MSHT20aN3LO - Approximate N3LO PDFs with Theoretical Uncertainties

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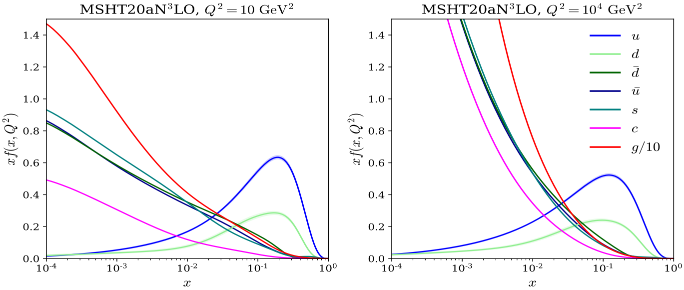
In collaboration with J. McGowan, L.A. Harland-Lang and R.S. Thorne.
More information in article: 2207.04739.

Overview

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.

  $\Rightarrow$ we can address both in one go! $\Rightarrow$ **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: 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 $P^{(3)}_{ab}(x)$	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 $A^{(3)}_{ab,H}(x)$	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) $C^{VF,(3)}_{H,a}$	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: 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)

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

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

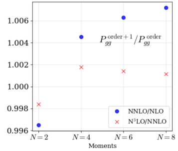
Experimental Nuisance parameters

- 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 $\sigma_{\theta'}$:

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

- 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



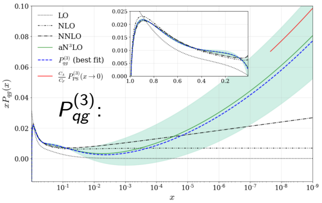
- Reminder - needed for PDF evolution, we know:
  - Even low-integer N Mellin Moments (4-8) - constrain intermediate and high x via $\int_0^1 dx\, x^{N-1} P(x)$.
  - Form at low x from resummation - LL log coefficients. (For $P_{gg}^{(3)}$ also NLL known)
- How do we incorporate this information?
  -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

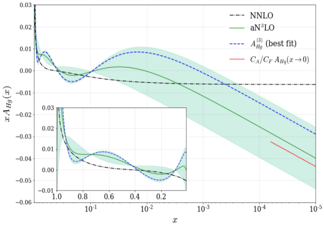
- So overall:

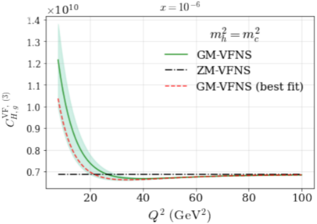
$$P_{ab}^{(3)}(x) = \sum_{i=1}^{k} A_i f_i(x) + f_e(x, \rho_{ab})$$



Transition Matrix Elements and DIS Coefficient Functions

- Transition matrix elements - needed to transition between number of flavours of PDFs at heavy quark masses, enter also structure functions:
  - Several transition matrix elements known completely - $A_{Hq}^{PS,(3)}$, $A_{gq,H}^{(3)}$.
  - Remaining not completely known ($A_{Hg}^{(3)}$, $A_{qq,H}^{NS,(3)}$, $A_{gg,H}^{(3)}$) deal with as for Splitting functions $\Rightarrow$ 1 nuisance parameter each - 3 in total from here.
- DIS Coefficient Functions - needed for N3LO Structure Functions:
  - Interpolate between high and low Q^2 known/approximated forms, include transition matrix elements to ensure cancellation of discontinuities.
  - Approximations to low-Q^2 FFNS coefficient functions $C_{H,\{q,g\}}$ have unknown NLL small x term $\Rightarrow$ 2 theory nuisance parameters c_q^{NLL}, c_g^{NLL}.





Hadronic K-factors

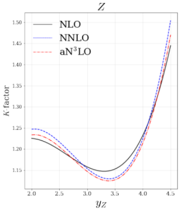
- N3LO calculations becoming available but not yet for PDF fits:
  - Higgs - ggF, VBF and VH [24,25,26,27] - doesn't go in PDFs.
  - Drell-Yan - Inclusive and some differential calculations [28,29,30,31] - not yet for relevant fiducial cross-sections or in form usable for PDFs.
  - Top (aN3LO) - soft 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:

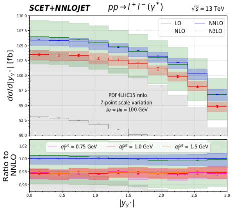
$$K^{N3LO/LO} = K^{NNLO/LO}(1+a_1\mathcal{N}^2\alpha_S^2(K^{NLO/LO}-1)+a_2\mathcal{N}\alpha_S(K^{NNLO/LO}-1))$$

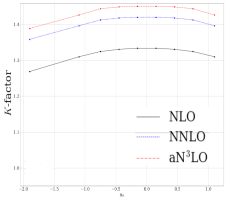
- Default prior is $a_1, a_2 = 0$, i.e. no N3LO correction.
- Categorise all hadronic processes into 5 types - jets (or dijets), Drell-Yan, top, vector boson p_T/jets, and dimuon.
- 2 theory nuisance parameters each $\Rightarrow$ 10 theoretical parameters added.

