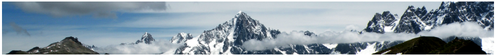
MSHT20aN3LO

- Approximate N3LO PDFs with Theoretical Uncertainties

Thomas Cridge

Les Houches PhysTeV 2023, 16th June 2023



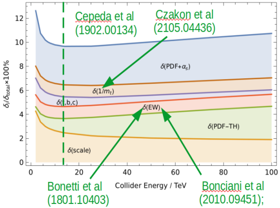
In collaboration with J. McGowan, L.A. Harland-Lang and R.S. Thorne.

More information in article: Eur. Phys. J. C 83 (2023) 3, 185, arXiv:hep-ph/2207.04739.

Motivation

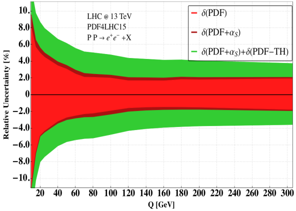
- As experiments become more precise, need to improve accuracy and precison of theoretical predictions $\Rightarrow$ N3LO.
- Progress for N3LO cross-sections: Higgs (ggF, VBF, VH), DY(NC, CC).

Higgs - ggF:



LHC Higgs XSWG 2019

Drell-Yan - NC:



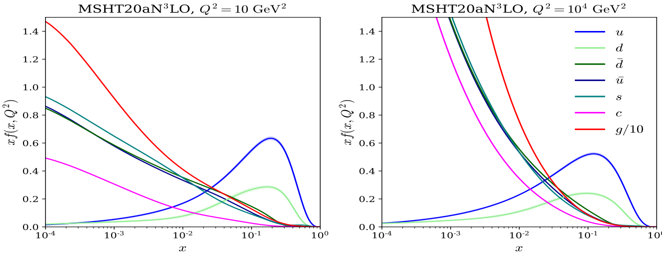
Duhr, Mistelberger 2111.10379

- PDF uncertainties $\delta(\mathrm{PDF})$ large $\Rightarrow$ hope to reduce at higher orders.
- Mismatch between N3LO σ and NNLO PDF $\Rightarrow$ $\delta(\mathrm{PDF} + \mathrm{th})$.
- PDFs at N3LO are becoming a bottleneck.
- PDF theoretical uncertainties are needed for missing/incomplete higher orders (MHOUs) to assess accuracy and uncertainties.

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**.
- Include known N3LO effects already into PDFs and to parameterise remaining unknown pieces via theory nuisance parameters.
- Variation of these remaining unknown N3LO pieces then provides a theoretical uncertainty within an approximate N3LO fit (aN3LO).



What do we need to know for N3LO PDFs?

- Need 4 ingredients. Current Knowledge (schematic summary):

Theory	Utility	Order required	What's known?
1. 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]
2. 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].
3. 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)[13,16−17], ZM-VFNS (high Q^2) N3LO coefficient functions known exactly[18]. Therefore GM-VFNS interpolation not completely known.
4. Hadronic Cross-sections (K-factors)	Determine cross-sections at N3LO	N3LO	Very little (none in usable form for PDFs)

- None of these are completely known, but a lot of information already.
- How to construct approximate N3LO PDFs given theory info. not fully known? Include known info. + theory nuisance parameters.

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)

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

Experimental Nuisance parameters

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

- 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'.

- Why this approach and theory nuisance parameters (TNPs):
  1. TNPs probe precisely the missing pieces, not lower orders.
  2. Allow inclusion of known N3LO pieces without risk of MHOU probing known info.
  3. Can be updated as and when new N3LO info is available.
  4. Scale variations in PDF fit and predictions need to be correlated.

Splitting Functions: What do we know and include?

- 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): Constrain high/intermediate x.

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

  Intermediate x $\longrightarrow$ $f_2(x) = \ln x$, $f_3(x) = 1$ or x or x^2,

  Higher x $\longrightarrow$ $f_4(x) = \ln^4(1-x)$ or $\ln^3(1-x)$ or $\ln^2(1-x)$ or $\ln(1-x)$,

  Try different functions for each f_i, include in uncertainty.

- Exact information included in $f_e(x, \rho_{ab})$ - LL terms at low x included.

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

(For $P_{gg}^{(3)}$ also NLL known)

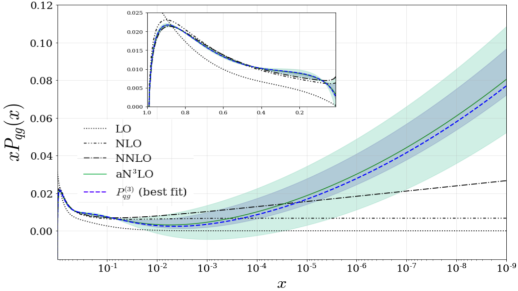
- Coefficient of low x NLL is dominant missing piece, include with theory nuisance parameter ρ_{ab} to incorporate MHOU: $\Rightarrow \rho_{qg}\frac{\ln 1/x}{x}$.

