PDF4LHC15 combined PDFs, compressed PDFs, and LHAPDF

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Introduction

This talk (mostly) on behalf of the PDF4LHC15 group.
They did the work, not me!

Talk outline:

- a potted history of the notorious PDF4LHC procedure
- recent developments in the recommendation ⇒ PDF4LHC15 PDFs
- construction of "compressed PDFs"
- *status of LHAPDF*

Credit: most of what I show will be "Frankenstein'd" from Juan Rojo & Albert de Roeck at QCD@LHC last month!

PDF4LHC uncertainty

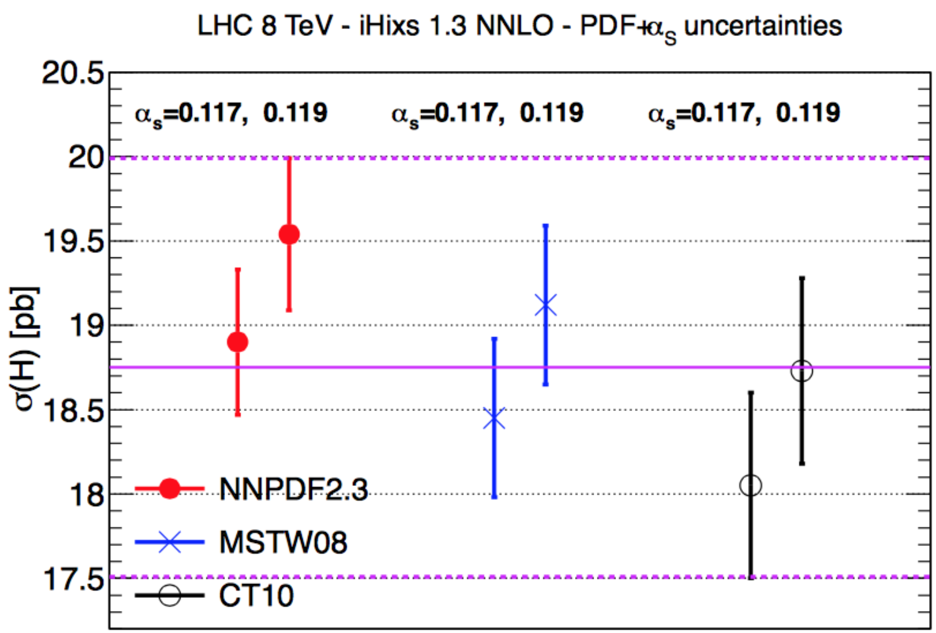
PDF4LHC…

- PDF4LHC originated from the HERA/LHC workshops organized in the period 2004-2008
- Forum for PDF discussions with all PDF fitting groups and experiments
- First recommendation in 2010: arXiv:1101.0538 (under some duress of the Higgs cross section group ☺)
- This recommendation (see later) was a bit tedious: revised and being improved now…
- New recommendation being finalized, which should be a easier for the user, without (noticable) loss of precision

2010 Recommendation

THE OLD PDF4LHC RECOMMENDATION

HIGGS IN GLUON FUSION



Using the full envelope was conservative but statically not optimal

- TAKE THE ENVELOPE OF RESULTS
- RED CONSERVATIVE WAY OF HANDLING DISCREPANCIES
- GGH: DISCREPANCY NOT UNDERSTOOD DESPITE INTENSIVE BENCHMARKING

Usages of PDFs

Note: basically two kinds of usages:

- For the assessment of the PDF uncertainty in comparing predictions to theory (top cross section, jets, W-rapidity distributions)

  Use the individual PDF sets (CT, NNPDF, MMHT, HERAPDF, ABM, JR, CJ…)

- For assessment of the PDF uncertainty as in searches, discovery, acceptance, measurements (eg Higgs, SUSY, …)

  Use the PDF4LHC prescription

History of the PDF4LHC Recommendation

- 2010: take the envelope of the 3 (most) global fits to available data: MSTW08, CTEQ6.6, NNPDF2.0

  Of these, only MSTW08 had an NNLO version
- In 2013 this was updated by taking the latest versions of the PDFs: CT10, MSTW2008 and NNPDF2.3

  All have NNLO versions
- A lot of extensive benchmarking of these and other PDF sets was done as input to these studies eg arXiv:1101.0536
- More details can be found on the PDF4LHC web

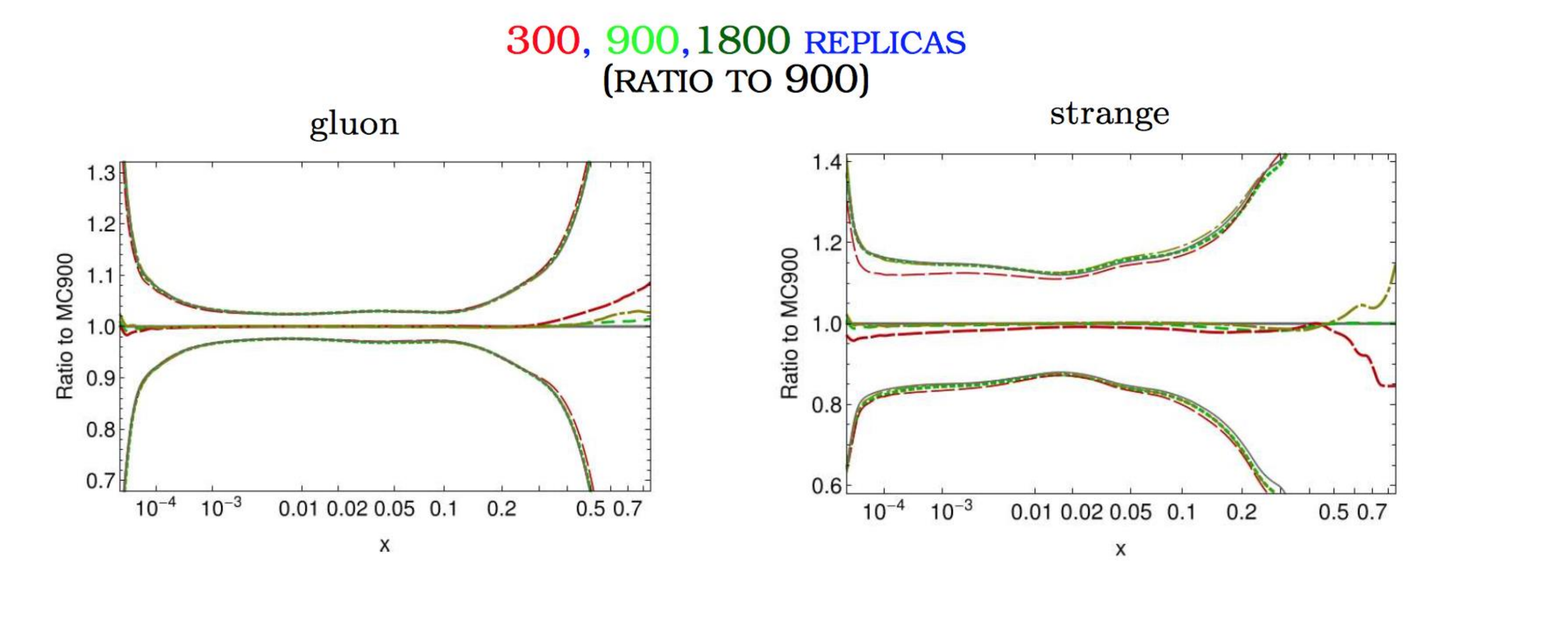
  http://www.hep.ucl.ac.uk/pdf4lhc/
- The making of the envelope was left to the user. The new recommendation will be more “user friendly”

Updated Recommendation

- Criticism: use of only 3 PDF (motivated in arXiv:1101.0538)
- Criticism: complicated for the user, having to make the envelope for each observable. Some signal programs are not adapted well to do that in an efficient way.
- Criticism: not statistically rigorous/robust
- Response: Use the transition from Run-I to Run-II for a more statistically rigorous procedure. Ideas developed in o.a. Forte arXiv:1011.5247, G Watt PDF4LHC meeting 4/2013
- Idea: create a "combined-PDF" set based on N input PDFs with its uncertainty band, using the MC replica method. This is what the user can use directly. Correlations between the PDFs should be kept. The user should have a simple procedure.
- Compress the set to reduce the number of replicas

Current Combination of PDFs

The present combination is based on Monte Carlo set combination of CT14, MMHT and NNPDF3.0
A total of 900 replicas (300 per PDF set) ensures a % level of accuracy on all quantities. We use this as a baseline



MC replicas and reduction of the replicas and getting Hessian representation discussed by J. Rojo in the previous talk

The New PDF4LHC Prescription

- Perform a Monte Carlo Combination of the underlying PDF sets (see NNPDF)
- Sets entering the combination must satisfy common requirements
- Deliver combined PDF sets in Hessian and MC representation.
- Monte Carlo: a reduced set of PDF replicas is delivered
- Hessian: central set and error sets are delivered
- α_s : PDFs are delivered for a central value of α_s of and for 1-sigma error.
- Hence the user gets combined sets he/she can directly use
- This scheme also allows to include more PDF families

Requirements for Inclusion

- PDF sets to be included in the combination must satisfy requirements which make the compatible
- Details are on the indico of the PDF4LHC workshop of April
- A few examples (see document for the full list)
  - Provide results at NLO and NNLO with NNLO α_s of evolution benchmarked against HOPPET and QCDNUM
  - Baseline set for $\alpha_s = 0.118$ and sets with α_s variation
  - Use a general-mass variable flavor number scheme with up to 5 flavors
  - For direct combination with current technology fits must be based on approximately common global sets of data. Reweighting will be necessary otherwise.
- HERAPDFs expressed interest to be included

Three Sets Proposed

From the user-community we also got feedback for the need for different sets for different applications… Hence we provide three sets

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

- These are available at NLO and NNLO and for standard $\alpha_s = 0.118$ and $\delta\alpha_s = \pm 0.0015$ variations
- Available in LHAPDF repository