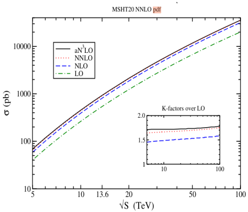
Hadronic K-factors

1. **Drell-Yan** (lower left 2 plots)
   - Fit prefers a $\approx 1\%$ decrease in the N3LO k-factors relative to NNLO.
   - Improved perturbative convergence with aN3LO PDFs.
   - In agreement with recent N3LO results (which used NNLO PDFs)[30].









2. **Top** (upper right two plots)
   - 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].

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.

Impact on fit and PDFs

More information in article: 2207.04739, J. McGowan, TC, L.A. Harland-Lang, R.S. Thorne.

Perform aN3LO fit - fit quality:

- Perform aN3LO fit with identical 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 $\Delta\chi^2 = -160.1$.
  - 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	1069.4/864	-18.5	+0.7
Dimuon datasets	125.0/170	-1.2	+0.5
Top datasets	75.1/71	-4.2	-2.5
p_T jets datasets	138.0/144	-77.2	-54.7
Jet datasets	963.6/739	+21.5	+42.2
Total	4961.2/4363	-160.1	-93.3

- Over half of fit improvement occurs without N3LO k-factors freedom.
- Many 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)
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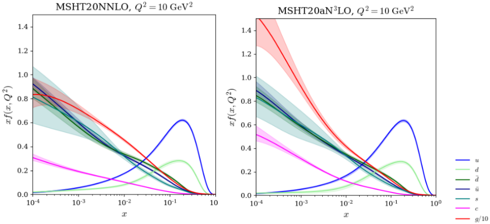
Total	4961.2/4363	-160.1	-93.3

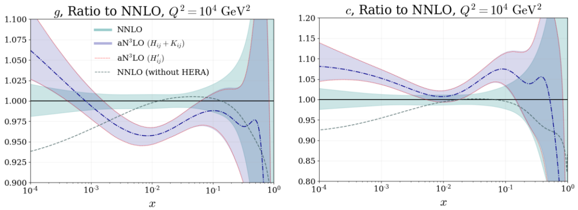
- Biggest improvement in DIS datasets, where most N3LO information known and included.
- Drell-Yan, dimuon, top improvements more from N3LO k-factor freedom; DY and top in approximate agreement with recent results.
- p_T jets improves significantly, mostly without N3LO k-factors - ATLAS 8 TeV Zp_T large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

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.
- Heavy quarks - c and b (perturbatively generated) raised due to increase in gluon at lower x and raised A_{Hg} at high x.



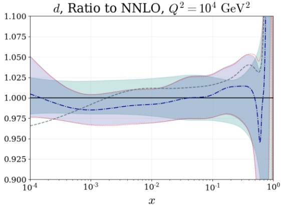
Green is NNLO, baseline for ratio.

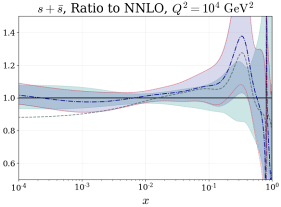
Blue dashed is aN3LO central + correlated k-factors in uncertainties.

Red line uncertainties with k-factors uncorrelated on aN3LO central.

Grey dashed is NNLO fit without HERA data.

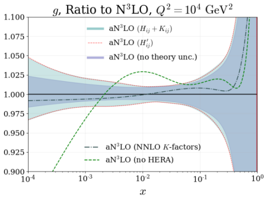
MSHT20aN3LO PDFs:

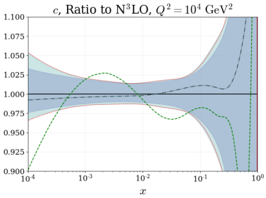




Green is NNLO, baseline for ratio.
Blue dashed is aN3LO central + correlated k-factors in uncertainties.
Red line uncertainties with k-factors uncorrelated on aN3LO central.
Grey dashed is NNLO fit without HERA data.

- Increase in $s + \bar{s}$ and light quarks at high x, aN3LO more similar to "no HERA" fit - eased tension.
- Gluon uncertainty enlarged at low x from splitting functions.
- Charm uncertainty enlarged, from both A_{Hg} at high x and gluon.
- Correlated and uncorrelated k-factors give consistent uncertainties.





