MSHT20aN3LO
- Approximate N3LO PDFs with Theoretical Uncertainties

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DESY

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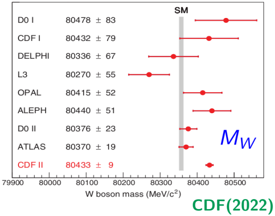
Fermilab LPC Physics Forum Seminar

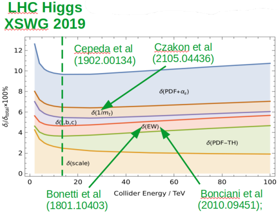
In collaboration with J. McGowan, L.A. Harland-Lang and R.S. Thorne.
More information in article: Eur. Phys. J. C 83 (2023) 3, 185, arXiv:hep-ph/2207.04739.

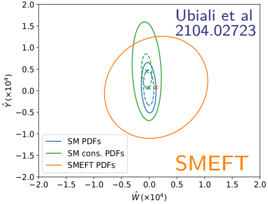
Particle Physics and Parton Distribution Functions

- Experiments are becoming ever more precise. LHC will measure several important processes at percent-level, e.g. Drell-Yan, Higgs.
- Key goal in the next few years is improving accuracy and precison of theoretical predictions, including percent-level theoretical predictions.
- Parton Distribution Functions (PDFs) are key part of this, whether DIS or hadronic collisions. PDFs provide dominant/large uncertainties for:

1. Precision SM
2. Higgs
3. BSM physics





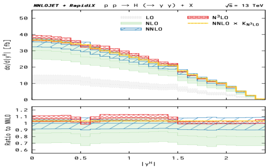


- To improve accuracy and precision, higher orders needed ⇒ N3LO.

Particle Physics and N3LO Progress

- Progress in recent years $\Rightarrow$ some N3LO results now known for σ, e.g.:

1. Higgs - Differential for ggF (y_H, etc) and VBF (p_T^H, y_H), inclusive VH:



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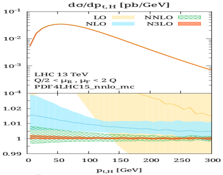
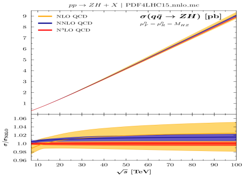
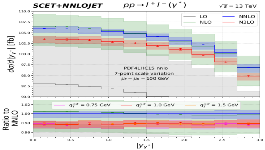


Dreyer et al 1606.00840



Baglio et al 2209.06138

2. DY - NC and CC inclusive, also some differential results appearing:



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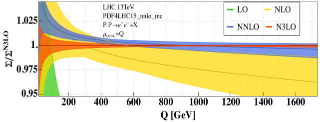
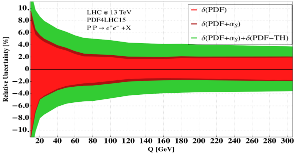




Duhr, Mistelberger 2111.10379

- In all cases here however there are only NNLO PDFs to use.
- PDFs at N3LO are becoming a bottleneck (+ theory uncertainties are needed), but not enough theoretical info. $\Rightarrow$ this talk is a solution . . .

Outline

1. Overview
2. Current knowledge of N3LO
3. Methodology
4. Impacts on fit and PDFs
5. Effect on cross-sections
6. Other results using aN3LO PDFs
7. Usage
8. Conclusions

In collaboration with MSHT group: Shaun Bailey, Lucian Harland-Lang, Alan Martin, Jamie McGowan and Robert Thorne.

Overview

MSHT20 PDFs

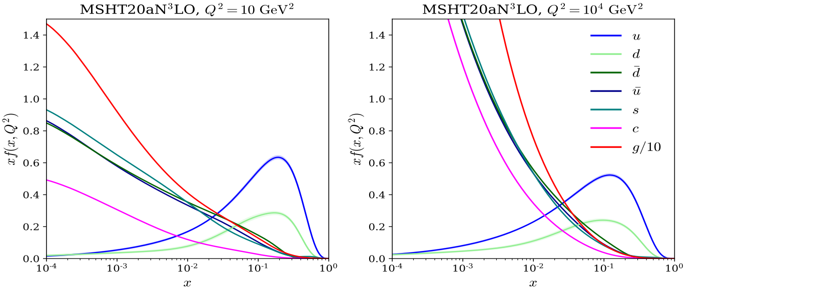
- Several PDF analysis groups - ABM, ATLASPDF, CJ, CT, HERAPDF, JAM, MSHT, NNPDF, etc. $\Rightarrow$ MSHT20 PDFs in this talk!
- MSHT20 - New PDF set for precision LHC era - arXiv:2012.04684 .
- Significant developments on all three fronts:.
  1. Theoretical - Vast majority of processes included have full NNLO QCD theory, with NLO EW where relevant.
  2. Experimental - New datasets, more precise, more differential.
  3. Methodological - Extended parameterisation allows fitting accuracy $< 1\%$ if data allows, better knowledge of central values and uncertainties.
- Global fit $\Rightarrow$ 61 different datasets - DIS structure functions, neutrinos, fixed target, Tevatron, LHC. More than 4000 datapoints included over wide range of (x, Q^2): $10^{-4} \lesssim x \lesssim 0.8$ and $2\ \mathrm{GeV}^2 \lesssim Q^2 \lesssim 10^6\ \mathrm{GeV}^2$.
- Key way to improve PDF precision and accuracy is to include higher orders, i.e. N3LO and theoretical uncertainties $\Rightarrow$ world-first:

MSHT20aN3LO PDFs

PDFs at higher order with theoretical uncertainties

- As PDFs become more precise two issues are more pressing:
  1. Moving to higher orders (N3LO).
  2. Inclusion of theoretical uncertainties.

  ⇒ we can address both in one go! ⇒ **MSHT20aN3LO PDFs.**
- Idea is to include known N3LO effects already into PDFs and to parameterise remaining unknown pieces via nuisance parameters.
- Variation of these remaining unknown N3LO pieces then provides a theoretical uncertainty within an approximate N3LO fit (aN3LO).



Current Knowledge of N3LO

More information in article: Eur. Phys. J. C 83 (2023) 3, 185, arXiv:hep-ph/2207.04739, J. McGowan, TC, L.A. Harland-Lang, R.S. Thorne.

What do we need to know for N3LO PDFs?

- Full N3LO PDFs need all N3LO pieces for both PDFs and included cross-sections to be known, not yet possible as several pieces missing.
- Need to know:
  - Splitting functions - at 4-loop to evolve PDFs in (x, Q^2):

$$P(x, \alpha_s) = \alpha_S P^{(0)}(x) + \alpha_S^2 P^{(1)}(x) + \alpha_S^3 P^{(2)}(x) + \alpha_S^4 P^{(3)}(x) + \ldots$$

  - Transition Matrix Elements - at 3-loop to change number of PDF flavours at heavy quark mass (m_h) thresholds.

$$f_\alpha^{n_f+1}(x, Q^2) = [A_{\alpha i}(Q^2/m_h^2) \otimes f_i^{n_f}(Q^2)](x)$$

  - Coefficient Functions for DIS - at 3-loop to determine structure functions along with transition matrix elements.

$$F_2(x, Q^2) = \sum_{\alpha \in H,q,g; \beta \in q,H} (C_{\beta,\alpha}^{VF,n_f+1} \otimes A_{\alpha i}(Q^2/m_h^2) \otimes f_i^{n_f}(Q^2))$$

  - Hadronic cross-section k-factors - at N3LO.

$$\sigma = \sigma_0 + \sigma_1 + \sigma_2 + \sigma_3 + \ldots \equiv \sigma_{N3LO} + \ldots$$

What do we already know for N3LO PDFs?

- None of these are completely known, but a lot of information already - leading theoretical uncertainty governed by remaining unknown pieces.
- Current Knowledge after a lot of effort (schematic summary):

Theory	Utility	Order required	What's known?
Splitting functions $P_{ab}^{(3)}(x)$	PDF evolution	4-loop	Mellin moments[3−5], leading small-x behaviour[3,6−11], plus some leading large-x in places[3]
Transition matrix elements $A_{ab,H}^{(3)}(x)$	Transitions between number of flavours in PDFs at mass thresholds	3-loop	Mellin moments[12], leading small-x behaviour[13−14], plus some leading large-x in places[14,15].
Coefficient functions (NC DIS) $C_{H,a}^{VF,(3)}$	Combine with PDFs and Transition Matrix Elements to form Structure Functions (NC DIS)	N3LO	Some approximations to FFNS (low Q^2) coefficient functions at α_S^3 (with exact LL pieces at low x, NLL unknown)[16−18], ZM-VFNS (high Q^2) N3LO coefficient functions known exactly[19]. Therefore GM-VFNS not completely known.
Hadronic Cross-sections (K-factors)	Determine cross-sections at N3LO	N3LO	Very little (none in usable form for PDFs)

- Knowledge of lower orders can guide us for remaining unknown pieces.

Methodology

More information in article: Eur. Phys. J. C 83 (2023) 3, 185, arXiv:hep-ph/2207.04739, J. McGowan, TC, L.A. Harland-Lang, R.S. Thorne.

How can we incorporate N3LO knowledge into PDFs?

- Consider usual PDF fit probability:

Theory — Data — Hessian matrix - contains uncorrelated (s_k) and correlated uncertainties (β_k)

$$P(T|D) \propto \exp(-\chi^2) \propto \exp\left(-\frac{1}{2}(T-D)^T H_0 (T-D)\right)$$

$$\propto \exp\left(-\frac{1}{2}\sum_{k=1}^{N_{pt}} \frac{1}{s_k^2}\left(D_k - T_k - \sum_{\alpha=1}^{N_{corr}} \beta_{k,\alpha}\lambda_\alpha\right)^2 + \sum_{\alpha=1}^{N_{corr}} {\lambda_\alpha}^2\right)$$

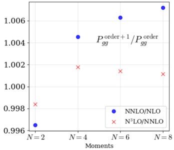
Experimental Nuisance parameters

- Include known N3LO pieces (tu) + parameterise remaining unknown pieces ⇒ theory nuisance parameters (θ').
- Now theory $T' = T + tu + (\theta - t)u = T_0' + \theta' u$, i.e. use known info. to shift theory to N3LO central value then allow to vary by θ'.
- Assign θ' a Gaussian prior probability $P(\theta')$, standard deviation $\sigma_{\theta'}$:

$$P(\theta') = \frac{1}{\sqrt{2}\pi\sigma_{\theta'}} \exp\left(-\theta'^2/2\sigma_{\theta'}^2\right)$$

- Key questions:
  1. How do we determine the priors? - From known info. and lower orders.
  2. Where do we include the theory nuisance parameters? - Next few slides.

Splitting Functions



- Reminder - needed for PDF evolution, we know:
  - Even low-integer N Mellin Moments (4-8) - constrain intermediate and high x via $\int_0^1 dx\, x^{N-1} P(x)$.
  - Form at low x from resummation - LL log coefficients. (For $P_{gg}^{(3)}$ also NLL known)
- How do we incorporate this information?
  - Mellin moments provide constraints - parameterise $P_{ab}^{(3)}(x)$ with functions $f_{1,\ldots,k}$ where $k =$ No. of known moments.

    E.g. $P_{qg}^{(3)}(x)$ (k=4): Try different functions for each f_i, include in uncertainty.

    Lower x ⟶ $f_1(x) = \frac{1}{x}$ or $\ln^4 x$ or $\ln^3 x$ or $\ln^2 x$,

    Intermediate x ⟶ $f_2(x) = \ln x$,

    $f_3(x) = 1$ or x or x^2,

    Higher x ⟶ $f_4(x) = \ln^4(1-x)$ or $\ln^3(1-x)$ or $\ln^2(1-x)$ or $\ln(1-x)$,
  - Exact information included in $f_e(x, \rho_{ab})$ - LL terms at low x included, coefficient of low x NLL is variational (theory nuisance) parameter ρ_{ab}.

$$f_e(x, \rho_{qg}) = \frac{C_A^3}{3\pi^4}\left(\frac{82}{81} + 2\zeta_3\right)\frac{1}{2}\frac{\ln^2(1/x)}{x} + \rho_{qg}\frac{\ln 1/x}{x}$$

⇒ 1 Theory Nuisance Parameter per Splitting Function - 5 total from here.