- Which ones to use when: Part of the recommendation being documented eg
  - _MC set: contains also non-gaussian effects. Important for searches at high masses. ..
  - _30 set: very good precision and probably usable for most experimental needs
  - _100 superior precision, eg for TH Higgs cross section uncertainty determinations…

PDF compression methods

Outline

To estimate the **total PDF uncertainty** associated to LHC processes, such as Higgs cross-sections or New Physics searches, a **combination of the results from individual PDF sets** is required

PDF4LHC11 → **Envelope Method**

- Cumbersome to implement: **a posteriori combination** of cross-sections from different PDF sets
- **Statistical interpretation** unclear. Over-conservative: too much weight given to **outliers**

PDF4LHC15 → **Monte Carlo Combination**

- Statistically meaningful combination

MC reduction → **CMC-PDFs**

Hessian reductions → **MC2H**, **Meta-PDFs**

MC2H → **SM-PDFs**

Combination tailored to **specific processes**

Monte Carlo Combination of PDF sets

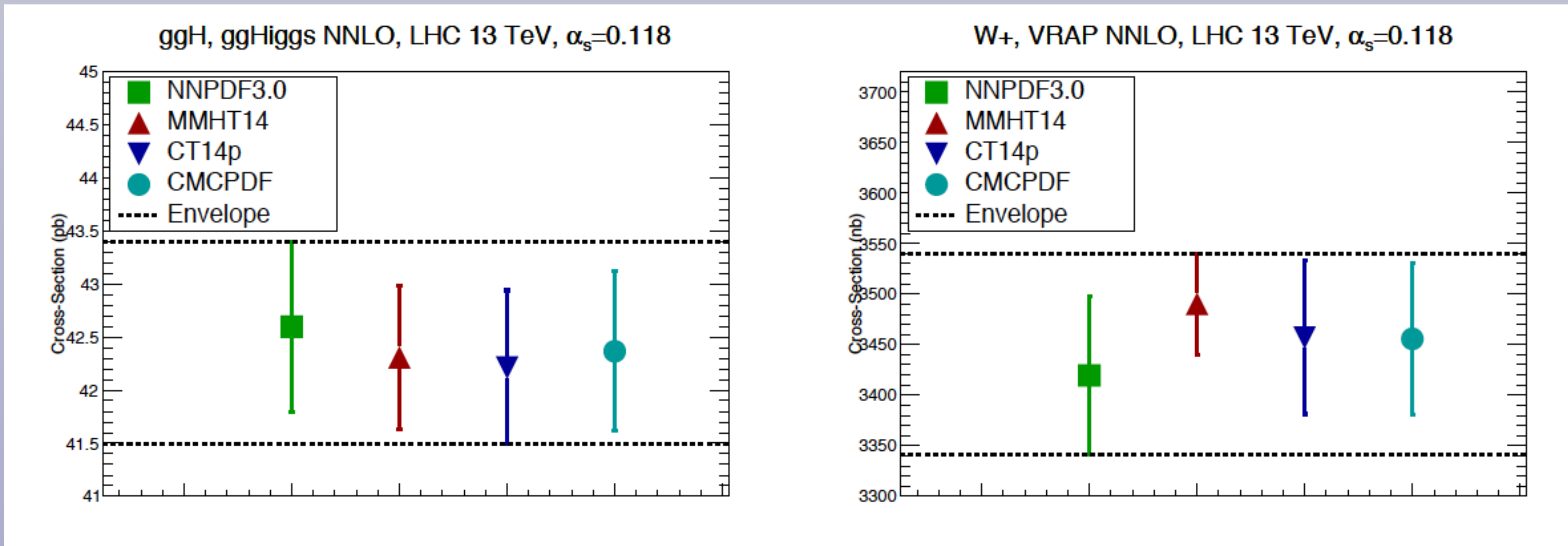
Watt and Thorne, arXiv:1205.4024
Forte, arXiv:1011.5247
Forte and Watt, arXiv:1301.6754
Carrazza, Latorre, J. R., Watt, arXiv:1504.06459

Monte Carlo combination

- First of all, select the **PDF sets that enter the combination**. Must be reasonably consistent among them for a meaningful combination
- Transform the **Hessian PDF sets into their Monte Carlo representation:**

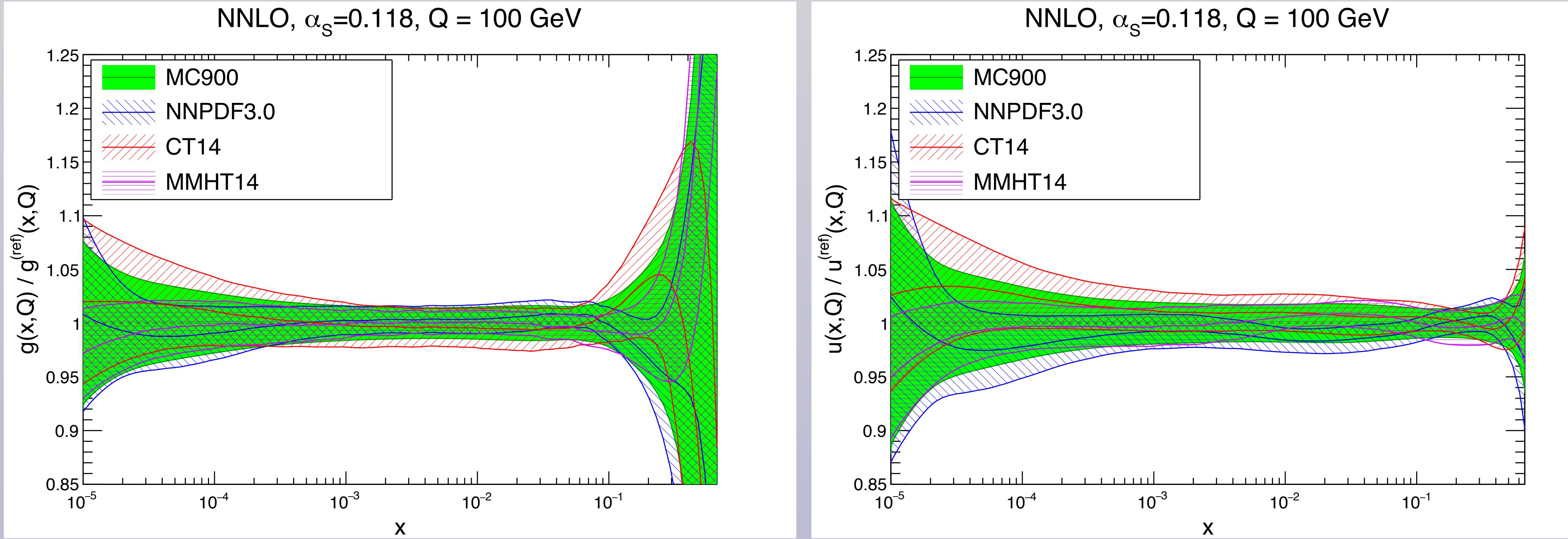
$$F^k = F(q_0) + \frac{1}{2}\sum_{j=1}^{N_{\rm eig}} \left[F(q_j^+) - F(q_j^-) \right] R_j^k \,, \quad k = 1, \ldots, N_{\rm rep} \,,$$

- 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, with smaller uncertainties, compared to the **original PDF4LHC envelope** (proper treatment of outliers)



The combined Monte Carlo PDF set

- Combine most recent releases of the three global sets: **NNPDF3.0, CT14, MMHT14**



- **900 MC replicas** required to stabilise the combination: these define the **MC900 prior**
- Too many for practical applications: need to find a strategy to **reduce the number of replicas** in which the MC combination is based
- In addition, for many important application, a **Hessian representation** would be required