Overall:

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

Splitting Functions

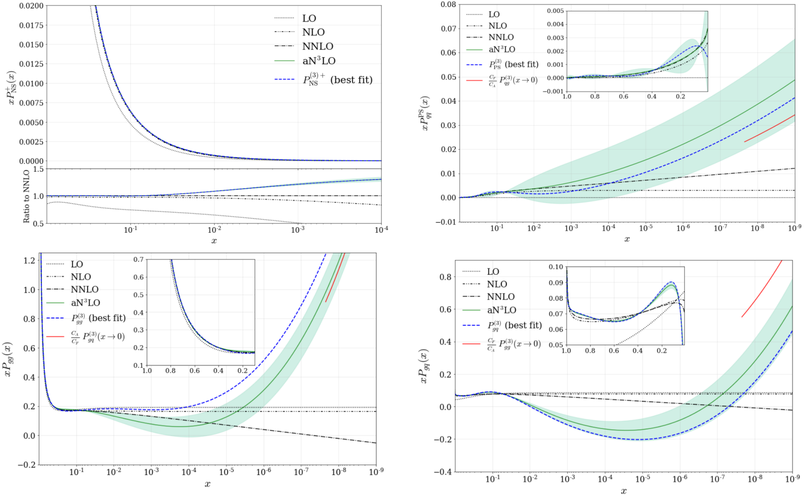
- Overall result for $P_{qg}^{(3)}$:



- 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.

Splitting Functions - Repeat for others:

1 Theory Nuisance Parameter per Splitting Function $\Rightarrow$ 5 from here.



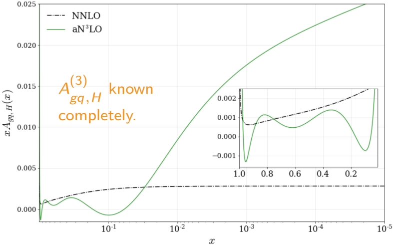
- $P_{qq}^{NS}(x)$ has small uncertainty as more info known (e.g. 8 Mellin moments, more exact info.), also less affected by small x as non-singlet.

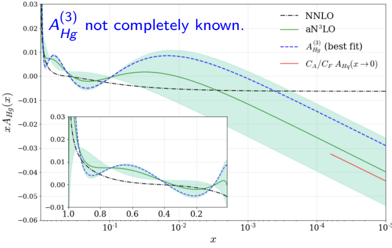
Transition Matrix Elements

- Several transition matrix elements known completely - $A_{Hq}^{PS,(3)}$, $A_{gq,H}^{(3)}$.
- For others 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.
- 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}, $a_{qq,H}^{NS}$, $a_{gg,H}$.

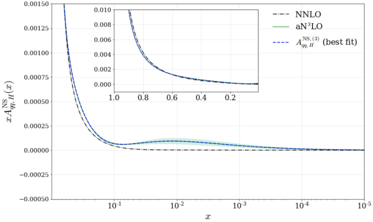
J. Blümlein et al 2107.06267.

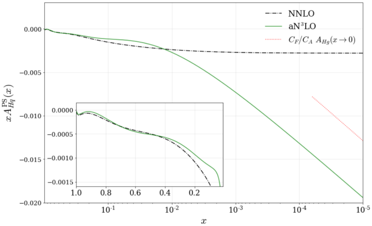
J. Ablinger et al 2211.05462.

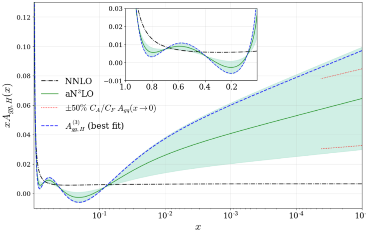




Transition Matrix Elements:







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

DIS Coefficient Functions

- Needed to produce N3LO Structure Functions, 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 $A_{Hg}^{(3)}$:

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

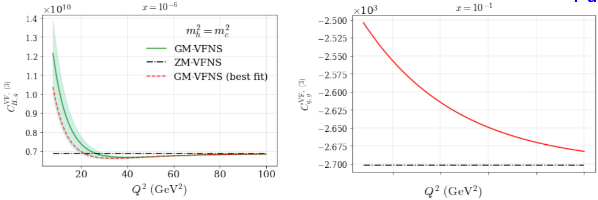
DIS Coefficient Functions

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

- 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}:

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

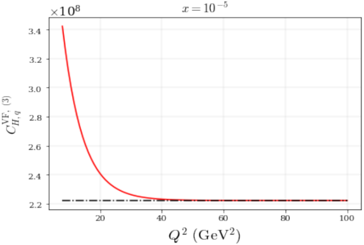
$\Rightarrow$ 2 Theory Nuisance Parameters from here.

