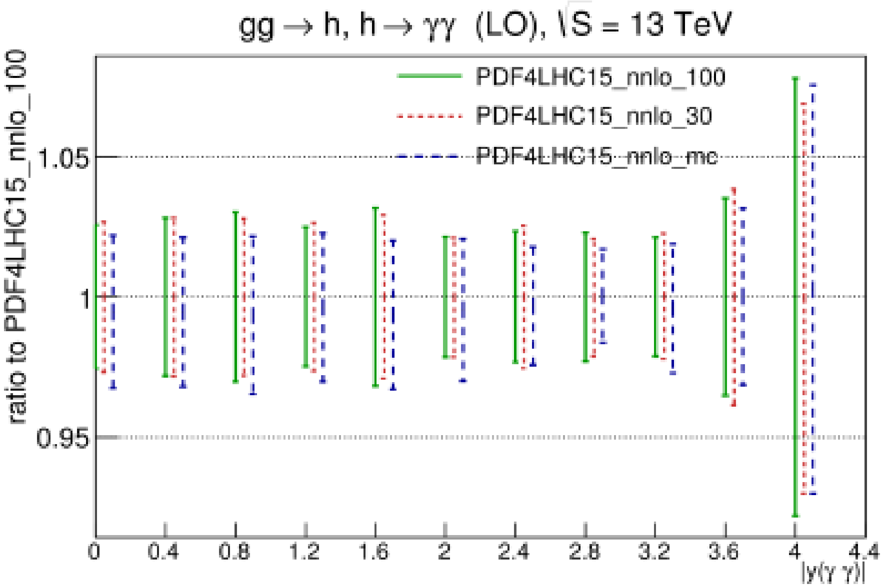
Compared PDFs: PDF4LHC15_100, _30, _MC, ABM’12, CT14, HERA2.0, MMHT14, NN3.0

Both full (MCFM) and fast (ApplGrid) calculations. AppGrlids are generated with minimal cuts and can be downloaded.

MCFM: compare PDF and Monte-Carlo integration errors

Differences of PDF4LHC PDFs do not matter in many cases when MC errors are negligible