The combined Monte Carlo PDF set

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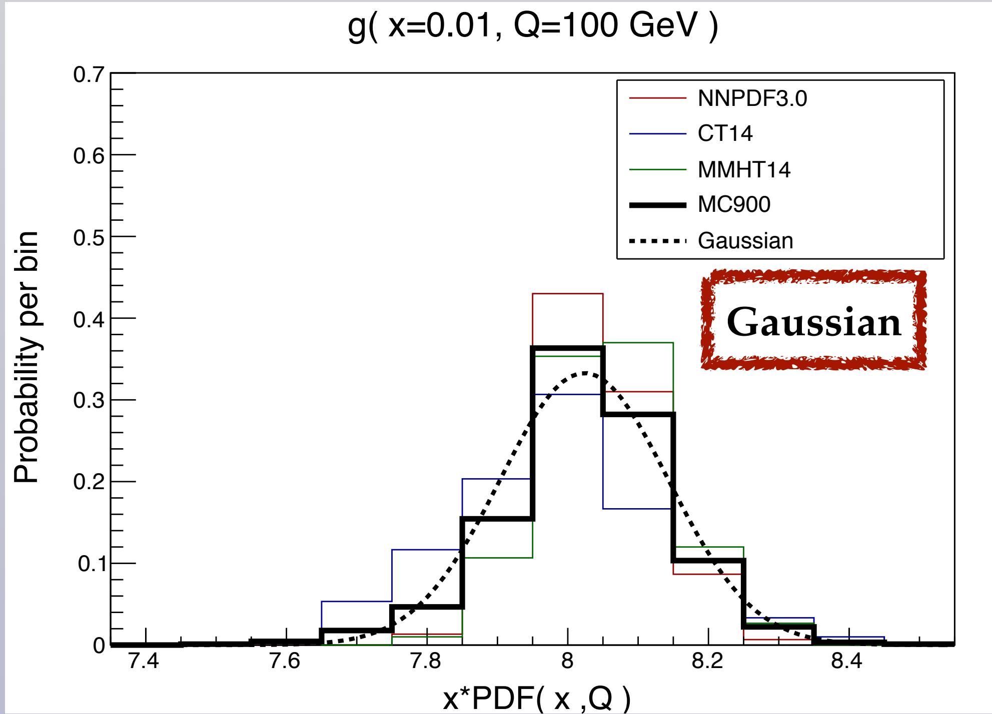
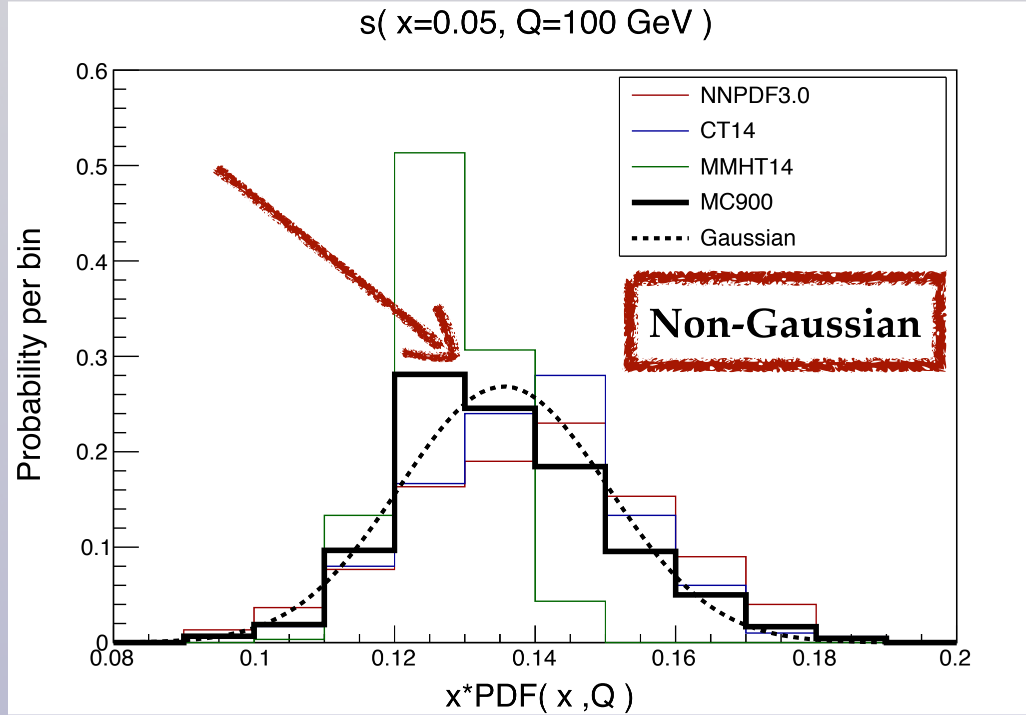




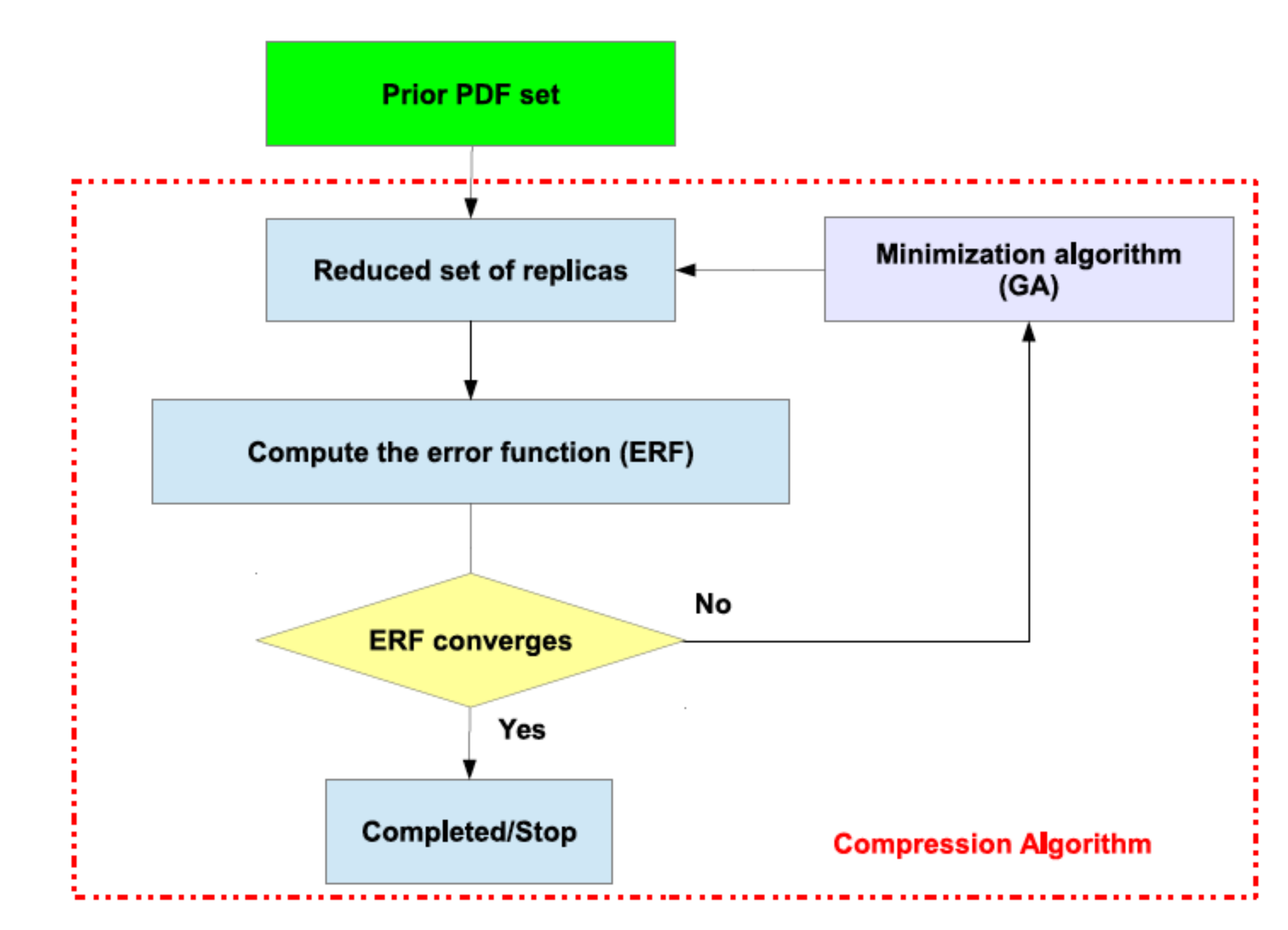
- The **MC combination** is usually **Gaussian** (in the data region) but in many cases **non-Gaussian features** are observed (in extrapolation regions, or for poorly constrained flavors)
- Specially important for **BSM searches**, which rely on PDFs in regions where **PDF errors are large**

CMC-PDFs

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

Compressed Monte Carlo 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



$$\mathrm{ERF} = \sum_k \frac{1}{N_k} \sum_i \left(\frac{C_i^{(k)} - O_i^{(k)}}{O_i^{(k)}} \right)^2 ,$$

$$ERF_{CV} = \frac{1}{N_{\mathrm{CV}}} \sum_{i=-n_f}^{n_f} \sum_{j=1}^{N_x} \left(\frac{f_i^{\mathrm{CV}}(x_j, Q) - g_i^{\mathrm{CV}}(x_j, Q)}{g_i^{\mathrm{CV}}(x_j, Q)} \right)^2$$

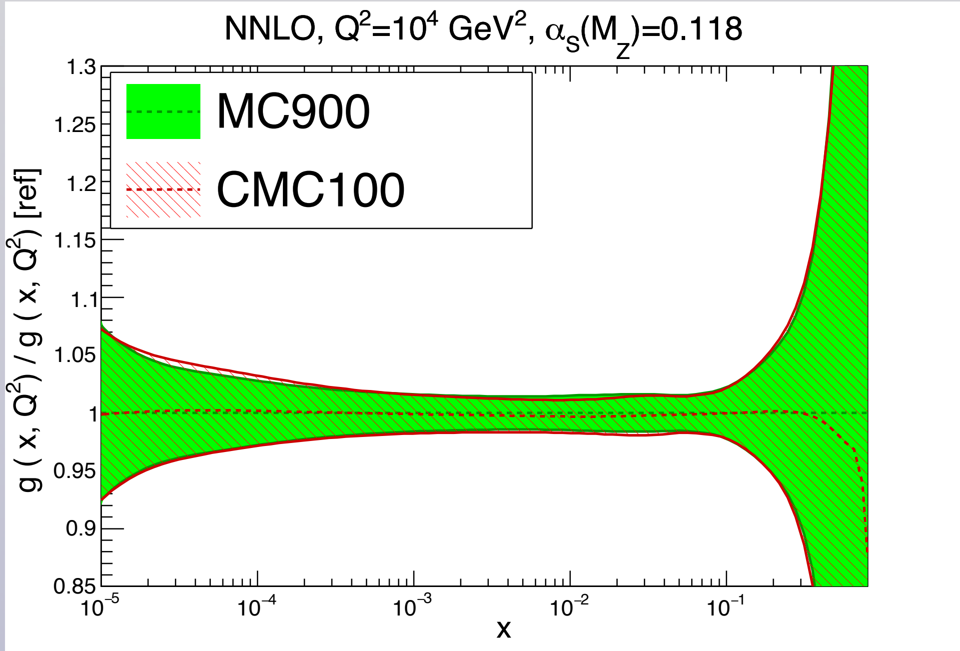
$$f_i^{\mathrm{CV}}(x_j, Q) = \frac{1}{N_{\mathrm{rep}}} \sum_{r=1}^{N_{\mathrm{rep}}} f_i^r(x_j, Q)$$

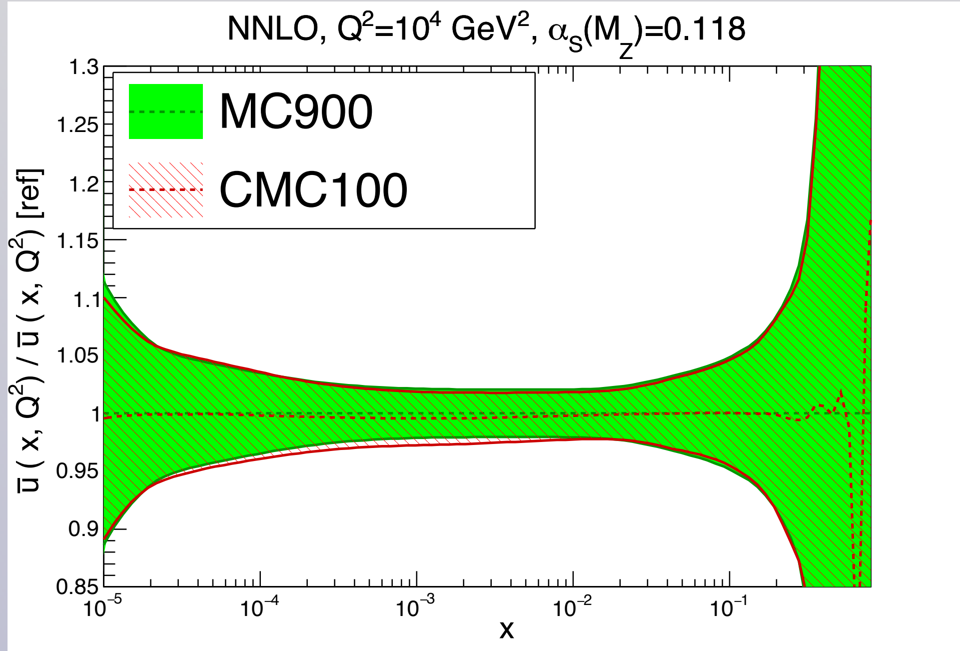
Similar for **variances, correlations, skewness, kurtosis** and the **Kolmogorov** distance

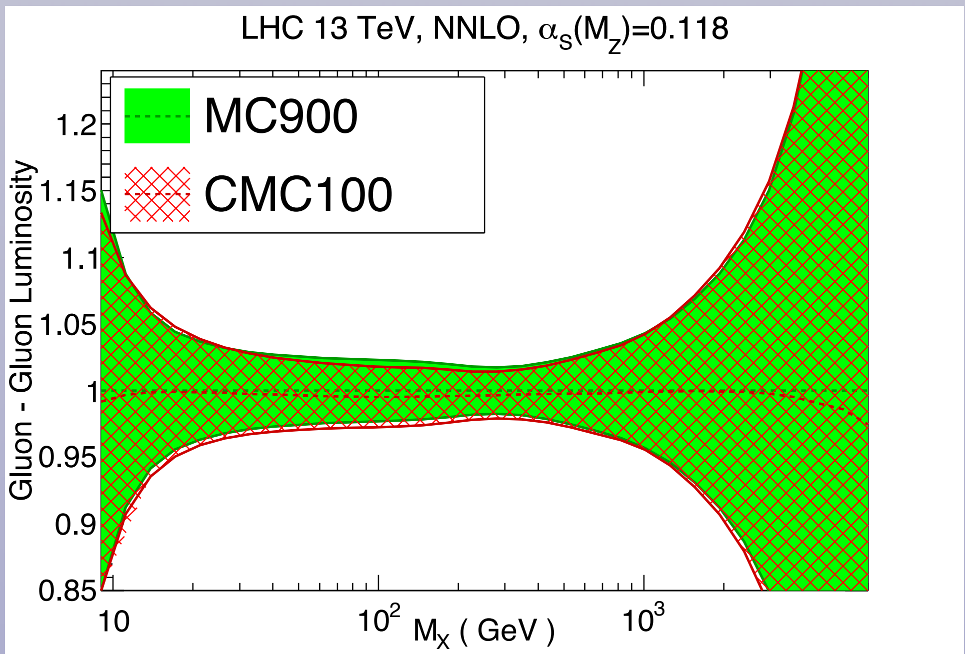
Minimise **distance between prior and compressed sets** using Genetic Algorithms applied to an **Error Function,** which ensures the reproduction of all statistical properties of the prior