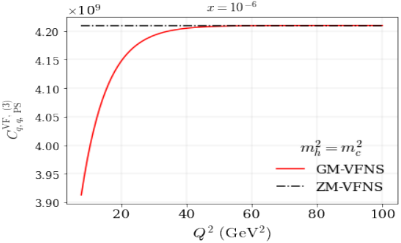


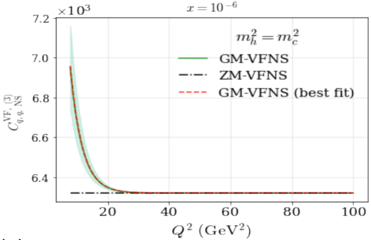
- $C^{VF,(3)}_{Hq}$ and $C^{VF,(3)}_{Hg}$ have uncertainties from c_q^{NLL} and c_g^{NLL} parameters, $C^{VF,(3)}_{Hg}$ and $C^{VF,(3)}_{qq,NS}$ inherit uncertainty from $A^{(3)}_{Hg}$ and $A^{(3)}_{qq,NS}$.

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

- N3LO calculations becoming available but not yet for PDF fits:
  - Higgs - ggF, VBF and VH [25,26,27,28] - doesn't go in PDFs.
  - Drell-Yan - Inclusive and some differential calculations [29,30,31,32] - not yet for relevant fiducial cross-sections or in form usable for PDFs.
  - Top (aN3LO) - soft gluon resummation approximation[33].
- 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:

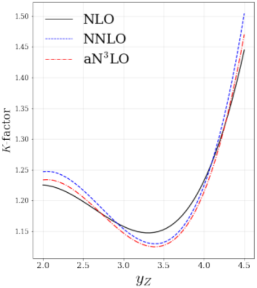
$$K^{N3LO/LO} = K^{NNLO/LO}(1 + a_1 \mathcal{N}^2 \alpha_S^2 (K^{NLO/LO} - 1) + a_2 \mathcal{N} \alpha_S (K^{NNLO/LO} - 1))$$

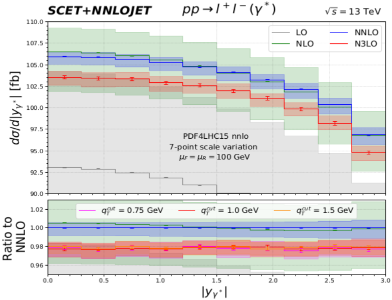
- Default prior is $a_1, a_2 = 0$, i.e. no N3LO correction.
- Categorise all hadronic processes into 5 types - jets (or dijets), Drell-Yan, top, vector boson p_T/jets, and dimuon.
- 2 theory nuisance parameters each $\Rightarrow$ 10 theoretical parameters added.

Hadronic K-factors - 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:[31].





- Key point: Method allows N3LO info. on any piece to be incorporated as it becomes available, rather than needing to wait for all info. - e.g. can include N3LO k-factors as they become available for PDFs.

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).

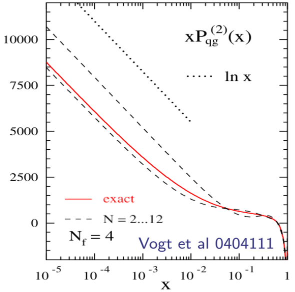
Origin	Parameters	Number of Added Parameters
Splitting Functions - $P_{qg}^{(3)}$, $P_{qq}^{NS,(3)}$, $P_{qq}^{PS,(3)}$, $P_{gq}^{(3)}$, $P_{gg}^{(3)}$	ρ_{qg}, ρ_{qq}^{NS}, ρ_{qq}^{PS}, ρ_{gq}, ρ_{gg}	5
Transition Matrix Elements - $A_{Hg}^{(3)}$, $A_{qq,H}^{NS,(3)}$, $A_{gg,H}^{(3)}$	a_{Hg}, $a_{qq,H}^{NS}$, $a_{gg,H}$	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	$Dimuon_{NLO}$, $Dimuon_{NNLO}$	

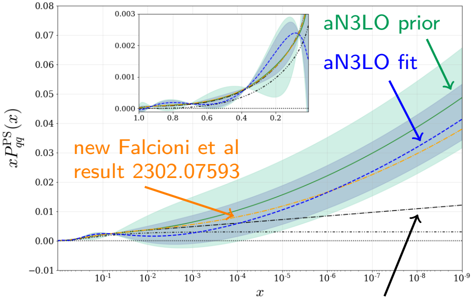
- Using `MSHT20an3lo_as118` eigenvectors as usual naturally incorporates MHOUs at aN3LO into the PDF uncertainties.

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

Validation of Methodology :

- Approach of using small-x limits and Mellin moments to approximate exact results is used by groups which calculate the higher order pieces.
- Moreover, similar approaches were used at NLO and matched eventual full NNLO result well[19–24] (e.g. by MRST and others).