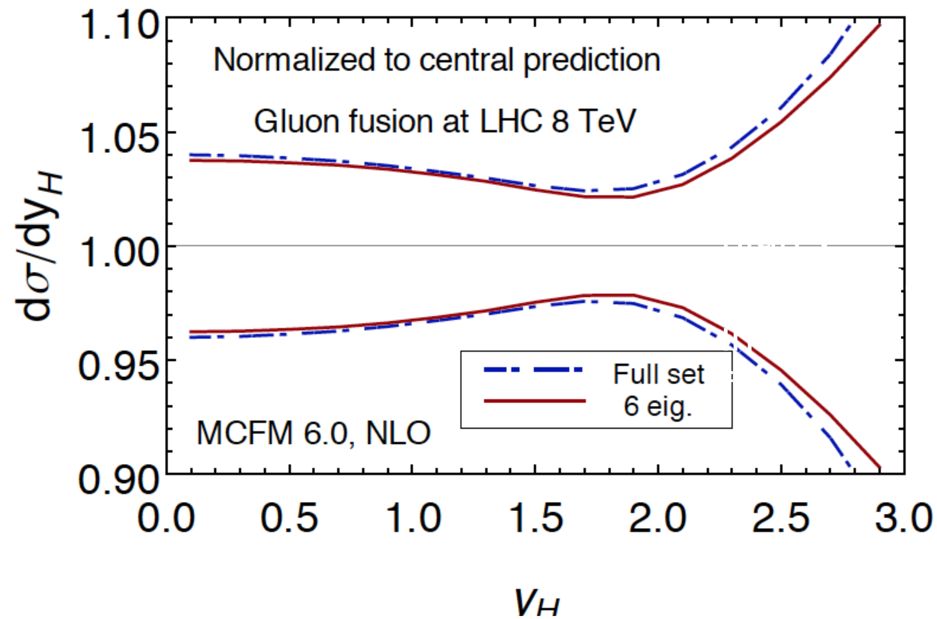


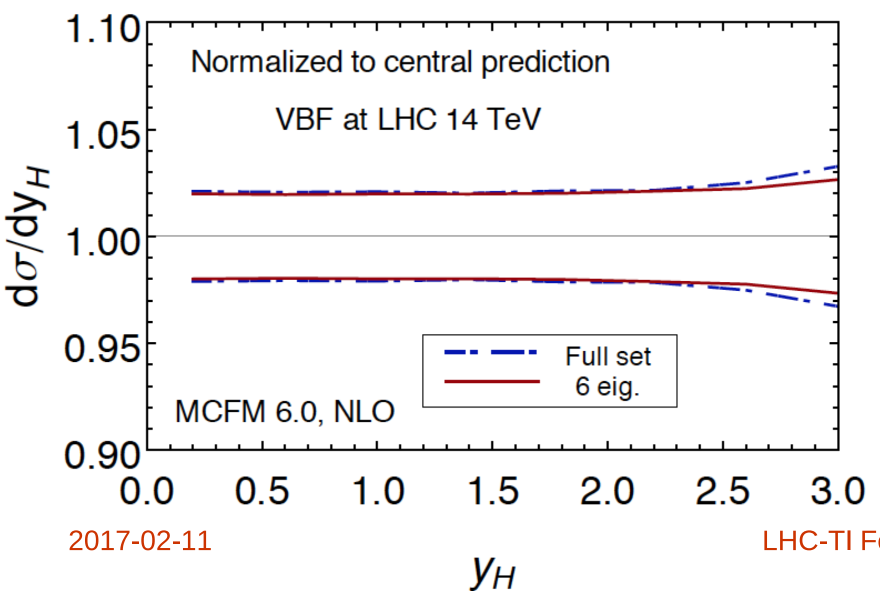
$gg \to H$ **at LO.** Simple process. 10^6 events, PDF reweighting, ~30 min per each PDF family

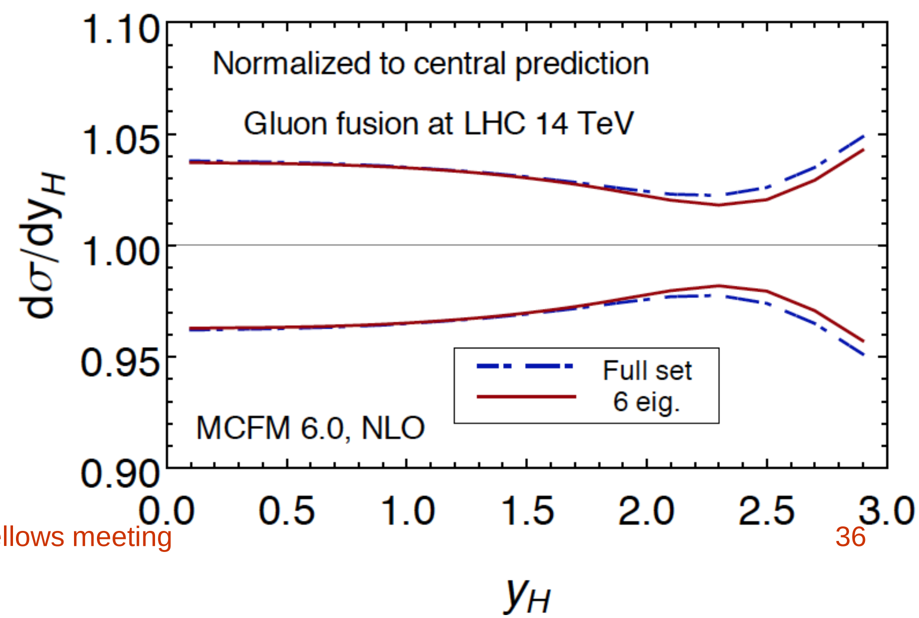
MC fluctuations in PDF errors are of the same order as the primordial differences

6-member Higgs eigenvector set

- For a given class of observables, the _30 set can be **diagonalized** to reproduce the bulk of the uncertainties and correlations with ~6 eigenvector sets







