PDF4LHC21

Combination of CT18, MSHT20, NNPDF3.1 global PDF fits for LHC Run III

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On behalf of PDF4LHC21 Combination Group
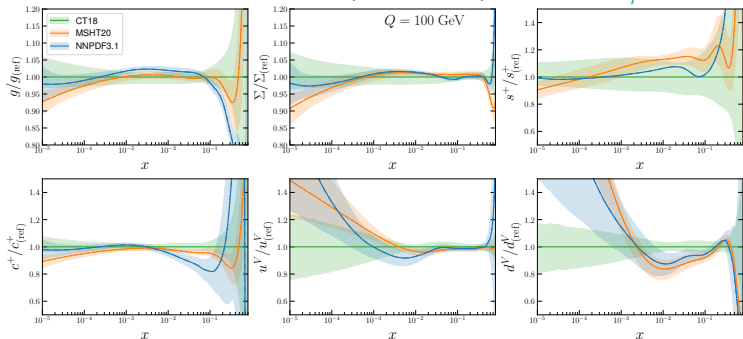
DIS2022

UCL

More information in article: PDF4LHC Working Group arXiv:2203.05506.
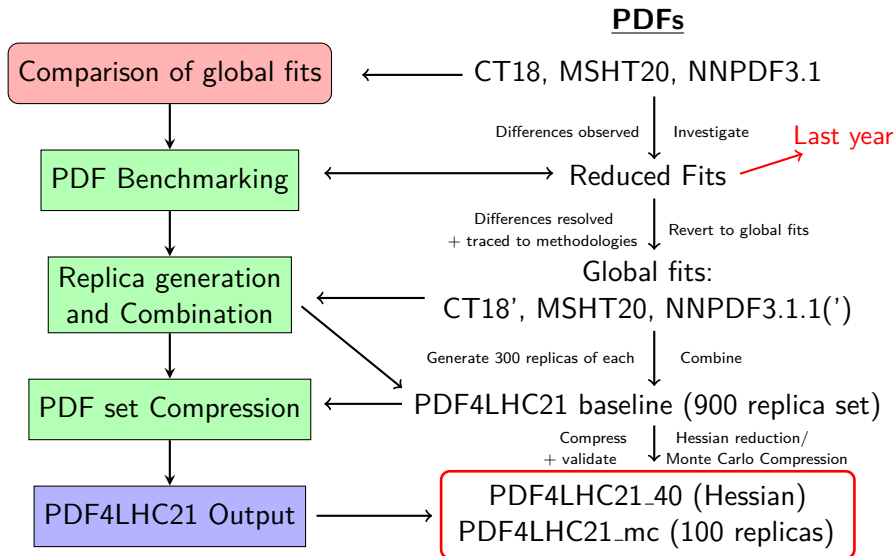
Introduction

Introduction - PDF Landscape

- New data, methodological improvements + theoretical progress $\Rightarrow$ PDFs now known more accurately and precisely than ever before.
- New PDF sets released - CT18, MSHT20, NNPDF3.1/4.0 and others.

- PDF agreement of global fits generally good, however differences exist in some areas.
- Combine PDFs to produce PDF4LHC21 set. Important to understand any differences $\Rightarrow$ extra contribution to combined uncertainty.

PDF4LHC21 Approach

PDFs

Comparison of global fits ⟵ CT18, MSHT20, NNPDF3.1

Differences observed | Investigate → Last year

PDF Benchmarking ⟷ Reduced Fits

Differences resolved + traced to methodologies | Revert to global fits

Global fits:
CT18', MSHT20, NNPDF3.1.1(')

Replica generation and Combination

Generate 300 replicas of each | Combine

PDF set Compression ⟵ PDF4LHC21 baseline (900 replica set)

Compress + validate | Hessian reduction/ Monte Carlo Compression

PDF4LHC21 Output ⟶ PDF4LHC21_40 (Hessian)
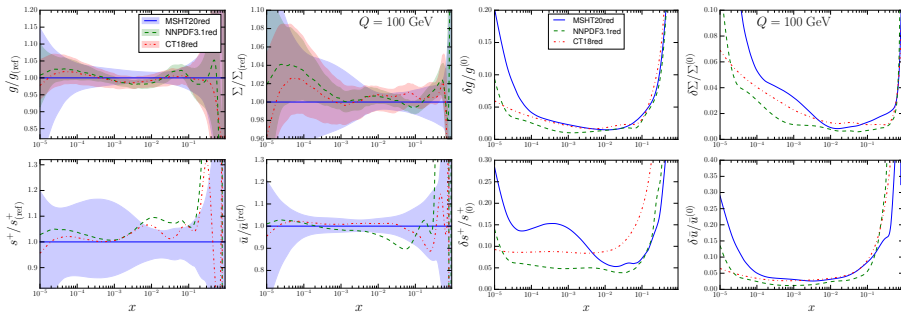PDF4LHC21_mc (100 replicas)

PDF Benchmarking

(reminder)

PDF Benchmarking: Reduced Fits

- Use fits to reduced common datasets and common theory settings.

- Very good agreement within uncertainties, including gluon.
- Similar size uncertainties in data regions, differences outside this, reflecting remaining methodological and other choices.
- Agreement much improved relative to global PDFs.
- Same data and theory settings → consistent PDFs. Smaller remaining differences, e.g. in errors, reflect methodological choices.
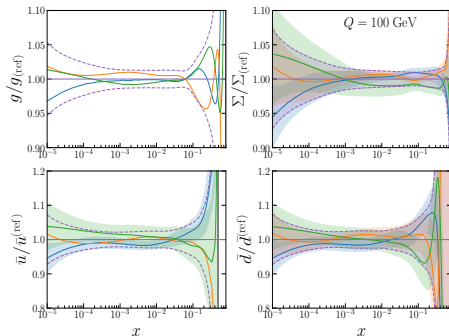
PDF4LHC21 Combination

PDF4LHC21 Combination

- Differences in PDFs reflect genuine freedom in PDF determination from data, theory, methodology $\Rightarrow$ spread in PDFs should therefore contribute to a combined PDF uncertainty.
- Continue with PDF4LHC21 combination of **global PDF fits**, with common $\alpha_S(M_Z^2) = 0.118$ and $m_c, m_b = 1.4, 4.75 \text{GeV}$. $\longrightarrow$ MSHT default values
- Each group determines their *own settings and datasets* for their global PDF fit contribution to combination. Several known, explained differences $\rightarrow$ high x gluon, (fitted) charm, strangeness.
- Combine **300 replicas of CT18', MSHT20, NNPDF3.1'** (aka NNPDF3.1.1) to give *baseline PDF4LHC21* set of 900 replicas.
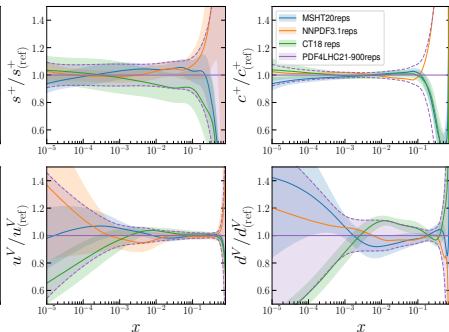
CT18'	MSHT20	NNPDF3.1'
- CT18 global PDF set but with m_c, m_b changed to common values.	- Default, public MSHT20 global PDF set.	- Update of NNPDF3.1. - Common m_c, m_b set. - Global PDF set, version in between NNPDF3.1/4.0.

PDF4LHC21 input *global* PDF sets.

Global Fits Comparison: PDF4LHC21 input replicas

- Good consistency at level of global fits, gluon in good agreement across most of x range. Similar for singlet, $\bar{u}$, $\bar{d}$, u_V.
- See expected differences in high x gluon, in strangeness and charm. Some difference in d_V related to strangeness difference.
- Consistent within *indicative* PDF4LHC21 900 replica baseline combination uncertainties across all flavours and all x.