Splitting Functions

- So overall:

$$P^{(3)}_{ab}(x) = \sum_{i=1}^{k} A_i f_i(x) + f_e(x, \rho_{ab})$$

- A_i coefficients constrained by Mellin moments, with exact information included and ρ_{ab} coefficient of NLL varied to produce uncertainty:

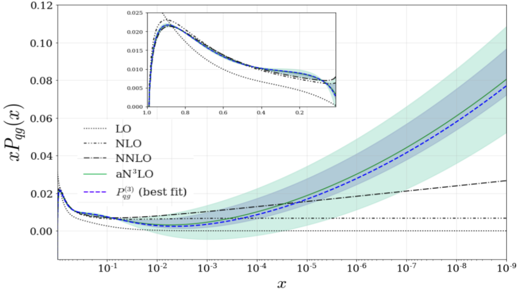
$$P^{(3)}_{qg}(x) = A_1 \ln^2 x + A_2 \ln x + A_3 x^2 + A_4 \ln(1-x) + \frac{C_A^3}{3\pi^4}\left(\frac{82}{81} + 2\zeta_3\right)\frac{1}{2}\frac{\ln^2(1/x)}{x} + \rho_{qg}\frac{\ln 1/x}{x}$$

- Set ρ_{ab} prior variation by requiring:
  1. Low x - Full function and small x description not in significant tension.
  2. High x - N3LO correction small and follows trend of NNLO at large x.
  3. Include effect of different $f_{1,\ldots,k}$ for Mellin moment constraints.

- Some subjectivity in precise range, but no more than in scale variation.
- Results checked to not depend sensitively on the prior chosen.
- Similar approaches were used at NLO before full NNLO known and matched eventual full NNLO result well[20,21,22,23] (e.g. by MRST).

Splitting Functions

- Overall result for $P_{qg}^{(3)}$:

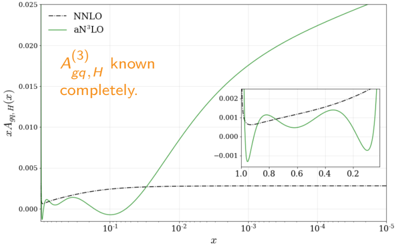


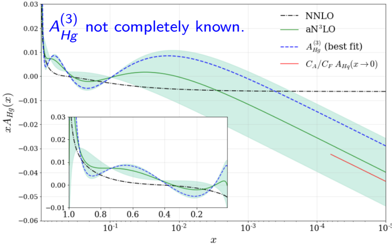
- Green Curve - central result of prior, not centred on NNLO.
- Blue Dashed - our best fit aN3LO, about which we produce uncertainties.
- Largest differences exist at low x relative to NNLO, more divergent pieces gained at N3LO.
- Differences relative to NNLO also at intermediate and high x, due to moment information.

Transition Matrix Elements

- Reminder - needed to transition between number of flavours of PDFs at heavy quark masses, enter also structure functions. We know:
  - Several transition matrix elements known completely - $A_{Hq}^{PS,(3)}$, $A_{gq,H}^{(3)}$, need to be approximated (without uncertainty) due to complex form.
  - Even low-integer N Mellin Moments (4-8) - constrain intermediate and high x via $\int_0^1 dx\, x^{N-1} P(x)$.
  - Form at low x, in some case low and high x limits.
- Deal with as for Splitting functions - for $A_{Hg}^{(3)}$, $A_{qq,H}^{NS,(3)}$, $A_{gg,H}^{(3)}$

$\Rightarrow$ 1 nuisance parameter each - 3 in total from here a_{Hg}, $a_{qq,H}^{NS}$, $a_{gg,H}$.





DIS Coefficient Functions

- Needed to produce N3LO Structure Functions, structure functions form large part of non-LHC data in PDF fits. We know:
  - Light flavour coefficient functions known, just need heavy flavour.
  - Expressions for heavy flavour in high and low Q^2 limits:
    1. Zero Mass ($Q^2 \to \infty$) case (ZM-VFNS) known exactly.
    2. Massive case $Q^2 \leq m_H^2$ (FFNS) approximations known.
- Need to interpolate to generate full General-Mass Variable Flavour Number Scheme (GM-VFNS) prediction for all Q^2.
- Include Transition Matrix Elements at aN3LO (last slide) so full cancellation of PDF discontinuties in the structure functions.
- Therefore some DIS coefficient functions inherit some uncertainty bands from these, e.g. $C_{H,g}^{VF,(3)}$ from $A_{Hg}^{(3)}$:

$$C_{H,g}^{VF,(3)} = C_{H,g}^{FF,(3)} - C_{H,g}^{VF,(2)} \otimes A_{gg,H}^{(1)} - C_{H,H}^{VF,NS+PS,(2)} \otimes A_{Hg}^{(1)} - C_{H,g}^{VF,(1)} \otimes A_{gg,H}^{(2)} - C_{H,H}^{VF,(1)} \otimes A_{Hg}^{(2)} - C_{H,H}^{VF,(0)} \otimes A_{Hg}^{(3)}$$

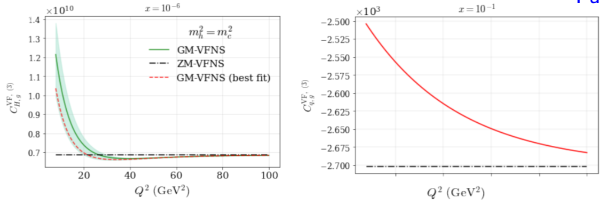
DIS Coefficient Functions

$$C^{VF,(3)}_{H,g} = C^{FF,(3)}_{H,g} - C^{VF,(2)}_{H,g} \otimes A^{(1)}_{gg,H} - C^{VF,NS+PS,(2)}_{H,H} \otimes A^{(1)}_{Hg} - C^{VF,(1)}_{H,g} \otimes A^{(2)}_{gg,H} - C^{VF,(1)}_{H,H} \otimes A^{(2)}_{Hg} - C^{VF,(0)}_{H,H} \otimes A^{(3)}_{Hg}$$

- Approximations to low-Q^2 FFNS coefficient functions $C_{H,\{q,g\}}$ include known LL small x terms and mass threshold info, but unknown NLL small x piece $\Rightarrow$ introduce theory nuisance parameters c_q^{NLL} and c_g^{NLL}:

$$C^{(3),NLL}_{H,i}(Q^2 \to 0) \propto c_i^{NLL}\left[-4\frac{1}{x} + c_i^{LL}\frac{\ln 1/x}{x}\right], \text{ for } i = q, g.$$

$\Rightarrow$ 2 Theory Nuisance Parameters from here.



- $C^{VF,(3)}_{Hq}$ and $C^{VF,(3)}_{Hg}$ have uncertainties from c_q^{NLL} and c_g^{NLL} parameters, $C^{VF,(3)}_{Hg}$ and $C^{VF,(3)}_{qq,NS}$ inherit uncertainty from $A^{(3)}_{Hg}$ and $A^{(3)}_{qq,NS}$.

Hadronic K-factors

- N3LO calculations becoming available but not yet for PDF fits:
  - Higgs - ggF, VBF and VH [24,25,26,27] - doesn't go in PDFs.
  - Drell-Yan - Inclusive and some differential calculations [28,29,30,31] - not yet for relevant fiducial cross-sections or in form usable for PDFs.
  - Top (aN3LO) - soft gluon resummation approximation[32].
- Overall, much less known than for other N3LO PDF fit ingredients.
- Parameterise N3LO k-factor as combination of NLO and NNLO k-factors, a_1, a_2 coeffs incorporating MHOUs into PDF uncertainties:

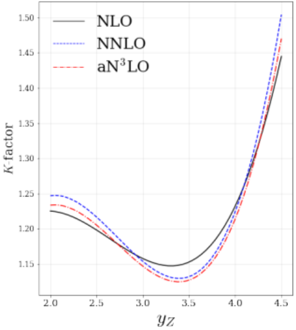
$$K^{N3LO/LO} = K^{NNLO/LO}(1 + a_1 \mathcal{N}^2 \alpha_S^2 (K^{NLO/LO} - 1) + a_2 \mathcal{N} \alpha_S (K^{NNLO/LO} - 1))$$

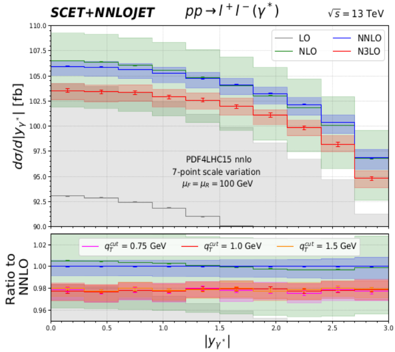
- Default prior is $a_1, a_2 = 0$, i.e. no N3LO correction.
- Categorise all hadronic processes into 5 types - jets (or dijets), Drell-Yan, top, vector boson p_T/jets, and dimuon.
- 2 theory nuisance parameters each ⇒ 10 theoretical parameters added.

Hadronic K-factors - Drell-Yan

1. **Drell-Yan**

- Fit prefers a $\approx 1\%$ decrease in the N3LO k-factors relative to NNLO.
- Improved perturbative convergence with aN3LO PDFs.
- In qualitative agreement with recent N3LO results for Neutral Current DY (which used NNLO PDFs)[30].

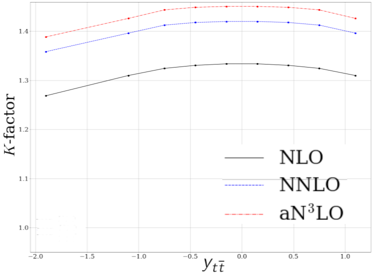


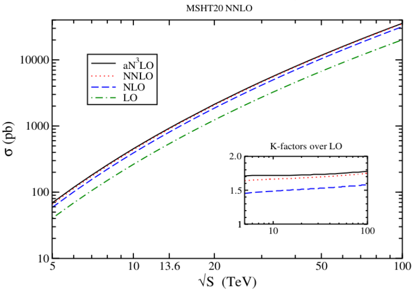


Hadronic K-factors - Top

2 Top

- Fit prefers a ≈ 4% increase in the aN3LO k-factors relative to NNLO.
- Improved perturbative convergence with aN3LO PDFs.
- Consistent with recent approximate N3LO result[32].





Theory Nuisance Parameter Summary

- So in total, we add 20 added theory nuisance parameters, on top of 51 central PDF parameters (which give 32 PDF uncertainty parameters).
- Now have 52 eigenvectors (32 as before + 20 new theory).

Origin	Parameters	Number of Added Parameters
Splitting Functions - $P_{qg}^{(3)}, P_{qq}^{NS,(3)}, P_{qq}^{PS,(3)}, P_{gq}^{(3)}, P_{gg}^{(3)}$	$\rho_{qg}, \rho_{qq}^{NS}, \rho_{qq}^{PS}, \rho_{gq}, \rho_{gg}$	5
Transition Matrix Elements - $A_{Hg}^{(3)}, A_{qq,H}^{NS,(3)}, A_{gg,H}^{(3)}$	$a_{Hg}, a_{qq,H}^{NS}, a_{gg,H}$	3
DIS Coefficient Functions - $C_{H,q}^{(3),NLL}, C_{H,g}^{(3),NLL}$	c_q^{NLL}, c_g^{NLL}	2
Hadronic K-factors -		
Drell-Yan	DY_{NLO}, DY_{NNLO}	
Top	Top_{NLO}, Top_{NNLO}	
Jets	Jet_{NLO}, Jet_{NNLO}	$5 \times 2 = 10$
p_T Jets	$p_T Jet_{NLO}, p_T Jet_{NNLO}$	
Dimuon	$Dimuon_{NLO}, Dimuon_{NNLO}$	

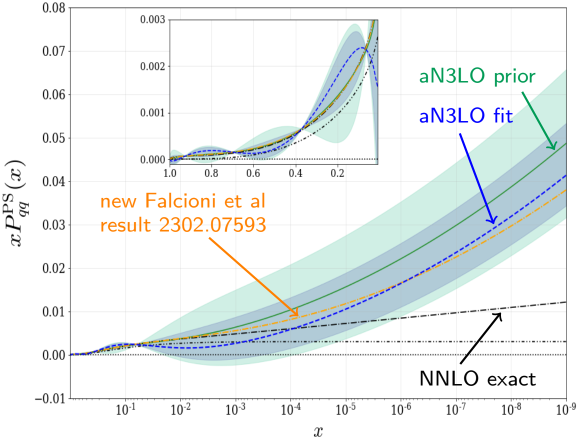
- Using `MSHT20an3lo_as118` eigenvectors as usual naturally incorporates MHOUs at aN3LO into the PDF uncertainties.

