



Combination of PDF uncertainties for LHC observables

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in collaboration with Jun Gao (Argonne),
Joey Huston (MSU)

Based on discussions of 2014-15 PDF4LHC
meetings and Benasque PDF workshop

Choosing a PDF for your practical computation

A. Accardi,
this workshop

	JLab	HERA I+II <i>Wichmann</i>	Tevatron new W,Z	LHC	di- μ	Nucl.	H ₁ TMC	Flex d	closure
NEW! HERAPDF2.0 → <i>Myronenko, Brandt</i>		✓	⊠						
NEW! CT14 → <i>Nadolski</i>			✓ ⊠⊠	✓	✓			✓	
NEW! MMHT14 → <i>Thorne</i>			✓ ⊠⊠	✓	✓	✓			
NEW! NNPDF3.0 → <i>Deans</i>				✓	✓				✓
[GJR14]	✓			✓	✓	✓	✓		
CJ12 * (→ CJ15) → <i>Melnitchouk</i>	✓	(✓)	(✓)		✗	✓	✓	✓	
ABM12 **					✓	✓	✓		

* NLO only ** No jet data ⊠ but see 1503.05221 ⊠⊠ no reconstructed W

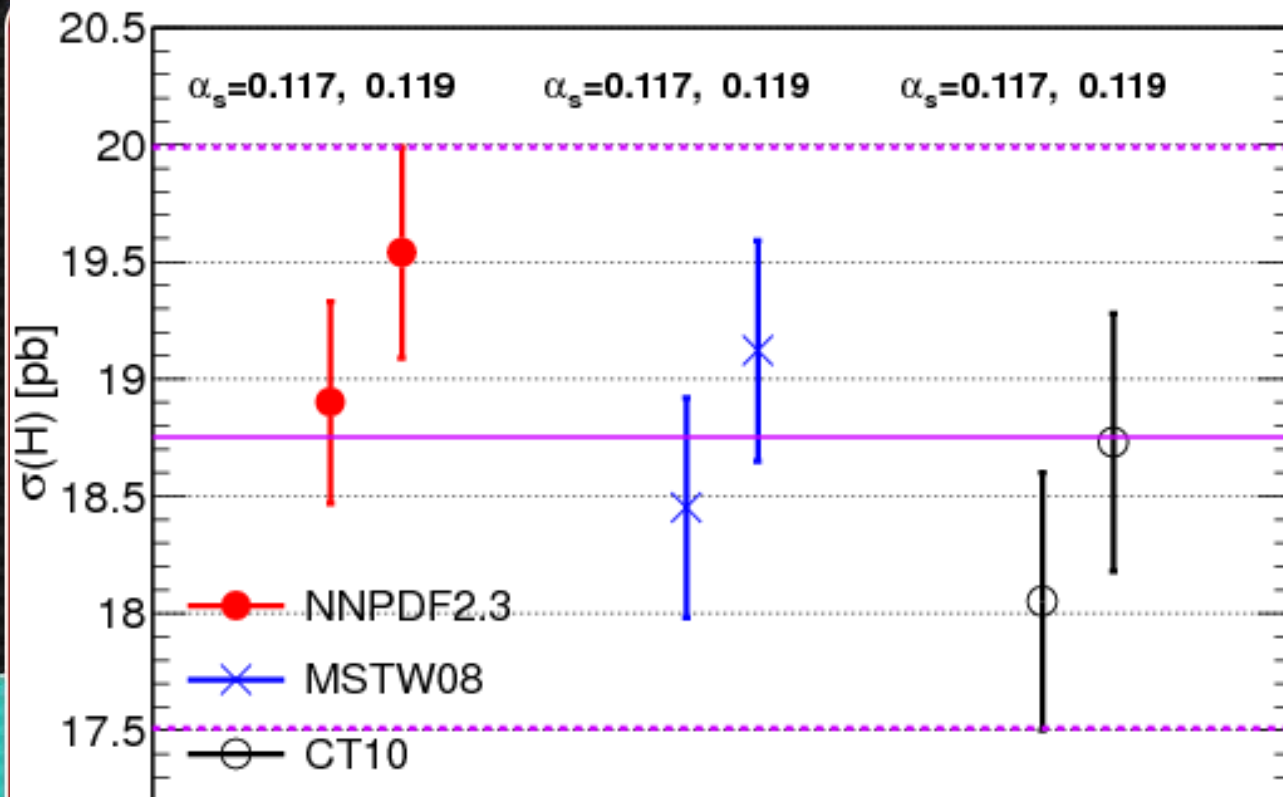
Several groups determine new PDF ensembles with various approaches. Which one(s) should be used in a given experimental study? Are all predictions compatible? Can/should one combine PDF uncertainties from various groups?

Recent progress

- These complex questions require to understand probability distribution in multi-parameter PDF space, affected by a host of theoretical and experimental factors
- Since 2012, consistency of NNLO global ensembles from CT, MSTW, NNPDF was validated by dedicated benchmarking of fitting codes
- Two methods (**meta-PDFs** and **compressed Monte-Carlo replicas**) were also developed for combination of the PDFs at the level of PDF parametrizations, rather than at the level of QCD observables

Status in 2012

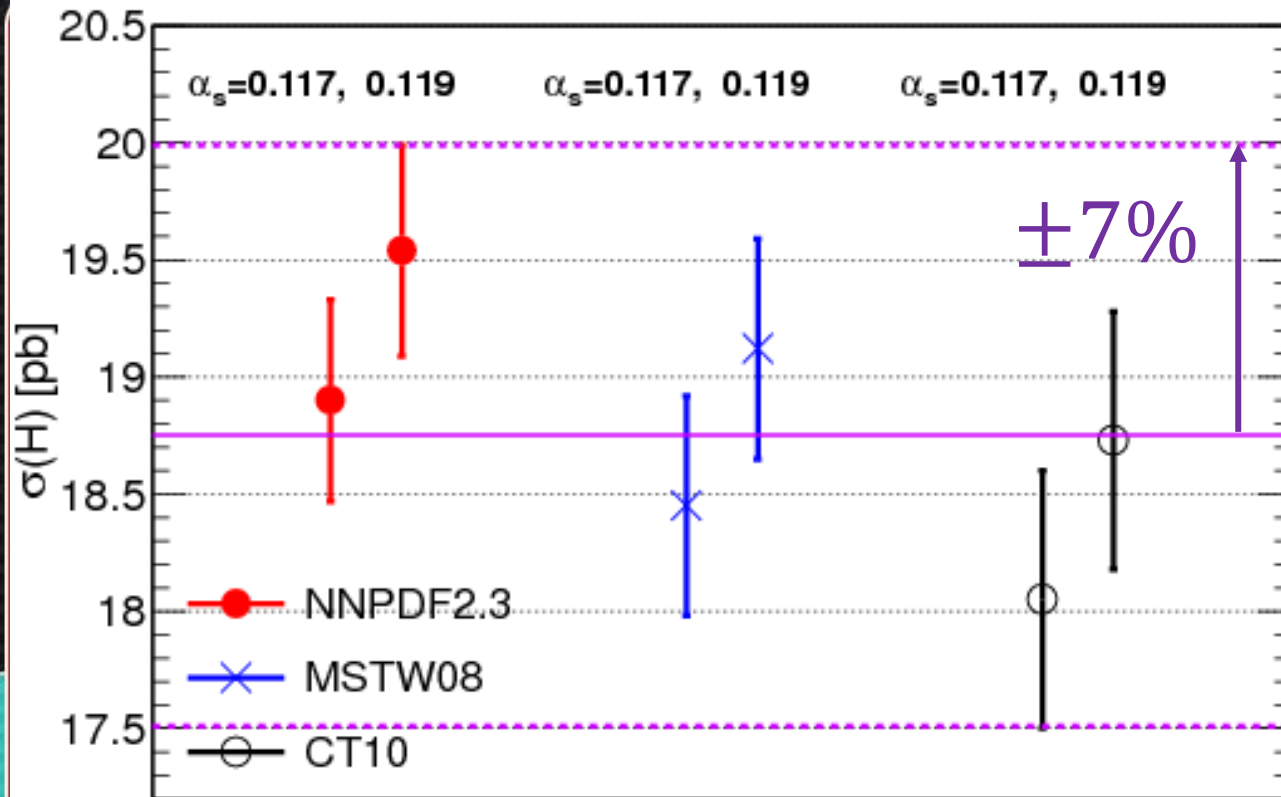
LHC 8 TeV - iHixs 1.3 NNLO - PDF+ α_s uncertainties



$$gg \rightarrow H_{SM}^0$$

Status in 2012

LHC 8 TeV - iHixs 1.3 NNLO - PDF+ α_s uncertainties

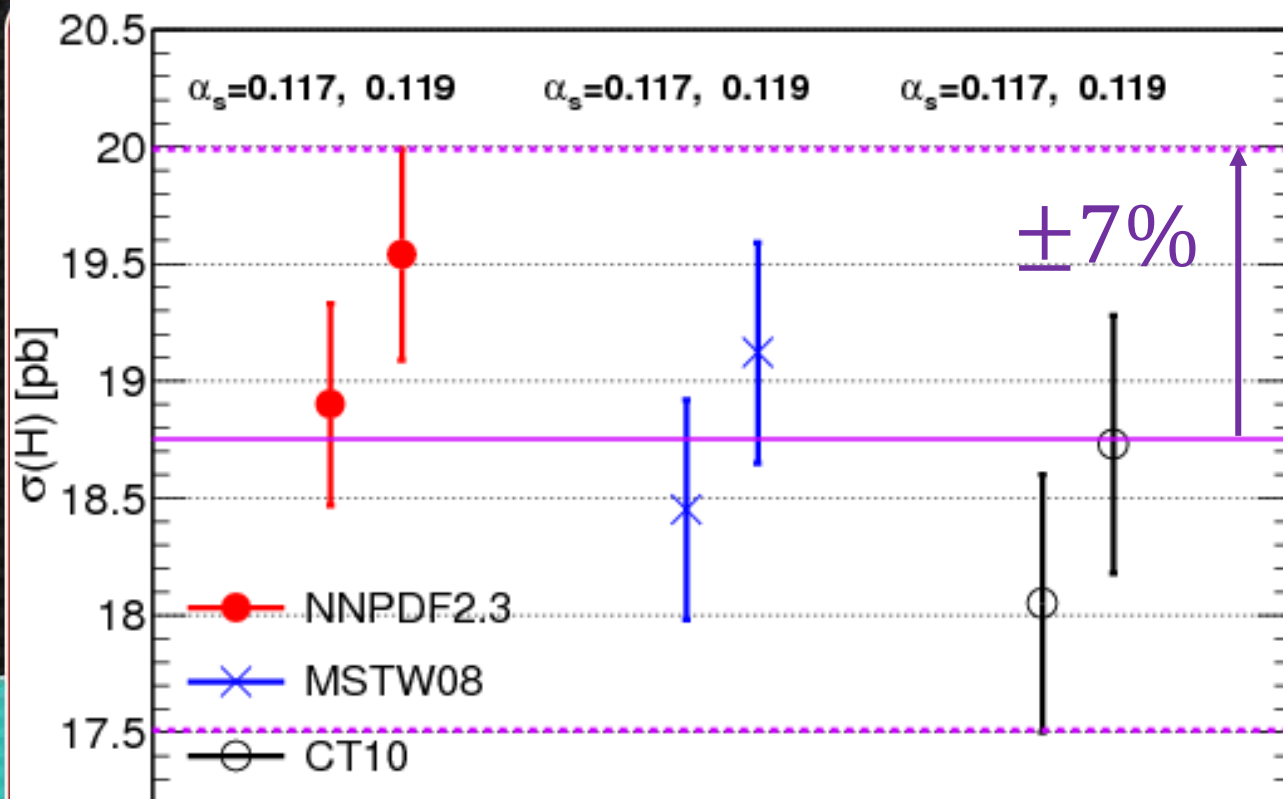


$$gg \rightarrow H_{SM}^0$$

PDF uncertainties from each group are $\approx 3\%$, but the central values are not fully compatible

Status in 2012

LHC 8 TeV - iHixs 1.3 NNLO - PDF+ α_s uncertainties

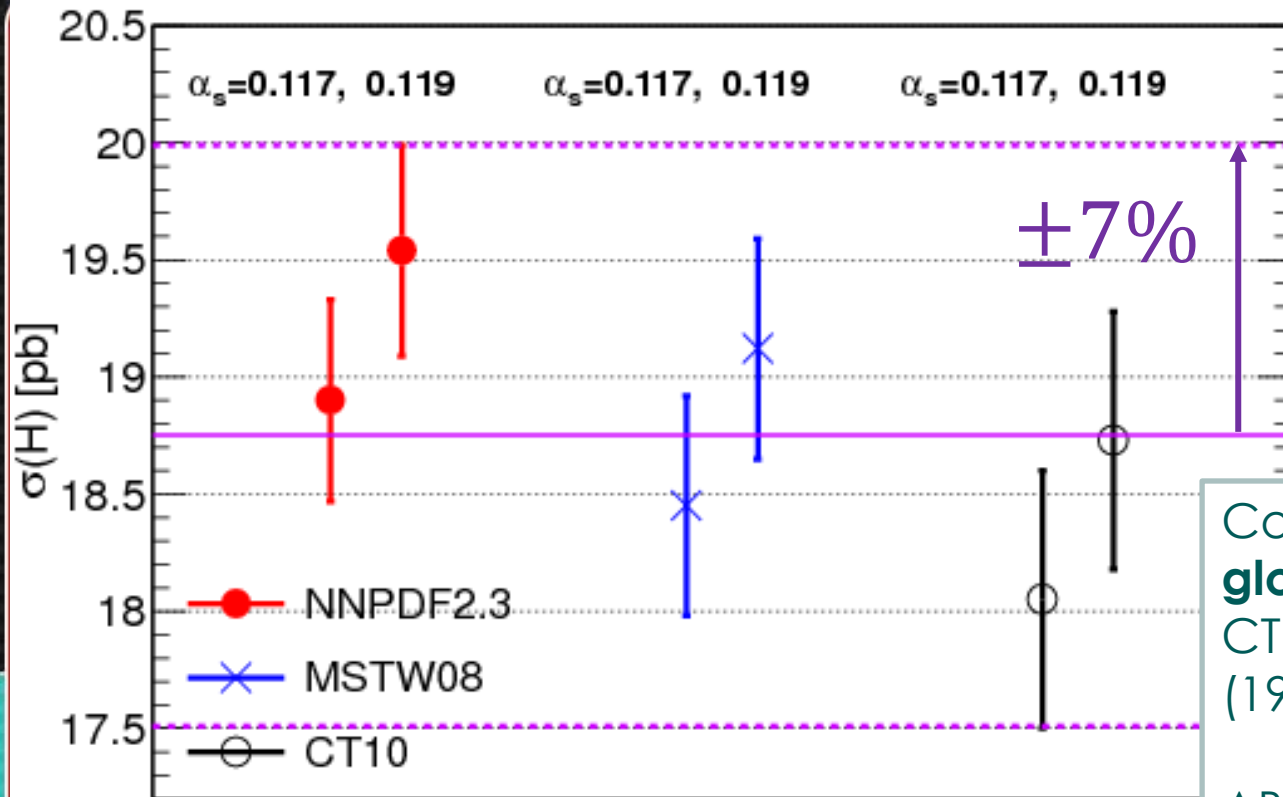


$$gg \rightarrow H_{SM}^0$$

1σ combined PDF+ α_s uncertainty, using PDF4LHC convention (Botje et al., arxiv:1101.0538)