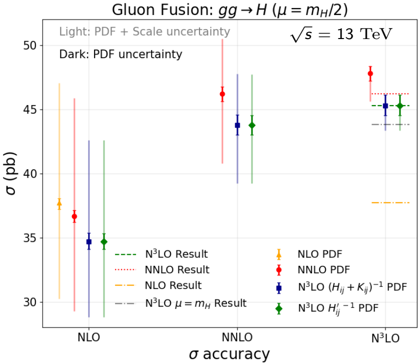
Blue band - no theoretical uncertainties included.
Green band is full MSHT20aN3LO uncertainty inc. theoretical uncertainties (correlated K-factors).
Red lines same as green bands but uncorrelated K-factors.
Grey dashed line is fit without N3LO K-factors.
Green dashed line is NNLO no HERA.

Effect on Cross-sections

More information in article: 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.

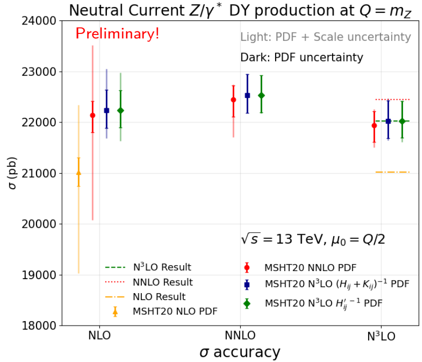
Results obtained using ggHiggs code[36].

- Increase in cross-section at N3LO compensated by reduction in PDFs at aN3LO ⇒ 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 Drell-Yan cross-sections:

Very preliminary!
Produced (in past week) 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.

Usage

More information in article: 2207.04739, J. McGowan, TC, L.A. Harland-Lang, R.S. Thorne.

Interpretation and Usage:

Available on LHAPDF (soon) and UCL website (now): `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.

Conclusions

More information in article: 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 uncertainties.
- This means we must include previously neglected effects - both higher orders and theoretical uncertainties.
- We have produced the 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 2207.04739.

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Backup Slides

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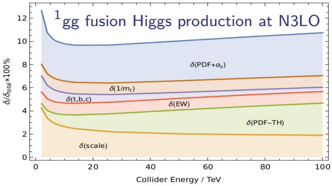
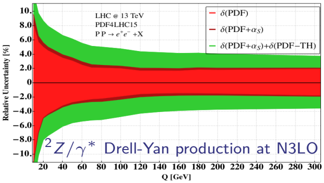
PDF Overview

- Significant developments on all three fronts - experimental, methodological, and theoretical.
- Current generation of PDFs, CT18, MSHT20, NNPDF3.1/4.0 are the most accurate and precise to date.
- However as experimental precision improves, demands placed on PDFs in terms of precision and accuracy are the most stringent ever.
- PDFs therefore remain dominant uncertainties for many processes.
- Requires efforts to both:
  1. Reduce current PDF uncertainties/differences - precision increase.
  2. Better understand and determine PDF uncertainties - accuracy increase.





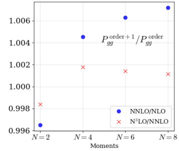
How can we incorporate N3LO knowledge into PDFs?

- After subbing in and rewriting obtain:

$$P(T|D) \propto \int d\theta' \exp\left(-\frac{1}{2}\left[(T' + \frac{\theta'}{\sigma_{\theta'}}u - D)^T H_0 (T' + \frac{\theta'}{\sigma_{\theta'}}u - D) + \theta'^2/\sigma_{\theta'}^2\right]\right)$$
$$\propto \int d\theta' \exp\left(-\frac{1}{2}M^{-1}(\theta' - \bar{\theta}')^2 - \frac{1}{2}(T' - D)^T H (T' - D)\right)$$
$$\propto \int d\theta' \exp\left(-\chi_1^2 - \chi_2^2\right)$$

- 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.

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:

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

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

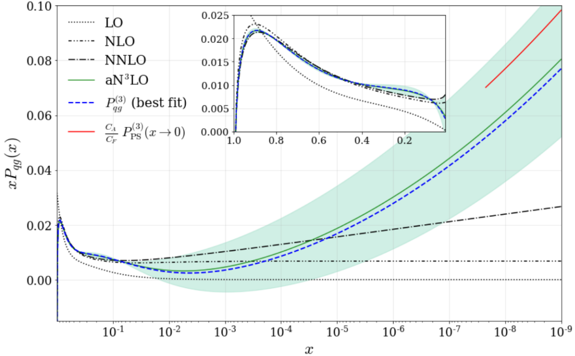
$$P_{qg}^{(3)}(x) = A_1 \ln^2 x + A_2 \ln x + A_3 x^2 + A_4 \ln(1-x) + \frac{C_A^3}{3\pi^4}\left(\frac{82}{81} + 2\zeta_3\right)\frac{1}{2}\frac{\ln^2(1/x)}{x} + \rho_{qg}\frac{\ln 1/x}{x}$$

- Set ρ_{ab} 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).