N.B. 2 slightly different cases - don't keep (default) or keep correlations of k-factors - "KCorr" set.

Further aN3LO information?:

What else could be added?:

- More information on high-x behaviour from threshold resummations.
- Cusp/virtual anomalous dimensions for P_{gg}, P_{qq}^{NS}. $\Rightarrow$ very high-x.
- N3LO k-factors as they become available for PDFs.
- New info on P_{qq}^{PS}:
  - more moments
  - further low and high x log coefficients and fitting remaining logs.



- Good agreement with our aN3LO result! Much better than NNLO!

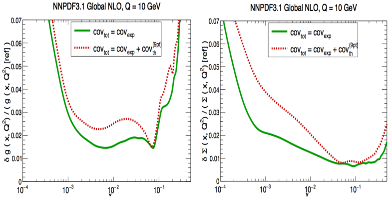
Other approaches for theoretical uncertainties in PDFs?

- Alternative is through scale variations.
- Vary renormalisation and factorisation scales in fit data to give a "theory covariance matrix" to incorporate into PDF uncertainties.
- Can also instead do a joint fit of PDF and scale uncertainties.
- So far both only NLO by NNPDF3.1, marginally increased PDF uncertainties and improved χ^2/N_{pts}.
- Specific issues include:
  1. Need to correlate PDF scale variations with theoretical predictions.
  2. Only varies terms appearing at lower order, not new terms.
  3. Does not incorporate already-known higher order information.

NNPDF 2207.07616

L.A. Harland-Lang, R.S. Thorne 1811.08434

NNPDF, 1905.04311, 1906.10698, 2105.05114



χ^2/N_{dat} in the NNPDF3.1 global fits	C	$C+S^{(9pt)}$	$C+S^{(7pt)}$	$C+S^{(3pt)}$	$C+S^{(9pt)}_{fit}$	$C+S^{(9pt)}_{samp}$
	1.139	1.109	1.129	1.139	1.113	1.220

Impact on fit and PDFs

More information in article: Eur. Phys. J. C 83 (2023) 3, 185, arXiv:hep-ph/2207.04739,
J. McGowan, TC, L.A. Harland-Lang, R.S. Thorne.

Perform aN3LO fit - fit quality:

- Perform aN3LO fit with <u>identical</u> dataset to MSHT20 NNLO PDF fit.
- Overall fit quality (4363 points)

χ^2/N_{pts}	LO	NLO	NNLO	aN3LO
	2.57	1.33	1.17	1.14

Smooth fit improvement with order and amount of improvement reducing with order - as we might hope.

- Improvement in fit quality from NNLO to aN3LO is $\Delta\chi^2 = -154.4$.
  - Much larger than number of parameters (20) introduced.

Dataset type	Total χ^2/N_{pts}	$\Delta\chi^2$ from NNLO	$\Delta\chi^2$ from NNLO (but no N3LO k-factors)
DIS datasets	2580.9/2375	-90.8	-86.2
Drell-Yan datasets	1065.4/864	-12.8	+10.4
Dimuon datasets	125.0/170	-1.2	+0.5
Top datasets	75.1/71	-4.2	-2.5
V p_T/ V + jets datasets	138.0/144	-77.2	-54.7
Inclusive Jets datasets	963.6/739	+21.5	+42.2
Total	4957.2/4363	-154.4	-83.6

- Over half of fit improvement occurs without N3LO k-factors freedom.
- N3LO theory changes not centred on NNLO, rather on known N3LO which can depart significantly, fit clearly preferring known N3LO info.

aN3LO Fit Quality Breakdown:

Dataset type	Total χ^2/N_{pts}	$\Delta\chi^2$ from NNLO	$\Delta\chi^2$ from NNLO (but no N3LO k-factors)
DIS datasets	2580.9/2375	-90.8	-86.2
Drell-Yan datasets	1065.4/864	-12.8	+10.4
Dimuon datasets	125.0/170	-1.2	+0.5
Top datasets	75.1/71	-4.2	-2.5
V p_T/ V + jets datasets	138.0/144	-77.2	-54.7
Inclusive Jets datasets	963.6/739	+21.5	+42.2
Total	4957.2/4363	-154.4	-83.6

- Biggest improvement in DIS datasets, where most N3LO information known and included.
- Drell-Yan, dimuon, top improvements more from N3LO k-factor freedom; DY and top in approximate agreement with recent results.
- V p_T/ V + jets improves significantly, mostly without N3LO k-factors - ATLAS 8 TeV Zp_T large improvement from $\chi^2/N = 1.81$ to 1.04.
- Zp_T constrains high x gluon, it saw similar improvement ($\Delta\chi^2 = -39.2$) at NNLO when HERA data removed - evidence aN3LO removes some tension between small x and high x data.
- Inclusive Jets gets worse - try dijets?

Dijet data:

N.B. This is all Leading Colour, we have looked preliminarily at Full Colour and not found significant PDF changes.

Preliminary!

- Inclusive jet data was the only class of processes where the fit worsened at aN3LO compared to NNLO.
- Dijets may have some advantages here - 3D measurement now possible, non-unitary nature of inclusive jets, etc
- We have also investigated dijets instead:
  - Obtain better fit quality at NNLO and aN3LO than inclusive jets.
  - Generally pull improves Zp_T fit and worsens top slightly.
  - Moreover, dijet fit quality improves further slightly at aN3LO.

Inclusive Jets	N_{pts}	χ^2/N_{pts}		Dijets	N_{pts}	χ^2/N_{pts}	
		NNLO	aN3LO			NNLO	aN3LO
ATLAS 7 TeV jets	140	1.58	1.54	ATLAS 7 TeV dijets	90	1.05	1.12
CMS 7 TeV jets	158	1.11	1.18	CMS 7 TeV dijets	54	1.43	1.39
CMS 8 TeV jets	174	1.50	1.56	CMS 8 TeV dijets	122	1.04	0.83
Total	472	1.39	1.43	Total	266	1.12	1.04

- Impact on PDFs and rest of data similar, particularly at aN3LO.
- N.B. Dijets very poorly fit at NLO (particularly CMS 8 TeV dijets) - need for NNLO.

More info. in backup slides.

Dijet data:

N.B. This is all Leading Colour, we have looked preliminarily at Full Colour and not found significant PDF changes.

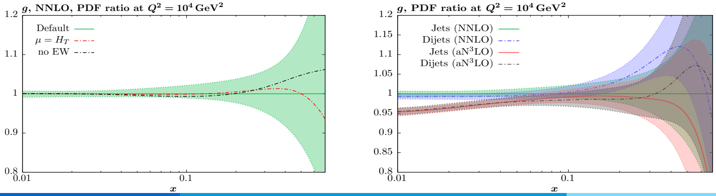
Preliminary!

- Extended study to also consider ATLAS 8 TeV jets.
- Alters gluon such that now inclusive jets also improve NNLO → aN3LO, albeit still significantly less than dijets.

Dataset Type	N_{pts}	NNLO		N3LO	
		Default	No EW	Default	No EW
Total jets	643	1.67	1.57	1.61	1.57
Total dijets	266	1.13	1.37	1.04	1.27

Total inclusive jets/ Total dijets fit qualities at NNLO and aN3LO with/without EW corrections.

- Dijets favours the inclusion of EW corrections (default), whereas inclusive jets disfavours them significantly ⇒ further support for dijets.
- Inclusive jet scale change $p_T^j \to H_T$ has little effect at NNLO/aN3LO.
- Difference in effect of dijets/inclusive jets on gluon is milder at aN3LO:



aN3LO vs NNLO, ATLAS 8 TeV Zp_T data:

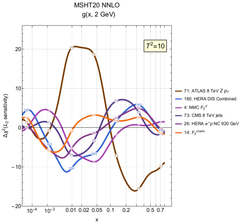
Preliminary!

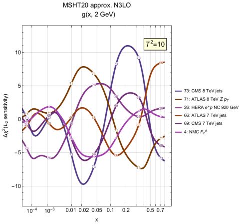
- ATLAS 8 TeV Zp_T data improved substantially in χ^2 at aN3LO :
- Fit different subsections of the data by altering the p_T^{cut}:

Order of fit/p_T^{cut} (GeV)	30 (default)	45	55	65	75	85	105
NNLO	1.86	1.68	1.67	1.42	1.39	1.42	1.21
aN3LO	1.04	0.95	1.01	0.84	0.86	0.87	0.81
N_{pts}	104	88	77	66	55	44	33

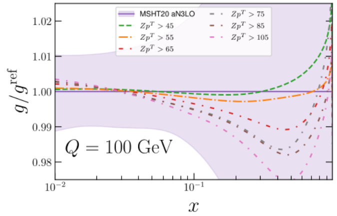
ATLAS 8 TeV Zp_T fit qualities with increasing the lower cut on the p_T^{ll}.

- Fit quality improves slowly as amount of data is reduced. More improvement at NNLO than aN3LO, but NNLO always worse.
- No obvious sign of a particular issue with any p_T region.
- Pulls on gluon NNLO vs aN3LO:





- Pulls with different p_T cut:



aN3LO Theory Nuisance Parameters:

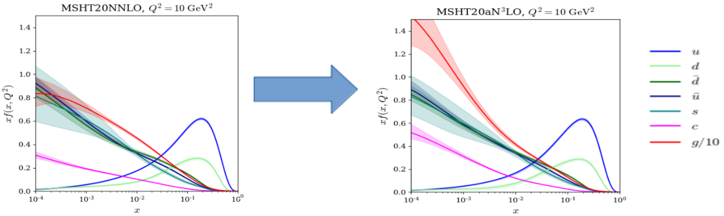
- Examine χ^2 penalties associated with moving theoretical nuisance parameters away from their priors in the aN3LO fit:

Low-Q^2 Coefficient			
$c_q^{\mathrm{NLL}} = -3.868$	0.004	$c_g^{\mathrm{NLL}} = -5.837$	0.844
Transition Matrix Elements			
$a_{Hg} = 12214.000$	0.601	$a_{qq,H}^{\mathrm{NS}} = -64.411$	0.001
$a_{gg,H} = -1951.600$	0.857		
Splitting Functions			
$\rho_{qq}^{NS} = 0.007$	0.000	$\rho_{gq} = -1.784$	0.802
$\rho_{qq}^{PS} = -0.501$	0.186	$\rho_{gg} = 19.245$	3.419
$\rho_{qg} = -1.754$	0.015		
K-factors			
$\mathrm{DY}_{\mathrm{NLO}} = -0.282$	0.080	$\mathrm{DY}_{\mathrm{NNLO}} = 0.079$	0.006
$\mathrm{Top}_{\mathrm{NLO}} = 0.041$	0.002	$\mathrm{Top}_{\mathrm{NNLO}} = 0.651$	0.424
$\mathrm{Jet}_{\mathrm{NLO}} = -0.300$	0.090	$\mathrm{Jet}_{\mathrm{NNLO}} = -0.691$	0.478
$p_T\mathrm{Jets}_{\mathrm{NLO}} = 0.583$	0.339	$p_T\mathrm{Jets}_{\mathrm{NNLO}} = -0.080$	0.006
$\mathrm{Dimuon}_{\mathrm{NLO}} = -0.444$	0.197	$\mathrm{Dimuon}_{\mathrm{NNLO}} = 0.922$	0.850
N^{3}LO Penalty Total	9.201 / 20	Average Penalty	0.460

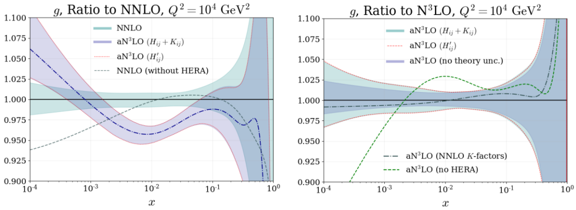
- All but one within prior chosen variation (penalty < 1), many penalties very small - conservative.
- Average penalty across the 20 parameters is 0.460.
- Results checked to not depend sensitively on the prior chosen.
- Fit able to describe data well with only small departures around prior.

aN3LO PDFs:

N.B. Inclusive jets included in default aN3LO fits not dijets.



- Gluon raises significantly at low x - from large logs in splitting functions, not present at NNLO. Reduction at $x \sim 10^{-2}$ due to splitting functions.
- Gluon uncertainty enlarged at low x from splitting functions.