- 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!.

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

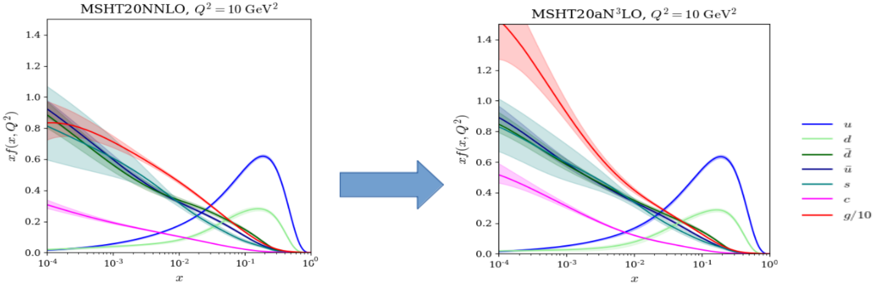
Smooth fit improvement with order and amount of improvement reducing with order - as we might hope.

- Improvement in fit quality from NNLO to aN3LO is $\Delta\chi^2 = -154.4$.
  - 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

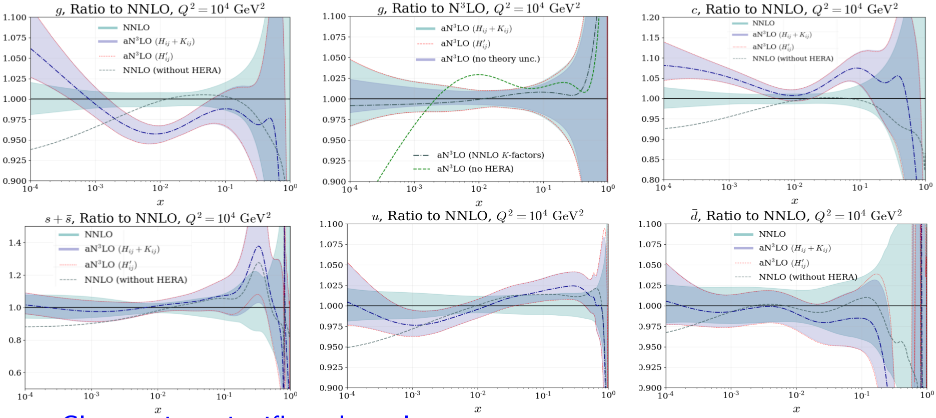
- Penalties on TNPs after fit are small $\Rightarrow$ prior set conservatively.
- Fit clearly prefers known N3LO info, even though it can depart significantly from NNLO.

aN3LO PDFs:



- Gluon raises significantly at low x. - from large logs in splitting functions, not present at NNLO.
- Heavy quarks - c and b (perturbatively generated) raised, due to increase in gluon at lower x and raised A_{Hg} at high x.
- Milder effects on other PDFs.
- Uncertainties may be enlarged at low x from MHOUs.

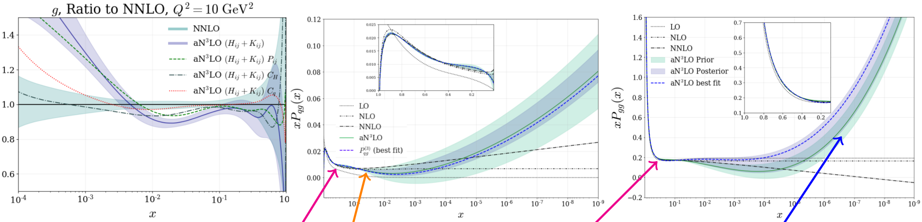
aN3LO PDFs:



- Gluon raises significantly at low x.
- Heavy quarks - c and b (perturbatively generated) raised.
- Milder effects on other PDFs.
- Uncertainties may be enlarged at low x from MHOUs.

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

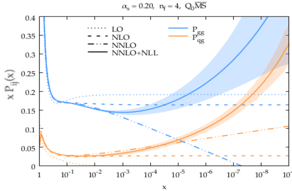
- Around $10^{-2} \lesssim x \lesssim 10^{-1}$ P_{ij}, C_H contribute $\approx$ equally. Also some C_q.
- At low x P_{ij} dominate, this contains much known N3LO information.