Global Fits Uncertainty Comparison: PDF4LHC21 input replicas
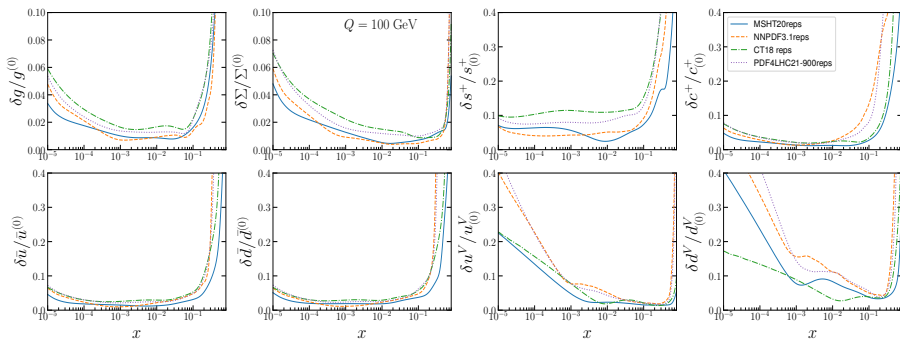
- Good general agreement with differences largely in extreme regions.
- Gluon uncertainty agrees in MSHT and NNPDF, larger in CT.
- Strangeness/Charm uncertainty higher in CT/NNPDF, as expected.
- Compare also with *indicative* PDF4LHC21 900 replica baseline combination uncertainties ⇒ see expected behaviour.

PDF4LHC21
Compression/Reduction

Compression/Reduction:

- Baseline PDF4LHC21 900 replica combined set is impractical $\Rightarrow$ wish to reduce its size for pheno applications, 2 methods:
  - ▶ Monte Carlo (MC) Compression - Extract subset of 900 replicas that reproduces statistical properties of baseline distribution.
  - ▶ Hessian Reduction - Convert 900 replica set to a Hessian set reproducing Gaussian features of baseline distribution.

- Examined and validated effects of compression/reduction on PDFs, PDF properties (mean, variance, correlations, etc) and on cross-sections to ensure faithful reproduction of baseline 900 replica distribution.

- Output is the PDF4LHC21 PDF sets for general usage:
  - ▶ PDF4LHC21_mc - Monte Carlo set with 100 replicas.
  - ▶ PDF4LHC21_40 - Hessian set with 40 eigenvectors.

# Monte Carlo Compression:

- 100 replicas determined to be optimal number to recover properties of full 900 replica distribution.
- Left: PDFs for 50, 100, 150 replicas. Right: Replica distribution 100 replicas vs full 900. Cross-secs and correlations in backup.
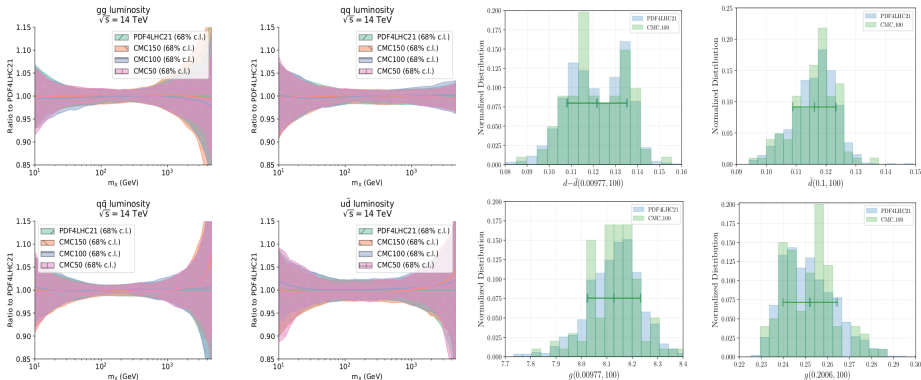
Hessian Reduction:

- META-PDF approach (MP4LHC package) used. Parameterises replicas with common form then produces Hessian matrix of this and removes least constrained eigenvectors.
- $N_{\mathrm{eig}} = 40$ observed to be optimal balance of reducing number of members and representing PDF baseline distribution with comparable accuracy to `PDF4LHC21_mc`.
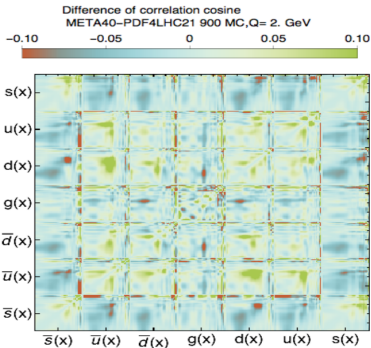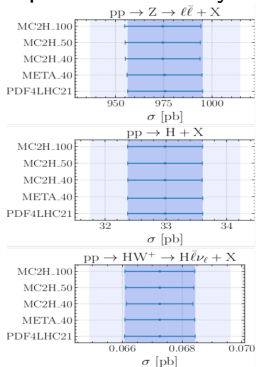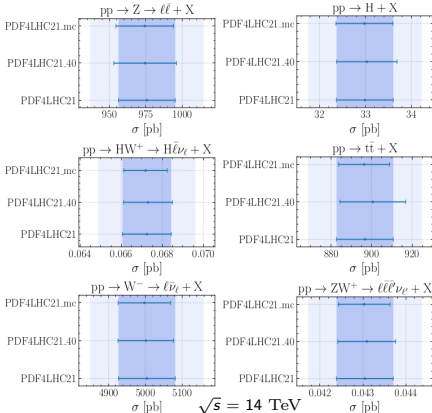
Comparison with baseline 900 set: PDFs

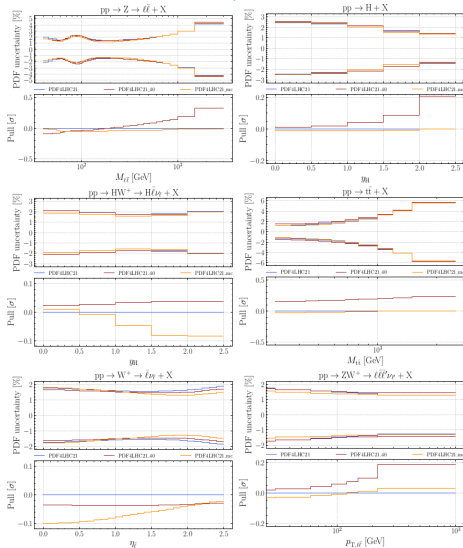- Central values (upper 2 rows) and uncertainties (lower 2 rows):
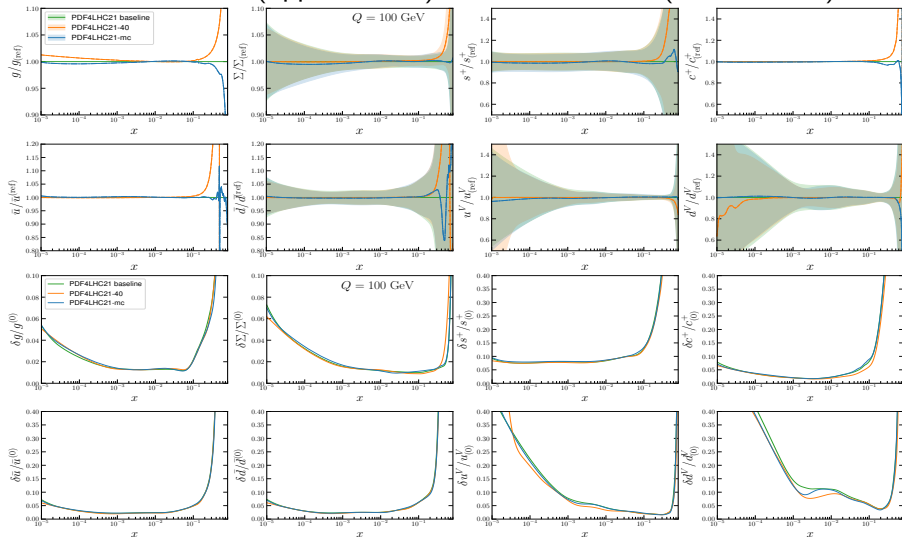
Comparison with baseline 900 set: σ, $d\sigma/d\mathcal{O}$

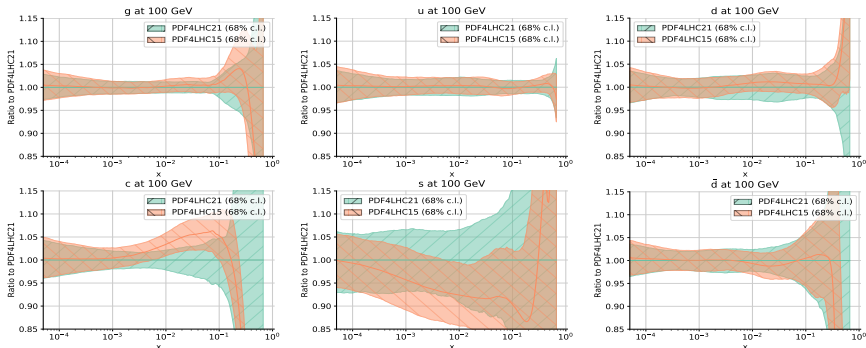- Very good agreement of baseline 900 replica set with MC 100 replica, Hessian 40 member sets.