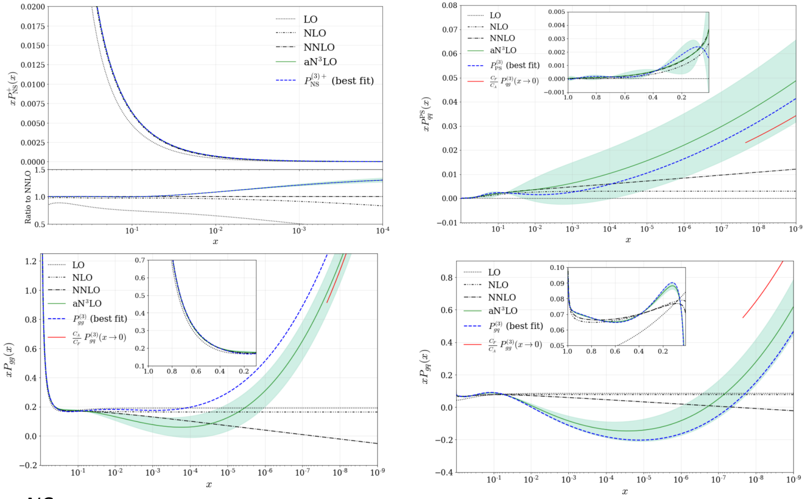
Splitting Functions

- 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, more divergent pieces gained at N3LO.
- Differences also at intermediate and high x, due to moment information.

Splitting Functions:

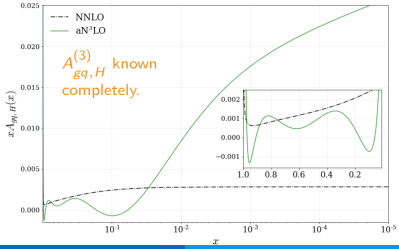


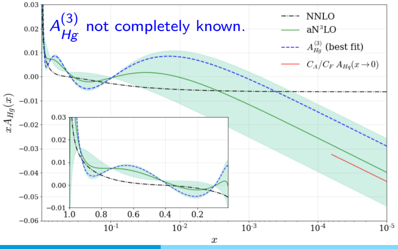
- $P_{qq}^{NS}(x)$ has small uncertainty as more info known (e.g. 8 Mellin moments, more exact info.), also less affected by small x as non-singlet.

Transition Matrix Elements

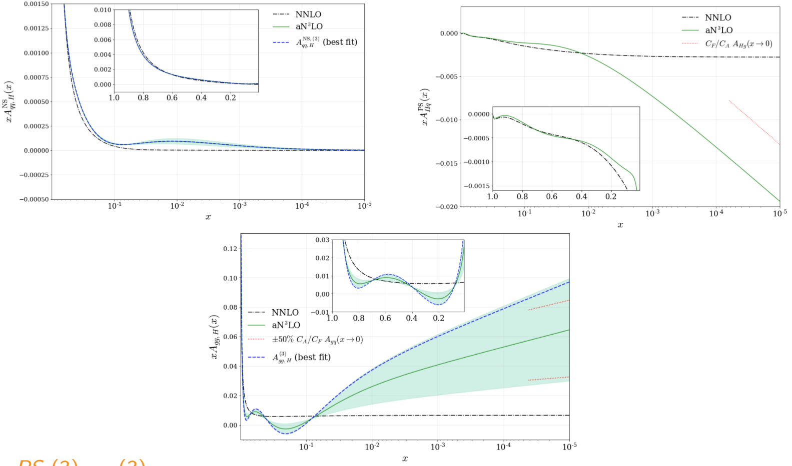
- Reminder - needed to transition between number of flavours of PDFs at heavy quark masses, enter also structure functions. We know:
  - Even low-integer N Mellin Moments (4-8)
    - constrain intermediate and high x via $\int_0^1 dx\, x^{N-1} P(x)$.
  - Form at low x, in some case low and high x limits.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





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

- 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 $A_{Hg}^{(3)}$:

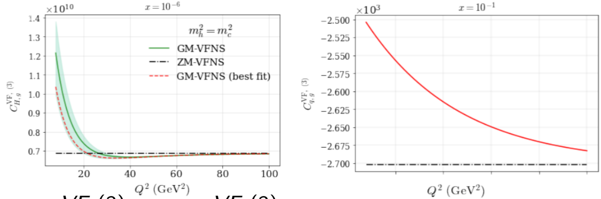
$$C_{H,g}^{VF,(3)} = C_{H,g}^{FF,(3)} - C_{H,g}^{VF,(2)} \otimes A_{gg,H}^{(1)} - C_{H,H}^{VF,NS+PS,(2)} \otimes A_{Hg}^{(1)} - C_{H,g}^{VF,(1)} \otimes A_{gg,H}^{(2)} - C_{H,H}^{VF,(1)} \otimes A_{Hg}^{(2)} - C_{H,H}^{VF,(0)} \otimes A_{Hg}^{(3)}$$

DIS Coefficient Functions

- Theoretical uncertainties included directly where relevant in some DIS coefficient functions, as well as those from transition matrix elements.
- 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}:

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

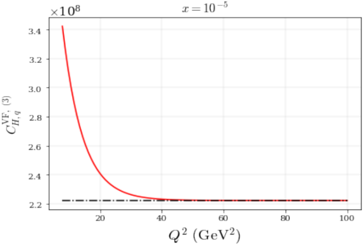
$\Rightarrow$ 2 Theory Nuisance Parameters from here.

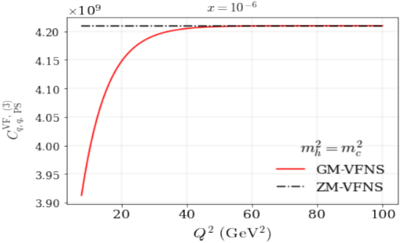


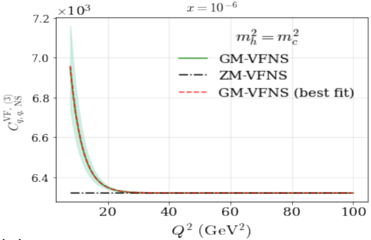
- Overall, $C_{Hq}^{VF,(3)}$ and $C_{Hg}^{VF,(3)}$ have uncertainties from added c_q^{NLL} and c_g^{NLL} parameters, $C_{Hg}^{VF,(3)}$ and $C_{qq,NS}^{VF,(3)}$ inherit uncertainty from $A_{Hg}^{(3)}$ and $A_{qq,NS}^{(3)}$. No theoretical uncertainties on $C_{qg}^{VF,(3)}$, $C_{qq,PS}^{VF,(3)}$.

DIS Coefficient Functions:

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



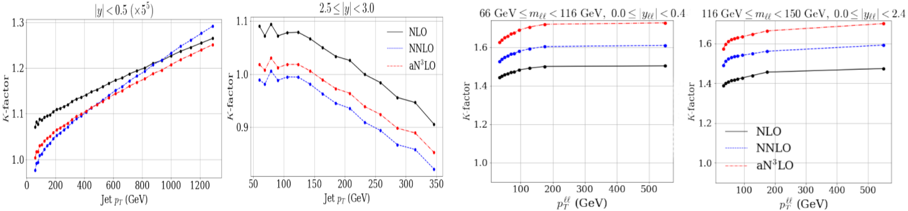




- $C_{Hq}^{VF,(3)}$ and $C_{Hg}^{VF,(3)}$ have uncertainties from c_q^{NLL} and c_g^{NLL} parameters, $C_{Hg}^{VF,(3)}$ and $C_{qq,NS}^{VF,(3)}$ inherit uncertainty from $A_{Hg}^{(3)}$ and $A_{qq,NS}^{(3)}$.

Hadronic K-factors

3. **Jets** (lower left 2 plots)
   - Fit prefers a mild shift of aN3LO k-factors relative to NNLO.
   - Good qualitative perturbative convergence.



4. **Vector boson + jets, Zp_T** (upper right two plots)
   - Fit prefers larger shifts here, NLO→NNLO and NNLO→aN3LO similar.
   - May be picking up sensitivity to all-order result via experimental data.
5. **Dimuon** - Semi-inclusive DIS
   - Already freedom to change BR($D \to \mu$) here, so limited sensitivity. BR reduces to 0.082 from 0.088 - within allowed 0.092 ± 0.01 range.

Dijet data:

Preliminary!

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

- 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 jets.
  - Generally pull improves Zp_T fit and worsens top slightly.
  - Moreover, dijet fit quality improves further slightly at aN3LO.

.	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	472	1.39	1.43	Total	266	1.12	1.04

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

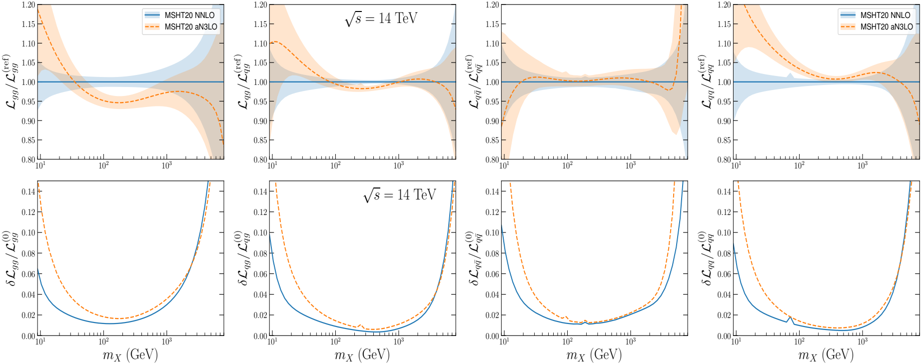
aN3LO Theory Nuisance Parameters:

- 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			
$a_{Hg} = 12214.000$ $a_{gg,H} = -1951.600$	0.601 0.857	$a_{qq,H}^{\mathrm{NS}} = -64.411$	0.001
Splitting Functions			
$\rho_{qq}^{NS} = 0.007$ $\rho_{qq}^{PS} = -0.501$ $\rho_{qg} = -1.754$	0.000 0.186 0.015	$\rho_{gq} = -1.784$ $\rho_{gg} = 19.245$	0.802 3.419
K-factors			
$\mathrm{DY_{NLO}} = -0.307$ $\mathrm{Top_{NLO}} = 0.041$ $\mathrm{Jet_{NLO}} = -0.300$ $p_T\mathrm{Jets_{NLO}} = 0.583$ $\mathrm{Dimuon_{NLO}} = -0.444$	0.094 0.002 0.090 0.339 0.197	$\mathrm{DY_{NNLO}} = -0.230$ $\mathrm{Top_{NNLO}} = 0.651$ $\mathrm{Jet_{NNLO}} = -0.691$ $p_T\mathrm{Jets_{NNLO}} = -0.080$ $\mathrm{Dimuon_{NNLO}} = 0.922$	0.053 0.424 0.478 0.006 0.850
N^{3}LO Penalty Total	9.262 / 20	Average Penalty	0.463

- All but one within prior chosen variation (penalty < 1), many penalties very small - conservative.
- Average penalty across the 20 parameters is 0.463.
- Fit able to describe data well with only small departures around prior N3LO knowledge.

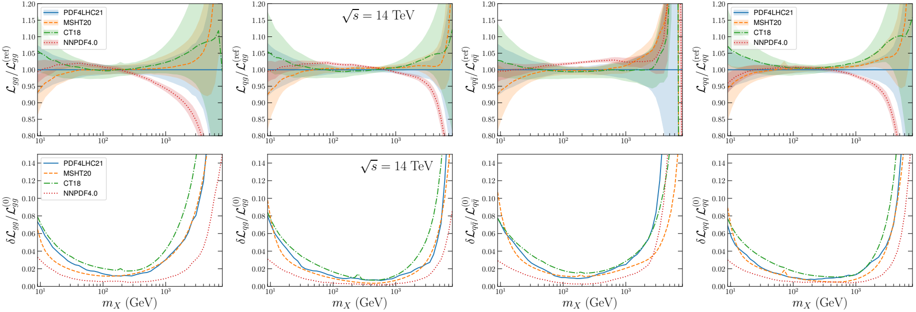
aN3LO PDF luminosities:



- 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.

Global Fits Luminosities Comparison:

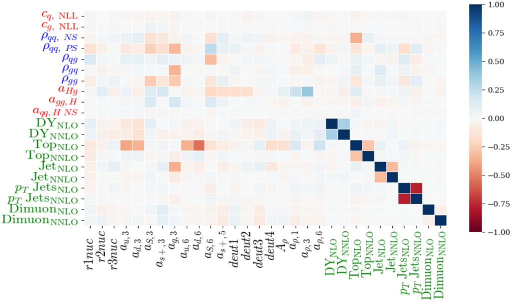
- Compare global fits at the level of the parton-parton luminosities:



- 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 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:

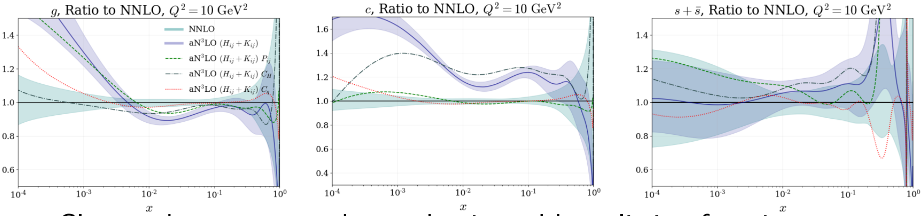
$$H'^{-1}_{ij} \rightarrow H^{-1}_{ij} + \sum_{p=1}^{N_p} K^{-1}_{ij,p}$$

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 effects on PDFs:

- For gluon, charm and strange consider effects of only aN3LO splitting functions, heavy or light flavour coefficient functions (and associated transition matrix elements) to breakdown effects on PDFs:



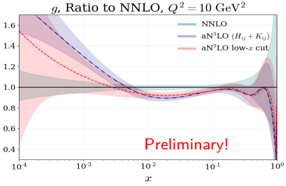
- Gluon enhancement at low x dominated by splitting functions.
- Gluon reduction around $x \sim 10^{-2}$ from combination of splitting functions and coefficient functions.
- Charm enhancement largely due to heavy flavour coefficient function (and transition matrix elements) in combination with increased gluon.
- Strange enhancement at high x reflects splitting functions and heavy flavour coefficient functions.

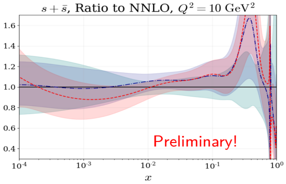
aN3LO PDFs - small x and high x: Preliminary!

- 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 in aN3LO fit.

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	-2.0	ATLAS 8 TeV W+jets	30	-1.7	-0.8
ATLAS 7 TeV jets	140	+6.5	+1.8	Top total	71	-4.4	+2.2
CMS 7 TeV jets	158	+3.8	+1.0	Total	3042	-61.6	-48.0

- Perform fits with small $x < 10^{-3}$ data removed:

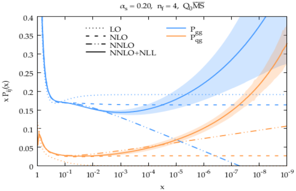


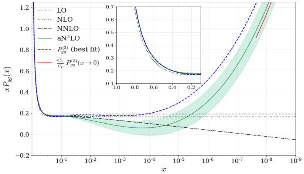


- Small x removal has limited effects on central values at high x.
- Small x uncertainties increase as expected.

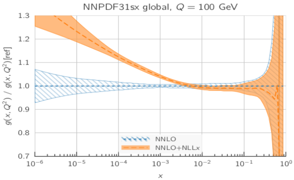
aN3LO at low x vs resummed:

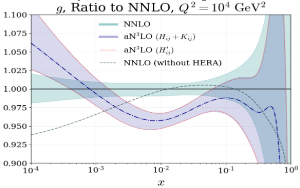
- We include LL low x resummed terms (and NLL with variable coefficient) in splitting functions - compare with resummed results[33]:





- 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].

Impact on Higgs cross-sections - ggF:

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

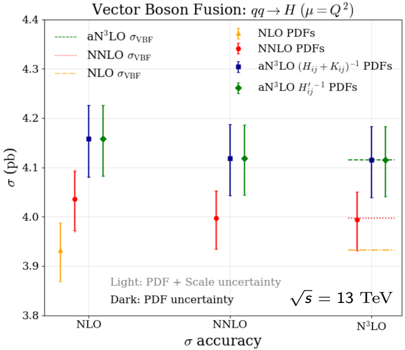
σ order	PDF order	$\sigma + \Delta\sigma_+ - \Delta\sigma_-$ (pb)	σ (pb) $+ \Delta\sigma_+ - \Delta\sigma_-$ (%)
	PDF uncertainties		
N^{3}LO	aN^{3}LO (no theory unc.)	$45.296 + 0.723 - 0.545$	$45.296 + 1.60\% - 1.22\%$
	aN^{3}LO ($H_{ij} + K_{ij}$)	$45.296 + 0.832 - 0.755$	$45.296 + 1.84\% - 1.67\%$
	aN^{3}LO (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^{3}LO	aN^{3}LO (no theory unc.)	$45.296 + 0.723 - 1.851$	$45.296 + 1.60\% - 4.09\%$
	aN^{3}LO ($H_{ij} + K_{ij}$)	$45.296 + 0.832 - 1.923$	$45.296 + 1.84\% - 4.25\%$
	aN^{3}LO (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:

- 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 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			
N^3LO	aN^3LO (no theory unc.)	$4.1150 + 0.0638 - 0.0724$	$4.1150 + 1.55\% - 1.76\%$
	aN^3LO $(H_{ij} + K_{ij})$	$4.1150 + 0.0682 - 0.0755$	$4.1150 + 1.66\% - 1.83\%$
	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			
N^3LO	aN^3LO (no theory unc.)	$4.1150 + 0.0638 - 0.0724$	$4.1150 + 1.55\% - 1.76\%$
	aN^3LO $(H_{ij} + K_{ij})$	$4.1150 + 0.0683 - 0.0755$	$4.1150 + 1.66\% - 1.83\%$
	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) $+ \Delta\sigma_+ - \Delta\sigma_-$ (%)
N^3LO	aN^3LO $n_f = 5$	4.1150 + 0.0683 - 0.0755	4.1150 + 1.66% - 1.83%
	aN^3LO $n_f = 4$	4.0270 + 0.0685 - 0.0765	4.0270 + 1.70% - 1.90%
	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.

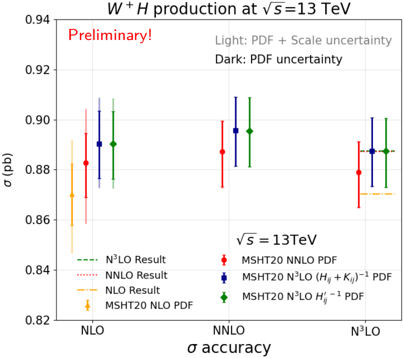
- PDF uncertainty increase from NNLO to aN3LO less than in ggF case.
- Scale dependence negligible at NNLO and aN3LO.
- Comparing $n_f = 3, 4$ see difference in NNLO and aN3LO predictions doubles once charm included.

Impact on *VH* cross-sections:

Very preliminary!

Produced (in past week) using the `n3loxs` code[27].

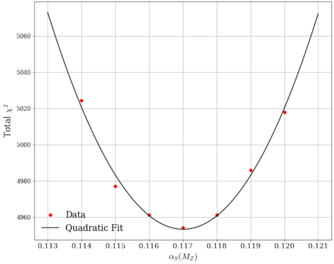
- Consider impact of our aN3LO PDFs on *VH* associated production at LHC, e.g. W^+H at 13 TeV:

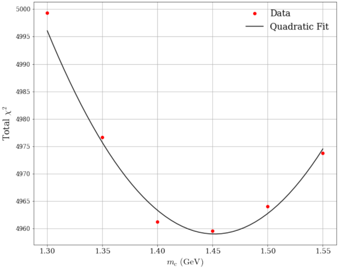


- Result with aN3LO PDFs raised slightly, reflects increased quarks at high x, antiquarks at low x and strange and charm.
- N3LO σ + aN3LO PDF result very close to NNLO σ + NNLO PDF result, increased stability in predictions.

Strong Coupling and heavy quarks:

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

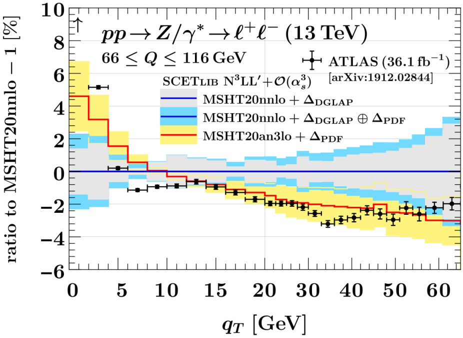




- aN3LO best fit: $\alpha_S(M_Z^2) = 0.1170$, overlaps with NNLO world average.
- NNLO best fit and uncertainty: $\alpha_S(M_Z^2) = 0.1174 \pm 0.0013$.
- NLO best fit and uncertainty: $\alpha_S(M_Z^2) = 0.120 \pm 0.0015$. TC et al, 2106.10289.
- m_c best fit ~ 1.45 GeV, compare with ~ 1.35 GeV at NNLO, so now better agreement with world average $m_c = 1.5 \pm 0.2\text{GeV}$.
- 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:

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

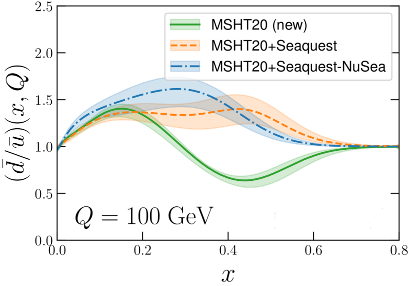


- aN3LO PDFs fit the measured ATLAS data better, likely due to indirect effects of gluon shape change....
- Credit: `SCETlib`, Johannes Michel - LHC EW WG meeting Sep 2022.

New data - Seaquest

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}: $0.65 \rightarrow 1.27$, 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.

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.