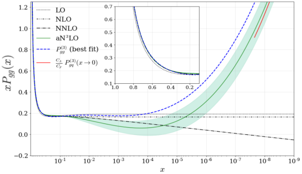


- Known Mellin moments tightly constrain high x splitting functions.
- At intermediate x increased P_{qg} and momentum sum rule affect gluon.
- At small x, LL and NLL (latter for P_{gg}) resummed pieces dominate.
- P_{gq} (not shown) has largest power of unknown log: $\log^2(1/x)/x$.
- Most singular 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 at low x vs resummed:

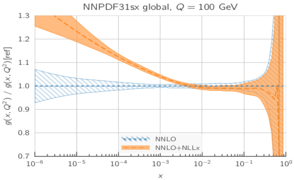
- We include up to (N)LL low x resummed terms (and (N)NLL with variable coefficient) in splitting functions - compare with resummed[35]:

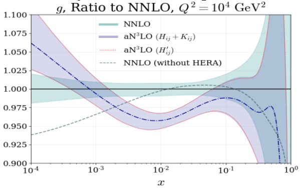




Compare blue solid (left) and dashed (right) lines for P_{gg}.

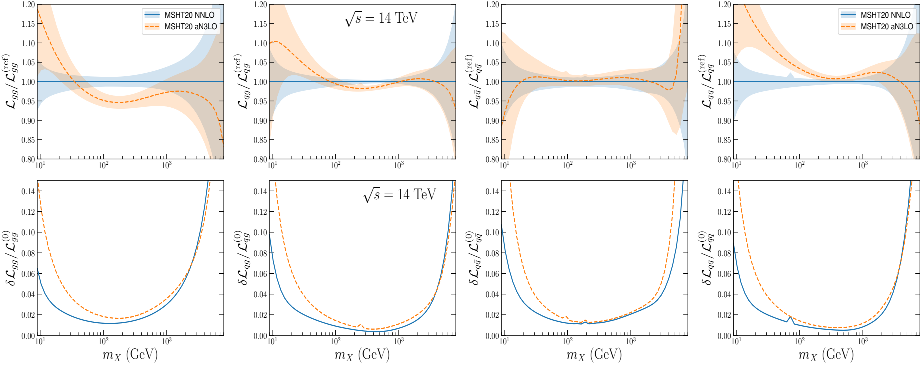
- Similar effects qualitatively (note scheme difference!) on P_{ij}s.
- Impact on gluon also shows similarities qualitatively to[34]:





- In MSHT20aN3LO have $\Delta\chi^2 = -91$ for DIS data from NNLO, with -68 in HERA, cf ~ -70 in both[35] and xFitter small x resummed study[36].

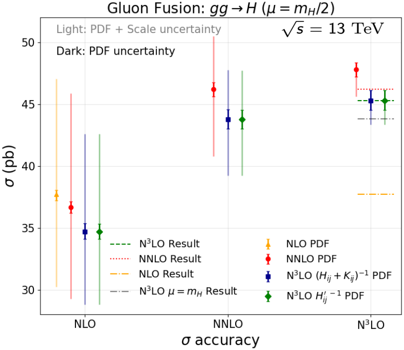
aN3LO PDF luminosities:



- 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.

Impact on Higgs cross-sections - ggF:

- Consider impact of our aN3LO PDFs on known N3LO Higgs production in gluon fusion[25,26] - 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.

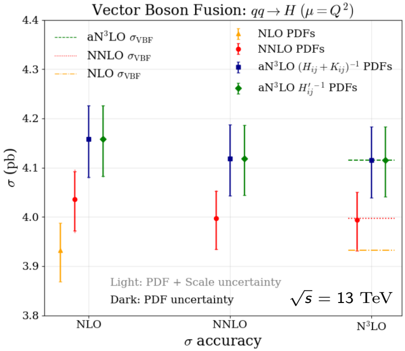
Results obtained using ggHiggs code[37].

- 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 (dark) enlarged - inclusion of MHOUs.

Preliminary!

Impact on Higgs cross-sections - VBF:

- Consider impact of our aN3LO PDFs on known N3LO Higgs production in vector boson fusion[27]:



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.

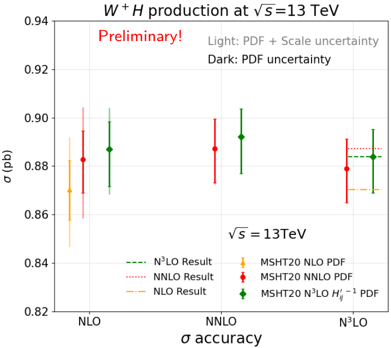
Results obtained using `proVBFH` code[27,38].

- 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 VH cross-sections:

Preliminary!

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



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.

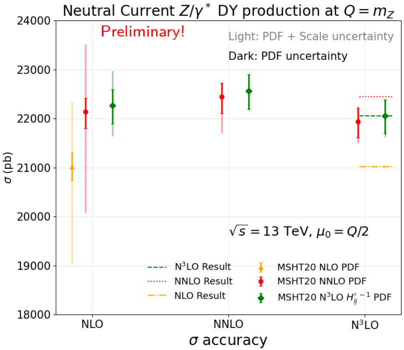
Results obtained using the `n3loxs` code[28].

- 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.

Preliminary!

Impact on Drell-Yan cross-sections:

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



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 the `n3loxs` code[28].

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

Conclusions:

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

- 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 also 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 ⇒ please ask us!

Selection of some references (others on slides)

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[2] Duhr, Mistelberger, 2111.10379.

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[27] F.A. Dreyer and A. Karlberg, 1606.00840.

[28] J. Baglio, C. Duhr, B. Mistlberger, R. Szafron, 2209.06138.

[29] C. Duhr, F. Dulat and B. Mistlberger, 2001.07717.

[30] C. Duhr, F. Dulat and B. Mistlberger 2007.13313.

[31] X. Chen et al., 2107.09085.

[32] C. Duhr and B. Mistlberger, 2111.10379.

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[36] H. Abdolmaleki et al, xFitter, 1802.00064.

[37] M. Bonvini, arXiv:1805.08785.

[38] M. Cacciari et al, 1506.02660.

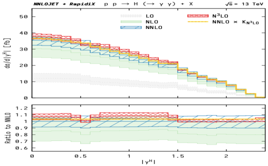
Backup Slides

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).

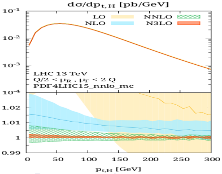
Particle Physics and N3LO Progress

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

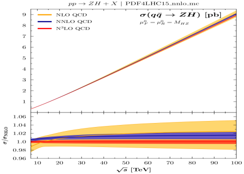
1. Higgs - Differential for ggF (y_H, etc) and VBF (p_T^H, y_H), inclusive VH:



Chen et al 2102.07607

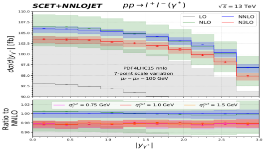


Dreyer et al 1606.00840

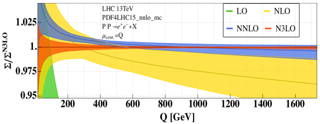


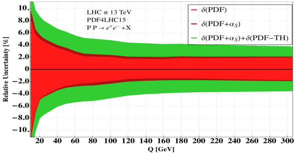
Baglio et al 2209.06138

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



Chen et al 2107.09085.





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. ⇒ this talk is a solution . . .

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

- Find penalties on theory nuisance parameters after fit are small and posterior errorbands reduced relative to prior $\Rightarrow$ prior set conservatively.
- All but one within prior chosen variation (penalty < 1).
- Results checked to not depend sensitively on the prior chosen.
- Fit able to describe data well with only small departures around prior.

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

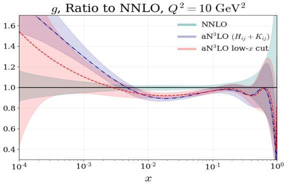
- Biggest improvement in DIS data $\Rightarrow$ most N3LO info. included.
- Drell-Yan, dimuon, top improvements more from N3LO k-factor freedom; DY and top in approximate agreement with recent results.
- V p_T/ V + jets improves significantly, mostly without N3LO k-factors - ATLAS 8 TeV Zp_T large improvement 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 only class which gets worse at aN3LO - try dijets?

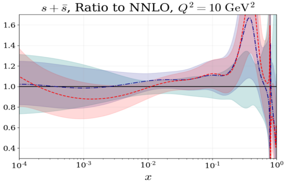
aN3LO PDFs - small x and high x:

- 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	$N_{\rm pts}$	$\Delta\chi^2$ no HERA vs full		Datasets	$N_{\rm pts}$	$\Delta\chi^2$ 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.

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.

Preliminary!

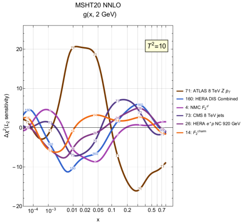
aN3LO vs NNLO, ATLAS 8 TeV Zp_T data:

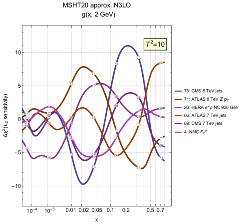
- ATLAS 8 TeV Zp_T data improved substantially in χ^2 at aN3LO :
- Fit different subsections of the data by altering the p_T^{cut}:

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

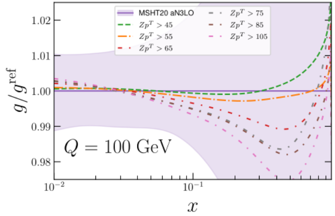
ATLAS 8 TeV Zp_T fit qualities with increasing the lower cut on the p_T^{ll}.

- 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:

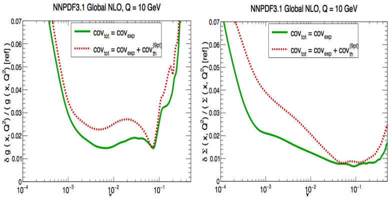


Other approaches for theoretical uncertainties in PDFs?