N.B. Can have small differences for Hessian 40 set as positivity imposed at large x (backup).

PDF4LHC21 Phenomenology

PDF4LHC21 vs PDF4LHC15*: PDF Central Values

*Note this is a comparison of the baseline 900 replica sets.

- Consistent for all flavours and x values.
- Remarkable agreement for $u, d, \bar{d}, \bar{u}$ and g for $x \lesssim 0.1$.
- High x gluon differs due to new data, lowered but within errorbands.
- Strange quark notably raised for $x \gtrsim 10^{-3}$ due to ATLAS high precision W, Z data in NNPDF3.1' and MSHT20.
- Charm raised at (very) high x due to NNPDF3.1' fitted charm.

In PDF4LHC15 all groups had perturbative charm.

PDF4LHC21 vs PDF4LHC15: PDF Uncertainties
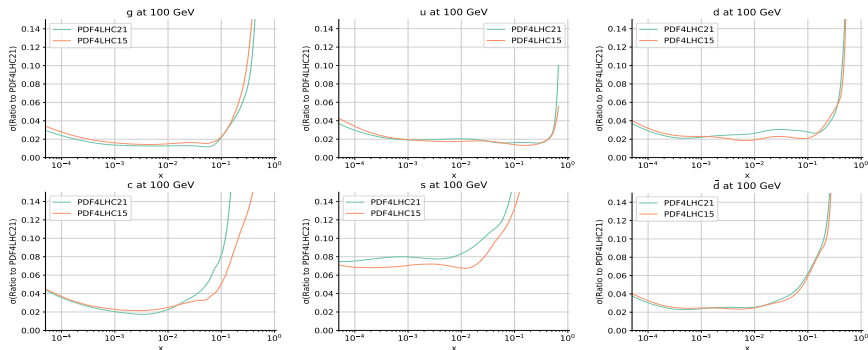
- PDF errorbands similar, reduced in some places, raised in others.
- Gluon errorband reduced across all x even though individual groups disagreement increased because individual groups' errorbands reduced.
- Uncertainties increase where disagreement between three input sets have worsened, e.g. for strangeness or for charm at $x \gtrsim 10^{-2}$.
- s disagreement affects d PDF at $x \sim 10^{-2}$ increasing its uncertainty.

PDF4LHC21 vs PDF4LHC15: PDF Luminosities
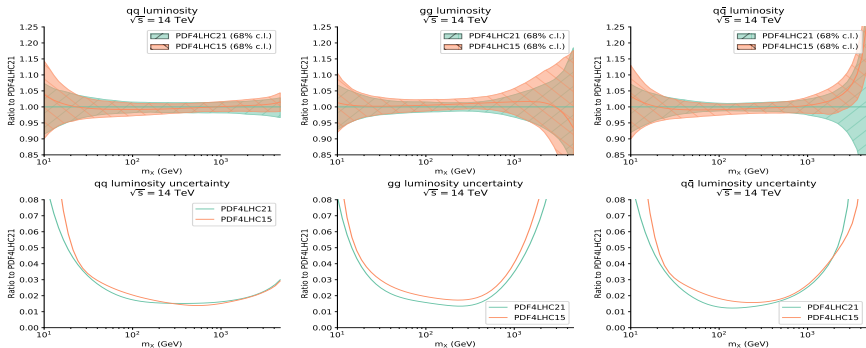
- Central values agree, PDF4LHC15 central value always in errorband.
- qq luminosity particularly stable, as are gg and gq for $m_X < 1$ TeV.
- $q\bar{q}$ luminosity shows greatest change, PDF4LHC21 over(under-)shoots PDF4LHC15 for $m_X \sim 100$ GeV$(m_X \gtrsim 1$ TeV$)$.
- Uncertainties reduced relative to PDF4LHC15, gg luminosity now systematically more precise over all m_X.

PDF4LHC21 vs PDF4LHC15: Inclusive Cross-sections
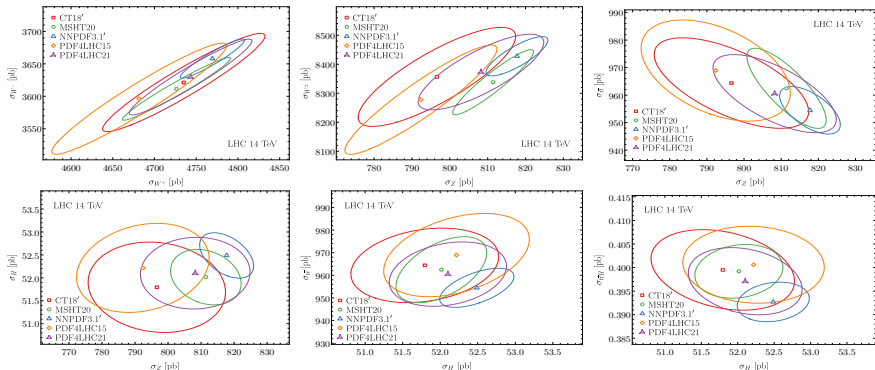
- Shows 1σ error ellipses for pairs of inclusive cross-sections.
- In all cases error ellipses of PDF4LHC21 and PDF4LHC15 overlap with central value of latter (almost) within ellipse of former.
- Error ellipses of PDF4LHC21 systematically reduced in size cf PDF4LHC15 $\Rightarrow$ more precise for LHC cross-sections.
- Also demonstrates correlations of processes.

PDF4LHC21 Sets + Usage

PDF4LHC21 PDF Sets

Already available at https://www.hep.ucl.ac.uk/pdf4lhc/[†], and also on LHAPDF, IDs 93000-93700.

LHAPDF6 grid name	Pert. order	n_f^{max}	ErrorType	N_{mem}	$\alpha_s(m_Z^2)$
PDF4LHC21	NNLO	5	replicas	900	0.118
PDF4LHC21_mc	NNLO	5	replicas	100	0.118
PDF4LHC21_40	NNLO	5	symmhessian	40	0.118
PDF4LHC21_mc_pdfas	NNLO	5	replicas+as	102	mem 0:100 → 0.118 mem 101 → 0.117 mem 102 → 0.119
PDF4LHC21_40_pdfas	NNLO	5	symmhessian+as	42	mem 0:40 → 0.118 mem 41 → 0.117 mem 42 → 0.119
PDF4LHC21_mc_nf4	NNLO	4	replicas	100	0.118
PDF4LHC21_40_nf4	NNLO	4	symmhessian	40	0.118
PDF4LHC21_mc_pdfas_nf4	NNLO	4	replicas+as	102	mem 0:100 → 0.118 mem 101 → 0.117 mem 102 → 0.119
PDF4LHC21_40_pdfas_nf4	NNLO	4	symmhessian+as	42	mem 0:40 → 0.118 mem 41 → 0.117 mem 42 → 0.119

List of PDF4LHC21 output PDF sets available in LHAPDF format.

- Main two for usage will be PDF4LHC21_40 and PDF4LHC21_mc.
- α_S variations also provided so can determine PDF+α_S uncertainty.
- No NLO/LO sets provided, very poor fits observed, use individual groups' PDF sets.

PDF4LHC21_mc vs PDF4LHC21_40:

- Both main PDF4LHC21 sets - `PDF4LHC21_mc`, `PDF4LHC21_40` reflect central values and uncertainties of three input PDF sets.
- Both carefully checked to ensure they reproduce excellently the baseline 900 replica combination, nonetheless small differences exist:

PDF4LHC21_mc	PDF4LHC21_40
➤ **Monte Carlo set** of 101 members (100 replicas + central value)	➤ **Hessian set** of 41 members (40 symmetric eigenvectors + central value)
➤ Reproduces *non-Gaussian features* of combination as well as mean, variances, correlations, etc.	➤ Reproduces *Gaussian features* of combination - i.e. mean, variances, correlations.
➤ Central value and replicas <u>may go negative</u> at large x. Note this occurred also in PDF4LHC15.	➤ <u>Positivity imposed</u>, central value remains positive, although errorband may include negative values.