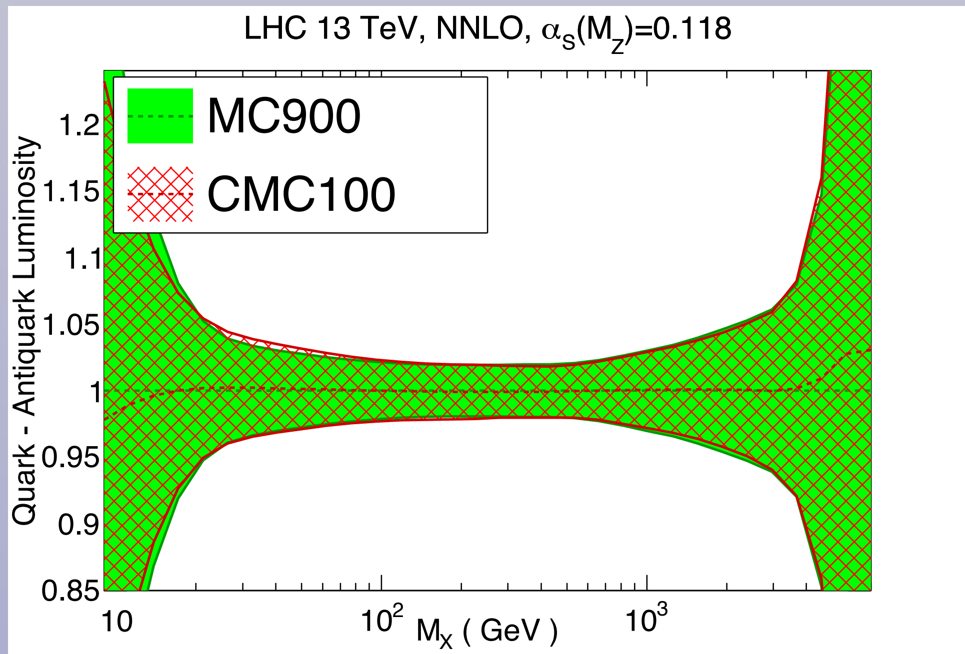
CMC-PDFs

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



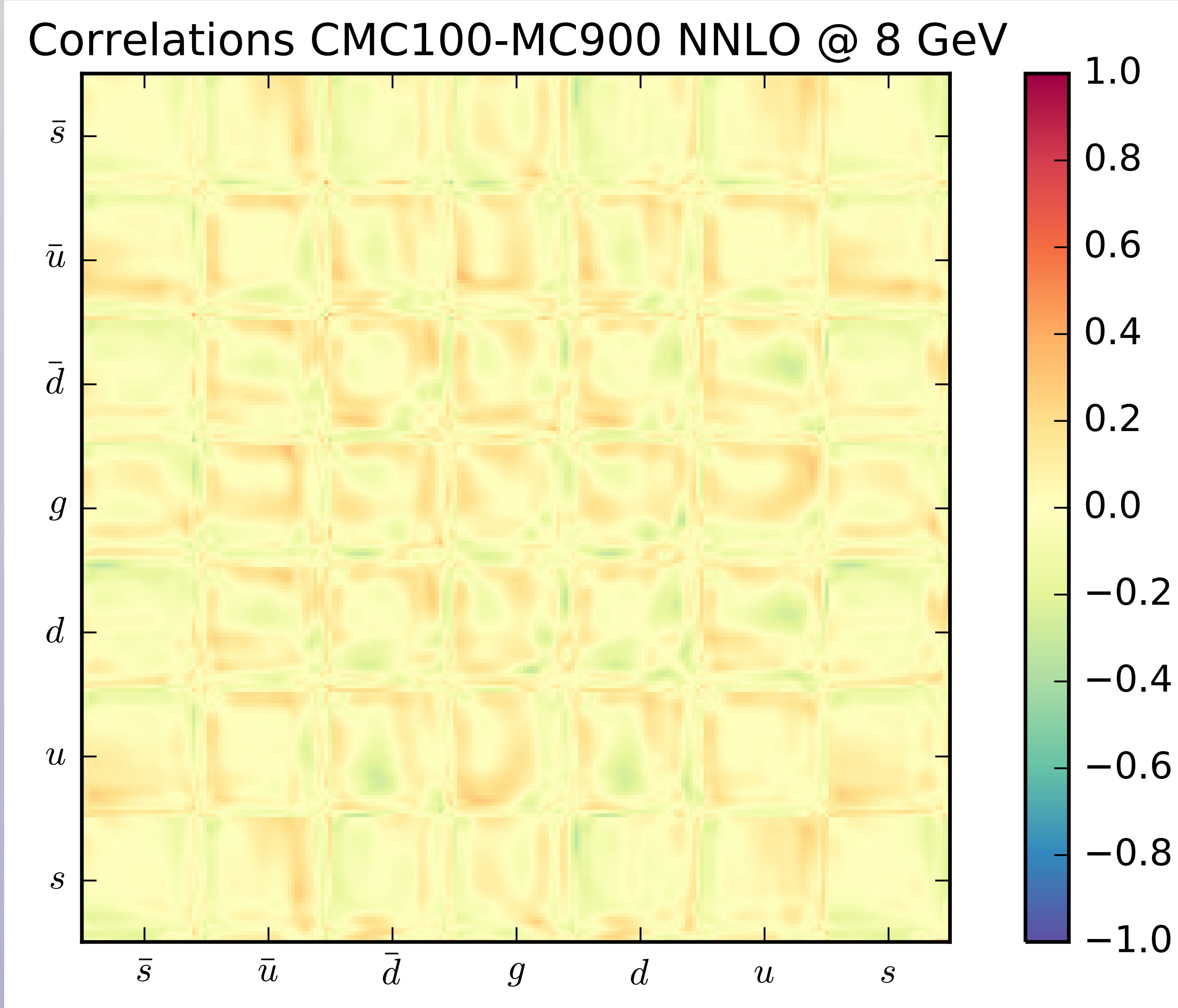






CMC-PDFs

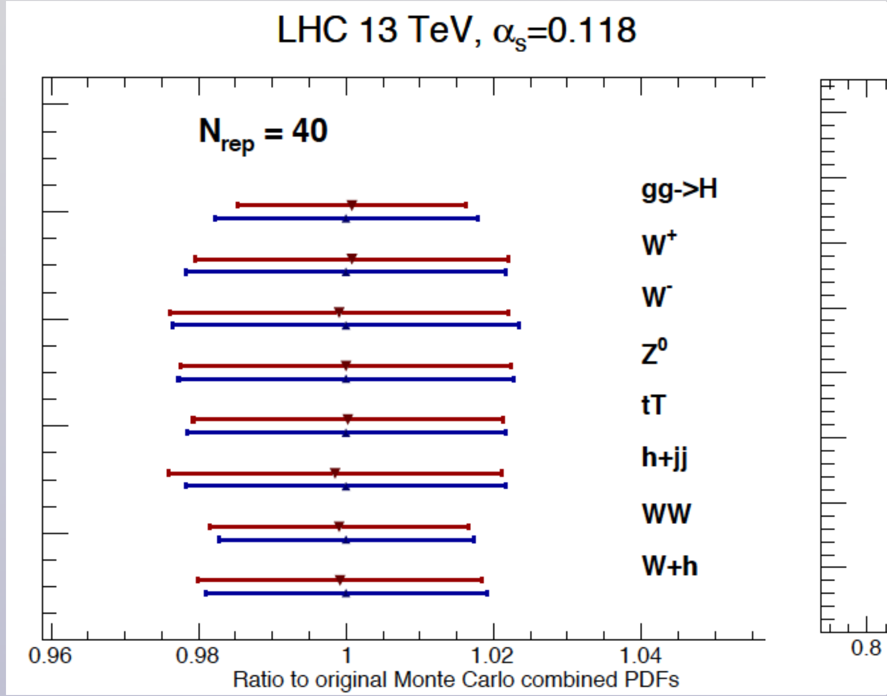
Reasonable agreement as well for the **correlations between different PDF flavours**

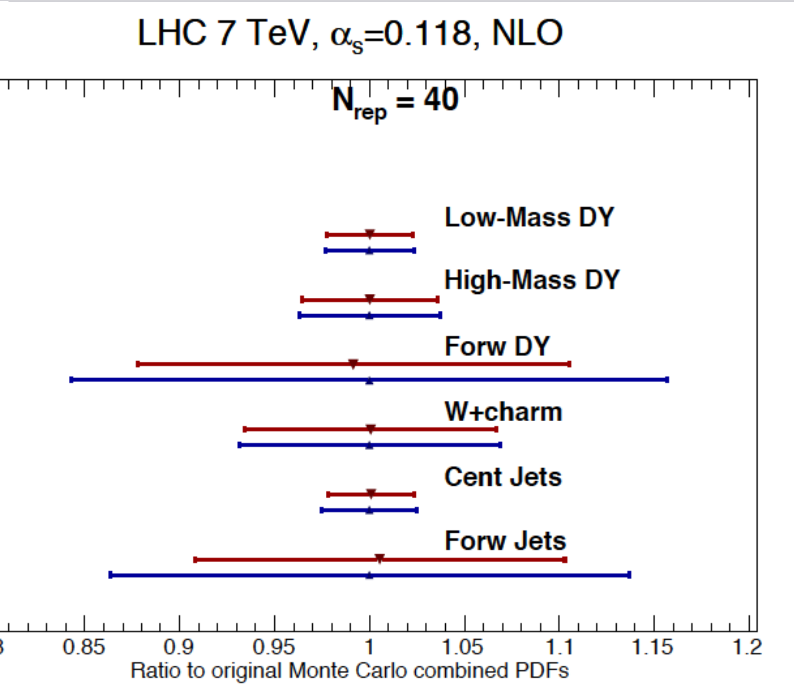


In this contour plot, the **differences in the correlation coefficients of MC900 and CMC100** between different PDF flavours are represented

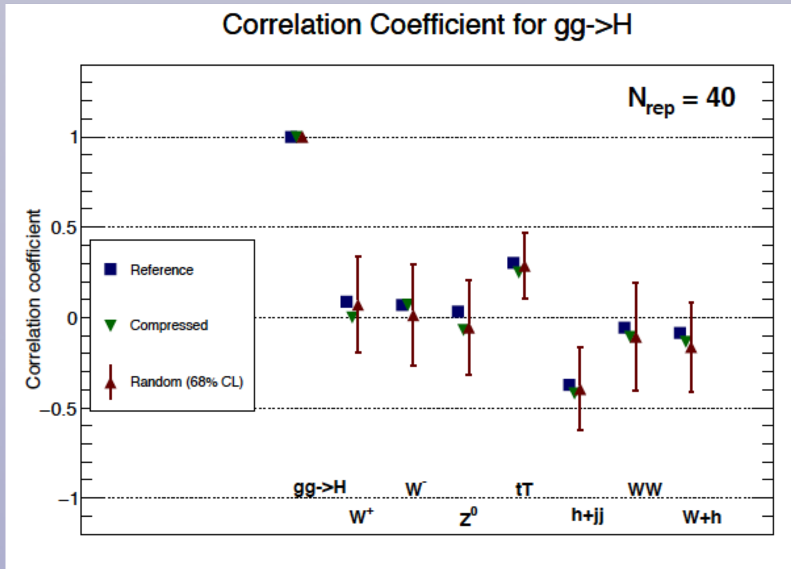
Correlation coefficients are computed at **Q = 8 GeV**, and in the **range of x of [10^{-5},0.9]** logarithmically spaced

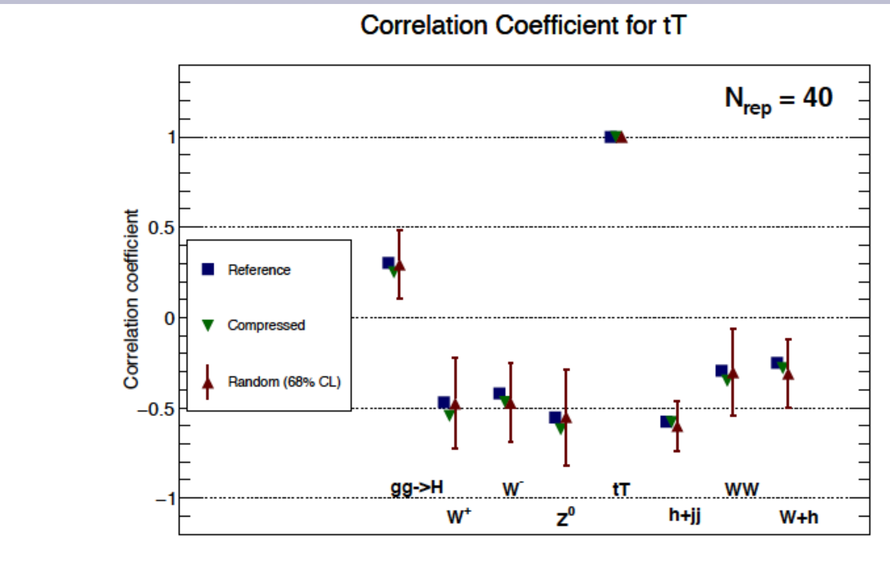
LHC Phenomenology





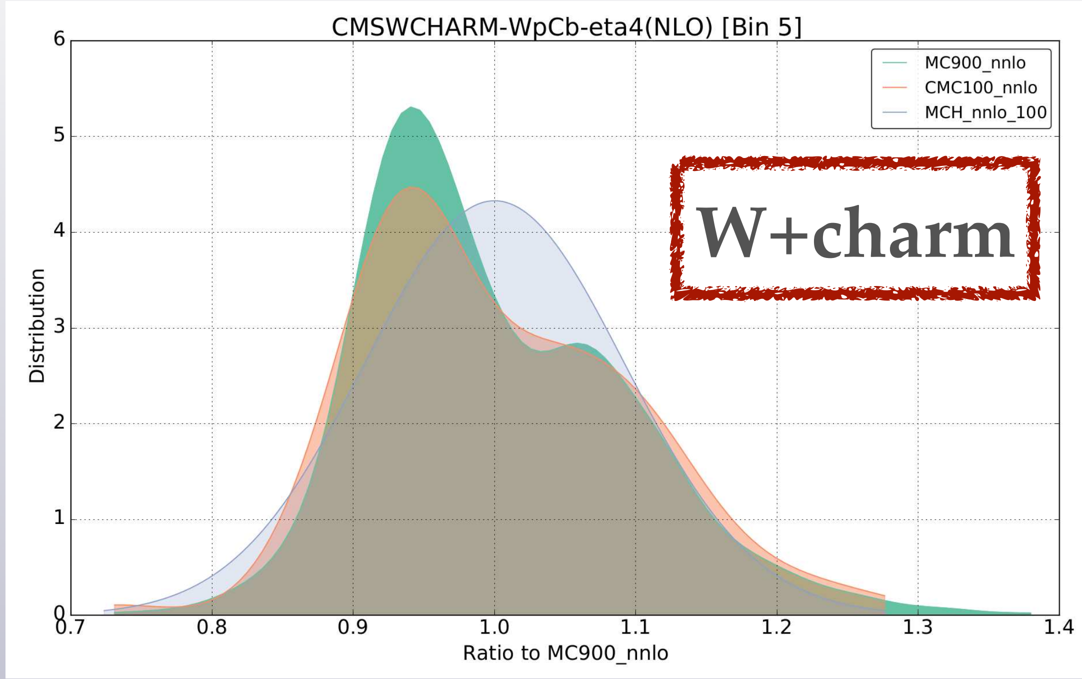
As expected from good agreement at the PDF level, CMC-PDFs also validated for **LHC inclusive cross-sections and diff distributions,** including **correlations**



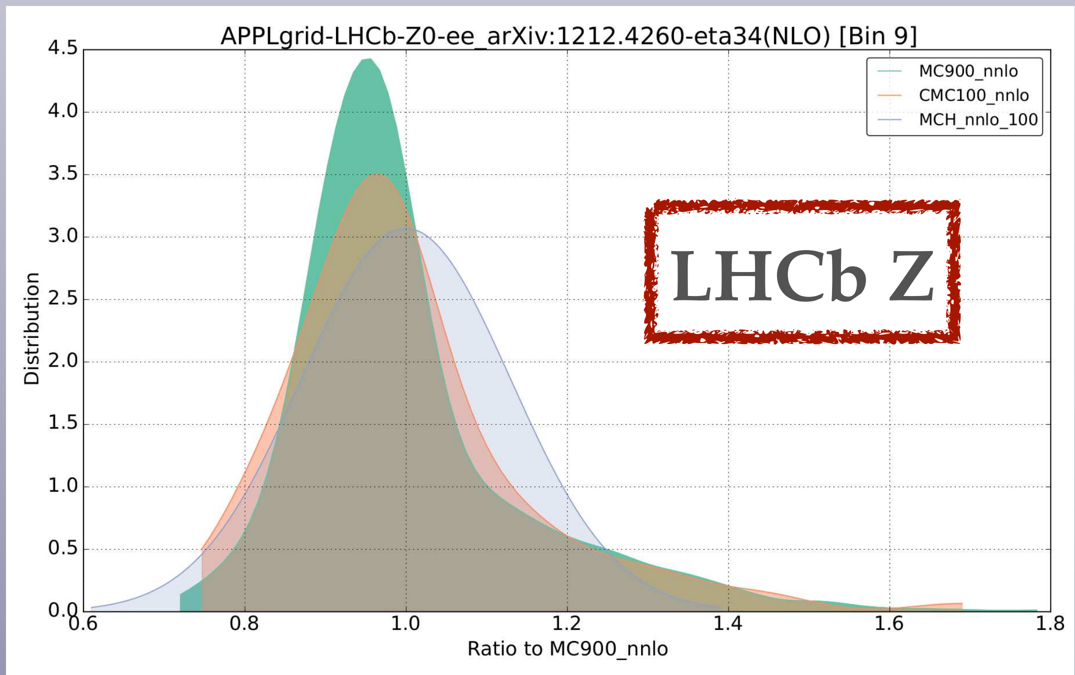


Agreement between MC900 and CMC significantly better than **random selection of same number of replicas**

Non-Gaussian features in LHC cross-sections



CMC100 reproduces properly **non-Gaussian features in MC900**, such as a **double-hump distribution** (in W+charm) and a **skewed distribution** (for forward Z)



Any **Hessian reduction fails** by construction to reproduce such features mc²hessian

MC2Hessian and Meta-PDFs

Meta-PDFs: Gao and Nadolsky, arXiv:1401.0013

MC2H: Carrazza, Forte, Kassabov, Latorre and J. R., arXiv:1505.06736

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**

MC900 → **Hessian reductions** → **MC2H**

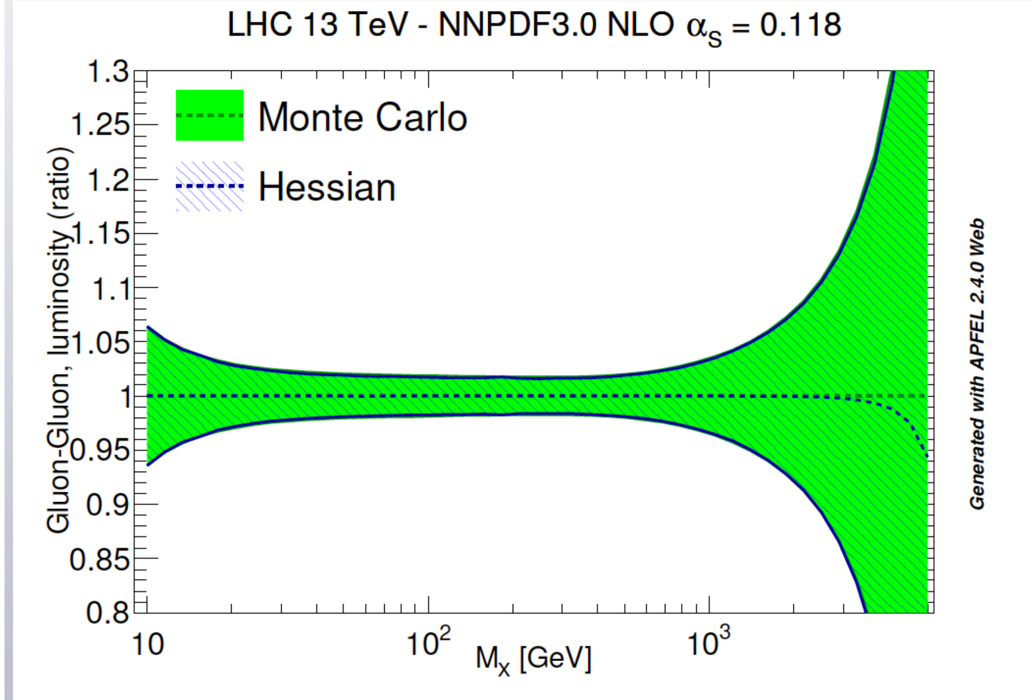
- **MC replicas** as expansion basis
- **Principal Component Analysis (PCA)** to reproduce PDF covariance matrix with arbitrary precision
- Standard linear algebra problem: **Singular Value Decomposition**

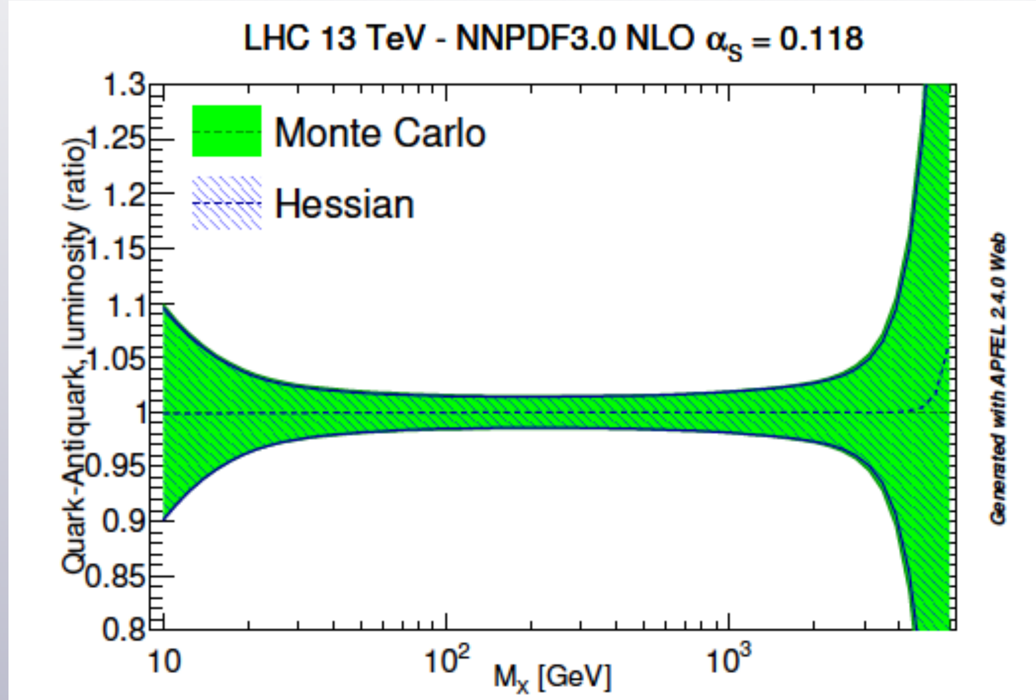
MC900 → **Hessian reductions** → **Meta-PDFs**

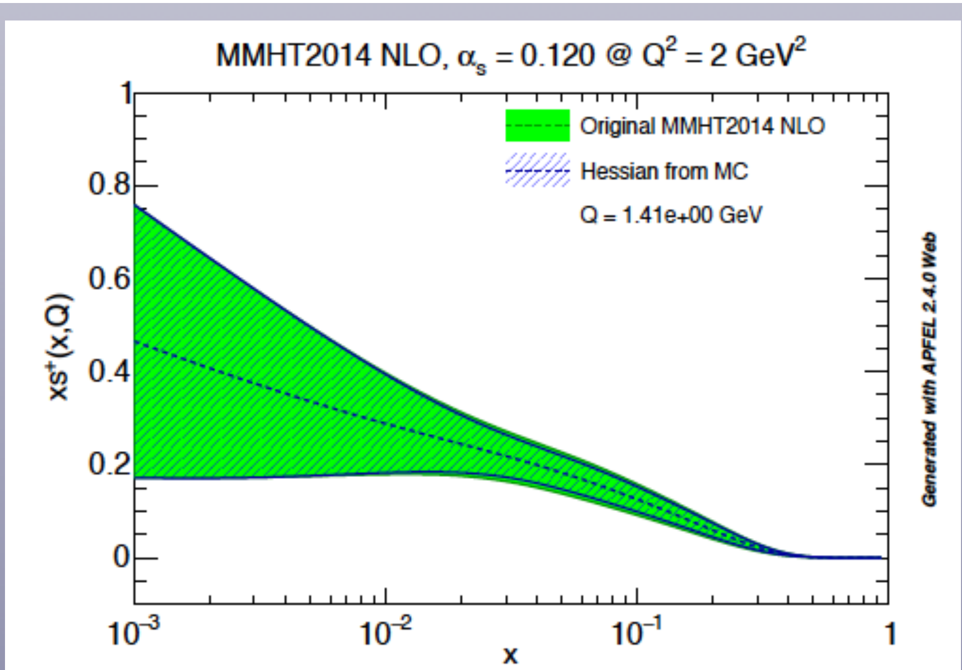
- **MC replicas** are fitted to a common **meta-parametrization**
- **MC900** defines the **68% CL of the parameters** of the fitted function form
- Linear expansion in these fit parameters