process	$\sigma_{cen.}$	δ_{Full}	$\delta_{Diag.}$	$\sigma^{\alpha_s}_{0.116}$	$\sigma^{\alpha_s}_{0.12}$
$gg \to H$ [pb]	18.77	$^{+0.48}_{-0.46}$	$^{+0.48}_{-0.44}$	18.11	19.4
	43.12	$^{+1.13}_{-1.07}$	$^{+1.13}_{-1.04}$	41.68	44.6
VBF [fb]	302.5	$^{+7.8}_{-6.7}$	$^{+7.6}_{-6.7}$	303.1	301.
	878.2	$^{+19.7}_{-17.9}$	$^{+19.2}_{-17.3}$	877.3	878.
HZ [fb]	396.3	$^{+8.4}_{-7.3}$	$^{+8.1}_{-7.4}$	393.0	399.
	814.3	$^{+14.8}_{-13.2}$	$^{+13.8}_{-13.0}$	806.5	823.
$HW^{\pm}$ [fb]	703.0	$^{+14.4}_{-14.4}$	$^{+14.3}_{-14.1}$	697.4	708.
	1381	$^{+28}_{-22}$	$^{+26}_{-22}$	1368	139
HH [fb]	7.81	$^{+0.33}_{-0.30}$	$^{+0.33}_{-0.30}$	7.50	8.1
	27.35	$^{+0.78}_{-0.72}$	$^{+0.78}_{-0.68}$	26.48	28.2
$t\bar{t}$ [pb]	248.4	$^{+9.1}_{-8.2}$	$^{+9.2}_{-8.1}$	237.1	259.
	816.9	$^{+21.4}_{-19.6}$	$^{+21.4}_{-18.4}$	785.5	848.
$Z/\gamma^*(l^+l^-)$ [nb]	1.129	$^{+0.025}_{-0.023}$	$^{+0.024}_{-0.023}$	1.113	1.14
	1.925	$^{+0.043}_{-0.041}$	$^{+0.040}_{-0.037}$	1.897	1.95
$W^+(l^+\nu)$ [nb]	7.13	$^{+0.14}_{-0.14}$	$^{+0.14}_{-0.13}$	7.03	7.2
	11.64	$^{+0.24}_{-0.23}$	$^{+0.22}_{-0.21}$	11.46	11.8
$W^-(l^-\bar{\nu})$ [nb]	4.99	$^{+0.12}_{-0.12}$	$^{+0.12}_{-0.11}$	4.92	5.0
	8.59	$^{+0.21}_{-0.20}$	$^{+0.19}_{-0.18}$	8.46	8.7
W^+W^- [pb]	4.14	$^{+0.08}_{-0.08}$	$^{+0.08}_{-0.07}$	4.04	4.2
	7.54	$^{+0.15}_{-0.14}$	$^{+0.14}_{-0.12}$	7.39	7.5
ZZ [pb]	0.703	$^{+0.016}_{-0.014}$	$^{+0.015}_{-0.014}$	0.695	0.71
	1.261	$^{+0.026}_{-0.024}$	$^{+0.024}_{-0.022}$	1.256	1.27
W^+Z [pb]	1.045	$^{+0.019}_{-0.018}$	$^{+0.019}_{-0.017}$	1.039	1.06
	1.871	$^{+0.033}_{-0.031}$	$^{+0.029}_{-0.027}$	1.850	1.89
W^-Z [pb]	0.788	$^{+0.020}_{-0.019}$	$^{+0.019}_{-0.018}$	0.780	0.79
	1.522	$^{+0.034}_{-0.032}$	$^{+0.033}_{-0.031}$	1.509	1.54