- Non-Gaussian features seen in slide 11 more relevant in regions where there are disagreements or lack of data.
- Positivity may be useful in certain applications, e.g. event generation.
- For each `PDF4LHC21_40...` set there is also a 'nopos' set.

N.B. See backup slides for more on positivity at large x.

PDF4LHC21 Usage Recommendations

N.B. As well as PDF4LHC21 paper, please cite individual groups' input PDF papers.

- Guidance largely follows PDF4LHC15, examples not exhaustive:

Case	Recommendation	Rationale
Comparison between data and theory for **SM measurements**	**Individual sets** (and use several of them)	If measurements have potential to constrain PDFs then best to compare with individual sets, particularly given high precision of some measurements. Same applies to extraction of precision (SM) parameters.
Searches for **BSM phenomena** or measurements of **SM observables of lower precision**	Use **PDF4LHC21_40** or **PDF4LHC21_mc**	Reduces computational burden and provides estimates of central values/uncertainties that agree with the 3 input PDF sets. May wish to consider extra individual PDF sets if particularly sensitive to PDFs or PDF uncertainties. <u>Hessian set PDF4LHC21_40</u> - *Advantage when speed is desirable* as 40 members, *Positivity* in $x \rightarrow 1$ limit also may be beneficial for some applications. <u>Monte Carlo set PDF4LHC21_100</u> - Reproduces also *non-Gaussian aspects* of baseline 900 replica set, however can go *negative at very large x*. Non-Gaussian features more likely in extrapolation regions so MC set may be beneficial here.
Theoretical Computations	**PDF4LHC21_40 and PDF4LHC21_mc** can be used	PDF4LHC21 combination includes information from all 3 input global fits and combines PDF uncertainty before theoretical calculation is done. Its uncertainty is moderately conservative and encloses the predictions of all 3 groups.

- Key point $\rightarrow$ PDF4LHC21 doesn't preclude use of individual PDF sets.
- Also if large discrepancies are observed $\Rightarrow$ we advise exploring wider range of individual PDF sets.

Conclusions

Summary

- PDF4LHC21 PDF sets now available for use by the community[†].

- Combined 300 replicas of CT18', MSHT20 and NNPDF3.1' global NNLO PDF sets to form combination.

- PDF4LHC21 combination is consistent with all three input PDF sets and with PDF4LHC15.

- PDF4LHC21 uncertainties reflect both those of the 3 groups and offsets in their central values where there are differences.

- Formed compressed sets for general usage → PDF4LHC21_mc, PDF4LHC21_40. Extensively checked and validated at level of both PDF properties and cross-sections.

- PDF4LHC21 has generally mildly reduced uncertainties relative to PDF4LHC15, particularly clear for luminosities and cross-sections.

- This includes reduction in gg luminosity uncertainty over all m_X, including at Higgs mass + systematically smaller error ellipses.

Backup Slides

Introduction - PDF Landscape

- PDFs of paramount importance for interpretation of LHC physics at Run III and beyond.
- Over the now > 6 years since PDF4LHC15, there have been many changes in the PDFs.
- Substantial new data, greater precision, new channels, more differential.
- Many theoretical improvements $\Rightarrow$ full NNLO predictions, methodological improvements (parameterisations, algorithms, etc).
- PDFs now known more accurately and precisely than ever before, but some differences emerging.
- Need to understand differences ahead of a new PDF4LHC21 combination $\Rightarrow$ benchmarking needed.
- We consider 3 global PDF fits, which include much of the recent datasets: MSHT20, CT18, NNPDF3.1.

Work undertaken through many useful discussions, many thanks to all members involved.
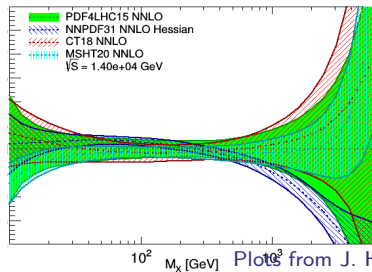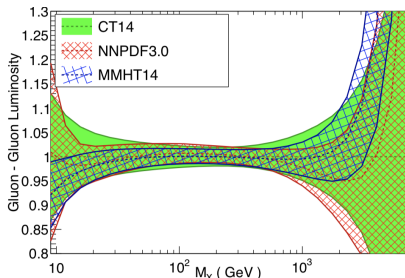
Introduction - Changes in PDFs

Gluon
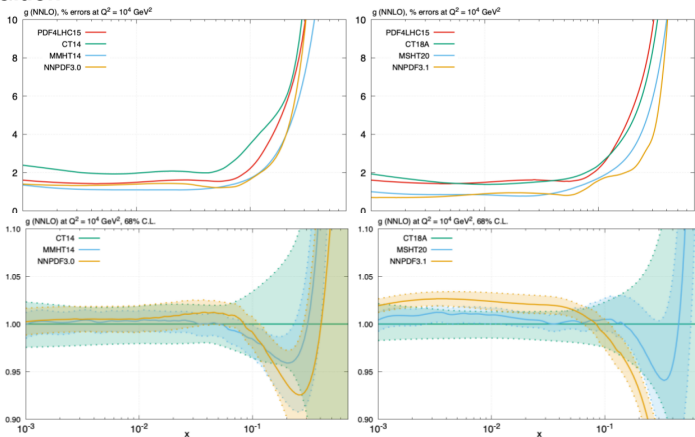
- Reduction in PDF uncertainties seen across all 3 groups.   Plots from L. Harland-Lang
- Central value agreement not as good, some differences emerging.

Note: CT18A shown for ease of comparison, however CT18 is the default set.

Introduction - Changes in PDFs

N.B. Different baseline for ratio in two plots and different colours.

Plots from J. Huston

- Central value spread effects gluon-gluon luminosity.
- If these were to be combined à la PDF4LHC15, there will be some contribution to uncertainty from spread as well as the uncertainties.
- Motivates understanding these differences and their origin ⇒ PDF4LHC21 benchmarking.
- New PDFs CT18, MSHT20, NNPDF3.1 ⇒ need to undertake benchmarking exercise, ahead of new ⇒ PDF4LHC21 combination.

Introduction - New Datasets (MSHT20)