Status in 2012

LHC 8 TeV - iHixs 1.3 NNLO - PDF+ α_s uncertainties



$$gg \rightarrow H_{SM}^0$$

1 σ combined PDF+ α_s uncertainty, using PDF4LHC convention (Botje et al., arxiv:1101.0538)

Combination of three **global** PDF ensembles CT10, MSTW08, NNPDF2.3 (190 error sets)

ABM, CJ, GJR, HERA PDF predictions not included

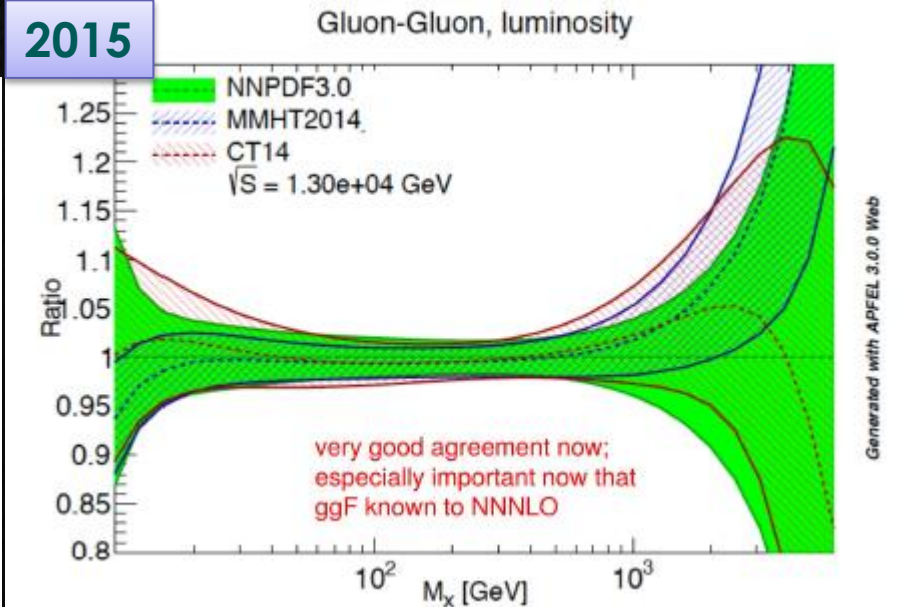
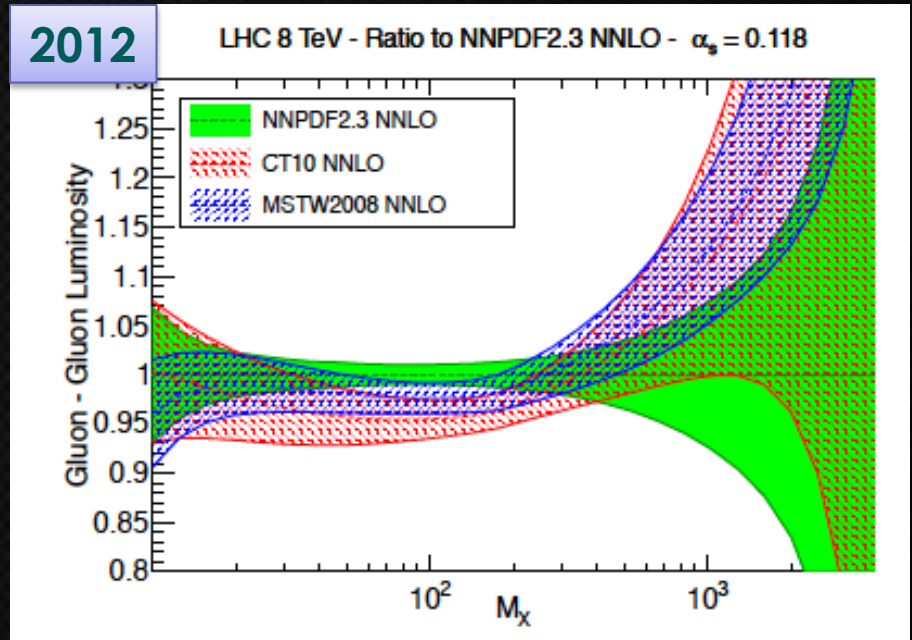
Roll forward to 2015

- Agreement between CT14, MMHT14, NNPDF3.0 improved for most flavors. Now very good agreement between $gg \rightarrow H$ cross section via VBF, for many other observables

$\sigma(gg \rightarrow H^0)$ at NNLO

	CT14	MMHT2014	NNPDF3.0
8 TeV	18.66 pb	18.65 pb	18.77 pb
	-2.2%	-1.9%	-1.8%
	+2.0%	+1.4%	+1.8%
13 TeV	42.68 pb	42.70 pb	42.97 pb
	-2.4%	-1.8%	-1.9%
	+2.0%	+1.3%	+1.9%

J.Huston, PDF4LHC, April 2015



Why NNLO PDFs of the new generation are in better agreement than ever

Since 2012, PDF analysis groups carried out a series of benchmarking exercises for key processes of DIS and jet production in PDF fits

Methodologies of all groups were cross-validated and improved. On the CTEQ side, a numerical improvement was made in the treatment of massive quarks in charged-current DIS that becomes important when NNLO corrections are included.

Benchmark comparisons of PDF analyses

1. J. Gao et al., MEKS: a program for computation of inclusive jet cross sections at hadron colliders , arXiv:1207.0513

Codes for NLO jet production

2. R. Ball et al., Parton Distribution benchmarking with LHC data, arXiv:1211.5142

(N)NLO LHC cross sections

3. S. Alekhin et al., ABM11 PDFs and the cross section benchmarks in NNLO, arXiv:1302.1516; The ABM parton distributions tuned to LHC data; arXiv:1310.3059

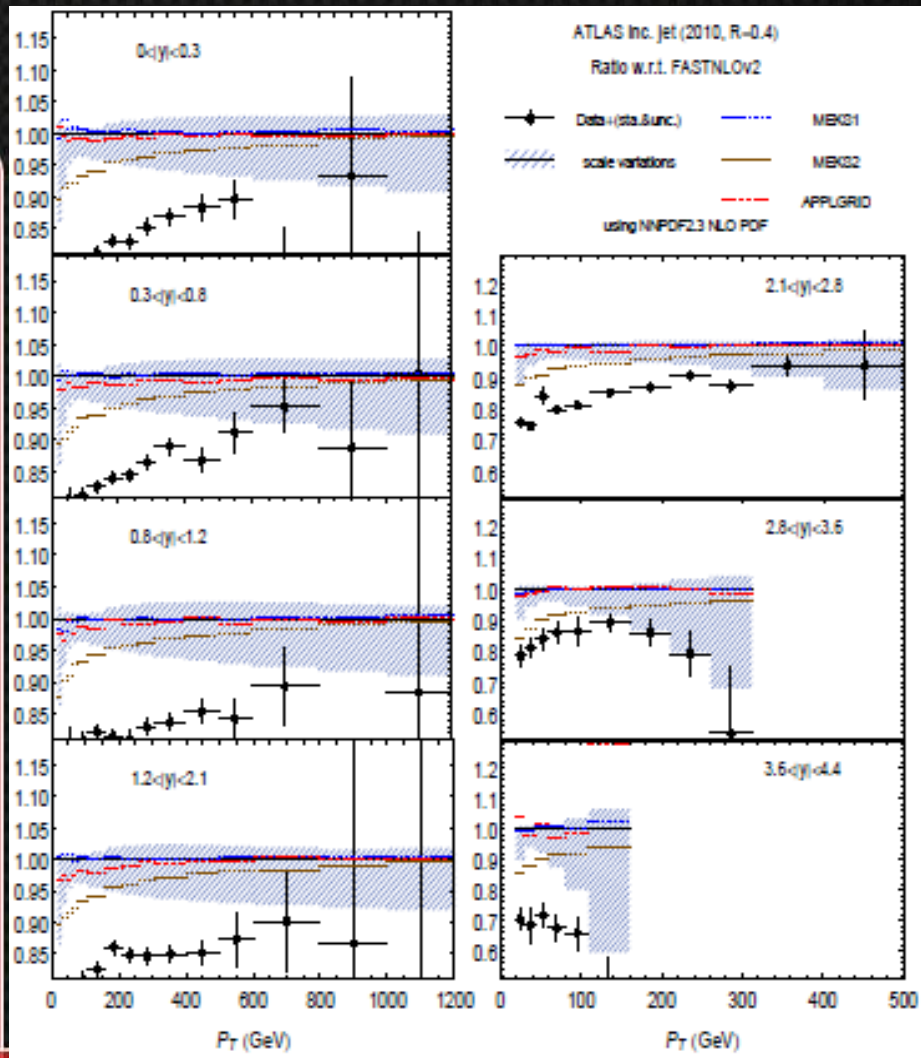
W/Z, $t\bar{t}$,...

4. A.Cooper-Sarkar et al., PDF dependence of the Higgs production cross section in gluon fusion from HERA data, 2013 Les Houches Proceedings, arXiv:1405.1067, p. 37

NC DIS;
CC DIS

5. S. Forte and J. Rojo, Dataset sensitivity of the $gg \rightarrow H$ cross-section in the NNPDF analysis, arXiv:1405.1067, p. 56

Advanced NLO predictions for incl. jet production

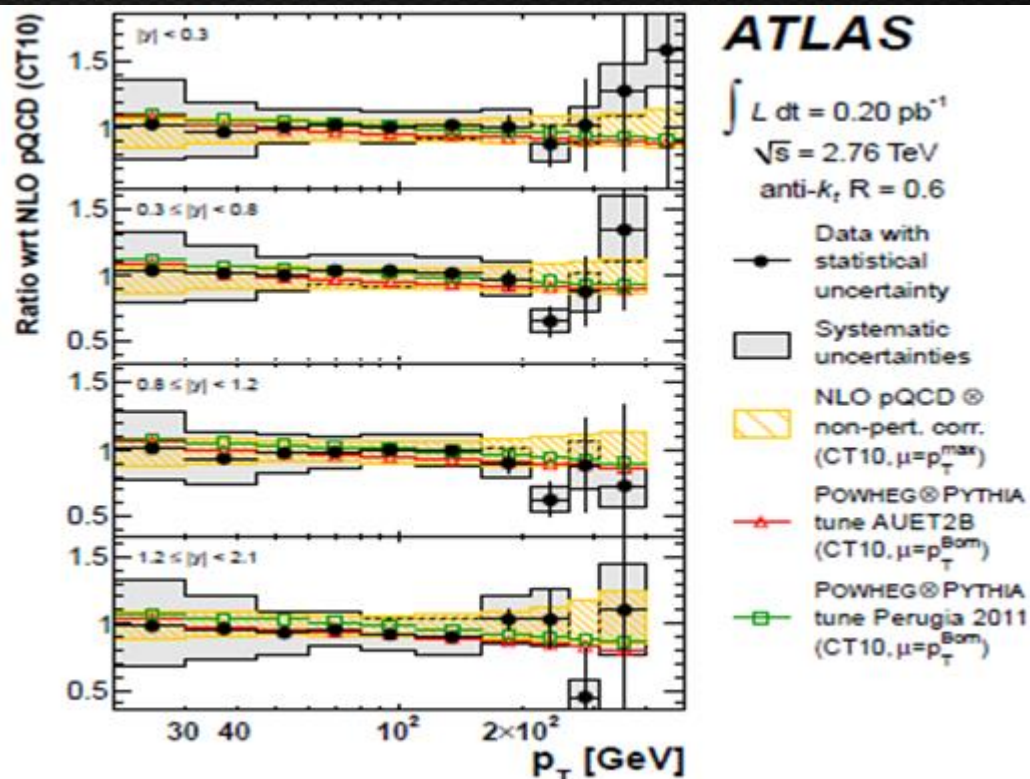


The need to have reliable predictions for LHC (di)jet production for PDF analysis inspired revisions/tuning of NLO theory calculations.

Through various tests, independent NLO codes (**NLOJet++/AppGrid/FastNLO** and **MEKS**) **AND** NLO event generators (**MC@NLO** and **Powheg, slide 2**) were brought into excellent agreement (non-trivial!)