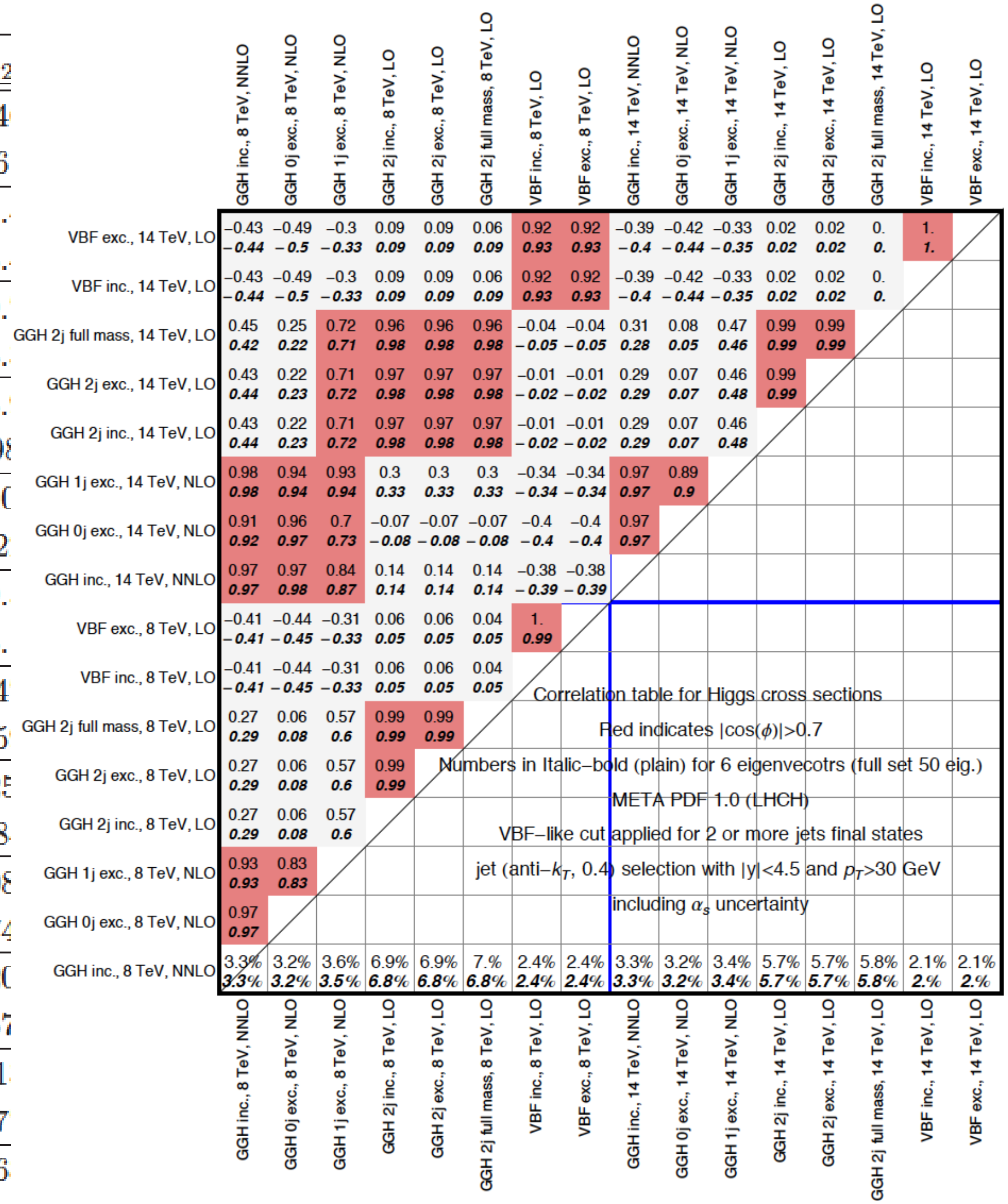


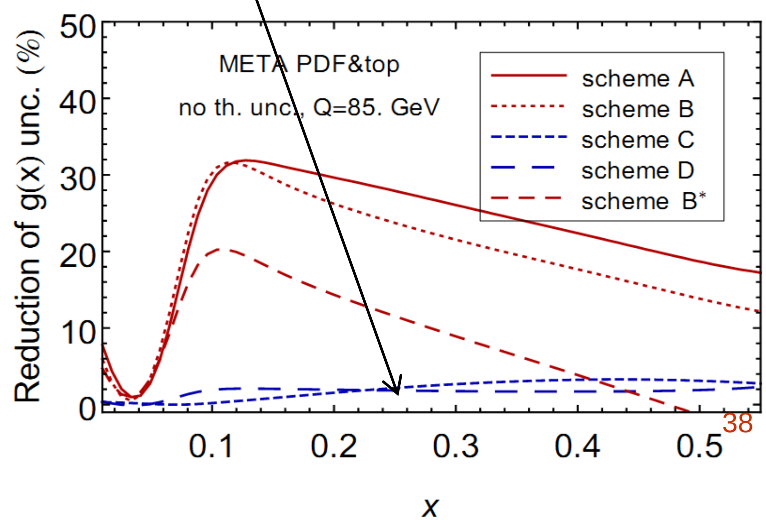
FIG. 7: Same as Fig. 5, with α_s uncertainties included by adding in quadrature.

Ongoing work: inclusion of new LHC data

- $W/Z,\ t\bar{t}$ differential
  - applgrid at NLO with NNLO/NLO K-factors
  - Understand tensions between ATLAS and CMS
- Inclusive jets
  - will continue to use NLO and fastNLO/applgrid to include 8 and 13 TeV ATLAS/CMS jet data sets
  - NNLO corrections were shown to be small when correct scale is used; no need for rapidity cuts
  - will adapt to NNLO format when available
- Photon/W/Z+charm
  - some theoretical work ongoing before inclusion in global PDF fit
  - framework for charm will continue to be perturbative charm, without an intrinsic component

- In general, we are working on improving the speeds of NLO and NNLO fits
- PDF reweighting is being explored, but has to take into account tolerance issues
- For example, for global PDF fits like MMHT or CT, reduction in χ^2 for $t\bar{t}$ total cross section (1303.7215) less significant than suggested by re-weighting

Jun Gao



Backup slides