LHCb W, Z data at
high rapidity

CMS W+c

Precision DY data

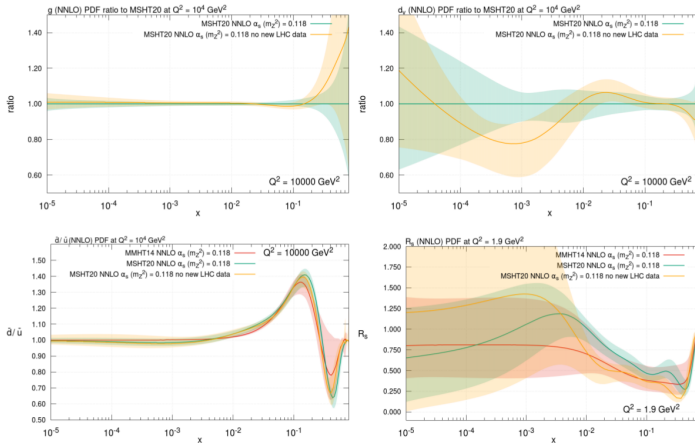$\Rightarrow$ Flavour
Decomposition

LHC Jet, Zp_T, $t\bar{t}$
data

$\Rightarrow$ High x gluon

Data set	Points	NLO χ^2/N_{pts}	NNLO χ^2/N_{pts}
DØ W asymmetry	14	0.94 (2.53)	0.86 (14.7)
$\sigma_{t\bar{t}}$ [93]- [94]	17	1.34 (1.39)	0.85 (0.87)
LHCb 7+8 TeV $W + Z$ [95,96]	67	1.71 (2.35)	1.48 (1.55)
LHCb 8 TeV $Z \to ee$ [97]	17	2.29 (2.89)	1.54 (1.78)
CMS 8 TeV W [98]	22	1.05 (1.79)	0.58 (1.30)
CMS 7 TeV $W + c$ [99]	10	0.82 (0.85)	0.86 (0.84)
ATLAS 7 TeV jets $R = 0.6$ [18]	140	1.62 (1.59)	1.59 (1.68)
ATLAS 7 TeV $W + Z$ [20]	61	5.00 (7.62)	1.91 (5.58)
CMS 7 TeV jets $R = 0.7$ [100]	158	1.27 (1.32)	1.11 (1.17)
ATLAS 8 TeV Z p_T [75]	104	2.26 (2.31)	1.81 (1.59)
CMS 8 TeV jets $R = 0.7$ [101]	174	1.64 (1.73)	1.50 (1.59)
ATLAS 8 TeV $t\bar{t} \to l + j$ sd [102]	25	1.56 (1.50)	1.02 (1.15)
ATLAS 8 TeV $t\bar{t} \to l^+l^-$ sd [103]	5	0.94 (0.82)	0.68 (1.11)
ATLAS 8 TeV high-mass DY [73]	48	1.79 (1.99)	1.18 (1.26)
ATLAS 8 TeV W^+W^- + jets [104]	30	1.13 (1.13)	0.60 (0.57)
CMS 8 TeV $(d\sigma_{t\bar{t}}/dp_{T,t}dy_t)/\sigma_{t\bar{t}}$ [105]	15	2.19 (2.20)	1.50 (1.48)
ATLAS 8 TeV W^+W^- [106]	22	3.85 (13.9)	2.61 (5.25)
CMS 2.76 TeV jets [107]	81	1.53 (1.59)	1.27 (1.39)
CMS 8 TeV $\sigma_{t\bar{t}}/dy_t$ [108]	9	1.43 (1.02)	1.47 (2.14)
ATLAS 8 TeV double differential Z [74]	59	2.67 (3.26)	1.45 (5.16)
Total, LHC data in MSHT20	1328	1.79 (2.18)	1.33 (1.77)
Total, non-LHC data in MSHT20	3035	1.13 (1.18)	1.10 (1.18)
Total, all data	4363	1.33 (1.48)	1.17 (1.36)

- Lots of new information constraining PDFs.   MSHT20, 2012.04684

Effect of new LHC data in MSHT20

Main effect on details of flavour, i.e. d_V shape, increase in strange quark for $0.001 < x < 0.3$ and $\bar{d}, \bar{u}$ details, though also partially from parameterisation change. Decrease in high-x gluon.

*MSHT20 2012.04684.   Slide from R. Thorne

PDF Benchmarking: Aim and Approach

- Desire to understand origin of differences:
  - ▶ Are they due to variations of experimental input, different theory settings, methodologies? Are these equally valid choices?
- Seek to remove as many differences in input/approach as possible:
  - ▶ Common input data - Small subset of datasets ⇒ reduced fits.
  - ▶ Common theory settings wherever possible.
  - ▶ Examine methodological differences in parallel as much as possible.
- Reduced fits offer *ease of comparison at expense of robustness*.
- To benchmark the reduced fits:
  - ▶ Compare PDFs directly to look for areas of difference.
  - ▶ Compare χ^2 to determine particular datasets showing differences.
 - ▶ Compare cross-sections and point-by-point theory predictions.

PDF Benchmarking: Datasets

- Chosen subset of datasets fit by all 3 groups in (almost) the same way, list is surprisingly small! Small reduced fit set.

- Take most conservative cuts applied by any group for consistency.

- Ensure enough datasets and a sufficient variety of dataset types are fit to have some (but incomplete) constraints on all PDF flavours.

- Overall list:
  - ▶ BCDMS proton and deuteron DIS data.
  - ▶ NMC deuteron to proton ratio in DIS.
  - ▶ E866 fixed target Drell-Yan ratio pd/pp data.
  - ▶ NuTeV dimuon cross-sections.
  - ▶ HERA I+II inclusive cross-sections from DIS.
  - ▶ D0 Z rapidity distribution.
  - ▶ ATLAS W, Z 7 TeV rapidity distribution, only Z peak and central.
  - ▶ CMS 7 TeV W asymmetry.
  - ▶ CMS 8 TeV inclusive jet data.
  - ▶ LHCb 7, 8 TeV W, Z rapidity distributions.

PDF Benchmarking: Theory Settings

- Choose common theory settings for simplicity:
  - ▶ Same heavy quark masses ($m_c = 1.4$GeV, $m_b = 4.75$GeV) and strong coupling $\alpha_S(M_Z^2) = 0.118$.
  - ▶ No strangeness asymmetry at input scale: $(s - \bar{s})(Q_0) = 0$.
  - ▶ Perturbative charm.
  - ▶ Positive definite quark distributions (lack of constraint may allow negative fluctuations).
  - ▶ No deuteron or nuclear corrections.
  - ▶ Fixed branching ratio for charm hadrons to muons.
  - ▶ NNLO corrections for dimuon data.

- <u>Note</u>: These are not the chosen settings for any group, but rather are a compromise to the least common denominator. Relevant for benchmarking but *we would not recommend them for a global fit*.

# Reduced Fits: CT18 reduced fit vs CT18A global fit
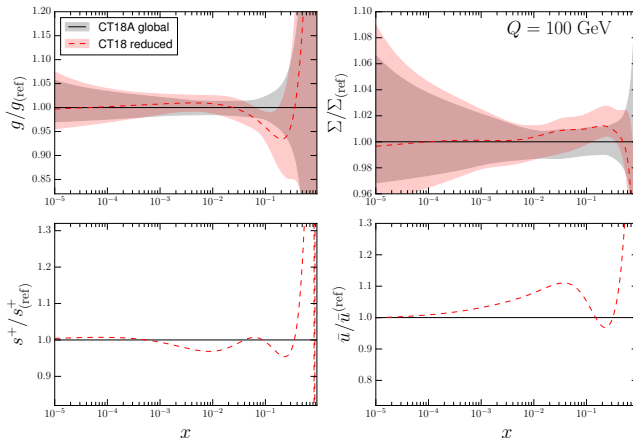
- Good compatibility with change in high x gluon shape and some increase in $\bar{u}$. Some changes in flavour decomposition.
- Some increase in *nominal* PDF uncertainties, particularly at low x.

# Reduced Fits: NNPDF reduced fit vs NNPDF3.1 global
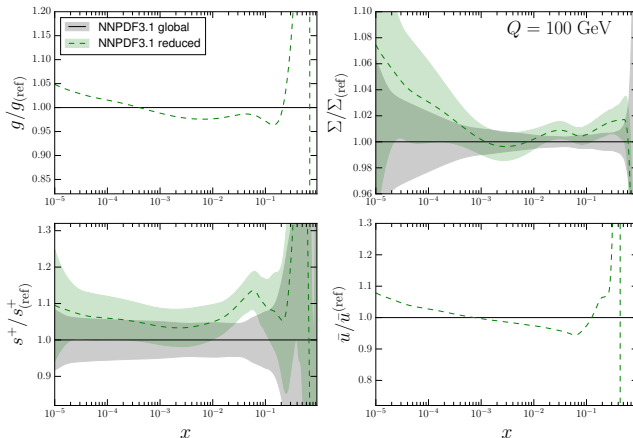
- Good compatibility, changes in strangeness (see later) and change in large x gluon (removal of top data, addition of CMS 8 TeV jet).
- Generally slightly increased uncertainties, particularly at low x.

# Reduced Fits: MSHT reduced fit vs MSHT20 global fit
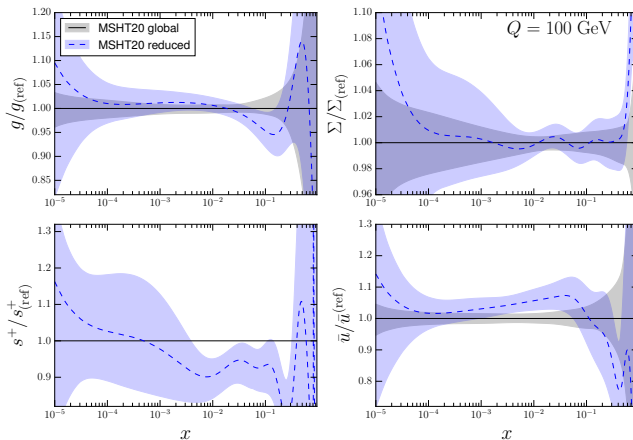
- Good compatibility, changes in strangeness (removal of 8 TeV ATLAS W, Z data), flavour decomposition and large x gluon.
- Marked increase in uncertainties of reduced fit, particularly outside of regions where there are data.