- An alternative is through scale variations.
- Vary renormalisation and factorisation scales in fit data to give a "theory covariance matrix" to incorporate into PDF uncertainties.

NNPDF, 1905.04311, 1906.10698, 2105.05114

- Can also instead do a joint fit of PDF and scale uncertainties. → NNPDF 2207.07616
- So far both only NLO by NNPDF3.1, marginally increased PDF uncertainties and improved χ^2/N_{pts}. Preliminary NNLO results shown at DIS23 (G. Magni).

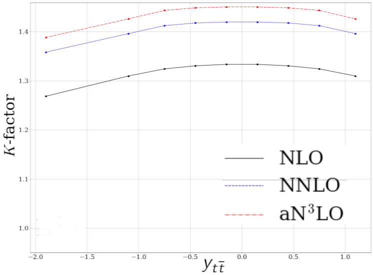


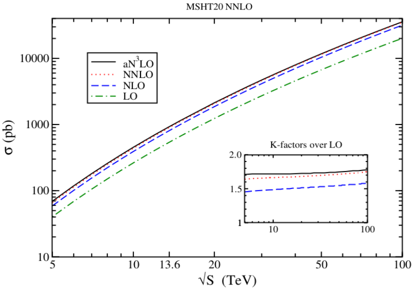
χ^2/N_{dat} in the NNPDF3.1 global fits	C	$C+S^{(9pt)}$	$C+S^{(7pt)}$	$C+S^{(3pt)}$	$C+S^{(9pt)}_{fit}$	$C+S^{(9pt)}_{samp}$
	1.139	1.109	1.129	1.139	1.113	1.220

- Specific issues include:
  1. Need to correlate PDF scale variations with theoretical predictions. (L.A. Harland-Lang, R.S. Thorne 1811.08434)
  2. Only varies terms appearing at lower order, not new terms.
  3. Does not incorporate already-known higher order information.

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].

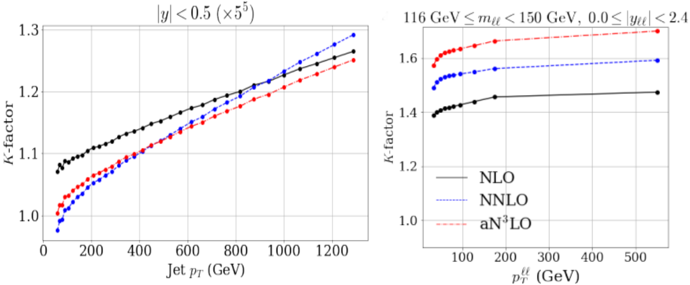




3. **Dimuon** - Semi-inclusive DIS
   - Already freedom to change BR($D \to \mu$) here, so limited sensitivity. BR reduces to 0.082 from 0.088 - within allowed 0.092 ± 0.01 range.

Hadronic K-factors

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

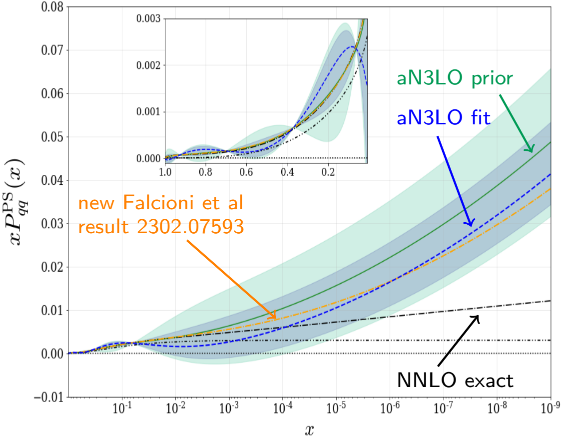


5. **Vector boson + jets, Zp_T** (upper right plot)
- Fit prefers larger shifts here, NLO→NNLO and NNLO→aN3LO similar.
- May be picking up sensitivity to all-order result via experimental data.

Further aN3LO information?:

<u>What else could be added?:</u>

- 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.
- $A_{gg,H}^{(3)}$ recently calculated. J. Ablinger et al 2211.05462.
- 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!

How can we incorporate N3LO knowledge into PDFs?