Results: NNPDF3.0 and MMHT14

- The MC2H algorithm succeeds in **producing a Hessian representation of a native MC set,** NNPDF3.0

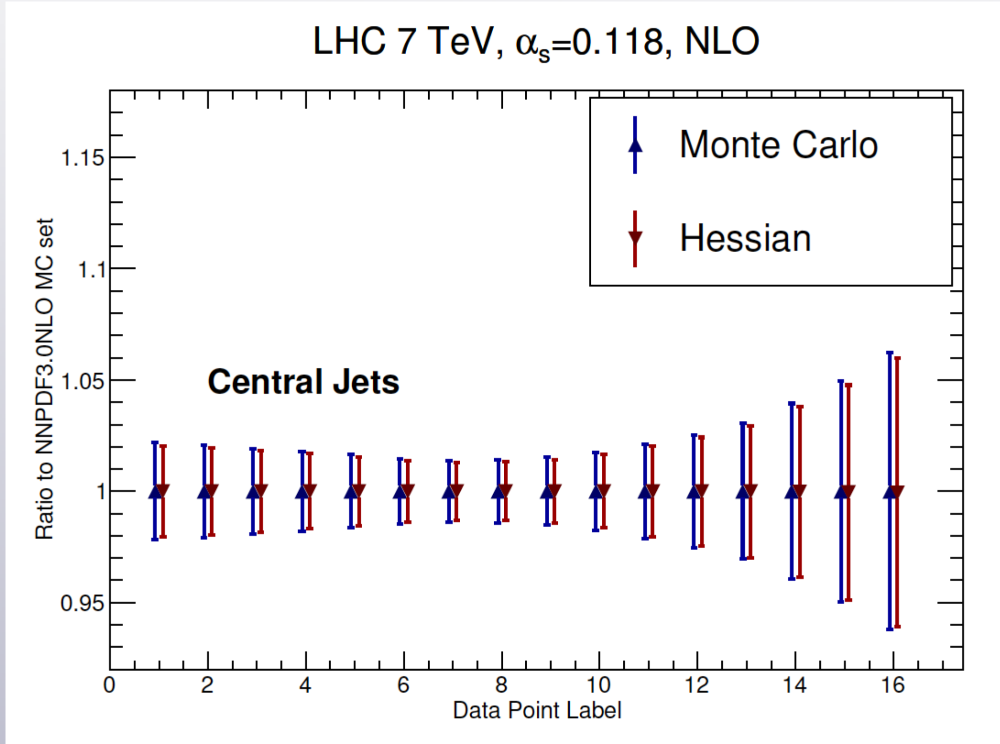


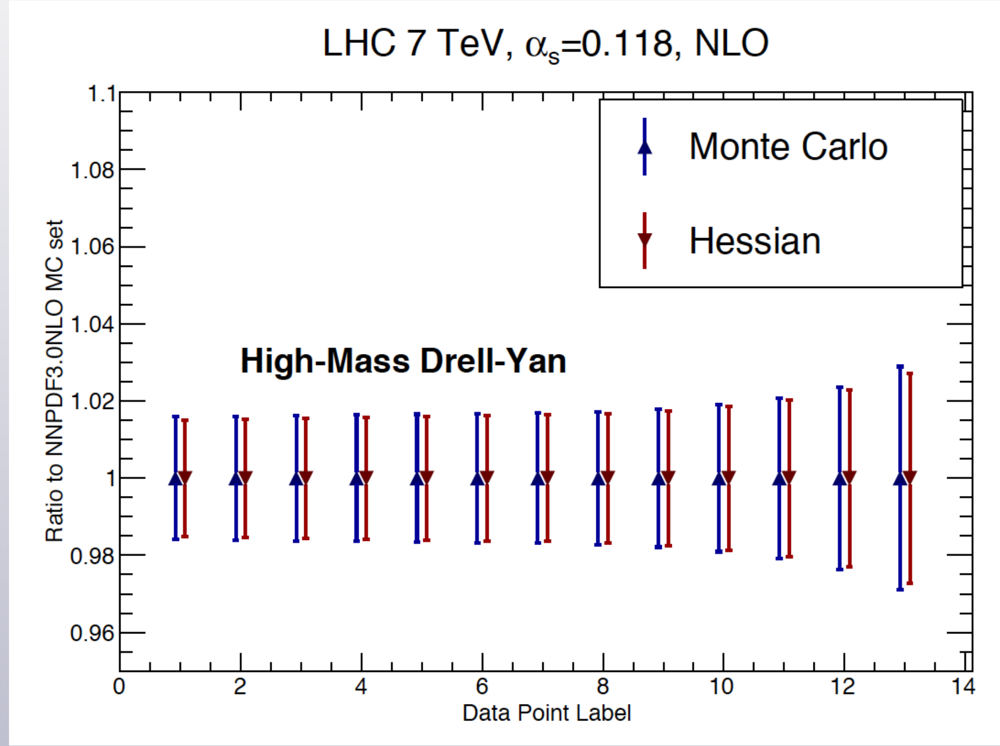


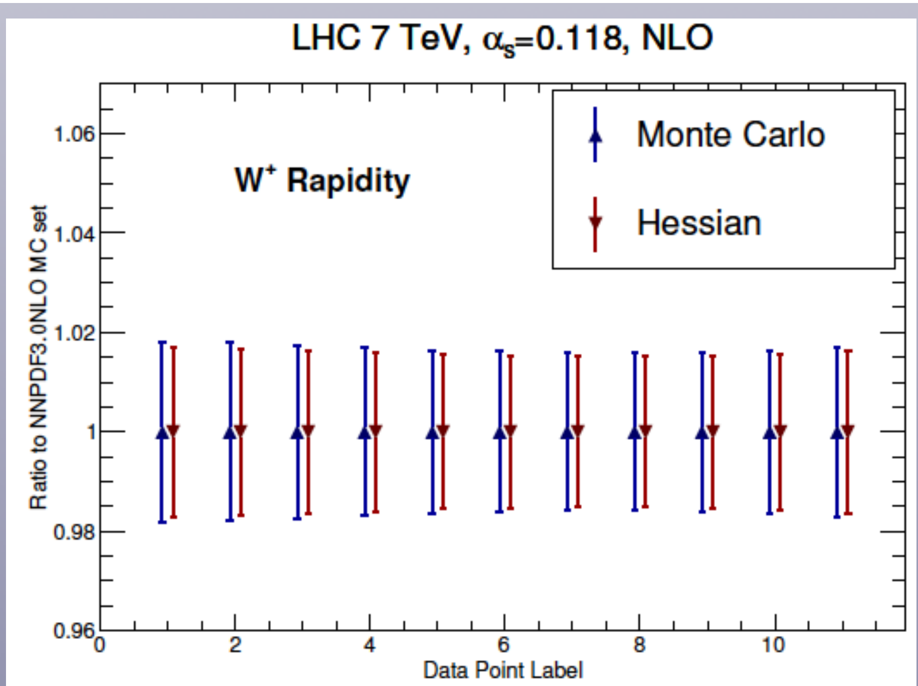


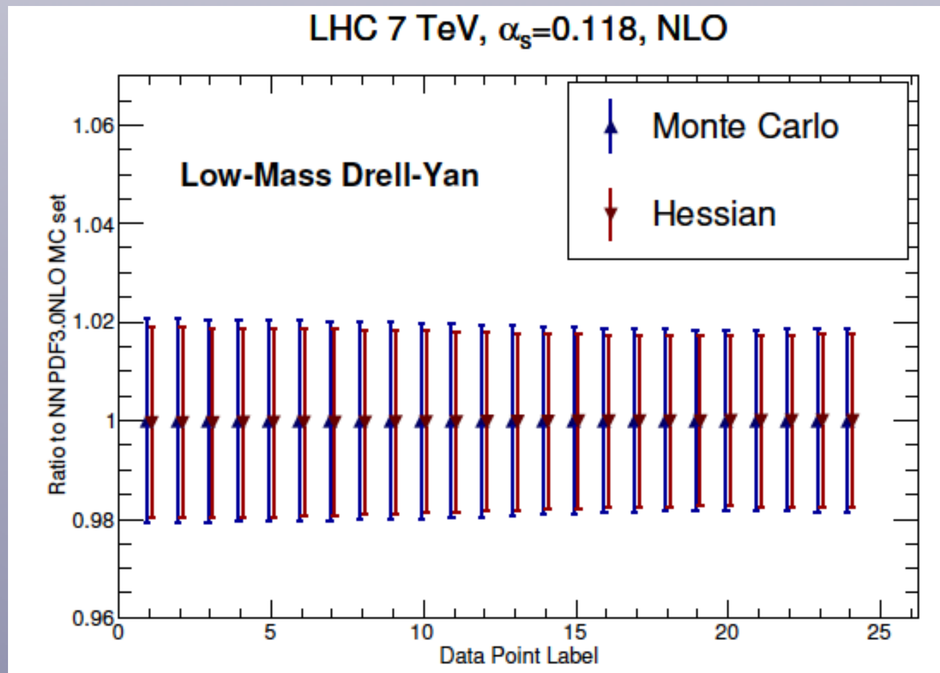
- Also verified that we can produce a **Hessian representation of a native Hessian set, MMH14**, via an **intermediate Monte Carlo representation**