Reduced Fits PDF Comparison
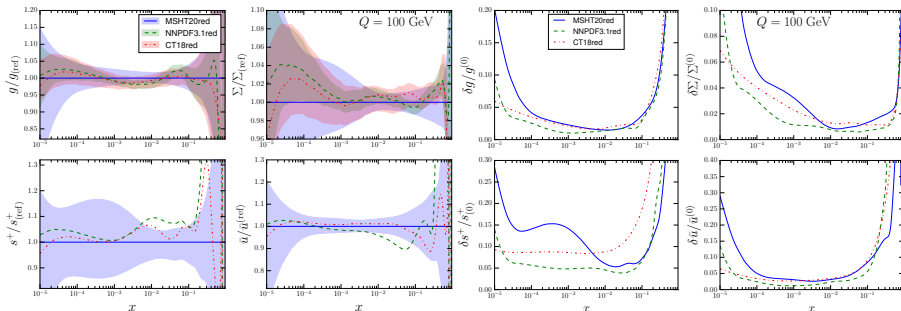
- Very good agreement within uncertainties, including gluon.

- Similar size uncertainties in data regions, differences outside this, parallel study into differences in uncertainty bands ongoing.

- Agreement much improved relative to global PDFs.

- Same data and theory settings → consistent PDFs. Smaller remaining differences, e.g. in errors, reflect methodological choices.

Reduced Fits: Luminosity comparison
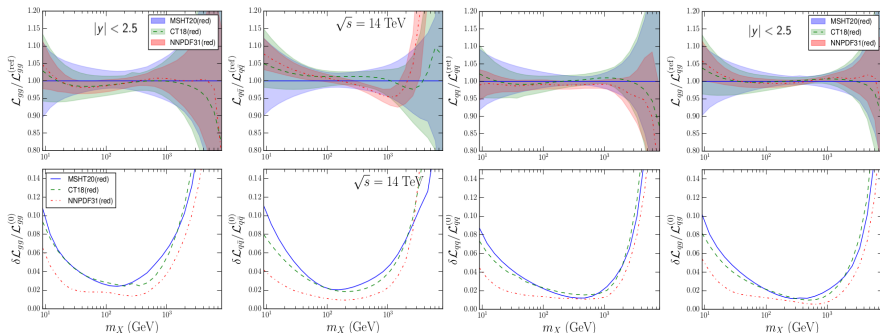
- Very good agreement in luminosities, gg agrees across whole of m_X.
- Differences in uncertainties, particularly at low masses and in gg.
- Same data and theory settings $\rightarrow$ consistent PDFs. Reduced fits well understood, benchmarking successful!
- Benchmarking with reduced fits has shown valid differences between PDFs from data, theory, methodology $\Rightarrow$ should enter combination.

PDF4LHC15 in Predictions Datasets χ^2 Comparison

- First make predictions with PDF4LHC15 PDFs, identifies any differences in theory/data between groups with fixed PDFs.

ID	Expt.	N_{pt}	χ^2/N_{pt} (CT)	χ^2/N_{pt} (MSHT)	χ^2/N_{pt} (NNPDF)
101	BCDMS F_2^p	$329/163^{\dagger\dagger}/325^{\dagger}$	1.35	1.2	1.51
102	BCDMS F_2^d	$246/151^{\dagger\dagger}/244^{\dagger}$	0.97	1.27	1.24
104	NMC F_2^d/F_2^p	$118/117^{\dagger}$	0.92	0.93	0.94
124+125	NuTeV $\nu\mu\mu + \bar{\nu}\mu\mu$	38+33	0.75	0.73	0.84
160	HERAI+II	1120	1.27	1.24	1.74
203	E866 $\sigma_{pd}/(2\sigma_{pp})$	15	0.45	0.54	0.59
245+250	LHCb 7TeV & 8TeV W,Z	29+30	1.5	1.34	1.76
246	LHCb 8TeV $Z \rightarrow ee$	17	1.35	1.65	1.25
248	ATLAS 7TeV W,Z(2016)	34	6.71	7.46	6.51
260	D0 Z rapidity	28	0.61	0.58	0.61
267	CMS 7TeV electron A_{ch}	11	0.45	0.5	0.73
269	ATLAS 7TeV W,Z(2011)	30	1.21	1.23	1.31
545	CMS 8TeV incl. jet	$185/174^{\dagger\dagger}$	1.53	1.89	1.78
Total	N_{pt}	—	2263	1991	2256
Total	χ^2/N_{pt}	—	1.31	1.36	1.62

PDF4LHC21 reduced fit dataset χ^2/N_{pt} with PDF4LHC15 PDF inputs, i.e. before fitting, ††MSHT †NNPDF.

- Similar overall quality of fit for MSHT and CT in χ^2/N, NNPDF significantly larger χ^2/N.
- Differences in some datasets:
  - Difference in NNPDF HERA χ^2 - flavour scheme, disappears in fit.

Table from T. Hobbs

Reduced Fits Datasets χ^2 Comparison

ID	Expt.	N_{pts}	χ^2/N_{pts} (CT)	χ^2/N_{pts} (MSHT)	χ^2/N_{pts} (NNPDF)
101	BCDMS F_2^p	329/163[††]/325[†]	1.06	1.00	1.21
102	BCDMS F_2^d	246/151[††]/244[†]	1.06	0.88	1.10
104	NMC F_2^d/F_2^p	118/117[†]	0.93	0.93	0.90
124+125	NuTeV $\nu\mu\mu + \bar{\nu}\mu\mu$	38+33	0.79	0.83	1.22
160	HERAI+II	1120	1.23	1.20	1.22
203	E866 $\sigma_{pd}/(2\sigma_{pp})$	15	1.24	0.80	0.43
245+250	LHCb 7TeV & 8TeV W,Z	29+30	1.15	1.17	1.44
246	LHCb 8TeV $Z \to ee$	17	1.35	1.43	1.57
248	ATLAS 7TeV W,Z(2016)	34	1.96	1.79	2.33
260	D0 Z rapidity	28	0.56	0.58	0.62
267	CMS 7TeV electron A_{ch}	11	1.47	1.52	0.76
269	ATLAS 7TeV W,Z(2011)	30	1.03	0.93	1.01
545	CMS 8TeV incl. jet	185/174[††]	1.03	1.39	1.30
Total	N_{pts}	—	2263	1991	2256
Total	χ^2/N_{pts}	—	1.14	1.15	1.20

PDF4LHC21 reduced fit dataset χ^2/N_{pts} after fitting, [††]MSHT [†]NNPDF.

Table from T. Hobbs

- Similar overall quality of fit in χ^2/N.
- Differences remaining in some datasets (as expected), investigated in benchmarking (backup slides) ⇒ reflect theory settings and methodological choices.
- Differences remaining in some datasets:
  - ▶ NuTeV agreement improved but difference remains, seen in $s + \bar{s}$.
 - ▶ Some differences in NNPDF fit quality to small datasets.

Flavour Decomposition - Strangeness and NuTeV

- One of the main differences between the first reduced sets was in the flavour decomposition and strangeness.
- NuTeV dimuon data key driver of this, complicated dataset:
  - ▶ Requires knowledge of charm hadron → muon branching ratio (BR).
  - ▶ Non-isoscalar nature of target.
  - ▶ Prefers non-zero strangeness asymmetry.
  - ▶ Acceptance corrections required.

- BR($c \rightarrow \mu$) anti-correlated with strangeness, 3 groups have different values:
  - ▶ NNPDF 0.087 ± 0.005
  - ▶ MSHT 0.092 ± 0.01 variable.
  - ▶ CT 0.099, normalisation uncertainty.