- After subbing in and rewriting obtain:

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

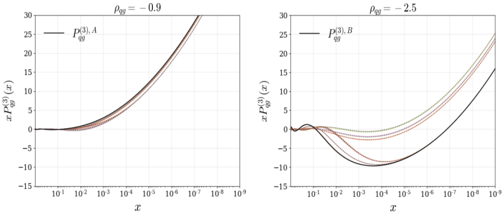
$$\propto \int d\theta' \exp\left(-\frac{1}{2}M^{-1}(\theta' - \bar{\theta}')^2 - \frac{1}{2}(T' - D)^T H (T' - D)\right)$$

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

- 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:

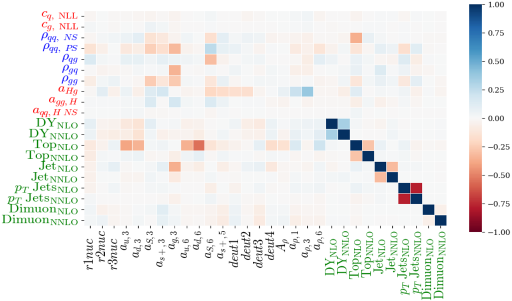
- Key part of the theoretical nuisance parameter framework for missing N3LO pieces is setting up the priors and penalties on their variations.
- Q. How do we do this? A. Conservatively!
- Set ρ_{ab} prior variation by requiring:
  1. At low x bound set once exact expression $f_e(x, \rho_{ab})$ exits 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:

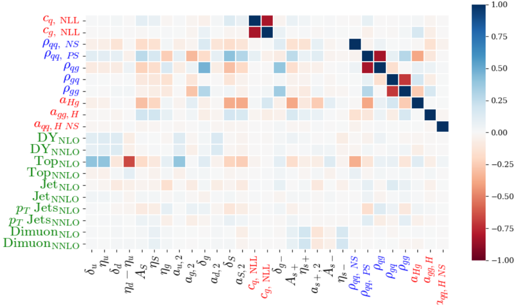
$$H'^{-1}_{ij} \rightarrow H^{-1}_{ij} + \sum_{p=1}^{N_p} K^{-1}_{ij,p}$$

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!

Dijet data:

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

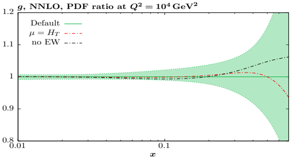
Preliminary!

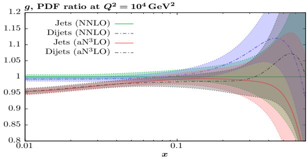
- Dijets may have some advantages here - 3D measurement now possible, non-unitary nature of inclusive jets, etc
- We have also investigated dijets instead:
  - Obtain better fit quality at NNLO and aN3LO than inclusive jets.
  - Moreover, dijet fit quality improves further slightly at aN3LO.
  - If add ATLAS 8 TeV jets, then incl. jets no longer worsens at aN3LO.

NNPDF, 2005.11327

Inclusive Jets	N_{pts}	χ^2/N_{pts} NNLO	χ^2/N_{pts} aN3LO	Dijets	N_{pts}	χ^2/N_{pts} NNLO	χ^2/N_{pts} aN3LO
Total	472	1.39	1.43	Total	266	1.12	1.04
Total (+ATLAS 8 TeV jets)	643	1.67	1.61	Total	266	1.12	1.04

- Inclusive jet scale change $p_T^j \to \hat{H}_T$ has little effect at NNLO/aN3LO.
- Difference in dijets/inclusive jets effect on gluon is milder at aN3LO:

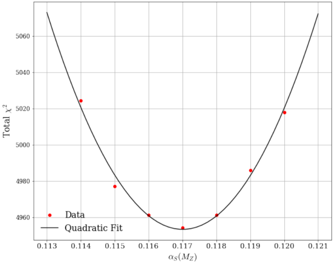


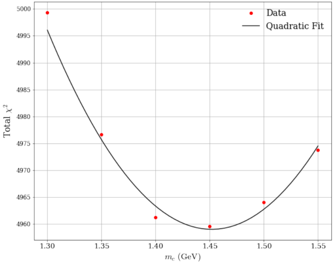


More info. in backup slides.

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 $\sim$ 1.45 GeV, compare with $\sim$ 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.

NLO and NNLO Cross-section Scale Variations

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

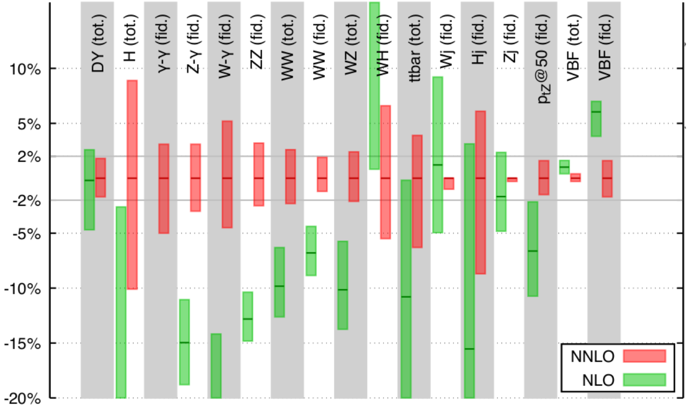


Image Credit: G. Salam

- 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		
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.

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	$n_f^{\max}$	$N_{\rm mem}$	$\alpha_S(m_Z^2)$	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.