Green is NNLO, baseline for ratio.

Blue dashed is aN3LO central + red lines give uncertainty bands.

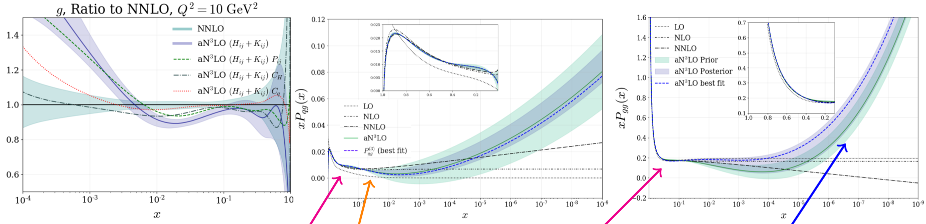
Grey/Green (left/right) dashed is NNLO fit without HERA data.

Dot-dashed (right) line is aN3LO with only NNLO k-factors.

Blue band on right - no theoretical uncertainties included.

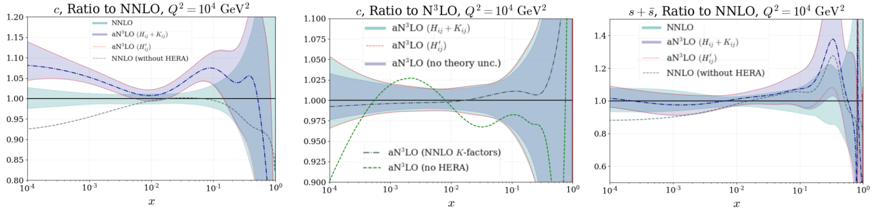
aN3LO PDFs - What causes the changes in the gluon?:

- Around $10^{-2} \lesssim x \lesssim 10^{-1}$ P_{ij}, C_H contribute ≈ equally. Also some C_q.
- At low x P_{ij} dominate, this contains much known N3LO information.



- Known Mellin moments tightly constrain high x splitting functions.
- At intermediate x increased P_{qg} and momentum sum rule affect gluon.
- At small x, LL and NLL (latter for P_{gg}) resummed pieces dominate. Uncertainty band from leading unknown coefficient (NLL or NNLL).
- Most singular NNLO term at small x in P_{gg} $(\alpha_S^3/x \log^2(1/x))$ is 0, so expect new N3LO piece $(\alpha_S^4/x \log^3(1/x))$ to cause significant change!

aN3LO PDFs:



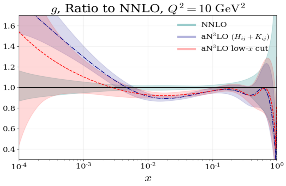
- Heavy quarks - c and b (perturbatively generated) raised due to increase in gluon at lower x and raised A_{Hg} at high x.
- Charm uncertainty enlarged, from both A_{Hg} at high x and gluon.
- Fit with no N3LO k-factors gives very similar PDFs to full aN3LO fit $\Rightarrow$ Effect of approximate N3LO fitted k-factors on PDFs is very mild.
- Increase in $s + \bar{s}$ and light quarks at high x, aN3LO more similar to "no HERA" fit - eased tension, now with enhanced high x quarks.
- Also seen in gluon on previous slides and in other light quarks.

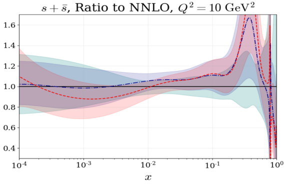
aN3LO PDFs - small x and high x:

- aN3LO fit seems to have reduced tension between small x and high x.
- Reflected in fit qualities - HERA improves by $\Delta\chi^2 =$ -68.4 at aN3LO.
- Effect of removing HERA from aN3LO vs NNLO is reduced for many high x datasets - reduced tension of HERA and high x data at aN3LO.

Datasets	N_{pts}	$\Delta\chi^2$ no HERA vs full		Datasets	N_{pts}	$\Delta\chi^2$ no HERA vs full	
		NNLO	aN3LO			NNLO	aN3LO
BCDMS $\mu p + d$ F_2	314	-7.6	+1.4	CMS 8 TeV jets	174	-1.8	-11.5
NMC $\mu p + d$ F_2	246	-20.6	-24.4	ATLAS 8 TeV Zp_T	104	-39.2	+12.8
DØ W asymmetry	14	-0.8	-2.1	ATLAS 8 TeV W+jets	30	-1.7	-0.8
ATLAS 7 TeV jets	140	+6.5	+1.8	Top total	71	-4.4	+1.4
CMS 7 TeV jets	158	+3.8	+1.0	Total	3042	-61.6	-49.0

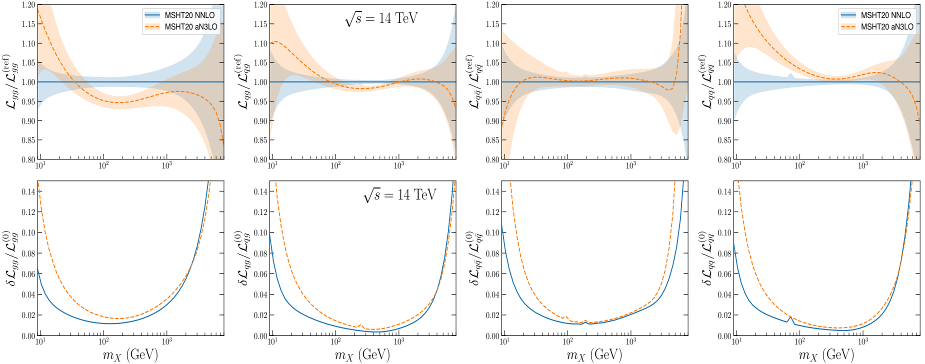
- Check by performing fits with small $x < 10^{-3}$ data removed:





- Small x removal has limited effects on central values at high x.
- Small x uncertainties increase as expected.

aN3LO PDF luminosities:



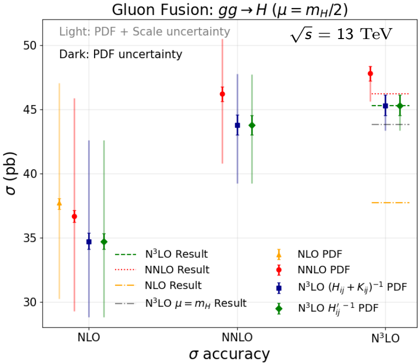
- PDF changes have implications for PDF luminosities for phenomenology.
- *gg* luminosity reduced around 100GeV and increased at 10GeV, *gg* uncertainty grows with inclusion of aN3LO and theoretical uncertainties.
- *qq* luminosity raised at low invariant masses from enhanced charm.
- Luminosity uncertainties enlarged (and more so at lower invariant masses) due to inclusion of aN3LO and PDF theory uncertainties.

Effect on Cross-sections

More information in article: Eur. Phys. J. C 83 (2023) 3, 185, arXiv:hep-ph/2207.04739,
J. McGowan, TC, L.A. Harland-Lang, R.S. Thorne.

Impact on Higgs cross-sections - ggF:

- Consider impact of our aN3LO PDFs on known N3LO Higgs production in gluon fusion[24,25] - shift down due to change in gluon:



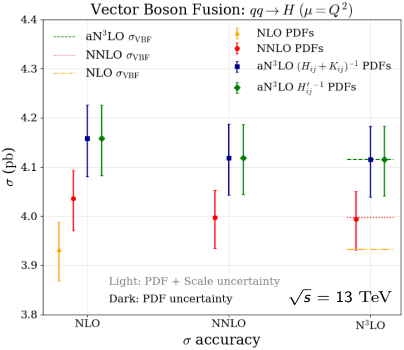
N.B. For scale variations - do μ_R and μ_F at NNLO but only μ_R at aN3LO as PDF uncertainty from MHOs (Missing Higher Orders) already in PDF eigenvectors.

Results obtained using ggHiggs code[36].

- Increase in cross-section at N3LO compensated by reduction in PDFs at aN3LO $\Rightarrow$ important to consider PDF and σ changes together.
- aN3LO result lies within uncertainty band of full NNLO.
- aN3LO PDF uncertainty bands enlarged - inclusion of MHOUs.

Impact on Higgs cross-sections - VBF:

- Consider impact of our aN3LO PDFs on known N3LO Higgs production in vector boson fusion[26]:



N.B. For scale variations - do μ_R and μ_F at NNLO but only μ_R at aN3LO as PDF uncertainty from MHOs already in PDF eigenvectors.

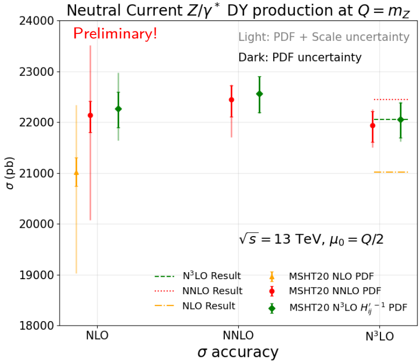
Results obtained using `proVBFH` code[26,37].

- Increase in σ using aN3LO PDFs, occurs due to enhanced charm and light quarks at high x.
- VBF more reliant on quark sector - changes less ($\sim$ 2.5%, cf $\sim$ 5% for ggF) with PDF order as more data constraints on quarks.

Impact on Drell-Yan cross-sections:

Preliminary!
Produced using the `n3loxs` code[27].

- Consider impact of our aN3LO PDFs on Drell-Yan production at LHC, e.g. Neutral current at m_Z at 13 TeV:

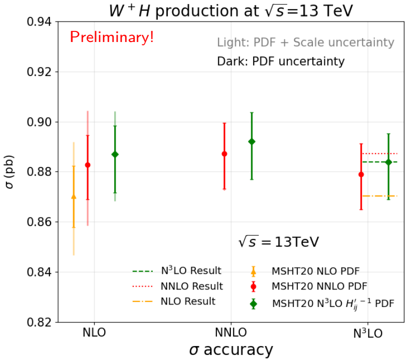


- Only small change in using aN3LO PDFs relative to NNLO PDFs.
- Prediction with NNLO and aN3LO PDFs are stable.
- PDF uncertainties dominate at NNLO and N3LO, indeed enlarged from MSHT20aN3LO with inclusion of MHOUs.

Impact on *VH* cross-sections:

Preliminary!
Produced using the n3loxs code[27].

- Consider impact of our aN3LO PDFs on *VH* associated production at LHC, e.g. W^+H at 13 TeV:



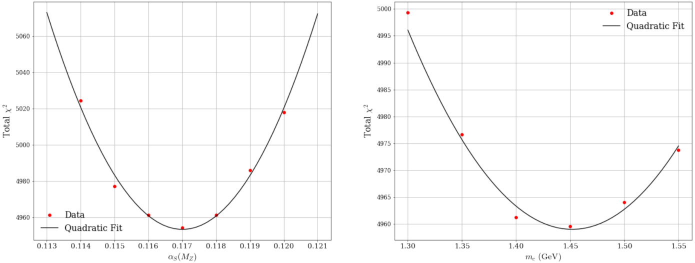
- Result with aN3LO PDFs raised slightly, reflects increased quarks at high x, antiquarks at low x and strange and charm.
- N3LO σ + aN3LO PDF result very close to NNLO σ + NNLO PDF result, increased stability in predictions.

Other results using our aN3LO PDFs:

More information in article: Eur. Phys. J. C 83 (2023) 3, 185, arXiv:hep-ph/2207.04739, J. McGowan, TC, L.A. Harland-Lang, R.S. Thorne.

Strong Coupling and heavy quarks:

- Both $\alpha_S(m_Z^2)$ and m_c show quadratic behaviour around minima.

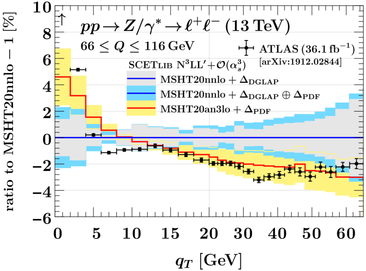


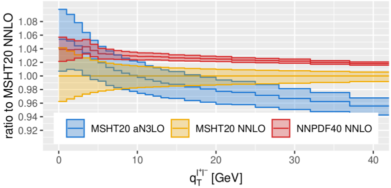
- aN3LO best fit: $\alpha_S(M_Z^2) = 0.1170$, overlaps with NNLO world average.
- NNLO best fit and uncertainty: $\alpha_S(M_Z^2) = 0.1174 \pm 0.0013$.
- NLO best fit and uncertainty: $\alpha_S(M_Z^2) = 0.120 \pm 0.0015$. TC et al, 2106.10289.
- m_c best fit ~ 1.45 GeV, compare with ~ 1.35 GeV at NNLO, so now better agreement with expectation $m_c^{\rm pole} = 1.5 \pm 0.2 \rm GeV$.
- Lower $\alpha_S(M_Z^2)$ and raised m_c suggest fit favouring slight suppression of gluon and charm.

aN3LO PDFs for Zp_T at low q_T:

Preliminary!

- MSHT20aN3LO PDFs already starting to be used by theory community - e.g. resummed (+ fixed order) predictions for Zp_T spectrum at low transverse momenta:





- Substantial aN3LO PDF effect on N3LL'/N4LL q_T spectrum. Left: SCETlib, Johannes Michel - LHC EW WG meeting Sep 2022. Right: CuTe-MCFM, Tobias Neumann CMS mW Hackathon Jan 2023.
- Left: aN3LO PDFs appear to fit the measured ATLAS data better, likely due to indirect effects of gluon shape change...?

Usage

More information in article: Eur. Phys. J. C 83 (2023) 3, 185, arXiv:hep-ph/2207.04739, J. McGowan, TC, L.A. Harland-Lang, R.S. Thorne.

Interpretation and Usage:

Available on LHAPDF and UCL website:
(http://www.hep.ucl.ac.uk/msht/)

- MSHT20an3lo_as118 PDFs available on MSHT website.
- The eigenvectors include theory uncertainties from MHOs in PDFs.
- We assume the dominant MHO uncertainty is from missing N3LO.

Recommendations:

1. If N3LO cross-sections are known use our aN3LO PDFs and their associated theoretical uncertainties.
2. For DIS processes, using our aN3LO PDF set is advised along with our aN3LO coefficient functions.
3. For the other 5 process categories in the fit (Drell-Yan, top, vector boson p_T, jets and dimuon), we fit K-factors and provide these fitted aN3LO K-factors to be used along with our aN3LO PDFs.
4. For processes not included in the fit - e.g. Higgs, the change of the aN3LO compared to the NNLO PDFs is representative of the potential theoretical uncertainty in the NNLO PDFs.

MSHT PDF sets available

All available at https://www.hep.ucl.ac.uk/msht/, and most also on LHAPDF.

- Overview of available MSHT20 PDF sets (this is a small selection!):

LHAPDF6 grid name	Order	$n_f^{\max}$	N_{mem}	$\alpha_S(m_Z^2)$	Description
MSHT20nnlo_as118	NNLO	5	65	0.118	Default NNLO set
MSHT20nlo_as120	NNLO	5	65	0.118	Default NLO set
MSHT20lo_as130	NNLO	5	65	0.118	Default LO set
MSHT20nnlo_as_largerange	NNLO	5	23	0.108-0.130	$\alpha_S(M_Z^2)$ variation NNLO set
MSHT20nlo_as_largerange	NLO	5	23	0.108-0.130	$\alpha_S(M_Z^2)$ variation NLO set
MSHT20nnlo_mcrange_nf5	NNLO	5	9	0.118	Charm mass variation (1.2-1.6 GeV) NNLO set
MSHT20nnlo_mbrange_nf5	NNLO	5	7	0.118	Bottom mass variation (4.0-5.5 GeV) NNLO set
MSHT20nnlo_nf3,4	NNLO	3, 4	65	0.118	NNLO set with max. 3 or 4 flavours
MSHT20qed_nnlo	NNLO	5	77	0.118	NNLO set with QED effects and γ PDF
MSHT20qed_nnlo_(in)elastic	NNLO	5	77	0.118	NNLO set with QED effects and (in)elastic γ
MSHT20qed_nnlo_neutron	NNLO	5	77	0.118	NNLO neutron set with QED effects and γ
MSHT20an3lo_as118	aN3LO	5	105	0.118	Approximate N3LO set with theoretical uncertainties also included
MSHT20an3lo_as118_KCorr	aN3LO	5	105	0.118	Approximate N3LO set with theoretical uncertainties also included, K-factors correlated
PDF4LHC21	NNLO	5	901	0.118	Baseline PDF4LHC21 set
PDF4LHC21_mc	NNLO	5	101	0.118	Replica compressed PDF4LHC21 set
PDF4LHC21_40	NNLO	5	41	0.118	Hessian compressed PDF4LHC21 set

Selection of some of the MSHT PDF sets available in LHAPDF format. Many more online!

Key:

- Default - $\alpha_S, m_{c,b}$ - QED - aN3LO - PDF4LHC21

- Feel free to contact us with questions about usage.

Conclusions

More information in article: Eur. Phys. J. C 83 (2023) 3, 185, arXiv:hep-ph/2207.04739, J. McGowan, TC, L.A. Harland-Lang, R.S. Thorne.

Conclusions:

- As demands on PDFs become stronger we must aim for both more precise and more accurate PDF central values and uncertainties.
- We have produced the world first approximate N3LO PDFs, including both higher order effects in PDFs and theoretical uncertainties.
- Method provides an intuitive and controllable way to include theoretical uncertainties into PDFs. Can be updated as more information becomes available on N3LO.
- Our aN3LO PDFs are available and we encourage their use: `MSHT20an3lo_as118`.
- Can be used if N3LO is known or where not to evaluate uncertainty due to missing higher orders in PDFs and include higher order effects.
- Full information is available in the article Eur. Phys. J. C 83 (2023) 3, 185, arXiv:hep-ph/2207.04739 .
- Any questions about them/their use $\Rightarrow$ please ask us!

Selection of some references (others on slides)

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[36] M. Bonvini, arXiv:1805.08785.

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Backup Slides

Note: For some of the more recent work, this project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (Grant agreement No. 101002090 COLORFREE).

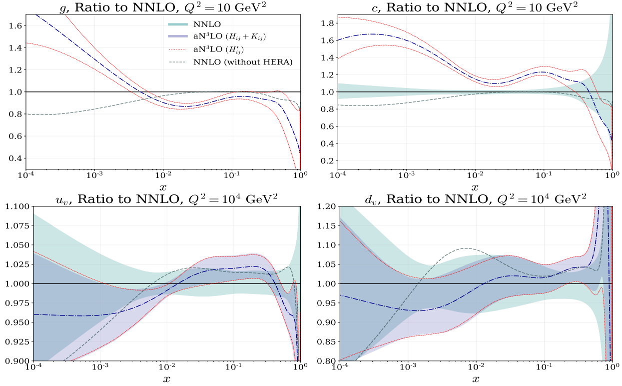
MSHT20aN3LO PDFs - Fit quality

- Smooth improvement and convergence in fit quality with increasing order.
- Fit quality improves by $\Delta\chi^2 = -150.4$ for 20 extra parameters.
- Reduction in tension between low and high x, HERA and fixed target fit better.
- ATLAS 8 TeV Zp_T improves significantly, reduction in tension with other data.
- Jets are only class of data with worsening of χ^2, looks better with dijet data (preliminary).

Order	LO	NLO	NNLO	aN3LO
χ^2/N_{pts}	2.57	1.33	1.17	1.14

Data set	Points	MSHT20aN3LO χ^2	$\Delta\chi^2$ from NNLO
HERA e^+p CC	39	49.7	-2.3
HERA e^-p CC	42	64.9	-5.3
HERA e^+p NC 820GeV	75	84.3	-5.6
HERA e^-p NC 460GeV	209	247.7	-0.6
HERA e^+p NC 920GeV	402	474.0	-38.7
HERA e^-p NC 575GeV	259	248.5	-14.5
HERA e^-p NC 920GeV	159	243.0	-1.4
CCFR $\nu N \to \mu\mu X$	86	68.3	+0.6
NuTeV $\nu N \to \mu\mu X$	84	56.7	-1.8
CMS double diff. DY	132	129.5	-15.1
ATLAS 7 TeV W, Z	61	94.5	-22.1
ATLAS 8 TeV W	22	58.0	+0.4
ATLAS 8 TeV Z	59	91.6	+15.7
ATLAS 8 TeV Zp_T	104	108.4	-80.0
CMS 7 TeV $W + c$	10	10.8	+2.2
ATLAS 8 TeV W+jets	30	18.8	+0.7
ATLAS 7 TeV jets	140	215.9	-5.6
CMS 7 TeV jets	158	186.8	+11.0
CMS 8 TeV jets	174	271.3	+10.0
CMS 2.76 TeV jets	81	109.8	+6.9
DIS data (total)	2375	2580.9	-90.8
Jets data (total)	739	963.6	+21.5
Top data (total)	71	75.1	-4.2
DY data (total)	864	1065.4	-12.8
p_T jets (total)	144	138.0	-77.2
Total	4363	4957.2	-154.4

MSHT20aN3LO PDFs - PDF changes



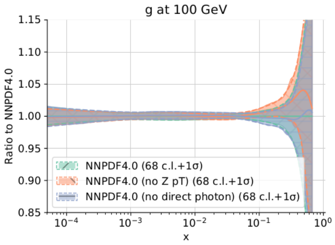
- Small-x low-Q^2 gluon enhanced due to large logs included at N3LO.
- Enhanced charm via enlarged $A^{(3)}_{Hg}$ and increased small-x gluon.
- Reduced quarks at intermediate/small-x accommodate small-x gluon.
- High-Q^2, intermediate/large-x light quarks largely follow NNLO no HERA fit, demonstrating eased tension with smaller x HERA data.

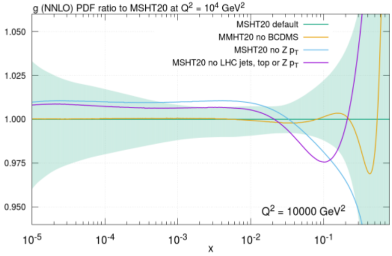
ATLAS 8 TeV Zp_T data:

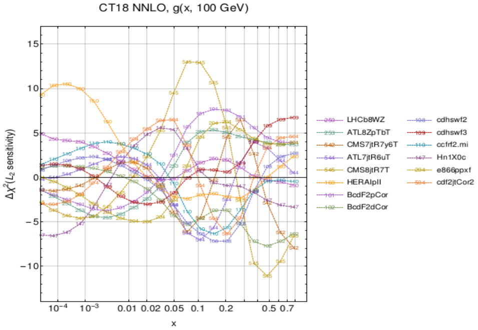
- ATLAS 8 TeV Zp_T data - precise data, large NNLO corrections.
- Different amounts of data used and different uncertainties applied.
- MSHT20 - Largest amount of data, double differential in $[p_T^{ll}, y_{ll}]$ in Z-peak mass bin, others single differential in y_{ll}. Fit quality $\chi^2/N_{pts} \sim 1.8$ for 104 points. k-factors fit and uncertainty extracted on them $\lesssim 0.5\%$ included.
- NNPDF cut high $p_T > 150\mathrm{GeV}$ data to remove sensitivity to EW corrections (although included). Add 1% uncorrelated uncertainty for k-factor MC errors + theory uncertainties + missing experimental errors. Fit quality $\chi^2/N_{pts} \sim 0.9$ for 92 points.
- CT fit only 3 mass bins $m_{ll} = \{[46, 66], [66, 116], [116, 150]\}\mathrm{GeV}$ bins single differential in $p_T^{ll} < 150 GeV$. Include a 0.5% uncorrelated uncertainty for k-factor MC errors + theory uncertainties. Fit quality $\chi^2/N_{pts} \sim 1.1$ for 27 points, argue other data not so constraining.
- Therefore different groups see different impacts and importance.

ATLAS 8 TeV Zp_T data:

- ATLAS 8 TeV Zp_T data - precise data, large NNLO corrections.
- Different amounts of data used and different uncertainties applied.
- Therefore different groups see different impacts and importance.

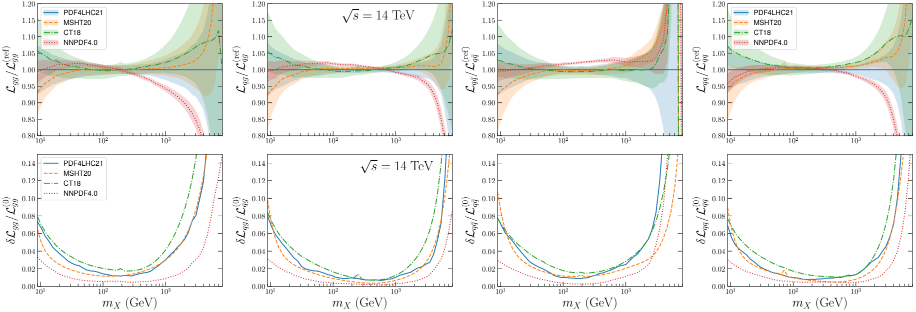






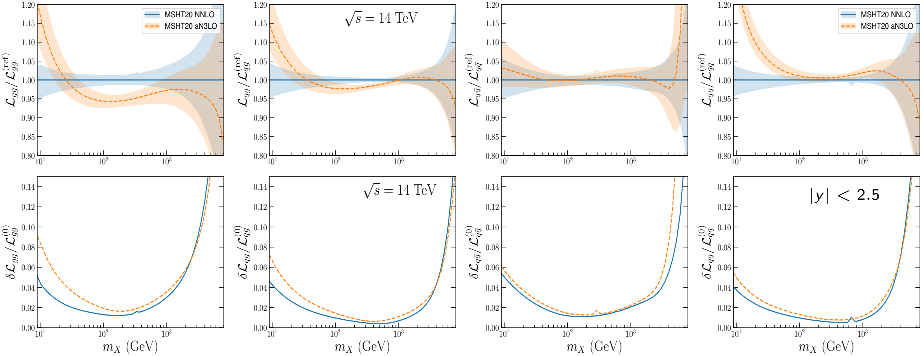
Global Fits Luminosities Comparison:

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



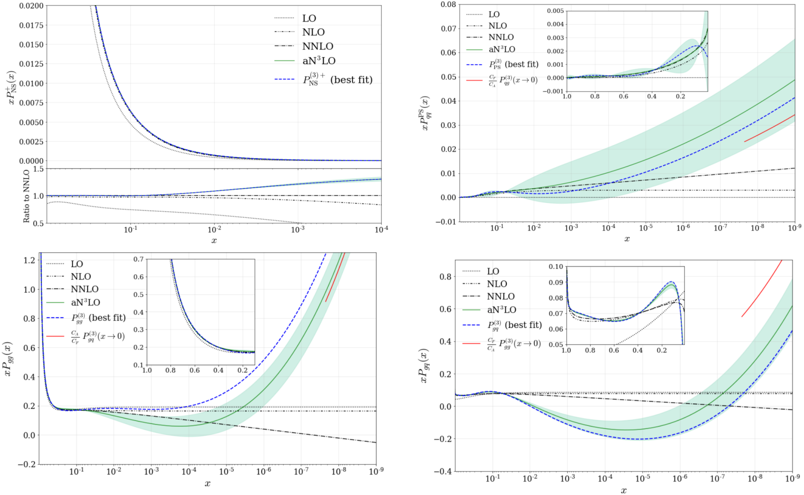
- Generally good agreement for central m_X, at least for qq, qg, gg luminosities. Exception is NNPDF4.0 higher for $q\bar{q}$.
- More marked differences at high m_X, largely unconstrained so more extrapolation driven.
- Significant differences in uncertainties reflect differences in methodology/data.

aN3LO PDF luminosities with rapidity cut:



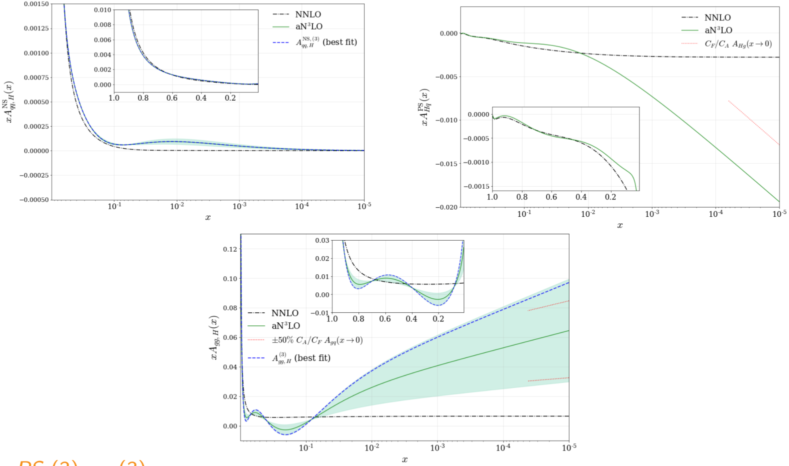
- *gg* luminosity reduced around 100GeV and increased at 10GeV, *gg* uncertainty grows with inclusion of aN3LO and theoretical uncertainties.
- *qq* luminosity raised at low invariant masses from enhanced charm.
- Luminosity uncertainties enlarged (and more so at lower invariant masses) due to inclusion of aN3LO and PDF theory uncertainties.
- Main effect of rapidity $|y| < 2.5$ cut is reducing low m_X uncertainties.

Splitting Functions:



- $P_{qq}^{NS}(x)$ has small uncertainty as more info known (e.g. 8 Mellin moments, more exact info.), also less affected by small x as non-singlet.

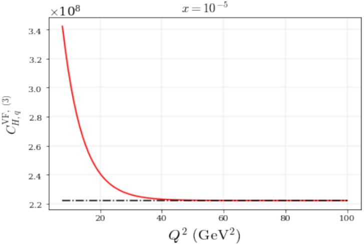
Transition Matrix Elements:

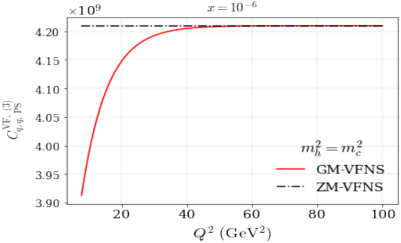


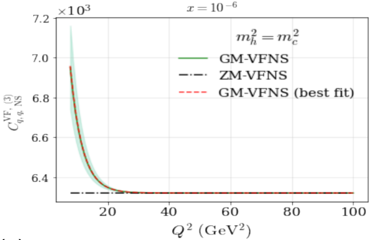
- $A^{PS,(3)}_{Hq}$, $A^{(3)}_{gq,H}$ known completely, need to be approximated (without uncertainty) due to complex form. $A^{(3)}_{Hg}$, $A^{NS,(3)}_{qq,H}$, $A^{(3)}_{gg,H}$ have one theory nuisance parameter each at low x.

DIS Coefficient Functions:

Note: Plots here only show uncertainties inherited from transition matrix elements, not $c^{NLL}_{q,g}$ parameters.





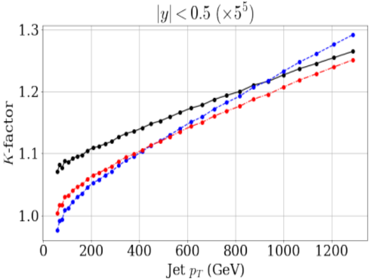


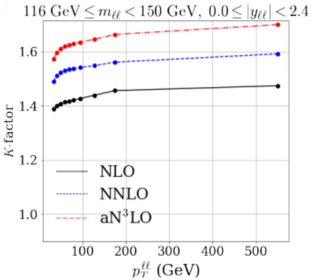
- $C^{VF,(3)}_{Hq}$ and $C^{VF,(3)}_{Hg}$ have uncertainties from c^{NLL}_q and c^{NLL}_g parameters, $C^{VF,(3)}_{Hg}$ and $C^{VF,(3)}_{qq,NS}$ inherit uncertainty from $A^{(3)}_{Hg}$ and $A^{(3)}_{qq,NS}$.

Hadronic K-factors

4. **Jets** (lower left plot)

- Fit prefers a mild shift of aN3LO k-factors relative to NNLO.
- Good qualitative perturbative convergence.





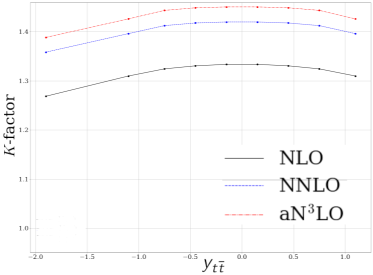
5. **Vector boson + jets, Zp_T** (upper right plot)

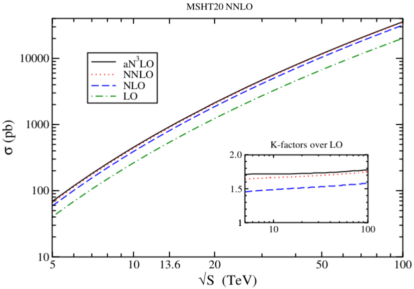
- Fit prefers larger shifts here, NLO→NNLO and NNLO→aN3LO similar.
- May be picking up sensitivity to all-order result via experimental data.

Hadronic K-factors - Top and Dimuon

2 Top

- Fit prefers a $\approx 4\%$ increase in the aN3LO k-factors relative to NNLO.
- Improved perturbative convergence with aN3LO PDFs.
- Consistent with recent approximate N3LO result[32].





3 Dimuon - Semi-inclusive DIS

- Already freedom to change BR$(D \rightarrow \mu)$ here, so limited sensitivity. BR reduces to 0.082 from 0.088 - within allowed 0.092 ± 0.01 range.

How can we incorporate N3LO knowledge into PDFs?

- After subbing in and rewriting obtain:

$$P(T|D) \propto \int d\theta' \exp\left(-\frac{1}{2}[(T' + \frac{\theta'}{\sigma_{\theta'}}u - D)^T H_0 (T' + \frac{\theta'}{\sigma_{\theta'}}u - D) + \theta'^2/\sigma_{\theta'}^2]\right)$$

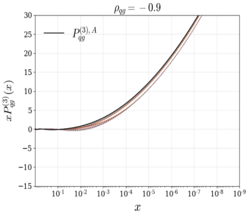
$$\propto \int d\theta' \exp\left(-\frac{1}{2}M^{-1}(\theta' - \bar{\theta}')^2 - \frac{1}{2}(T' - D)^T H (T' - D)\right)$$

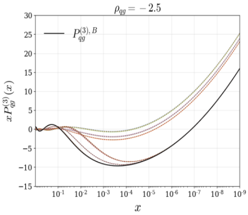
$$\propto \int d\theta' \exp\left(-\chi_1^2 - \chi_2^2\right)$$

- First term is posterior penalty when the theory strays from the best fit.
- Second term is χ^2 from fitting procedure with $H = (H_0^{-1} + uu^T)^{-1}$ now containing also additional theoretical uncertainties.
- In addition, *how we decompose H allows us to examine correlations of the theoretical nuisance parameters* - backup slides!
- Key questions:
  1. How do we determine the priors?
     - Summary from known information and intuition from lower orders.
  2. Where do we include the theory nuisance parameters? - Next few slides.

How to determine the priors:

- Key part of the theoretical nuisance parameter framework for missing N3LO pieces is setting up the priors and penalties on their variations.
- Q. How do we do this? A. Conservatively!
- Set ρ_{ab} prior variation by requiring:
  1. At low x bound set once exact expression $f_e(x, \rho_{ab})$ exits range of results from different (larger) x functional forms, e.g. see lower plots.
  2. At high x bound set if N3LO correction becomes too large (rare).
  3. Once functional form fixed, check range of prior and extend as necessary to incorporate different functional form variation.

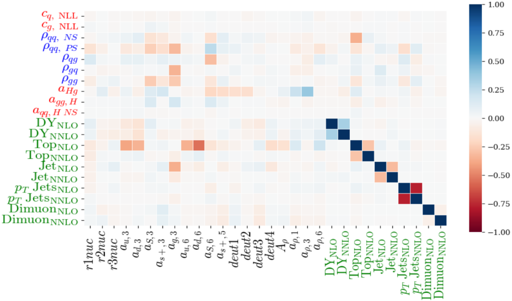




- Find penalties on theory nuisance parameters after fit are small and posterior errorbands reduced relative to prior ⇒ prior set conservatively.

aN3LO PDFs Correlations:

- Examine correlations of theory parameters and other PDF parameters.



- Given expected and observed very limited correlation of K-factors with other theory parameters, can separate them out:

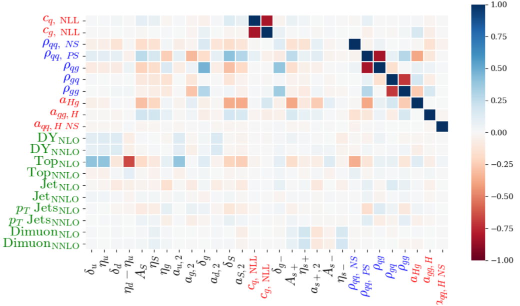
$$H'^{-1}_{ij} \rightarrow H^{-1}_{ij} + \sum_{p=1}^{N_p} K^{-1}_{ij,p}$$

Allows fit k-factors to be separated out - useful.

- Produce two PDF uncertainty sets - `MSHT20an3lo_as118_Kcorr` and `MSHT20an3lo_as118`, default is latter. Very little difference in PDF uncertainties!

aN3LO PDFs Correlations:

- Examine correlations of theory parameters and other PDF parameters.



- Given expected and observed very limited correlation of K-factors with other theory parameters, can separate them out:

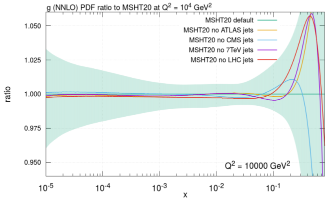
$$H_{ij}^{\prime -1} \rightarrow H_{ij}^{-1} + \sum_{p=1}^{N_p} K_{ij,p}^{-1}$$

Allows fit k-factors to be separated out - useful.

- Produce two PDF uncertainty sets - `MSHT20an3lo_as118_Kcorr` and `MSHT20an3lo_as118`, default is latter. Very little difference in PDF uncertainties!

New data - Dijets - Introduction

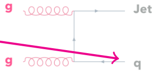
- High x gluon is of interest in PDFs, with tensions between datasets.
- MSHT20 - data on inclusive jets from ATLAS, CMS at 7 and 8 TeV, sensitive to high-x gluon. Different pulls.
- Known issues with systematic correlations in ATLAS 7, 8 TeV inclusive jets (latter therefore not included in MSHT20).



- Theoretical issues: scale choice, non-unitary nature of inclusive jets.
- Dijets also allow triple differential measurement, cf double differential for single inclusive jets. Schematically at LO:

$$x = \frac{p_T}{\sqrt{s}}\left(e^{y_j} + e^{y_j}\right)$$

Integrated over in inclusive jet case.



$\Rightarrow$ Single inclusive jets: $\frac{d\sigma}{dp_T^j\, d|y^j|}$, dijets: $\frac{d\sigma}{dp_T^{\mathrm{avg}}\, dy^*\, dy_b}$.

CMS 8 TeV dijets

Dijets when triple differential more sensitive to x-dependence.

Dijets vs Inclusive Jets - Fit Quality (NNLO)

Preliminary!

- Fit either 7+8 TeV inclusive jets or dijets on MSHT20 baseline.
- Inclusive jets have issues with systematic correlations and theoretical questions, e.g. scale choice, non-unitary nature, etc.
- Dijets may resolve some such issues, and triple differential measurement is more sensitive to PDF x-dependence.

Also investigated. at aN3LO ⇒ see later!

Dijets:

Dataset	N_{pts}	χ^2/N_{pts}
ATLAS 8 TeV Zp_T	104	1.65
Top differential data total	54	1.24
ATLAS 7 TeV dijets	90	1.05
CMS 7 TeV dijets	54	1.43
CMS 8 TeV dijets	122	1.04
Total dijets	266	1.12

Inclusive Jets:

Dataset	N_{pts}	χ^2/N_{pts}
ATLAS 8 TeV Zp_T	104	1.85
Top differential data total	54	1.12
ATLAS 7 TeV jets	140	1.53
ATLAS 8 TeV jets	171	1.45
CMS 7 TeV jets	158	1.22
CMS 8 TeV jets	174	1.80
Total inclusive jets	643	1.50

- Fit quality of dijets - 1.12, better than inclusive jets - 1.50.
- Clear improvement with order, NNLO needed for precise LHC data.

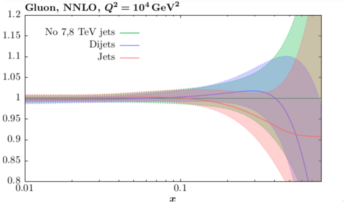
Dataset	N_{pts}	NLO	NNLO
ATLAS 7 TeV dijets	90	1.10	1.05
CMS 7 TeV dijets	54	1.71	1.43
CMS 8 TeV dijets	122	5.30	1.04
Total dijets	266	3.15	1.12

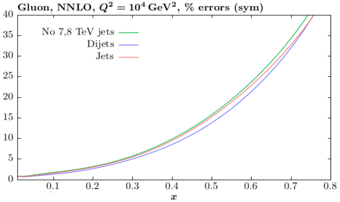
Dataset	N_{pts}	NLO	NNLO
ATLAS 7 TeV jets	140	1.69	1.53
ATLAS 8 TeV jets	171	2.37	1.45
CMS 7 TeV jets	158	1.38	1.22
CMS 8 TeV jets	174	1.65	1.80
Total inclusive jets	643	1.78	1.50

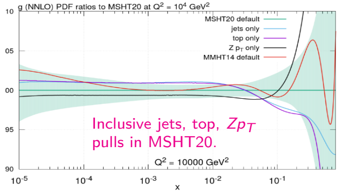
Dijets vs Inclusive Jets - PDFs (NNLO)

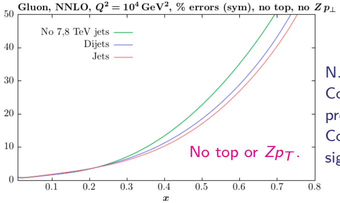
Preliminary!

- Impact on gluon PDF at high x, consistent but different pulls.
- Dijets have more impact on reducing gluon uncertainty at high x.









N.B. This is all Leading Colour, we have looked preliminarily at Full Colour and not found significant changes.

- Dijets increases high-x gluon, like Zp_T, inclusive jets reduces high x gluon, like top data. $\Rightarrow$ Interplay with other data.
- Without Zp_T or top, inclusive jets has greater impact on uncertainty.

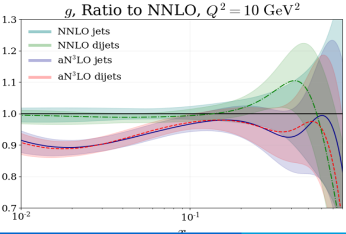
Dijet data aN3LO vs NNLO:

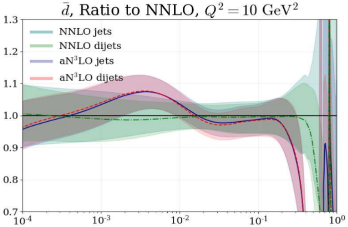
Preliminary!

- Obtain better fit quality at NNLO and aN3LO than jets.
- Dijet fit quality improves further slightly at aN3LO, unlike for jets.

.	N_{pts}	χ^2/N_{pts}		.	N_{pts}	χ^2/N_{pts}	
		NNLO	aN3LO			NNLO	aN3LO
ATLAS 7 TeV jets	140	1.58	1.54	ATLAS 7 TeV dijets	90	1.05	1.12
CMS 7 TeV jets	158	1.11	1.18	CMS 7 TeV dijets	54	1.43	1.39
CMS 8 TeV jets	174	1.50	1.56	CMS 8 TeV dijets	122	1.04	0.83
Total (jets)	472	1.39	1.43	Total (dijets)	266	1.12	1.04
Total	4363	1.17	1.14	Total	4157	1.14	1.10

- Effect of jets vs dijets on PDFs and rest of data similar at NNLO and aN3LO, and no significant change in uncertainty.



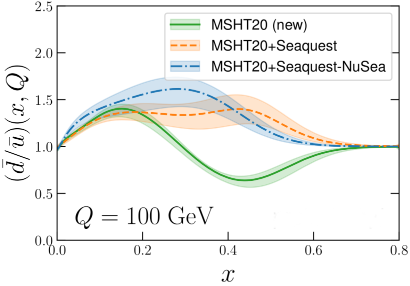


N.B. This is all Leading Colour, we have looked preliminarily at Full Colour and not found significant changes.

New data - Seaquest (NNLO)

Preliminary!

- Seaquest (E906) fixed target DY data - sensitivity to high x q, $\bar{q}$: $\Rightarrow \sigma_D/\sigma_H \sim 1 + \bar{d}/\bar{u}$. Direct measurement of $\bar{d}/\bar{u}$ at high x.
- Various models for $\bar{d}/\bar{u}$ at high x: Pauli blocking, pion cloud, etc.
- Previous questions of NuSea (E866) data preferring $\bar{d} < \bar{u}$ at $x \approx 0.4$.
- Clearly raises high x $\bar{d}/\bar{u}$. Tension with NuSea which pulls it down.

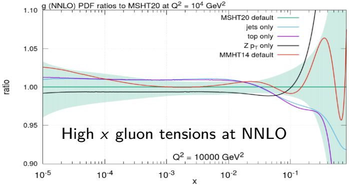


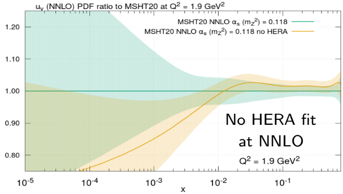
Dataset	N_{pts}	MSHT20	New
Seaquest	6	-	8.2
NuSea	15	9.8	19.0
Total (without Seaquest or NuSea)	4348	5102.3	5112.1

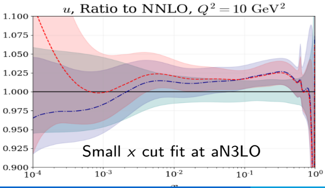
- NuSea χ^2/N_{pts}: $0.65 \to 1.27$, when Seaquest added.

- Rest of data also worsens in χ^2 by 9 points, with 4.5 in E866 absolute DY (rather than ratio), 4.4 in NMC n/p, 4.3 in DØ W asymmetry.

Dataset tensions at NNLO:







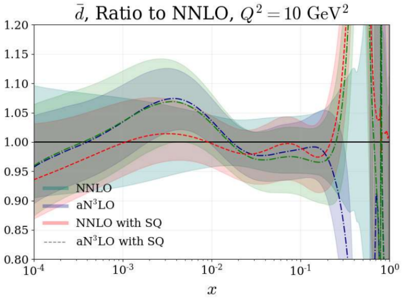
Fit qualities of fits excluding HERA data:

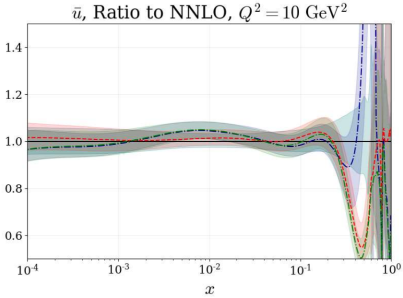
Dataset	N_{pts}	$\Delta\chi^2$ aN3LO	$\Delta\chi^2$ NNLO
BCDMS μp F_2	163	+1.4	−5.5
BCDMS μd F_2	151	−0.0	−2.1
NMC μp F_2	123	−7.8	−4.5
NMC μd F_2	123	−16.6	−16.1
E665 μd F_2	53	+1.3	+3.9
E665 μp F_2	53	+1.5	+4.3
E866 / NuSea pp DY	184	+2.3	+2.9
NuTeV $\nu N \to \mu\mu X$	84	−9.1	−9.5
DØ II $W \to \nu e$ asym.	12	+0.2	−3.9
ATLAS High-mass Drell-Yan	13	−0.9	−2.0
CMS double diff. Drell-Yan	132	−3.7	−10.3
LHCb 2015 W, Z	67	−6.5	−1.9
LHCb 8 TeV $Z \to ee$	17	−2.4	−1.8
CMS 8 TeV W	22	+0.1	+0.9
ATLAS 7 TeV jets	140	+1.8	+6.5
ATLAS 7 TeV high prec. W, Z	61	−1.3	+0.2
CMS 7 TeV jets	158	+1.0	+3.8
DØ W asym.	14	−2.0	−0.8
ATLAS 8 TeV Z p_T	104	+12.8	−39.2
CMS 8 TeV jets	174	−11.5	−1.8
ATLAS 8 TeV High-mass DY	48	+2.4	+3.7
ATLAS 8 TeV W + jets	30	−0.8	−1.7
CMS 8 TeV double diff. $t\bar{t}$	15	−0.8	+0.8
ATLAS 8 TeV W	22	−5.0	−3.0
CMS 2.76 TeV jet	81	−6.8	+0.0
CMS 8 TeV sing. diff. $t\bar{t}$	9	+2.0	−2.6
ATLAS 8 TeV double diff. Z	59	+5.7	+22.7
Total	3042	-48.0	−61.6

MSHT20aN3LO PDFs - Seaquest

Preliminary!

- At aN3LO, the $\bar{d}$ become negative above $x \sim 0.5$ with a minimum at $x \sim 0.6$. Nonetheless remains positive within uncertainties.
- Like at NNLO, adding the Seaquest data raises the $\bar{d}/\bar{u}$.



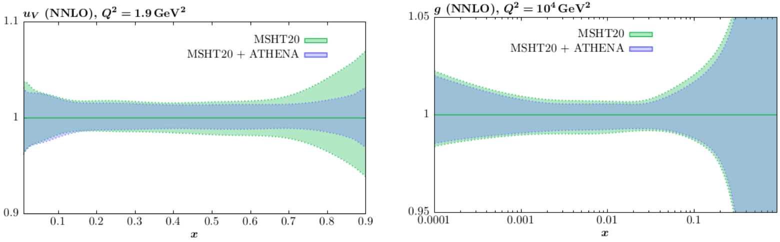


- Adding Seaquest $\Rightarrow$ NNLO and aN3LO $\bar{d}$, $\bar{u}$ again very similar.
- Effect on fit quality of adding Seaquest similar to NNLO, $\Delta\chi^2 = +6$ in rest of data, NuSea χ^2/N doubles from ~ 0.6 to ~ 1.3.

New data - EIC Pseudodata

Again note added on NNLO fit here.

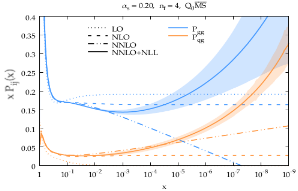
- Investigated impact of simulated EIC pseudodata with colleagues from ATHENA/EIC.
- Effects on unpolarised proton PDFs from high x lower Q^2 sensitivity.

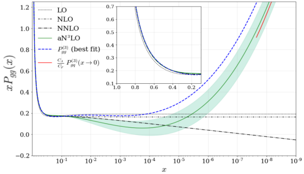


- Effect on up valence larger due to charge-squared coupling of virtual photon in DIS $\Rightarrow$ reduction in u_V uncertainty above $x \sim 0.5$.
- Smaller impact on other partons, gluon uncertainty nonetheless reduced across range of x.

aN3LO at low x vs resummed:

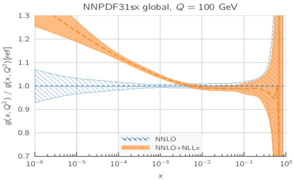
- We include up to (N)LL low x resummed terms (and (N)NLL with variable coefficient) in splitting functions - compare with resummed[33]:

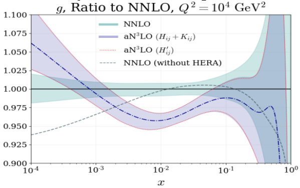




Compare blue solid (left) and dashed (right) lines for P_{gg}.

- Similar effects qualitatively (note scheme difference!) on P_{ij}s.
- Impact on gluon also shows similarities qualitatively to[34]:





- In MSHT20aN3LO have $\Delta\chi^2 = -91$ for DIS data from NNLO, with -68 in HERA, cf ~ -70 in both [34] and xFitter small x resummed study[35].

NLO and NNLO Cross-section Scale Variations

- For many processes NLO scale variations were not sufficient to incorporate NNLO result.

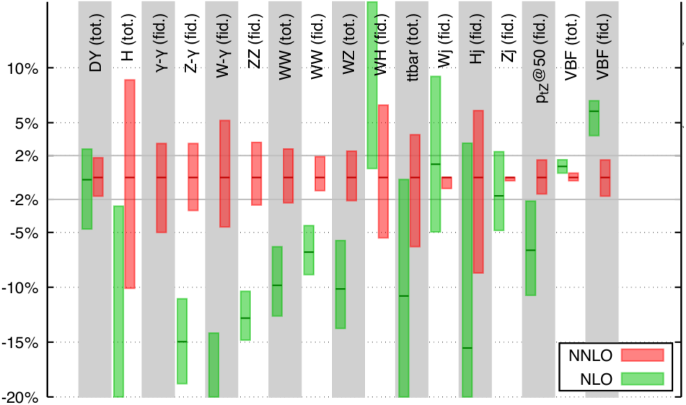


Image Credit: G. Salam

- Is there a better way to do this?

Impact on Higgs cross-sections - ggF:

- More information on impact of aN3LO PDFs on N3LO ggF Higgs production:

σ order	PDF order	$\sigma + \Delta\sigma_+ - \Delta\sigma_-$ (pb)	σ (pb) $+ \Delta\sigma_+ - \Delta\sigma_-$ (%)
		PDF uncertainties	
N^3LO	aN^3LO (no theory unc.)	$45.296 + 0.723 - 0.545$	$45.296 + 1.60\% - 1.22\%$
	aN^3LO $(H_{ij} + K_{ij})$	$45.296 + 0.832 - 0.755$	$45.296 + 1.84\% - 1.67\%$
	aN^3LO (H'_{ij})	$45.296 + 0.821 - 0.761$	$45.296 + 1.81\% - 1.68\%$
	NNLO	$47.817 + 0.558 - 0.581$	$47.817 + 1.17\% - 1.22\%$
NNLO	NNLO	$46.206 + 0.541 - 0.564$	$46.206 + 1.17\% - 1.22\%$
		PDF + Scale uncertainties	
N^3LO	aN^3LO (no theory unc.)	$45.296 + 0.723 - 1.851$	$45.296 + 1.60\% - 4.09\%$
	aN^3LO $(H_{ij} + K_{ij})$	$45.296 + 0.832 - 1.923$	$45.296 + 1.84\% - 4.25\%$
	aN^3LO (H'_{ij})	$45.296 + 0.821 - 1.926$	$45.296 + 1.81\% - 4.25\%$
	NNLO	$47.817 + 0.577 - 2.210$	$47.817 + 1.21\% - 4.62\%$
NNLO	NNLO	$46.206 + 4.284 - 5.414$	$46.206 + 9.27\% - 11.72\%$

Gluon fusion cross-section and uncertainties at $\mu = m_H/2$ at $\sqrt{s} = 13$ TeV.

- PDF uncertainty increase from NNLO to aN3LO $\Rightarrow$ inclusion of MHOs.
- Scale dependence reduced at N3LO. Central values for both scale choices $\mu = m_H/2$(shown) and $\mu = m_H$(not shown) lie within each others' errorbands.

Impact on Higgs cross-sections - VBF:

- More information on impact of aN3LO PDFs on N3LO VBF Higgs:

σ order	PDF order	$\sigma + \Delta\sigma_{+} - \Delta\sigma_{-}$ (pb)	σ (pb) $+ \Delta\sigma_{+} - \Delta\sigma_{-}$ (%)
PDF uncertainties			
$\mathrm{N^3LO}$	$\mathrm{aN^3LO}$ (no theory unc.)	$4.1150 + 0.0638 - 0.0724$	$4.1150 + 1.55\% - 1.76\%$
	$\mathrm{aN^3LO}$ $(H_{ij} + K_{ij})$	$4.1150 + 0.0682 - 0.0755$	$4.1150 + 1.66\% - 1.83\%$
	$\mathrm{aN^3LO}$ (H'_{ij})	$4.1150 + 0.0678 - 0.0742$	$4.1150 + 1.65\% - 1.80\%$
	NNLO	$3.9941 + 0.0558 - 0.0631$	$3.9941 + 1.40\% - 1.58\%$
NNLO	NNLO	$3.9974 + 0.0557 - 0.0633$	$3.9974 + 1.39\% - 1.58\%$
PDF + Scale uncertainties			
$\mathrm{N^3LO}$	$\mathrm{aN^3LO}$ (no theory unc.)	$4.1150 + 0.0638 - 0.0724$	$4.1150 + 1.55\% - 1.76\%$
	$\mathrm{aN^3LO}$ $(H_{ij} + K_{ij})$	$4.1150 + 0.0683 - 0.0755$	$4.1150 + 1.66\% - 1.83\%$
	$\mathrm{aN^3LO}$ (H'_{ij})	$4.1150 + 0.0678 - 0.0742$	$4.1150 + 1.65\% - 1.80\%$
	NNLO	$3.9941 + 0.0560 - 0.0631$	$3.9941 + 1.40\% - 1.58\%$
NNLO	NNLO	$3.9974 + 0.0576 - 0.0642$	$3.9974 + 1.44\% - 1.61\%$

Vector boson fusion cross-section and uncertainties at $\mu = Q^2$ at $\sqrt{s} = 13$ TeV.

σ order	PDF order	$\sigma + \Delta\sigma_{+} - \Delta\sigma_{-}$ (pb)	σ (pb) $+ \Delta\sigma_{+} - \Delta\sigma_{-}$ (%)
$\mathrm{N^3LO}$	$\mathrm{aN^3LO}$ $n_f = 5$	4.1150 + 0.0683 - 0.0755	4.1150 + 1.66% - 1.83%
	$\mathrm{aN^3LO}$ $n_f = 4$	4.0270 + 0.0685 - 0.0765	4.0270 + 1.70% - 1.90%
	$\mathrm{aN^3LO}$ $n_f = 3$	2.7248 + 0.0653 - 0.0673	2.7248 + 2.40% - 2.47%
NNLO	NNLO $n_f = 5$	3.9974 + 0.0557 - 0.0633	3.9974 + 1.39% - 1.58%
	NNLO $n_f = 4$	3.9118 + 0.0561 - 0.0634	3.9118 + 1.44% - 1.62%
	NNLO $n_f = 3$	2.6845 + 0.0539 - 0.0641	2.6845 + 2.01% - 2.39%

Vector boson fusion cross-section with increasing number of flavours at $\mu = Q^2$ at $\sqrt{s} = 13$ TeV.

- PDF uncertainty increase from NNLO to aN3LO less than in ggF case.
- Scale dependence negligible at NNLO and aN3LO.
- Comparing $n_f = 3, 4$ see difference in NNLO and aN3LO predictions doubles once charm included.

MSHT PDF sets available

All available at https://www.hep.ucl.ac.uk/msht/, and most also on LHAPDF.

- Overview of available MSHT20 PDF sets (this is a small selection!):

LHAPDF6 grid name	Order	$n_f^{\max}$	N_{mem}	$\alpha_S(m_Z^2)$	Description
MSHT20nnlo_as118	NNLO	5	65	0.118	Default NNLO set
MSHT20nlo_as120	NNLO	5	65	0.118	Default NLO set
MSHT20lo_as130	NNLO	5	65	0.118	Default LO set
MSHT20nnlo_as_largerange	NNLO	5	23	0.108-0.130	$\alpha_S(M_Z^2)$ variation NNLO set
MSHT20nlo_as_largerange	NLO	5	23	0.108-0.130	$\alpha_S(M_Z^2)$ variation NLO set
MSHT20nnlo_mcrange_nf5	NNLO	5	9	0.118	Charm mass variation (1.2-1.6 GeV) NNLO set
MSHT20nnlo_mbrange_nf5	NNLO	5	7	0.118	Bottom mass variation (4.0-5.5 GeV) NNLO set
MSHT20nnlo_nf3,4	NNLO	3, 4	65	0.118	NNLO set with max. 3 or 4 flavours
MSHT20qed_nnlo	NNLO	5	77	0.118	NNLO set with QED effects and γ PDF
MSHT20qed_nnlo_(in)elastic	NNLO	5	77	0.118	NNLO set with QED effects and (in)elastic γ
MSHT20qed_nnlo_neutron	NNLO	5	77	0.118	NNLO neutron set with QED effects and γ
MSHT20an3lo_as118	aN3LO	5	105	0.118	Approximate N3LO set with theoretical uncertainties also included
MSHT20an3lo_as118_KCorr	aN3LO	5	105	0.118	Approximate N3LO set with theoretical uncertainties also included, K-factors correlated
PDF4LHC21	NNLO	5	901	0.118	Baseline PDF4LHC21 set
PDF4LHC21_mc	NNLO	5	101	0.118	Replica compressed PDF4LHC21 set
PDF4LHC21_40	NNLO	5	41	0.118	Hessian compressed PDF4LHC21 set

Selection of some of the MSHT PDF sets available in LHAPDF format. Many more online!

Key:

- Default   - $\alpha_S, m_{c,b}$ - QED   - aN3LO   - PDF4LHC21

- Feel free to contact us with questions about usage.