$s + \bar{s}$(NNLO) PDF ratio to MSHT20 at $Q^2 = 10^4$ GeV^2

- Choose same BR fixed at 0.092 ⇒ better strangeness agreement, largely within uncertainties between all 3 groups.
- Also aids reduction in flavour decomposition differences.
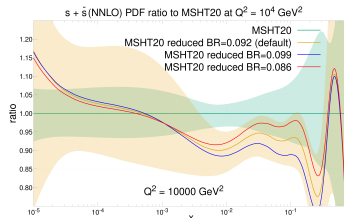
High x gluon

- High x gluon of interest to both reduced and global fits.

- 3 main datasets play a role here - jet data, top data, Zp_T data, different pulls:

- Not straightforward to fit some of them:
  - Difficulties fitting all bins.
  - Possible tensions.
  - Issue of correlated systematics.

- Global fit is a balance between these different pulls.

- MSHT, CT, NNPDF observe differences in the relative importance of these datasets and the quality of their individual fits
  - *does the same hold in reduced fits and can we understand this better in this context?*
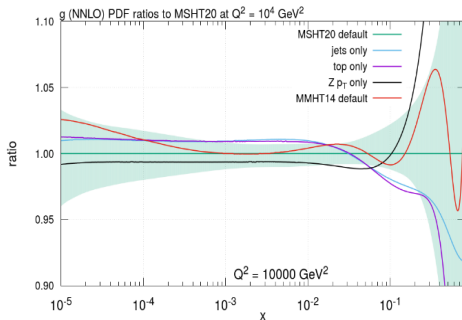
High x gluon - Jet tensions

- Not only tensions between different dataset types at high x, also tensions within dataset types, e.g. between different jet measurements.

- ATLAS 7 TeV jets pulls gluon down at high x, whereas CMS jets (mainly 8 TeV) pull gluon up.

- Global fit is a balance between these different pulls and those of Zp_T, $t\bar{t}$ datasets here.

g (NNLO) PDF ratio to MSHT20 at $Q^2 = 10^4$ GeV^2
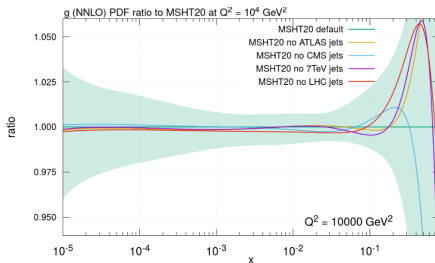
† MSHT20, TC, S. Bailey, L. Harland-Lang, A. Martin, R. Thorne 2012.04684

ATLAS 8 TeV multi-differential $t\bar{t}$ lepton+jets

- Comes differential in 4 variables with correlations - $m_{tt}, y_t, y_{tt}, p_t^T$.
- MSHT*, CT$^+$ difficulties fitting all 4 distributions simultaneously.
- MSHT, CT, ATLAS$^-$ cannot get good fit to y_t or y_{tt} individually.
- NNPDF3.0 however able to fit all 4 distributions well individually†.

Benchmarking:

- Adding to reduced fit, what happens?

Distribution/N	p_t^T/8	y_t/5	y_{tt}/5	m_{tt}/7	Total
MSHT PDF4LHC15 in	3.0	10.6	17.6	4.3	35.5
NNPDF PDF4LHC15 in	3.4	9.5	16.2	4.1	33.2
CT PDF4LHC15 in	3.1	10.1	15.3	4.2	32.7
MSHT fit uncorrelated	3.8	8.4	12.5	6.4	31.2
CT fit uncorrelated	3.4	12.9	17.3	6.1	39.7
NNPDF fit uncorrelated	7.2	3.9	5.1	2.5	18.7
MSHT fit correlated	-	-	-	-	130.6
NNPDF fit correlated	-	-	-	-	122.7
MSHT fit decorrelated	-	-	-	-	35.3

Before Fitting
All groups χ^2 in agreement, same pattern - poor χ^2 for rapidity data.

After Fitting (Uncorrelated)
MSHT and CT see poor fits to rapidities y_t, y_{tt} but NNPDF see good fits to rapidities, as in global fits.

After Fitting (Correlated)
MSHT and NNPDF both see very poor fit to all 4 distributions with correlations, as in global fits.

- Same behaviour as in global fits after fitting....

* S. Bailey & L.Harland-Lang 1909.10541. $^+$ Kadir et al 2003.13740.
† Czakon et al 1611.08609. $^-$ ATL-PHYS-PUB-2018-017.

Benchmarking ATLAS 8 TeV $t\bar{t}$ lepton+jets

- How can we explain these differences in global and reduced fits?
- Global fits have different fit environments - different weights and other datasets included, tensions may affect fit quality for this dataset:
  - ▶ NNPDF3.0 had little jet data - perhaps tensions cause issues in y_t, y_{tt}. NNPDF4.0 sees similar behaviour to other groups.
  - ▶ NNPDF reduced fit up-weights this dataset by putting all data in training (as small dataset) - perhaps up-weighting causes difference.
- Investigate weights and tensions in reduced fit environment:

| Dataset (N)	MSHT reduced (default CMS8j)	NNPDF reduced (default CMS8j)	MSHT reduced (CMS7j)	MSHT reduced (AT7j)	MSHT reduced (no jets)	MSHT reduced (CMS8j, double weight $t\bar{t}$)
χ^2/N	1.15	1.20	1.11	1.17	1.12	1.15
p_t^T (8)	3.8	7.2	4.0	4.6	4.5	4.2
y_t (5)	8.4	4.3	6.4	5.5	5.2	5.8
y_{tt} (5)	12.5	5.7	7.2	5.2	6.6	7.4
m_{tt} (7)	6.4	2.4	6.4	6.4	7.4	6.5
$t\bar{t}$ total	31.2	19.6	24.0	21.6	23.8	23.9

- Weights and tensions with other datasets notably affect fit quality, removing these differences ⇒ similar behaviour can be observed.

Global Fits Specific Comparisons: PDF4LHC21 input replicas

- Central value is average of those of the 3 global fits input.
- Central values agree closely ⇒ uncertainty is average of 3 groups:
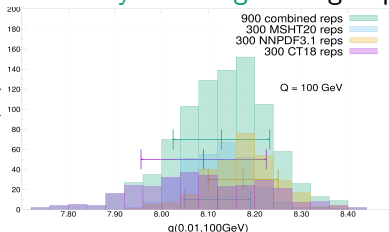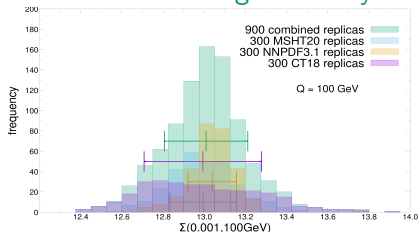
- Central values spread ⇒ uncertainty has component from spread.
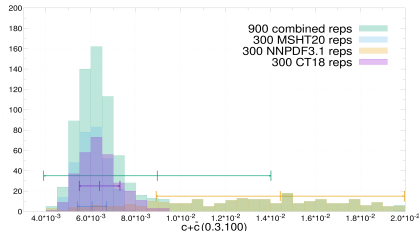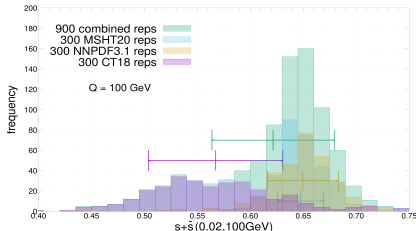
- Combination has expected properties in central values and errors.

Replica generation:

- The PDF4LHC21 baseline combination is a set of 900 replicas, constituted of 300 replicas from CT18', MSHT20 and NNPDF3.1'.

- CT18' and MSHT20 must therefore be transformed into Monte Carlo representations to generate their 300 replicas.

- Existing methods already available - basic idea is to sample probability distribution described by the eigenvectors randomly whilst preserving the central value as the average of the replicas.