The range of scale uncertainty was determined

Advanced NLO predictions for incl. jet production



P. Starovoitov, DIS'2013

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The range of scale uncertainty was determined

Benchmark comparisons of DIS cross sections

2013 Les Houches Proceedings, arXiv:1405.1067, p. 37 and 56

1. Detailed studies of reduced cross sections $\sigma_{r,NC}^{\pm}$ and structure functions $F_{1,2}$ from CT, HERA, MSTW, NNPDF

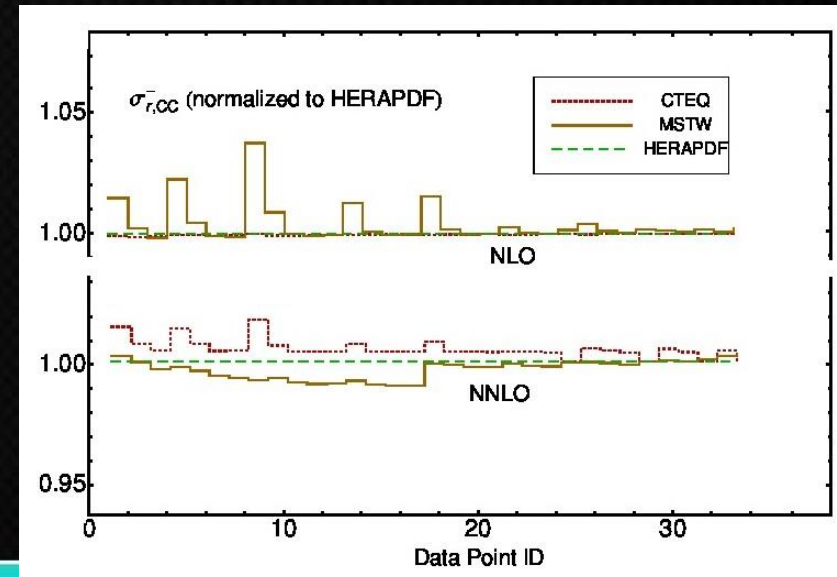
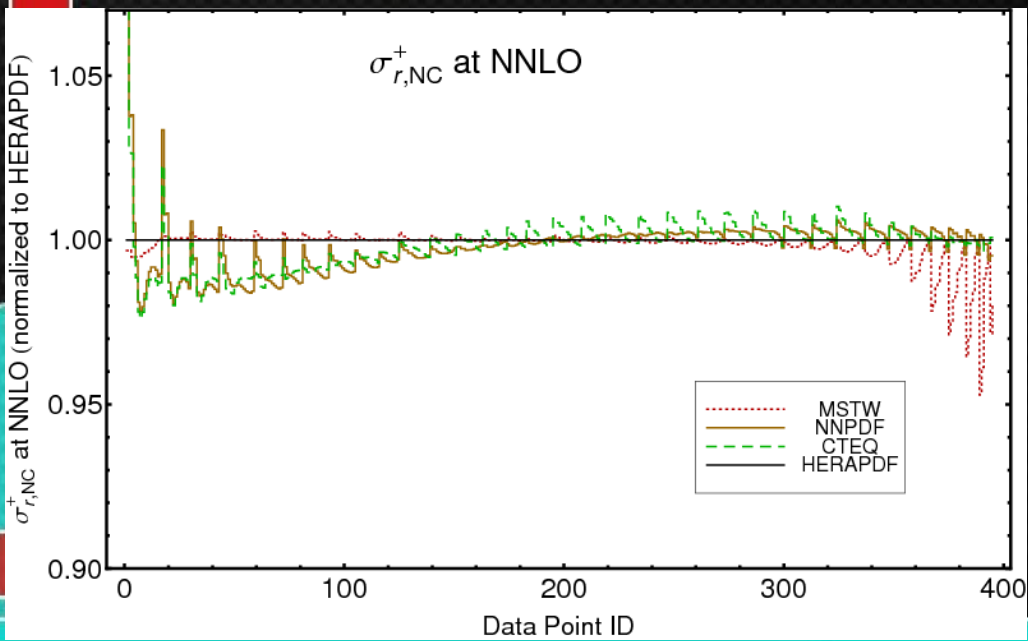
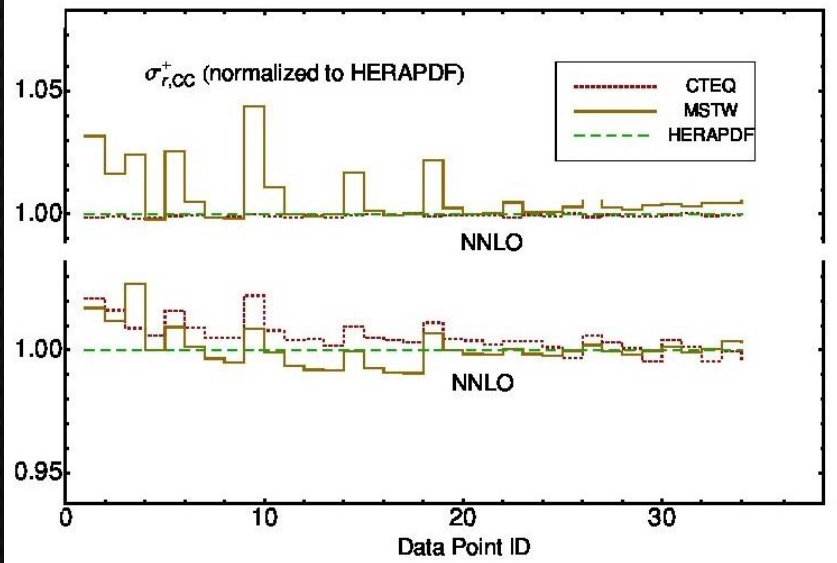
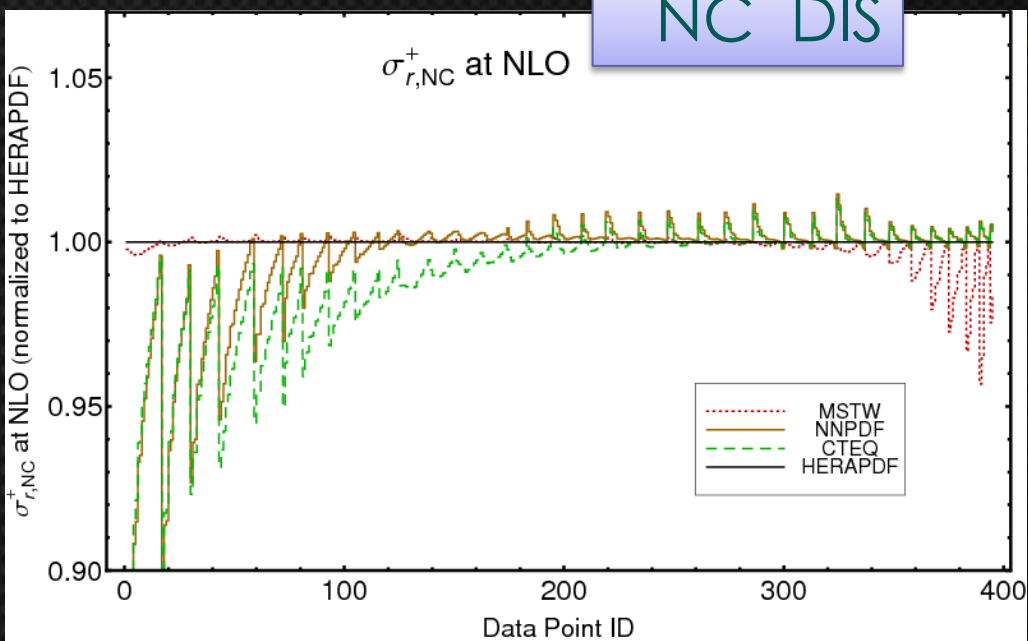
- for neutral-current DIS (published), charged-current DIS (in progress)
- at LO, NLO, and NNLO
- separately for light quarks and heavy quarks
- with Les Houches toy PDFs
- in various heavy-quark schemes

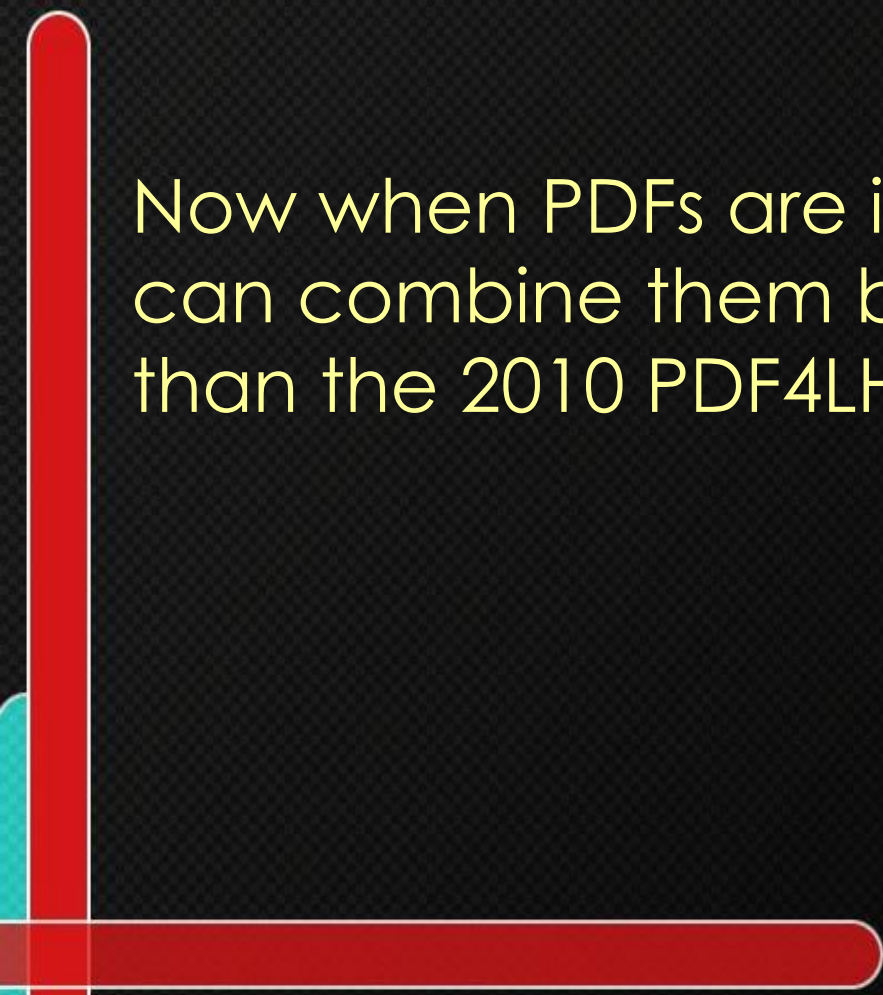
2. Fits to HERA data only, using 4 fitting codes

- with native and varied PDF parametrizations
- with various Q cuts
- with various treatment of systematic errors
- with varied heavy-quark masses

NC DIS

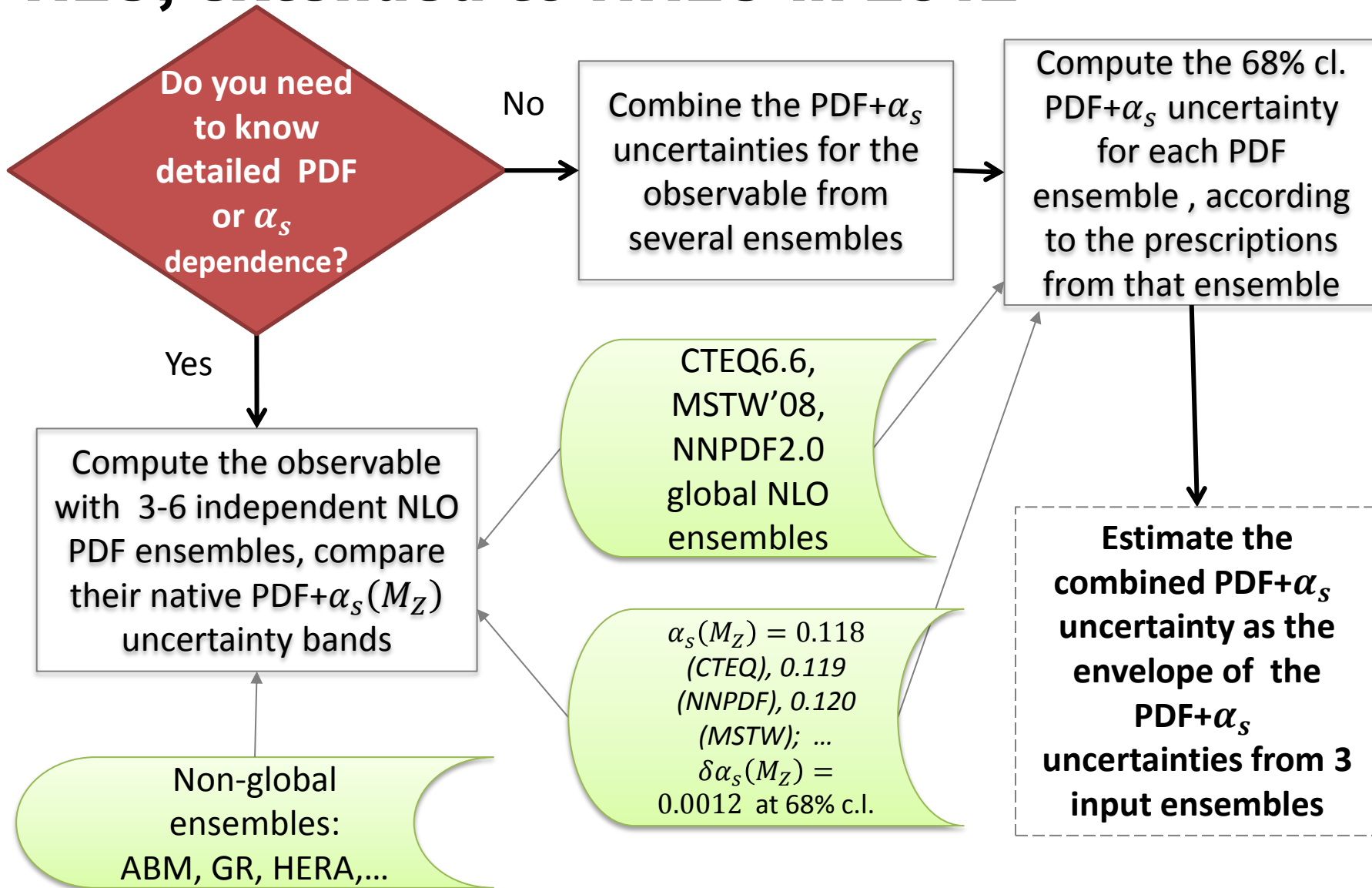
CC DIS



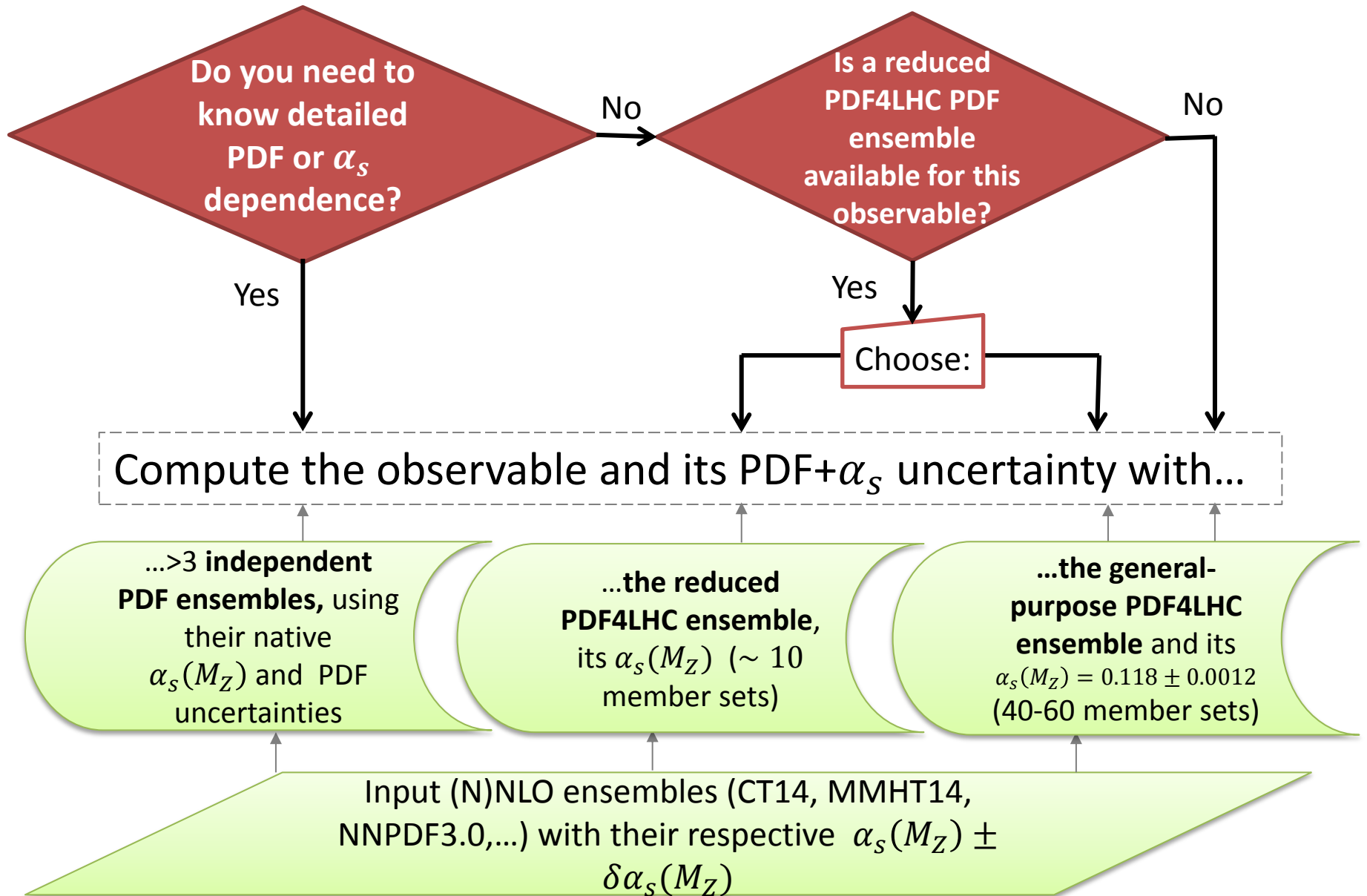
A decorative graphic on the left side of the slide consists of a vertical red bar with rounded ends, a horizontal red bar with rounded ends, and a horizontal cyan bar with rounded ends. The red bars are positioned above the cyan bar.

Now when PDFs are in good agreement, we can combine them by more efficient methods than the 2010 PDF4LHC prescription

2010 PDF4LHC recommendation for an LHC observable: NLO; extended to NNLO in 2012



2015: A concept for a new PDF4LHC recommendation



This procedure applies both at NLO and NNLO

Combination of the PDFs into the future PDF4LHC ensemble

PDFs from several groups are combined into a PDF4LHC ensemble of error PDFs **before** the LHC observable is computed. This simplifies the computation of the PDF+ α_s uncertainty and will likely cut down the number of the PDF member sets and the CPU time needed for simulations.

The same procedure is followed at NLO and NNLO. The combination was demonstrated to work for global ensembles (CT, MSTW, NNPDF). It still needs to be generalized to allow inclusion of non-global ensembles.

The PDF uncertainty at 68% c.l. is computed from error PDFs at central $\alpha_s(M_Z)$.

Two additional error PDFs are provided with either PDF4LHC ensemble to compute the α_s uncertainty using $\alpha_s(M_Z) = 0.118 \pm 0.0012$ at the 68% c.l.

Progress in developing the combination procedure

Two methods for combination of PDFs were extensively compared, with promising results:

1. Meta-parametrizations + MC replicas + Hessian data set diagonalization

(J. Gao, J. Huston, P. Nadolsky, 1401.0013)

2. Compression of Monte-Carlo replicas

(Carazza, Latorre, Rojo, Watt, 1504:06469)

Both procedures start by creating a combined ensemble of MC replicas from all input ensembles (G. Watt, R. Thorne, 1205.4024; S. Forte, G. Watt, 1301.6754). They differ at the second step of reducing a large number of input MC replicas (~ 300) to a smaller number for practical applications (13-100 in the META approach; 40 in the CMC approach). The core question is how much input information to retain in the reduced replicas in each Bjorken- x region.

META 1.0 PDFs: A working example of a meta-analysis

See arXiv:1401.0013 for details

1. Select the input PDF ensembles (CT, MSTW, NNPDF...)
2. Fit each PDF error set in the input ensembles by a common functional form ("**a meta-parametrization**")
3. Generate many Monte-Carlo replicas from meta-parametrizations of each set to investigate the probability distribution on the ensemble of all meta-parametrizations (as in Thorne, Watt, 1205.4024)
4. Construct a final ensemble of 68% c.l. **Hessian eigenvector sets** to propagate the PDF uncertainty from the combined ensemble of replicated meta-parametrizations into LHC predictions.

Only in
the META
set

Only in
the META
set

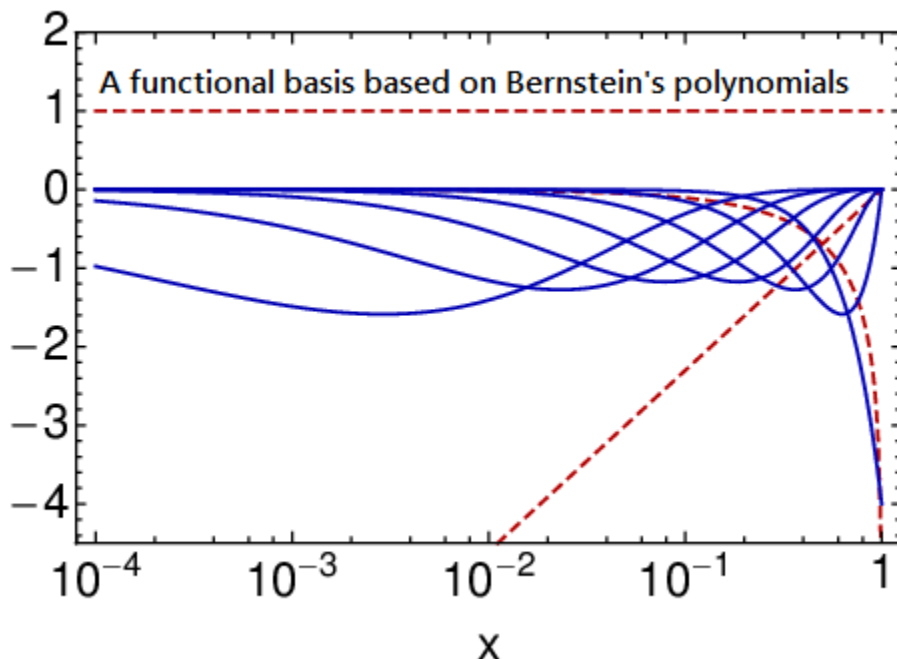
META2.0 PDFs: new functional forms

New

2014: Chebyshev polynomials (Pumplin, 0909.5176, Glazov, et al., 1009.6170, Martin, et al., 1211.1215)

2015: Bernstein polynomials \Rightarrow more faithful reproduction of the full ensemble of MC replicas

The initial scale of DGLAP evolution is $Q_0=8 \text{ GeV}$.



The meta-parametrizations are fitted to the input PDFs at $x > 3 \cdot 10^{-5}$ for all flavors ; $x < 0.4$ for \bar{u}, \bar{d} ; $x < 0.3$ for s, \bar{s} ; and $x < 0.8$ for other flavors. PDFs outside these x regions are determined entirely by extrapolation.

Reduction of the error PDFs

The number of final error PDFs can be much smaller than in the input ensembles

In the META2.0 study:

200 CT, MSTW, NNPDF error sets

⇒ 600 MC replicas for reconstructing the combined probability distribution

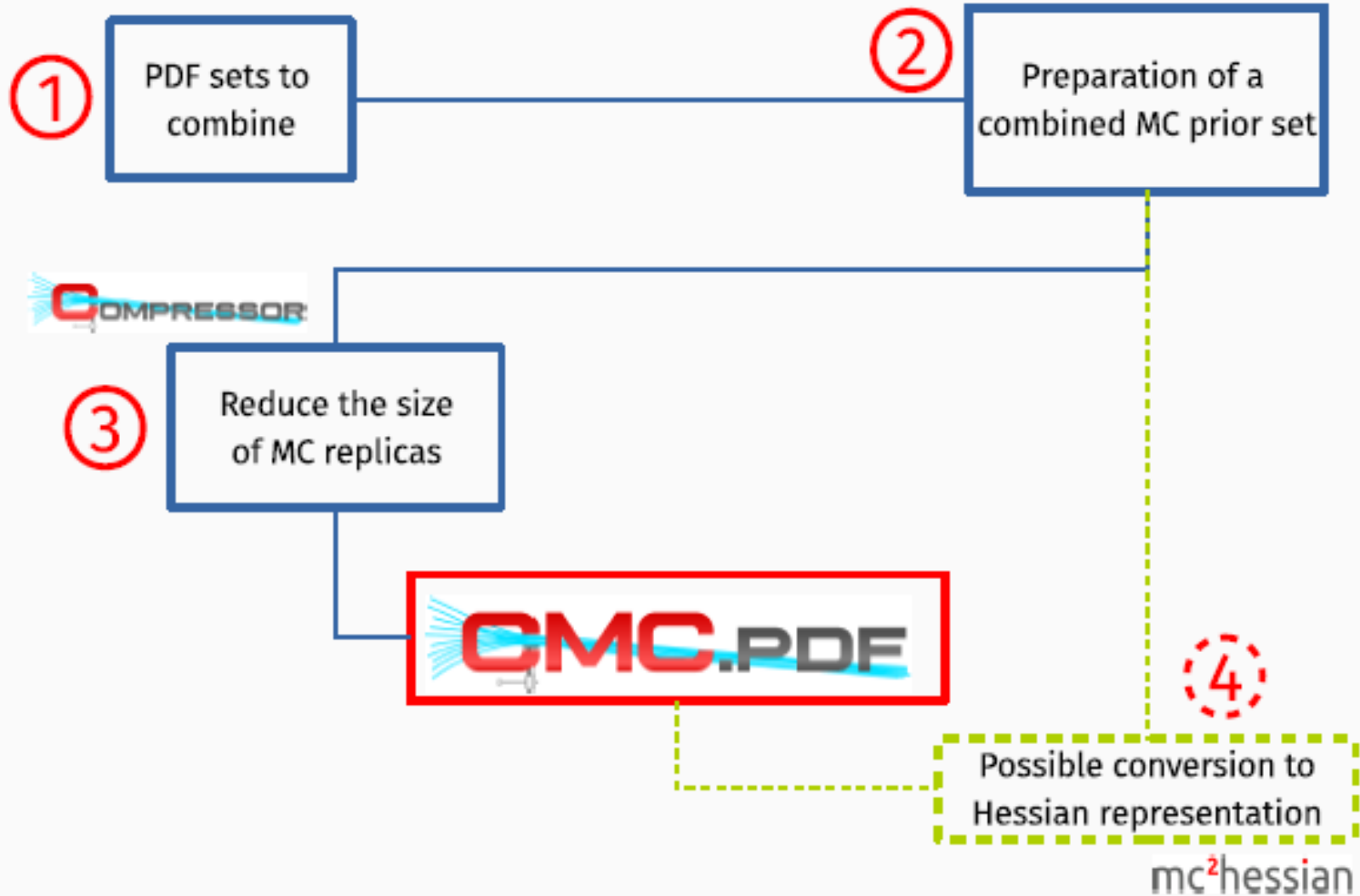
⇒ 40-100 Hessian META sets for most LHC applications (**general-purpose** ensemble META1.0)

⇒ 13 META sets for LHC Higgs production observables (**reduced ensemble** META LHCH)

New

CMC PDFs

S. Carrazza, Feb. 2015



We define **statistical estimators** for the MC prior set:

1. **moments:** central value, variance, skewness and kurtosis
2. **statistical distances:** the Kolmogorov distance
3. **correlations:** between flavors at multiple x points

These estimators are then **compared** to subsets of replicas **interactively** driven by an *error function*, i.e.

$$\text{ERF}_{\text{tot}} = \sum_n \frac{1}{N_n} \sum_i \left(\frac{C_i^{(n)} - O_i^{(n)}}{O_i^{(n)}} \right)^2$$

where n runs over the number of statistical estimators and

- N_i is a normalization factor extracted from random realizations
- $O_i^{(n)}$ is the value of the estimator for the prior
- $C_i^{(n)}$ is the corresponding value for the compressed set



Benchmark comparisons of CMC and META PDFs

CMC ensembles with 40 replicas and META ensembles with 40-100 replicas are compared with the full ensembles of 300-600 MC replicas.

Accuracy of both combination procedures is already competitive with the 2010 PDF4LHC procedure, can be further fine-tuned by adjusting the final number of replicas.

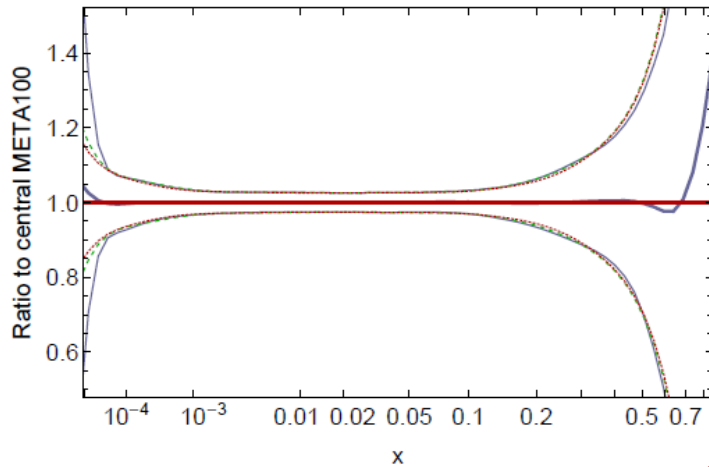
Error bands:

In the (x, Q) regions covered by the data, the agreement of 68%, 95% c.l. intervals is excellent. The definition of the central PDFs and c.l. intervals is ambiguous in extrapolation regions, can differ even within one approach. E.g., differences between mean, median, mode “central values”.

Reduction, META ensemble: 600 \rightarrow 100 \rightarrow 60 error sets

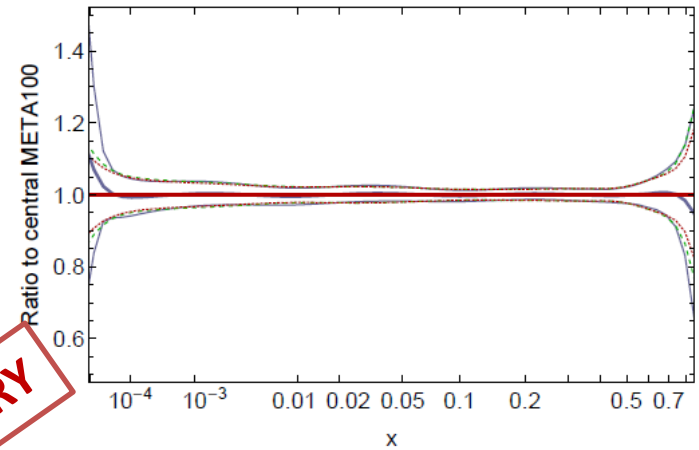
$g(x,Q)$ at $Q=8$ GeV at 68% c.l.

META600 (solid), META100 (dashed), META60 (dotted)



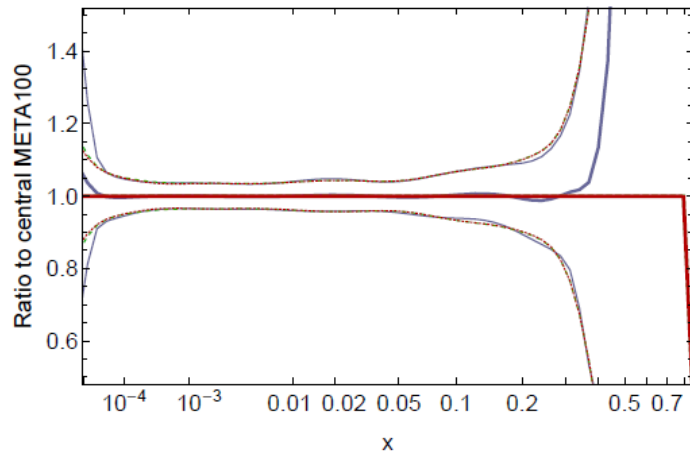
$u(x,Q)$ at $Q=8$ GeV at 68% c.l.

META600 (solid), META100 (dashed), META60 (dotted)



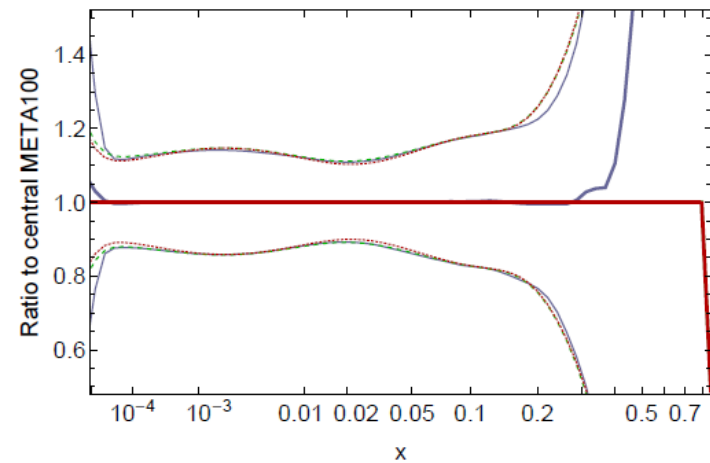
$\bar{d}(x,Q)$ at $Q=8$ GeV at 68% c.l.

META600 (solid), META100 (dashed), META60 (dotted)



$\bar{s}(x,Q)$ at $Q=8$ GeV at 68% c.l.

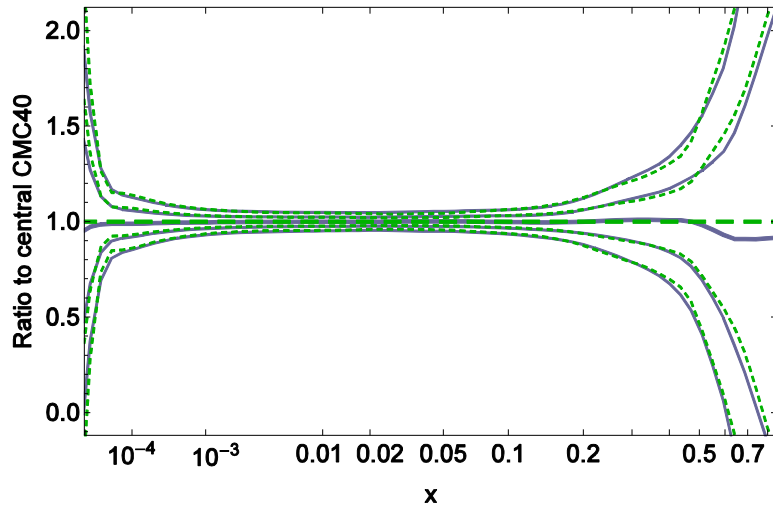
META600 (solid), META100 (dashed), META60 (dotted)



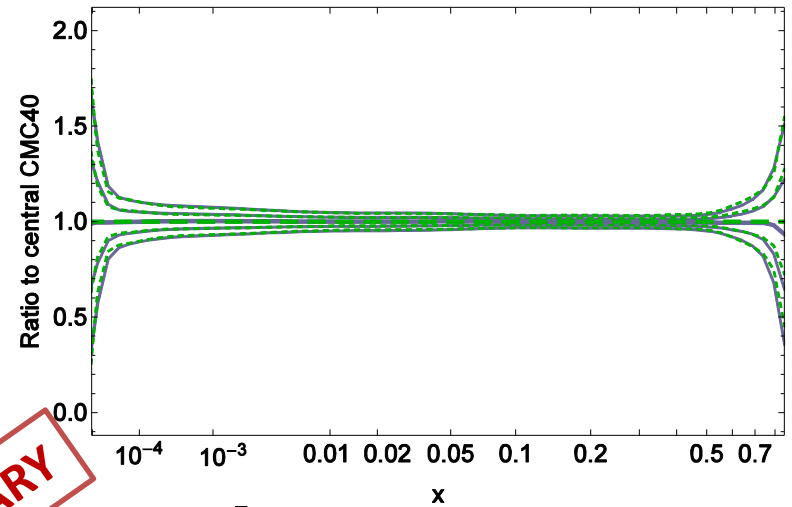
PRELIMINARY

Reduction, CMC ensemble: 300 \rightarrow 40 replicas

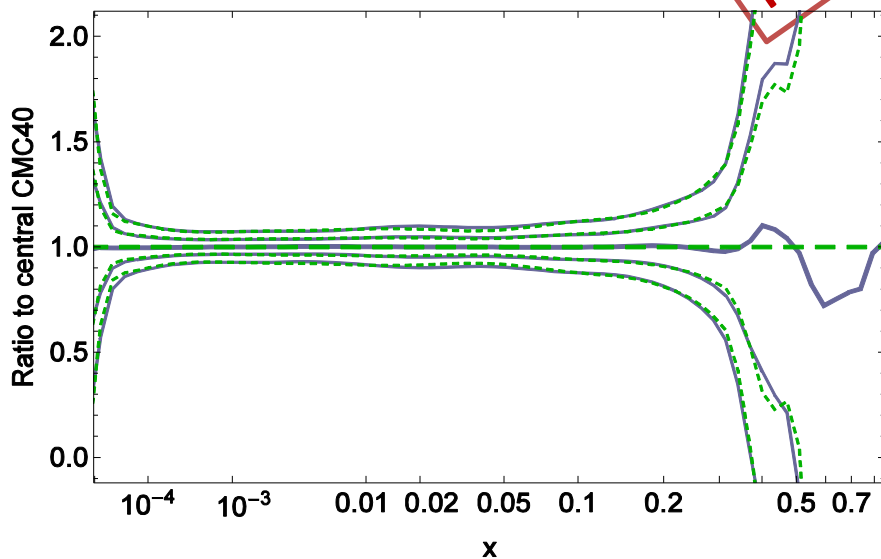
$g(x,Q)$ at $Q=8$ GeV at 1σ and 2σ
CMC40 (dashed), CMC300 (solid)



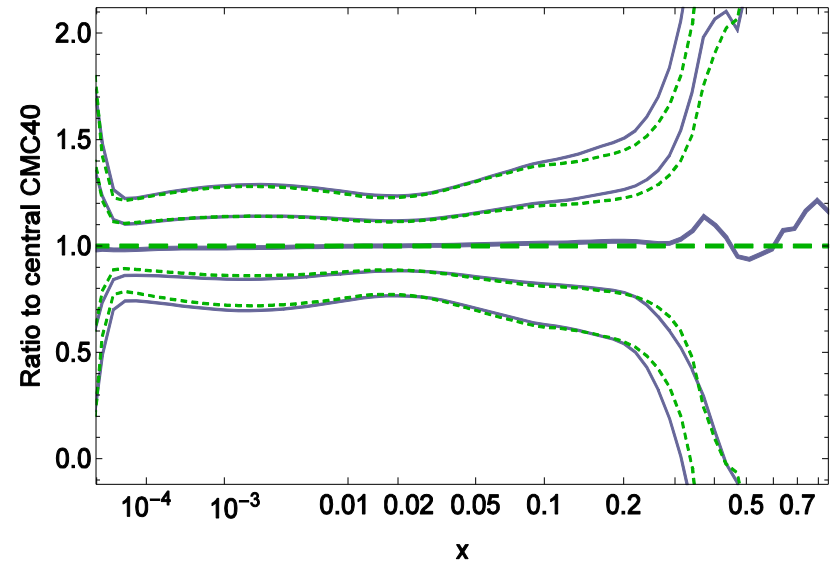
$u(x,Q)$ at $Q=8$ GeV at 1σ and 2σ
CMC40 (dashed), CMC300 (solid)



$d(x,Q)$ at $Q=8$ GeV at 1σ and 2σ
CMC40 (dashed), CMC300 (solid)



$\bar{s}(x,Q)$ at $Q=8$ GeV at 1σ and 2σ
CMC40 (dashed), CMC300 (solid)



PRELIMINARY

Benchmark comparisons, general observations II

PDF-PDF correlations:

Correlations of META300 and CMC300 ensembles differ by up to ± 0.2 as a result of fluctuations in replica generation

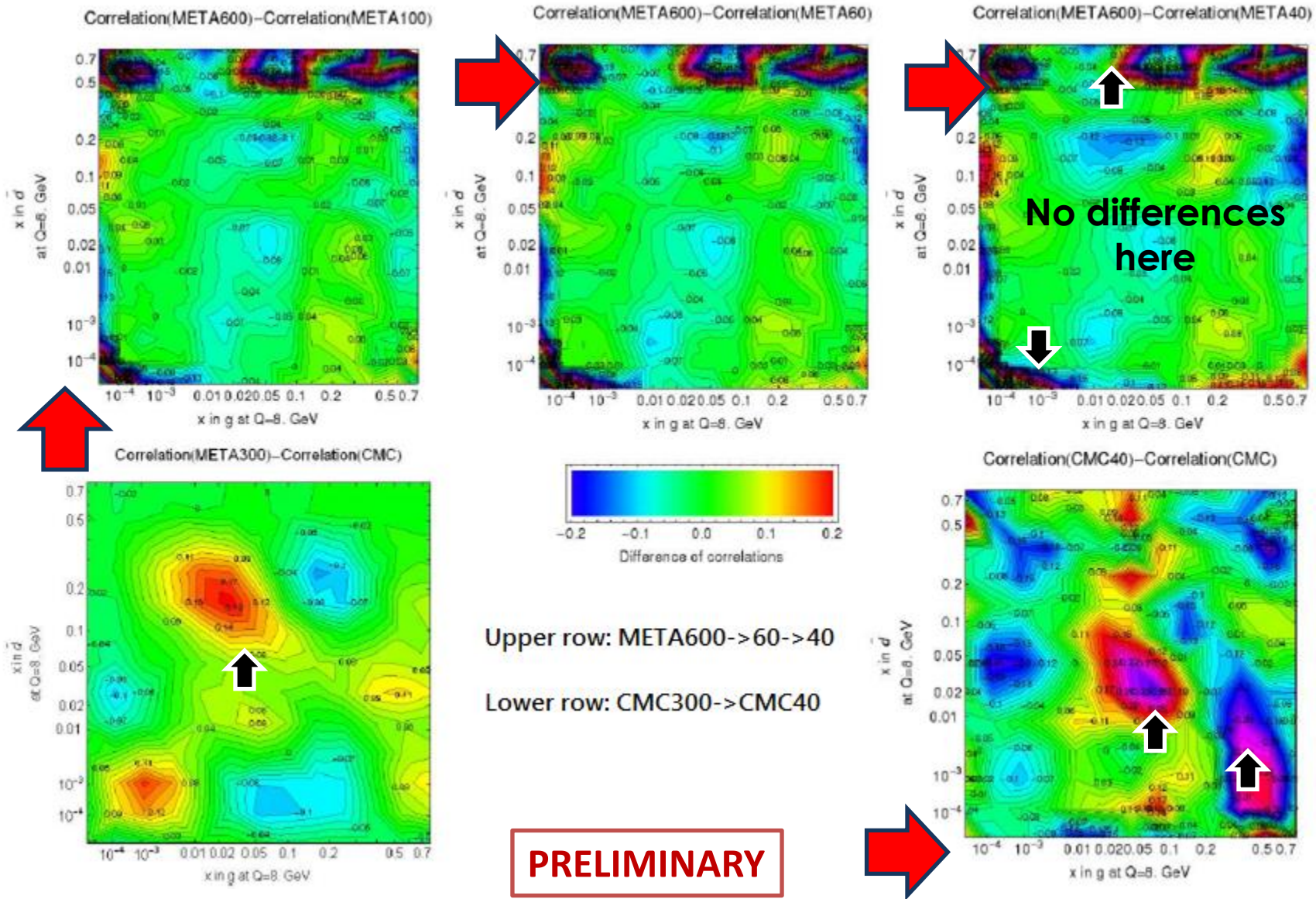
META40 PDFs faithfully reproduce PDF-PDF correlations of the META600 PDFs in the regions with data; fail to reproduce correlations in extrapolation regions \Rightarrow *next slide, upper row*

CMC40 PDFs better reproduce correlations of CMC300 in extrapolation regions; lose more accuracy in (x, Q) regions with data, but still within acceptable limits \Rightarrow *next slide, lower row*

These patterns of correlations persist at the initial scale

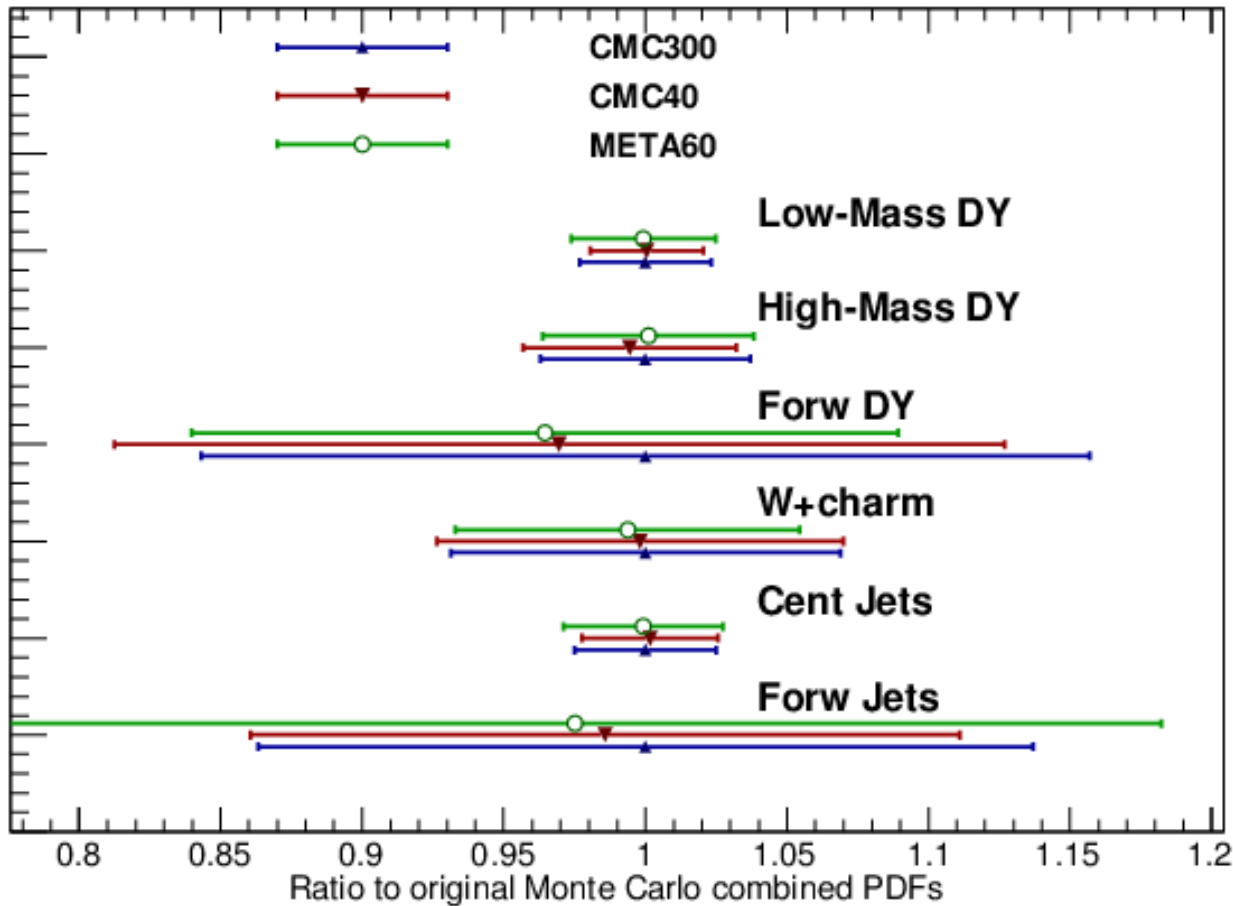
$Q_0 = 8 \text{ GeV}$ as well as at EW scales

PDF-PDF correlation, example: $\bar{d}(x, Q)$ vs $g(x, Q)$ at $Q = 8 \text{ GeV}$



Agreement at the level of benchmark cross sections

LHC 7 TeV, $\alpha_s=0.118$, NLO



CMC-META benchmark cross sections are consistent in the x regions constrained by data

There are moderate differences in extrapolation regions. Either reduced ensemble only partly captures non-Gaussianity of the full MC ensemble at such x

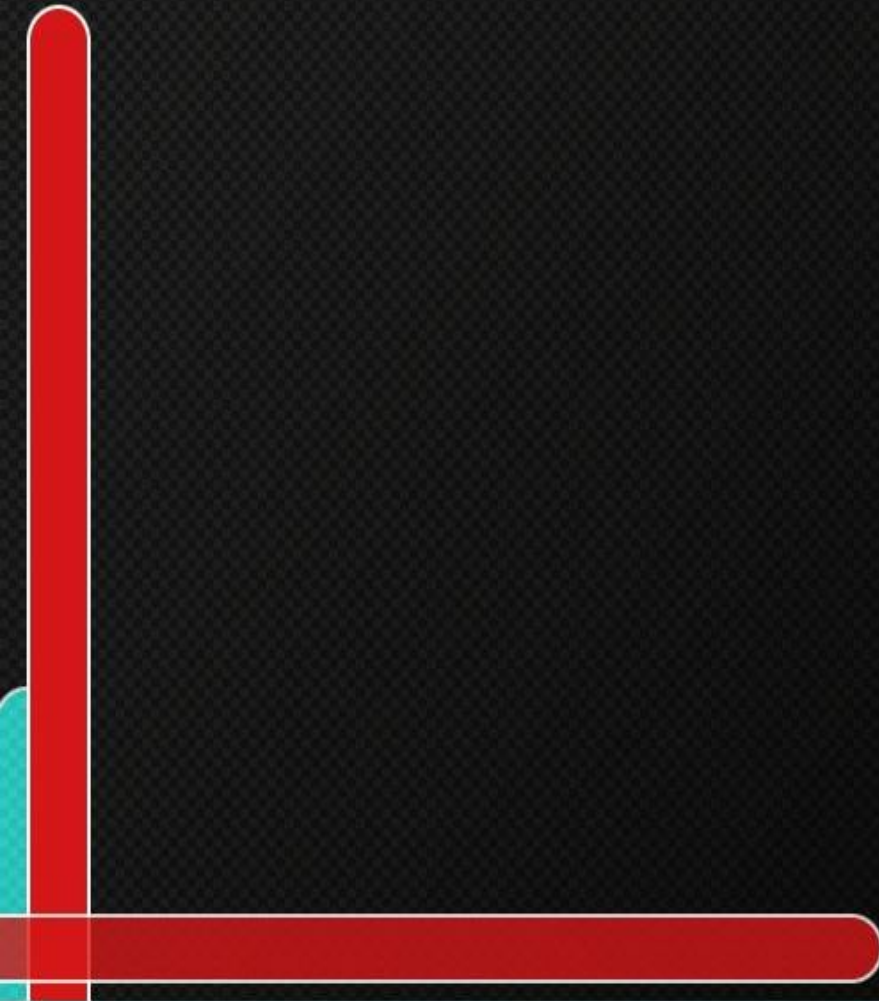
J. Rojo

To summarize, based on benchmark comparisons we recommend to use both CMC and META methods for combination of PDF uncertainties from global PDF ensembles

We will continue development of the meta-parametrization method, given its confirmed benefits:

- A general and intuitive method. Implemented in a public Mathematica module MP4LHC
- The PDF parameter space of all input ensembles is visualized explicitly.
- Data combination procedures familiar from PDG can be applied to each meta-PDF parameter
- Asymmetric Hessian errors can be computed, similar to CT14 approach
- Effective in data reduction; makes use of diagonalization of the Hessian matrix in the Gaussian approximation. Reproduces correlations between Higgs signals and backgrounds with just 13 META –LHCH PDFs.

Back-up slides



The logic behind the META approach

Emphasize simplicity and intuition

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

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

The Hessian analysis can be applied to the combination of all input ensembles in order to optimize uncertainties and eliminate “noise”

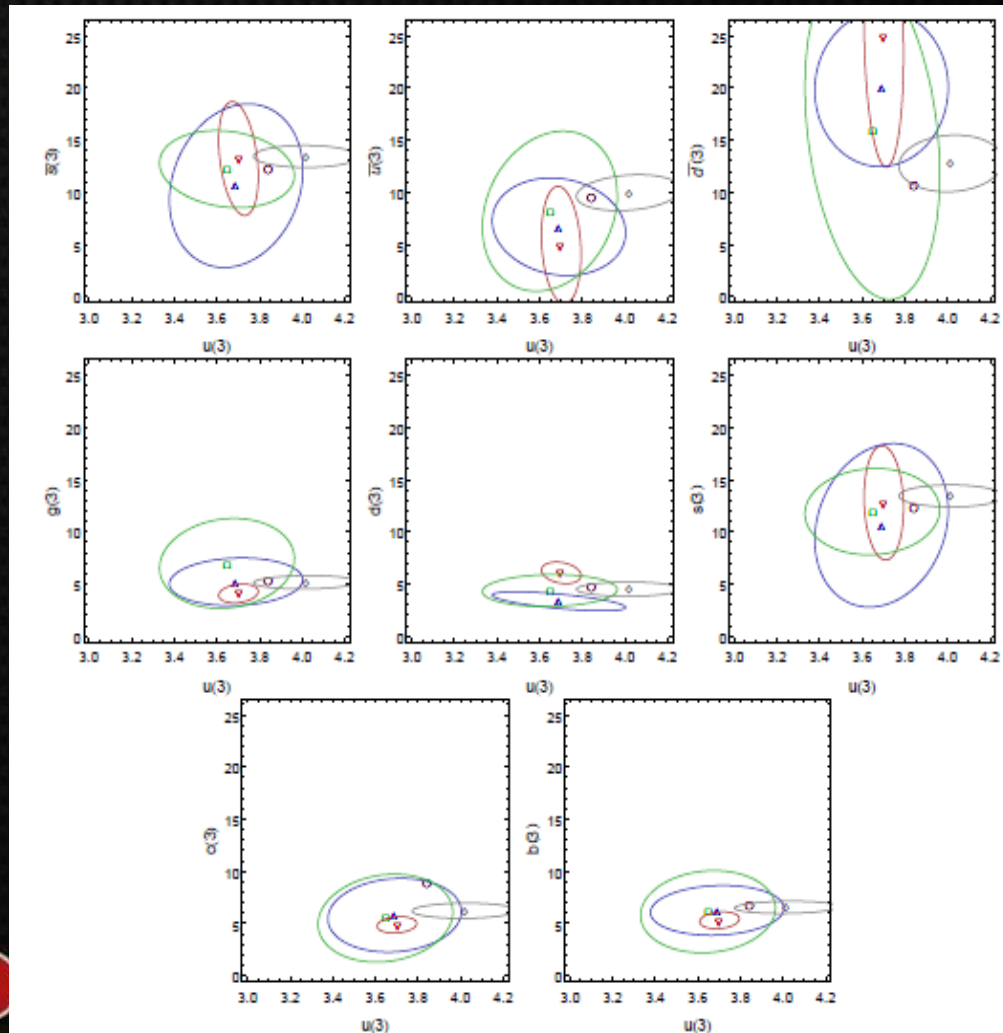


Figure 10: Fitted PDF parameters and 90% c.l. ellipses for CT10 (blue up triangle), MSTW08 (red down triangle), NNPDF2.3 (green square), HERAPDF1.5 (gray diamond) and ABM11 (magenta circle).

Meta-parameters of 5 sets and META PDFs

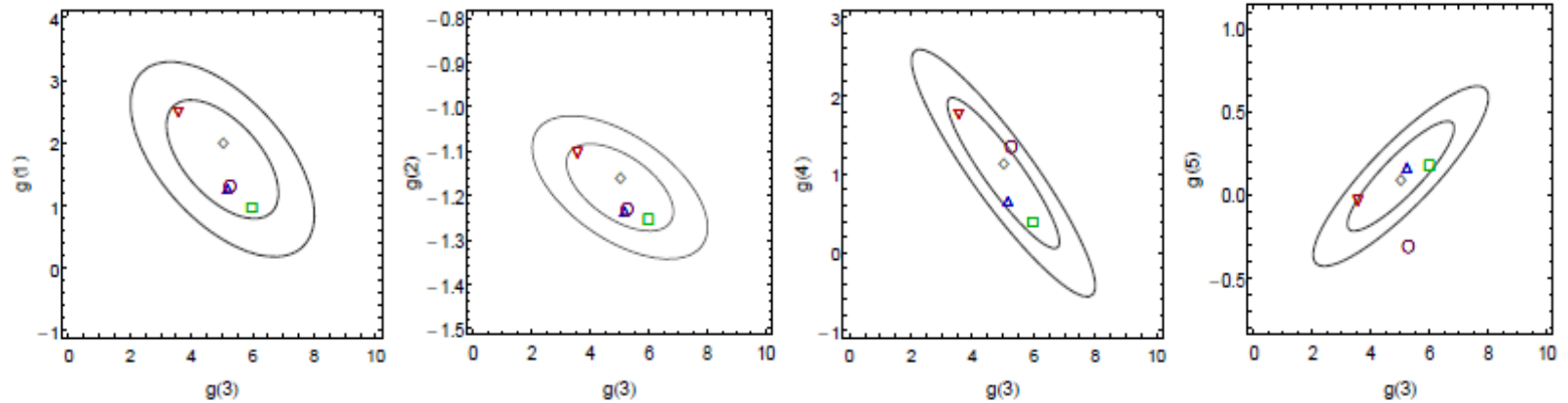


Figure 16: Comparison of META PDF confidence intervals with central NNLO PDFs of the input PDF ensembles in space of meta-parameters a_{1-5} for the gluon PDF. Up triangle, down triangle, square, diamond, and circle correspond to the best-fit PDFs from CT10, MSTW, NNPDF, HERAPDF, and ABM respectively. The ellipses correspond to 68 and 90% c.l. ellipses of META PDFs.

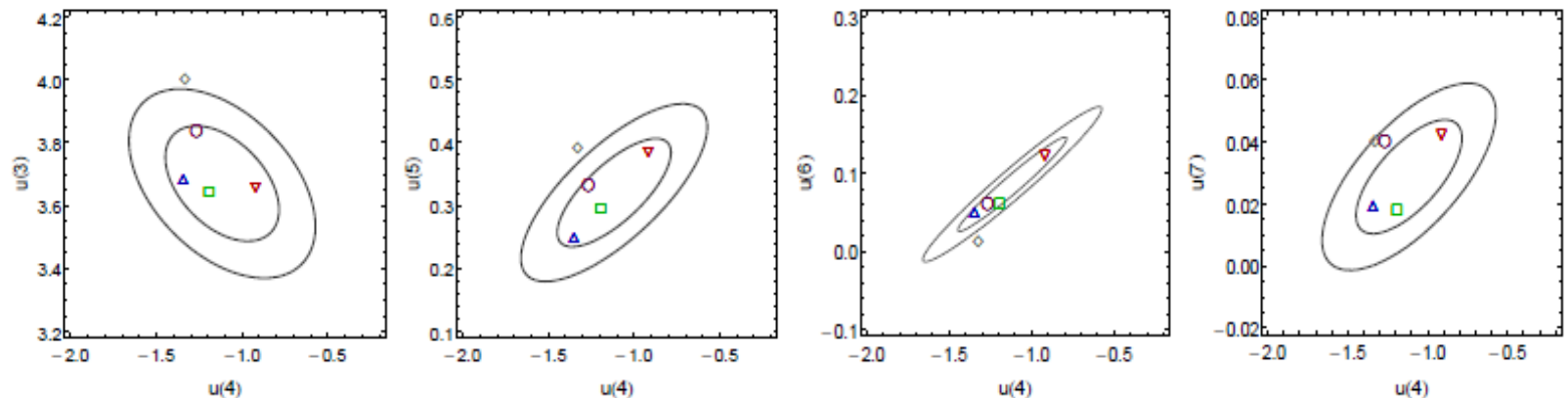


Figure 17: Same as Fig. 16, for a_{3-7} of the u quark PDF.

Merging PDF ensembles

The ensembles can be merged by averaging their meta-parameters. For CT10, MSTW, NNPDF ensembles, unweighted averaging is reasonable, given their similarities.

For any parameter a_i , ensemble g with N_{rep} initial replicas:

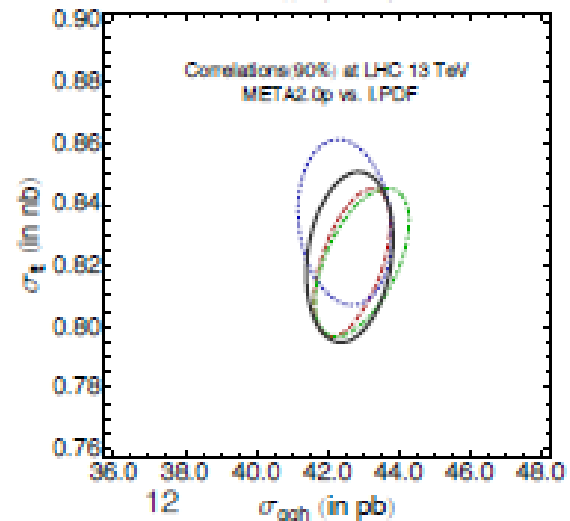
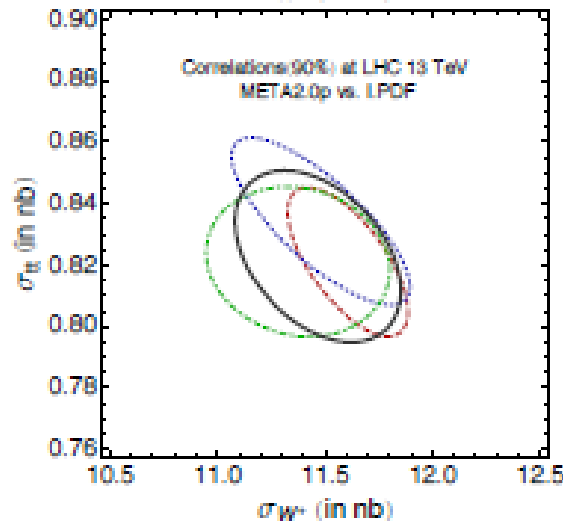
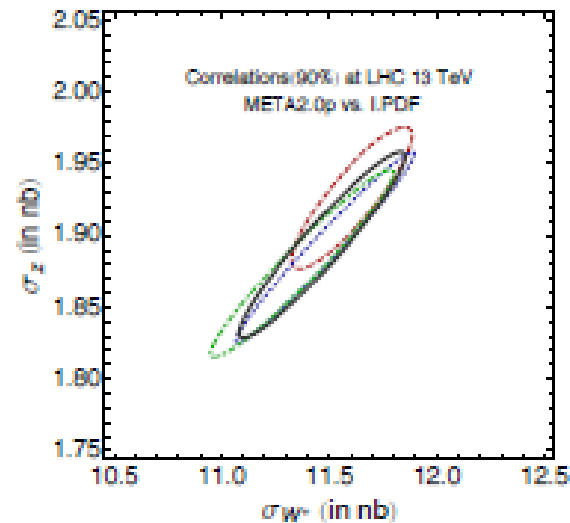
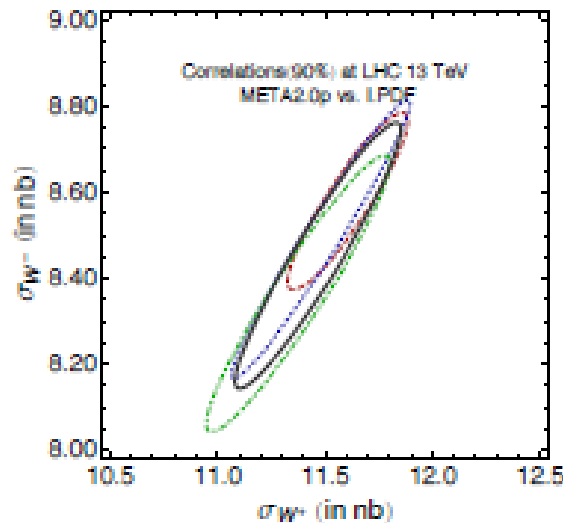
$$\langle a_i \rangle_g = \frac{1}{N_{rep}} \sum_{k=1}^{N_{rep}} a_i(k), \quad \leftarrow \text{Central value on } g$$

$$\text{cov}(a_i, a_j)_g = \frac{N_{rep}}{N_{rep} - 1} \langle (a_i - \langle a_i \rangle_g) \cdot (a_j - \langle a_j \rangle_g) \rangle_g,$$

$$(\delta a_i)_g = \sqrt{\text{cov}(a_i, a_i)_g}. \quad \leftarrow \text{Standard deviation on } g$$

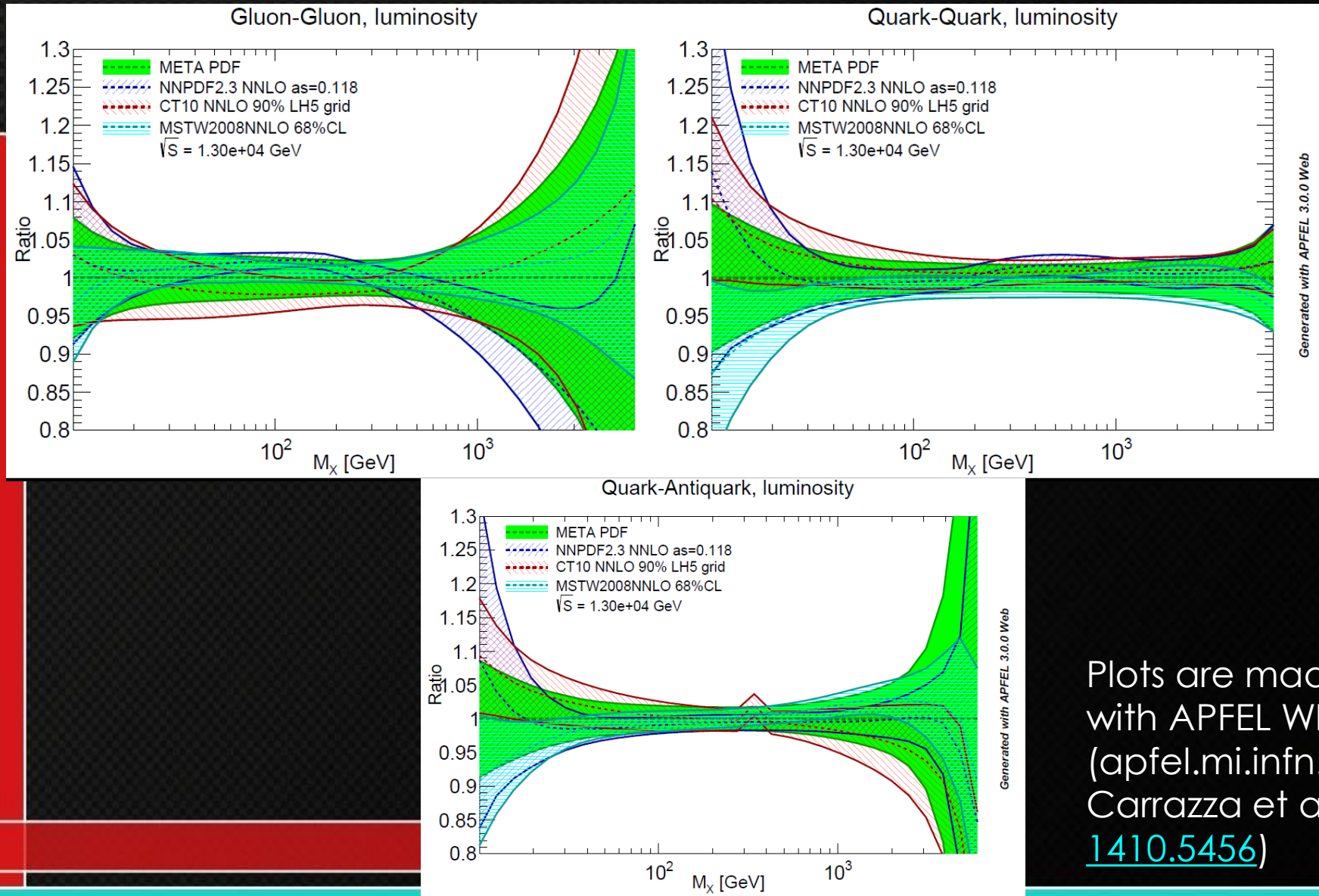
META2.0 predictions for LHC observables

- Currently only have results for META NNLO v2.0p, will add later for v2.1, inclusive observables at 13 TeV



- Blue, CT14p, red, MMHT14, green, NNPDF3.0, black, META2.0p, error ellipse at 90% cl; using Vrap0.9, iHixs1.3, and top++2.0

Some parton luminosities



Plots are made
with APFEL WEB
(apfel.mi.infn.it;
Carrazza et al.,
[1410.5456](https://arxiv.org/abs/1410.5456))

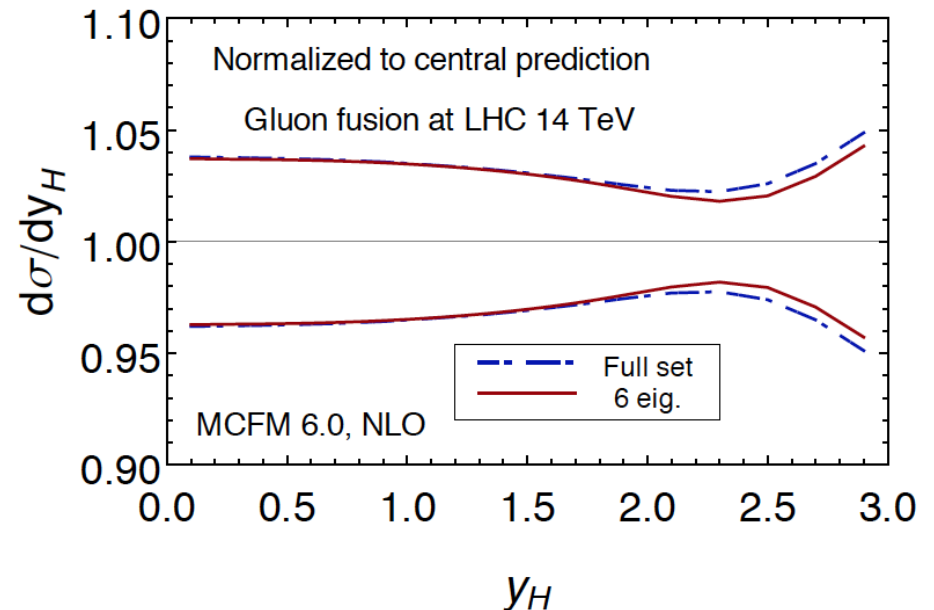
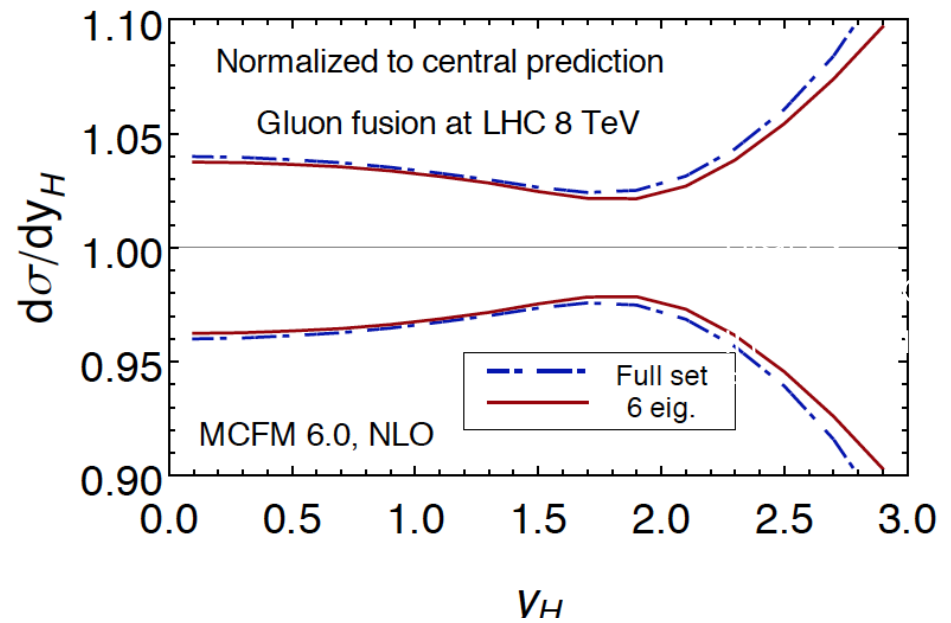
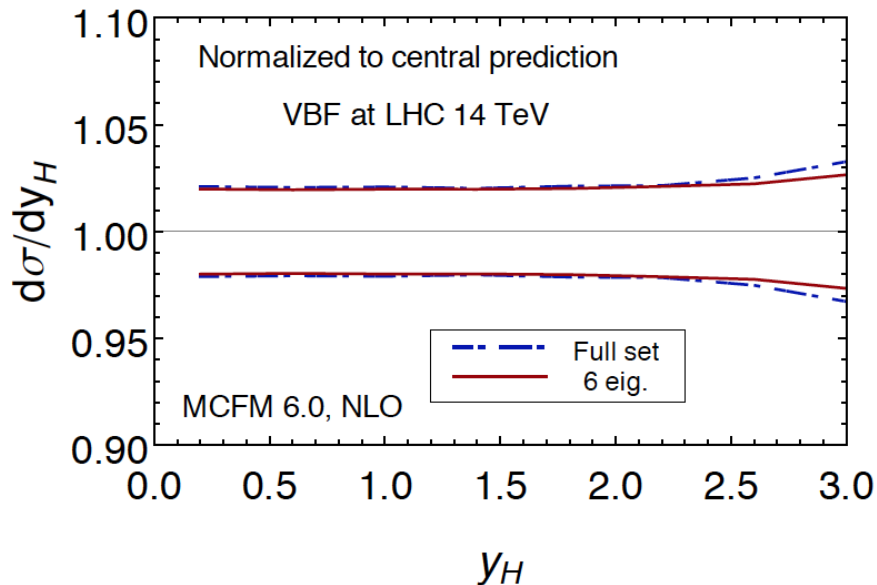
Reduced META ensemble

- Already the general-purpose ensemble reduced the number of error PDFs needed to describe the LHC physics; but we can further perform a data set diagonalization to pick out eigenvector directions important for Higgs physics or another class of LHC processes
- Select global set of Higgs cross sections at 8 and 14 TeV (46 observables in total; more can be easily added if there is motivation)

production channel	$\sigma(inc.)$	$\sigma(y_H > 1)$	$\sigma(p_{T,H} > m_H)$	scales
$gg \rightarrow H$	iHixs1.3 [32] at NNLO	MCFM6.3 [33] at LO	—	m_H
$b\bar{b} \rightarrow H$	iHixs at NNLO	—	—	m_H
VBF	VBFNLO2.6 [34] at NLO	same	same	m_W
HZ	VHNNLO1.2 [35] at NNLO	CompHEP4.5 [36] at LO	CompHEP at LO	$m_Z + m_H$
HW^\pm	VHNNLO at NNLO	—	—	$m_W + m_H$
HW^+	CompHEP at LO	same	same	$m_W + m_H$
HW^-	CompHEP at LO	same	same	$m_W + m_H$
$H + 1jet$	MCFM at LO	same	same	m_H
$Ht\bar{t}$	MCFM at LO	CompHEP at LO	CompHEP at LO	$2m_t + m_H$
HH	Hpair [37] at NLO	—	—	$2m_H$

Higgs eigenvector set

- The reduced META eigenvector set does a good job of describing the uncertainties of the full set for *typical* processes such as ggF or VBF
- But actually does a good job in reproducing PDF-induced correlations and describing those LHC physics processes in which g , \bar{u} , \bar{d} drive the PDF uncertainty (see next slide)



process	$\sigma_{cen.}$	δ_{Full}	$\delta_{Diag.}$	$\sigma_{0.116}^{\alpha_s}$	$\sigma_{0.12}^{\alpha_s}$
$gg \rightarrow H$ [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	301.4
	878.2	+19.7 -17.9	+19.2 -17.3	877.3	878.2
HZ [fb]	396.3	+8.4 -7.3	+8.1 -7.4	393.0	399.1
	814.3	+14.8 -13.2	+13.8 -13.0	806.5	823.2
HW^\pm [fb]	703.0	+14.4 -14.4	+14.3 -14.1	697.4	708.9
	1381	+28 -22	+26 -22	1368	1398
HH [fb]	7.81	+0.33 -0.30	+0.33 -0.30	7.50	8.10
	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	259.1
	816.9	+21.4 -19.6	+21.4 -18.4	785.5	848.2
$Z/\gamma^*(l^+l^-)$ [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	7.25
	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	5.08
	8.59	+0.21 -0.20	+0.19 -0.18	8.46	8.74
W^+W^- [pb]	4.14	+0.08 -0.08	+0.08 -0.07	4.04	4.20
	7.54	+0.15 -0.14	+0.14 -0.12	7.39	7.57
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

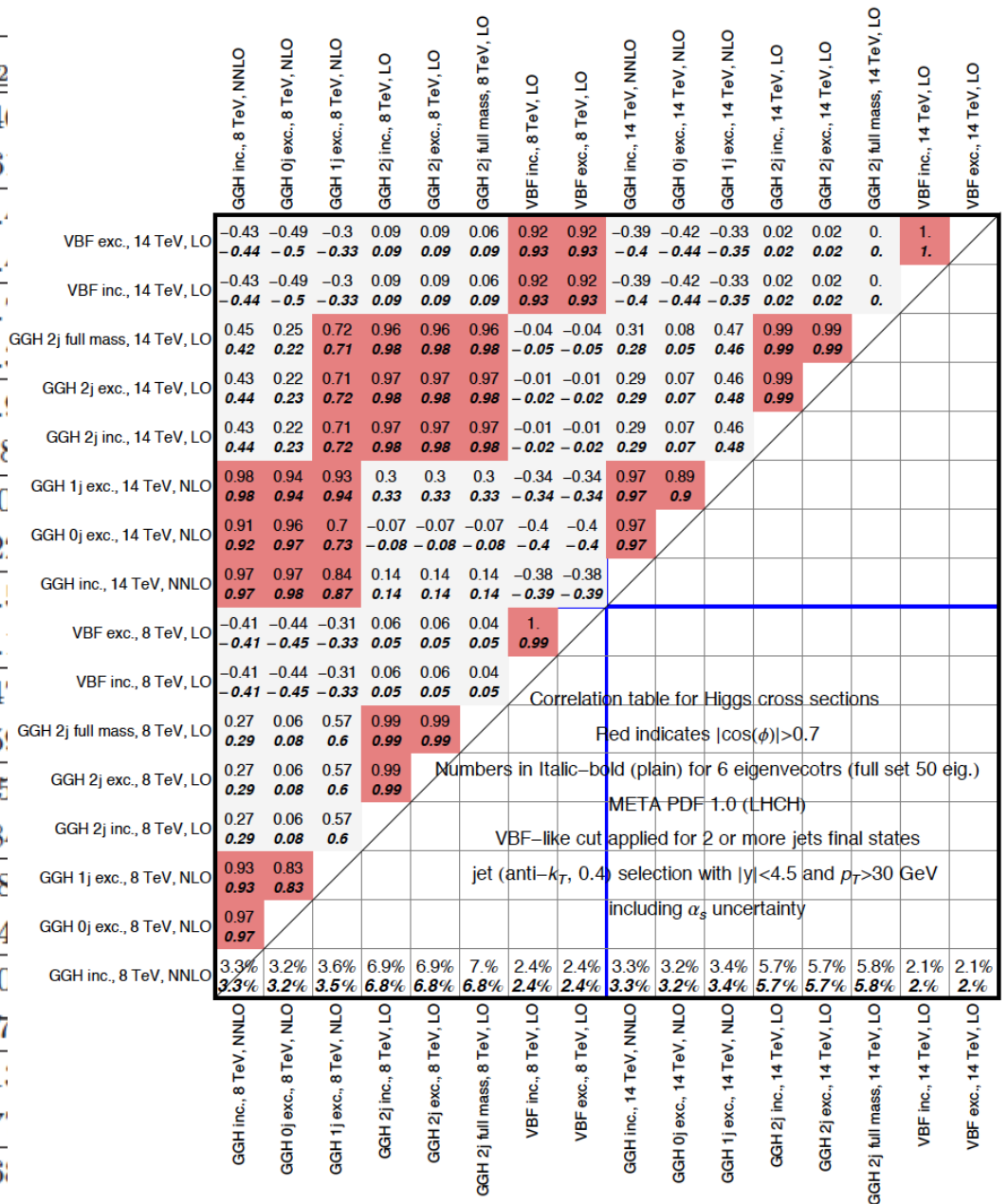
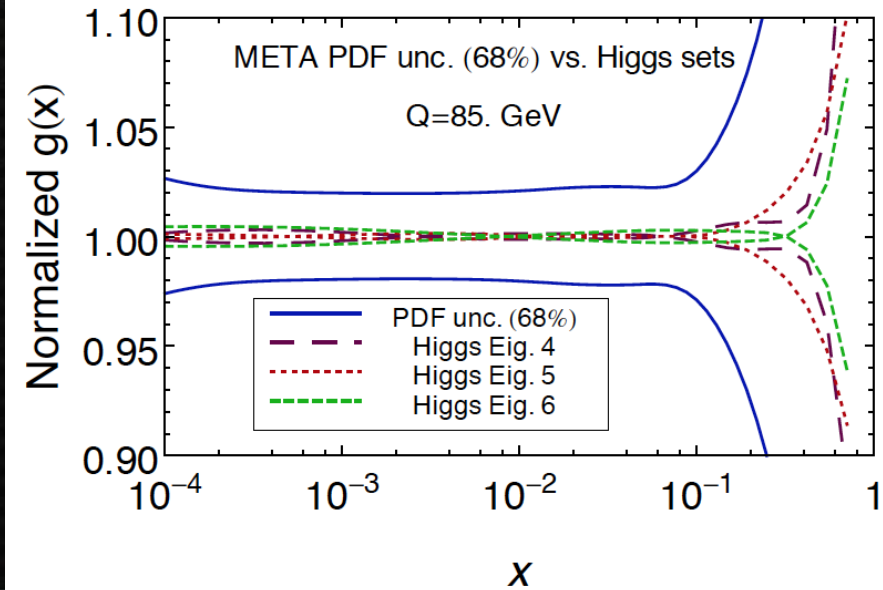
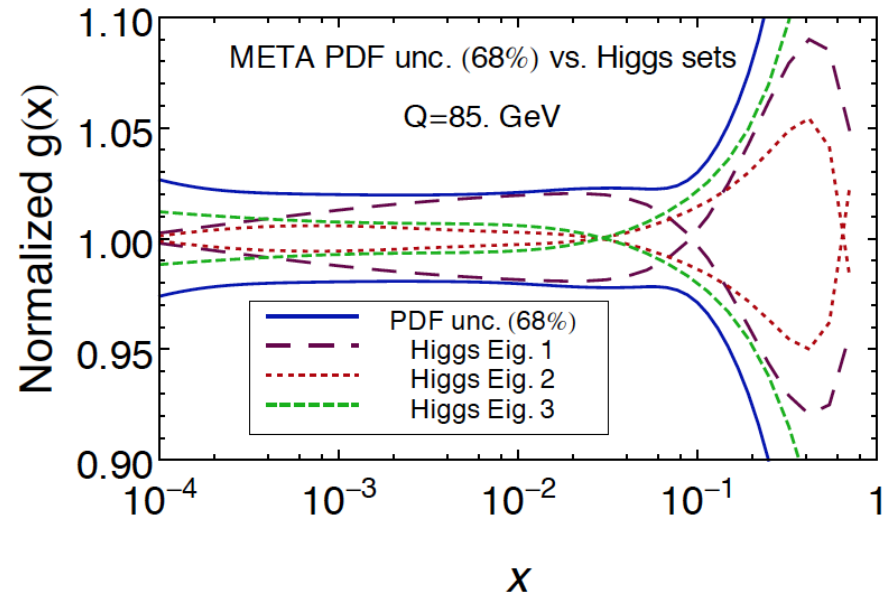


FIG. 7: Same as Fig. 5, with α_s uncertainties included by adding in quadrature.

Re-diagonalized eigenvectors...

...are associated with the parameter combinations that drive the PDF uncertainty in Higgs, W/Z production at the LHC

- Eigenvectors 1-3 cover the gluon uncertainty. They also contribute to \bar{u} , \bar{d} uncertainty.
- Eigenvector 1 saturates the uncertainty for most of the $gg \rightarrow H$ range.



u, d quark uncertainties are more distributed