MC2H LHC phenomenology



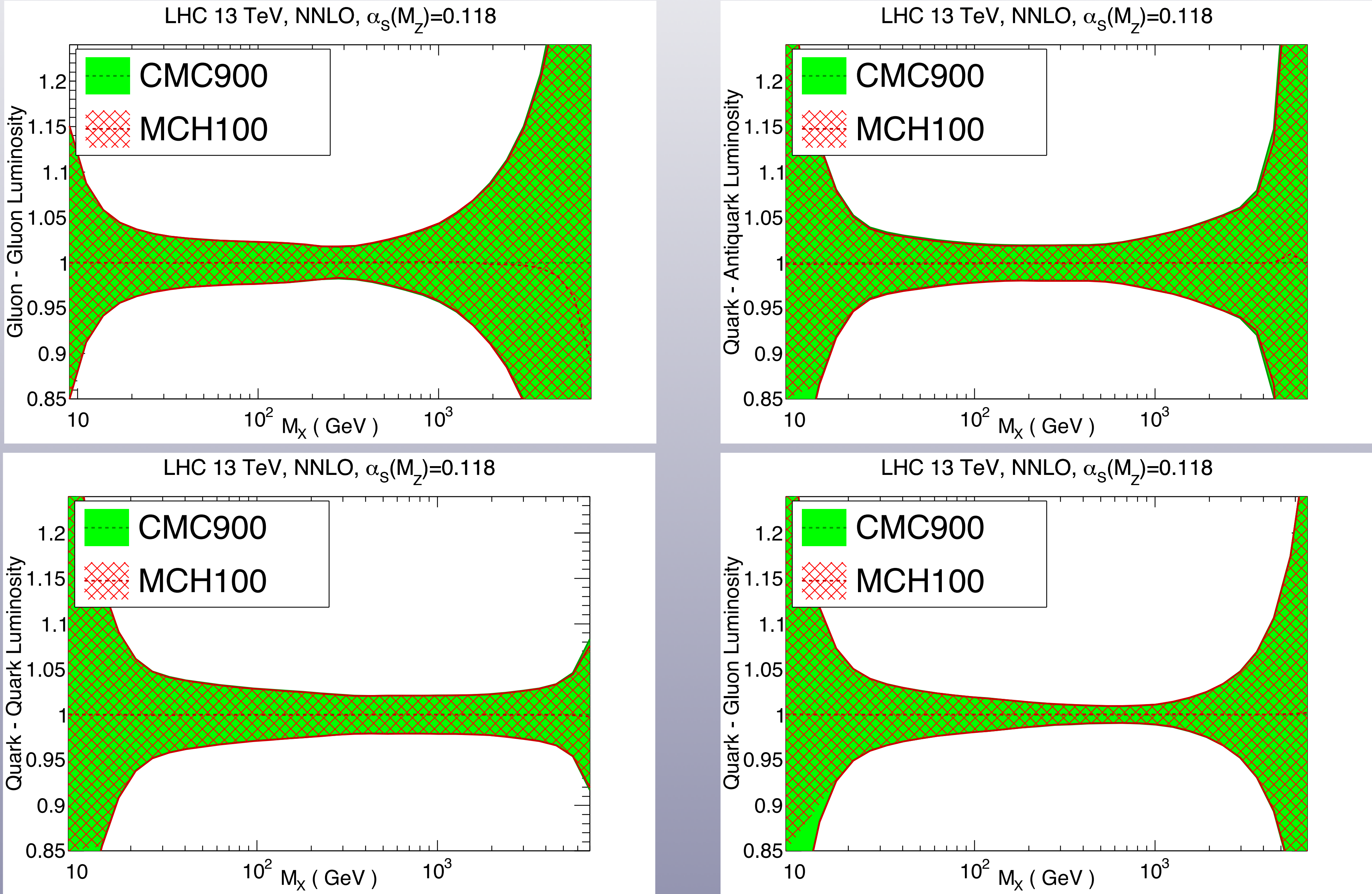






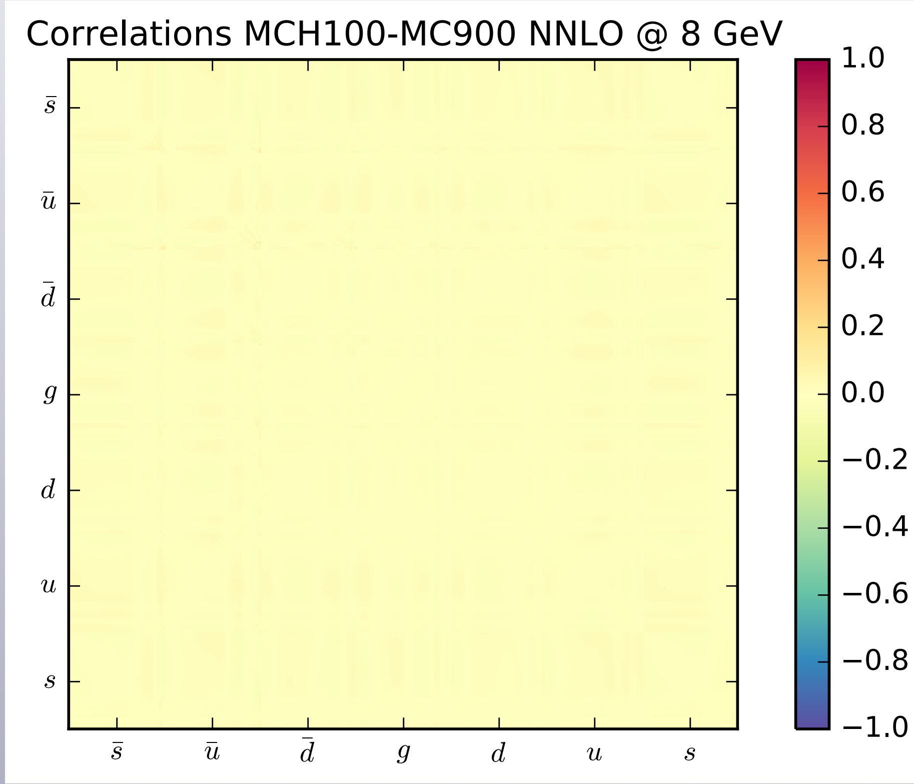
MC2H from MC900

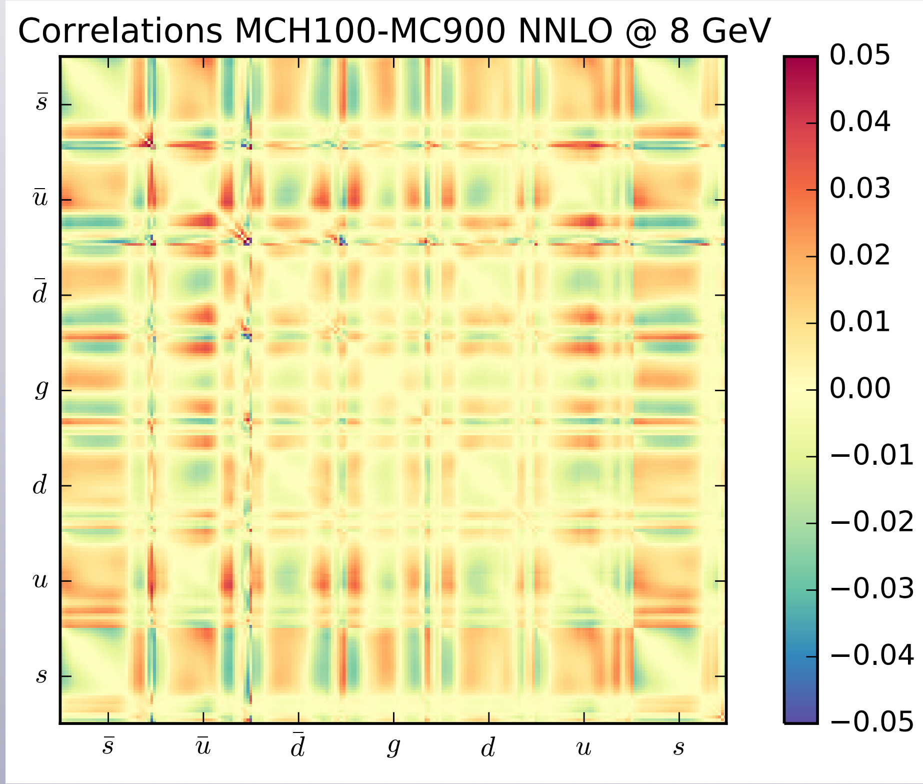
- A Hessian representation of the **MC900 PDF combination** has been constructed using **MC2H(PCA)**
- **Virtually perfect agreemen**t obtained for PDFs and luminosities as compared with MC900



Correlation matrix

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





Perfect?

Zooming in ...

Almost!

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

LHAPDF

Status of LHAPDF

LHAPDF evolved from PDFLIB in 2004. Learn from experience, avoid bulky data grids in library: generate evolution on the fly.

Over 10 years, this model fell apart: almost everything as grids, with hard coded evolution arrays. *Huge* memory footprint (2GB!) and correctness issues (especially in multiset mode).

Rewritten 2012-2014: LHAPDF6 rewritten in C++, ∼every design problem solved. [arXiv:1412.7420]

Memory negligible, speed-ups, arbitrary member IDs in PDG scheme, sets now pure data & release decoupled, powerful metadata, ID code management, new universal interpolation functions (including α_S), member is now central object, compatibility (and new) interfaces, and built-in uncertainty calculation.

Latest developments: not much! *The model is working…*

Upcoming features: new Fortran API for arbitrary flavours, composite PDFs for nuclear corrections, + extended errors.

Upcoming new PDFs: PDF4LHC15, as discussed + MMHT14 and PDF4LHC15 fixed flavour sets + HERAPDF 2.0 + nCTEQ15

Summary & outlook

- PDF4LHC procedure standard for computation of PDF uncertainties in *searches*
- But requires several sets, with distinct uncertainty schemes: cumbersome & expensive
- $\Rightarrow$ new proposal: use combined PDFs based on MC replicas of $\sim$compatible standard fits
- Compression to fewer MC replicas or to Hessian as standard: different compressions for different applications
- PDF4LHC15 sets will be released very soon, via LHAPDF6. Built-in uncertainty calculator to be extended, and more new sets coming.