- Watt-Thorne Method (MSHT20):

$$\mathcal{F}^{(k)} = \mathcal{F}(S_0) + \frac{1}{2} \sum_{j=1}^{N_{\text{eig}}} \left[\mathcal{F}\left(S_i^{(+)}\right) - \mathcal{F}\left(S_i^{(-)}\right) \right] R_j^{(k)}, \qquad k = 1 \ldots, N_{\text{rep}}$$

- CT (Hou et al) Method (CT18'):

$$X^{(k)} = X(S_0) + \sum_{i=1}^{N_{\text{eig}}} \left(\frac{X\left(S_i^{(+)}\right) - X\left(S_i^{(-)}\right)}{2} R_i^{(k)} + \frac{X\left(S_i^{(+)}\right) + X\left(S_i^{(-)}\right) - 2X(S_0)}{2} \left(R_i^{(k)}\right)^2 \right) + \Delta.$$

Global Fits Luminosities Comparisons:

- Compare global fits* at the level of the parton-parton luminosities:
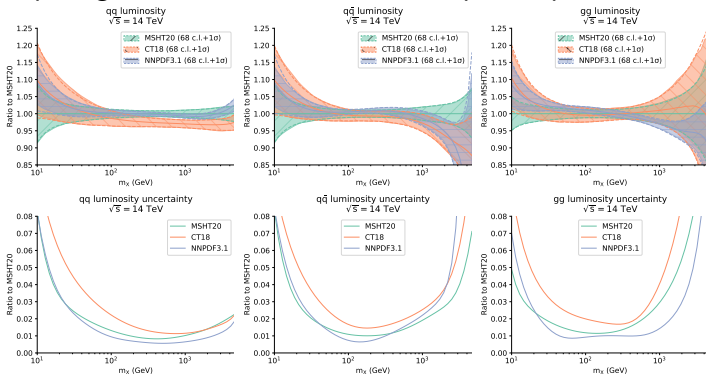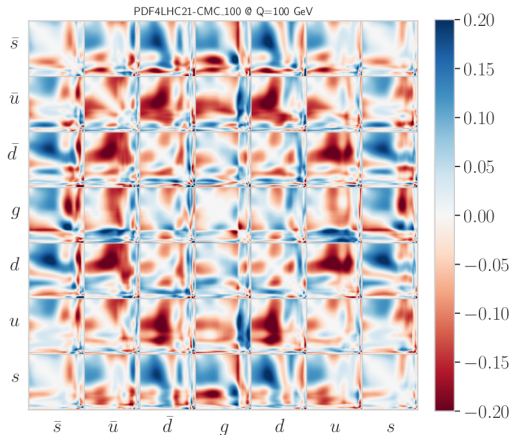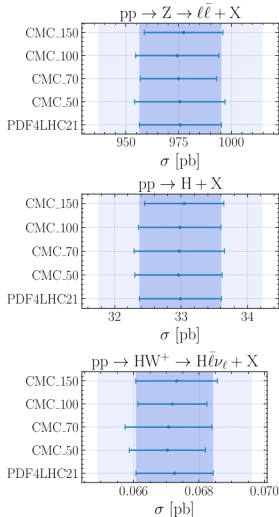

Plots from E. Nocera

- Very good agreement for all m_X for qq, $q\bar{q}$, gg luminosities.
- Exception is CT18 slightly lower for qq for $m_X \gtrsim 100\,GeV$.
- Differences in uncertainties reflect differences in methodology and data used.
  *Global fits have slight modifications in input sets of CT and NNPDF to PDF4LHC21.

Monte Carlo Compression:

Less than 100 MC replicas may distort
uncertainties for key LHC processes
and PDF correlations a little too much

Slide from E. Nocera.

Large x behaviour:

- PDF4LHC21 combination set can have a fraction of replicas at large x that become slightly negative for $g, u, d, s, \bar{u}, \bar{d}, \bar{s}$.
- g and $\bar{u}$ central value is < 0 at large x for $Q = 100\mathrm{GeV}$.
- Results from NNPDF imposing positivity on physical observables but not PDFs.
- Also converting Hessian set into replicas can give some -ve replicas.
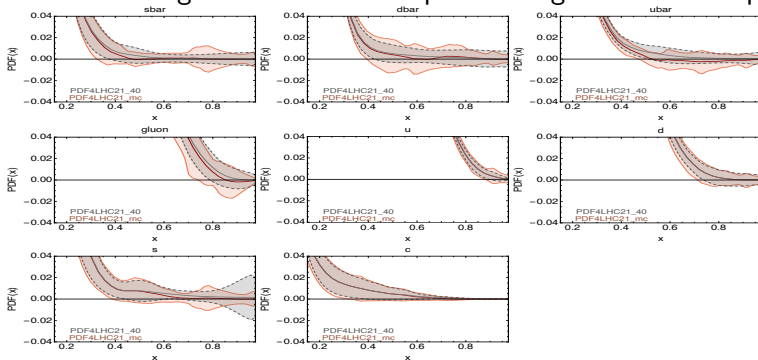
Large x behaviour:

- Same occurred in PDF4LHC15.
- As well as issues with negative PDFs in some applications, it can cause Hessian errorband to be reduced.
- PDF4LHC_40 set has positivity criterion applied to ensure positive central PDFs at large x by stretching parameterisation.
- Results in small difference in central values for (very) large x PDFs and sensitive cross-sections (e.g. sensitive to high x gluon), much smaller than errorbands.
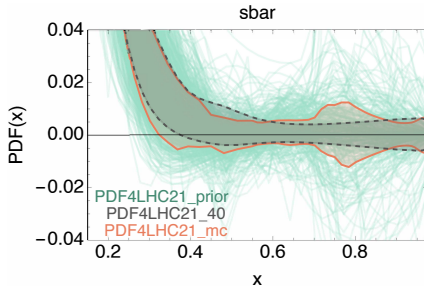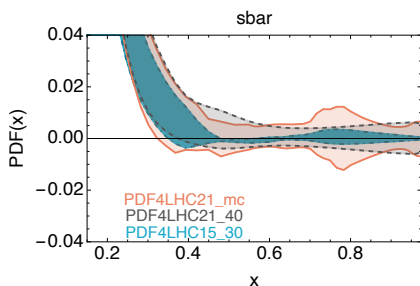
Large x behaviour:

- Small differences in central values for (very) large x PDFs and sensitive cross-sections.

- Resulting differences much smaller than errorbands.

- No positivity imposed in MC 100 replica set.

- Extra Hessian set without positivity is also provided PDF4LHC21_40_nopos.

- Errorband can still extent to negative values (as in MC case), in this case truncate at 0.
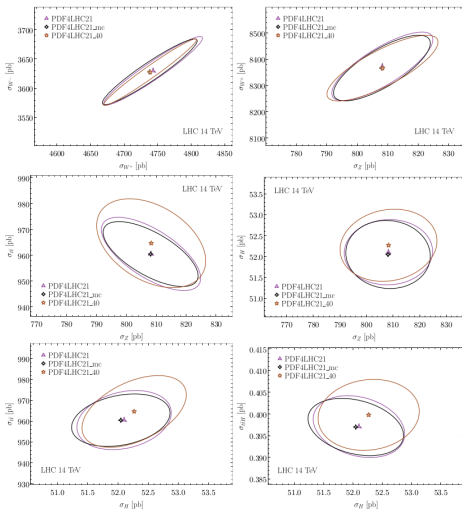
Negative cross-sections:

- As PDFs can go slightly negative at large x, one can obtain negative cross-sections in a few extreme cases.

- For MC replica set individual replicas can give -ve cross-sections.

- For Hessian reduced set (with default positivity) then central value is necessarily positive and gives positive cross-sections but uncertainty may stretch to negative values.

- In these cases simply truncate the lower uncertainty at 0.

- Extra Hessian set without positivity is also provided PDF4LHC21_40_nopos.

- Example case is High mass Drell-Yan:
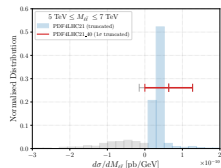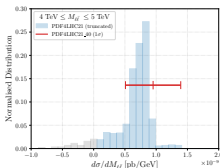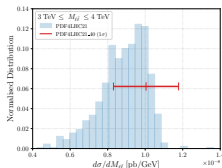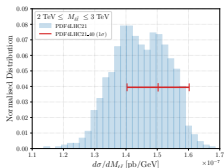
PDF4LHC21 and NNPDF4.0:

- NNPDF4.0 appeared relatively late in the PDF4LHC21 benchmarking/combination effort, therefore now included.
- Instead NNPDF3.1' (aka NNPDF3.1.1) is included which is intermediate between NNPDF3.1 and NNPDF4.0.
- Comparison of NNPDF3.1', NNPDF4.0 and PDF4LHC21 PDFs: