

# MSHT20aN3LO

- Approximate N3LO PDFs with Theoretical Uncertainties



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DESY

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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.

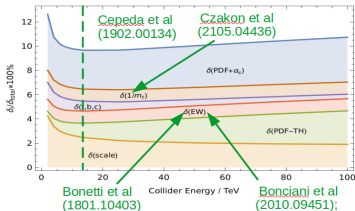
# Overview

# N3LO Calculations and PDFs

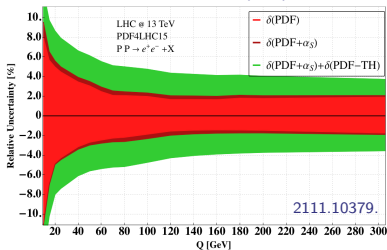
- Experiments are becoming ever more precise. LHC will measure several important processes at percent-level, e.g. Drell-Yan, Higgs.
- Key way to improve precision and accuracy of theoretical predictions is to include higher orders, i.e. N3LO QCD.
- Progress in recent years  $\Rightarrow$  some N3LO results now known for  $\sigma$ , e.g.

Higgs (ggF)

LHC Higgs  
XSWG 2019



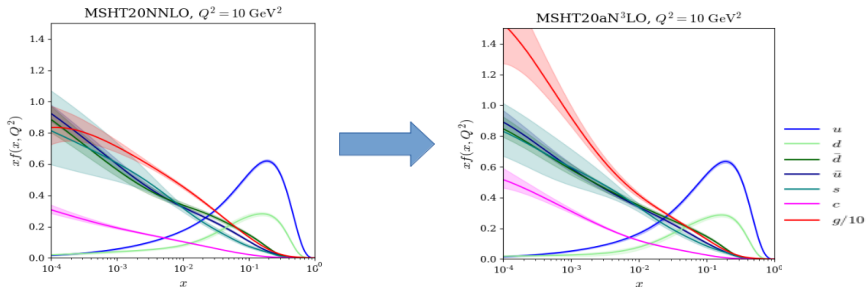
Drell-Yan (NC)



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

# PDFs at higher order with theoretical uncertainties

- Key way to **improve PDF precision and accuracy** is to include **higher orders**, i.e. **N3LO** and **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: Eur. Phys. J. C 83 (2023) 3, 185, arXiv:hep-ph/2207.04739,  
J. McGowan, TC, L.A. Harland-Lang, R.S. Thorne.

## What do we already 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**.
- Still, a **lot of information is known already** (schematic summary):

Theory	Utility	Order required	What's known?
Splitting functions $P_{ab}^{(3)}(x)$	PDF evolution	4-loop	Mellin moments <sup>3–5</sup> , leading small- $x$ behaviour <sup>3,6–11</sup> , plus some leading large- $x$ in places <sup>3</sup>
Transition matrix elements $A_{ab,H}^{(3)}(x)$	Transitions between number of flavours in PDFs at mass thresholds	3-loop	Mellin moments <sup>12</sup> , leading small- $x$ behaviour <sup>13–14</sup> , plus some leading large- $x$ in places <sup>14,15</sup> .
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 $\alpha_S^3$ (with exact LL pieces at low $x$ , NLL unknown) <sup>16–18</sup> , ZM-VFNS (high $Q^2$ ) N3LO coefficient functions known exactly <sup>19</sup> . Therefore GM-VFNS not completely known.
Hadronic Cross-sections (K-factors)	Determine cross-sections at N3LO	N3LO	Very little (none in usable form for PDFs)

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

# Methodology

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

# How can we incorporate N3LO knowledge into PDFs?

- Consider usual PDF fit probability: Theory Data Hessian matrix - contains uncorrelated ( $s_k$ ) and correlated uncertainties ( $\beta_k$ )

$$\begin{aligned}
 P(T|D) &\propto \exp(-\chi^2) \propto \exp\left(-\frac{1}{2}(\text{Theory} - \text{Data})^T H_0 (\text{Theory} - \text{Data})\right) \\
 &\propto \exp\left(-\frac{1}{2} \sum_{k=1}^{N_{pt}} \frac{1}{s_k^2} (D_k - T_k - \sum_{\alpha=1}^{N_{corr}} \beta_{k,\alpha} \lambda_\alpha)^2 + \sum_{\alpha=1}^{N_{corr}} \lambda_\alpha^2\right)
 \end{aligned}$$

Experimental Nuisance parameters

- Include known N3LO pieces ( $tu$ ) + parameterise remaining unknown pieces  $\Rightarrow$  theory nuisance parameters ( $\theta'$ ).
- 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  $\theta'$ .
- Assign  $\theta'$  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:
  - How do we determine the priors? - From known info. and lower orders.
  - Where do we include the theory nuisance parameters? - Next few slides.

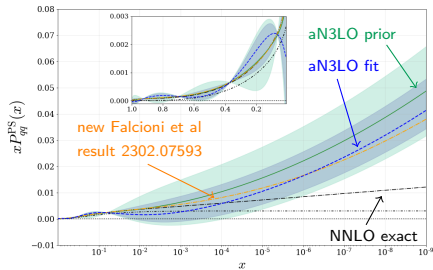
# Splitting Functions

1 Theory Nuisance Parameter per  
Splitting Function - 5 total from [here](#).

- What do we know and how do we incorporate this information?
  - Even low-integer  $N$  **Mellin Moments** (4-8)
    - constrain intermediate and high  $x$  via  $\int_0^1 dx x^{N-1} P(x)$ .
  - Parameterise  $P_{ab}^{(3)}(x)$  with functions  $f_{1,...,k}$  where  $k$  = No. of known moments.
  - Exact LL form at low  $x$  from resummation** - included in  $f_e(x, \rho_{ab})$  with coefficient of **low  $x$  NLL** is **variational (theory nuisance) parameter  $\rho_{ab}$** .

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

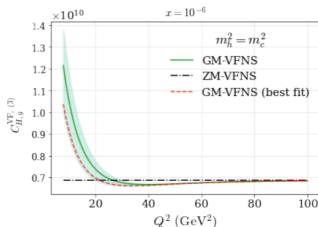
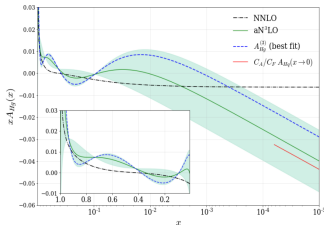
- New info on  $P_{qq}^{PS}$ :**
  - more moments ( $4 \rightarrow 10$ )
  - further low and high  $x$  log coefficients + fit further logs.



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

# 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.
  - ▶ **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:
  - ▶ **Drell-Yan** - Inclusive and some differential calculations <sup>28,29,30,31</sup> - not yet for relevant fiducial cross-sections or in form usable for PDFs.
  - ▶ **Higgs** - ggF, VBF and VH <sup>24,25,26,27</sup> - doesn't go in PDFs.
  - ▶ **Top** (aN3LO) - soft gluon resummation approximation<sup>32</sup>.
- 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 MHOU's into PDF uncertainties:

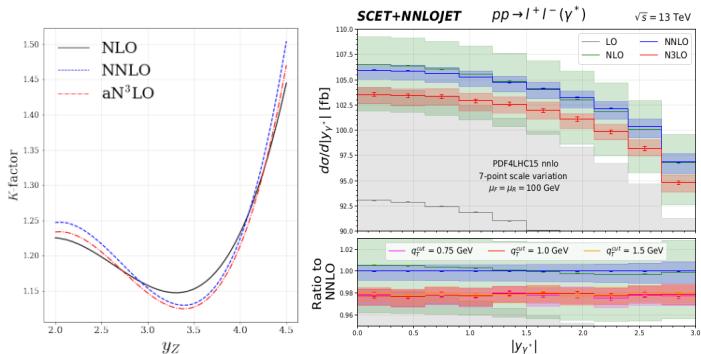
$$K^{N3LO/LO} = K^{NNLO/LO} (1 + a_1 \mathcal{N}^2 \alpha_S^2 (K^{NLO/LO} - 1) + a_2 \mathcal{N} \alpha_S (K^{NNLO/LO} - 1))$$

- **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

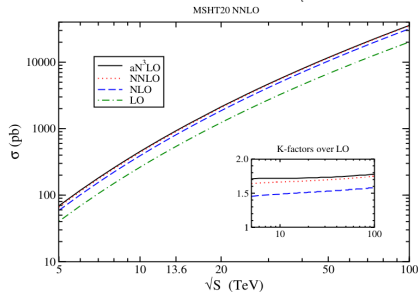
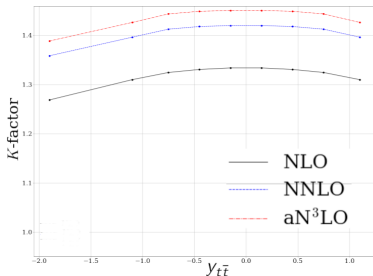
- Fit prefers a  $\approx 1\%$  decrease in the N3LO k-factors relative to NNLO.
- Improved perturbative convergence with aN3LO PDFs.
- In qualitative agreement with recent N3LO results for Neutral Current DY (which used NNLO PDFs)<sup>30</sup>.



# Hadronic K-factors - Top

## 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<sup>32</sup>.



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

- Using **MSHT20an3lo\_as118** eigenvectors as usual naturally incorporates MHOUs at aN3LO into the PDF uncertainties.

N.B. We will see the penalties on these parameters are almost all  $< 1 \Rightarrow$  conservative priors set.

# Impact on fit and PDFs

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

## Perform aN3LO fit - fit quality:

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

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

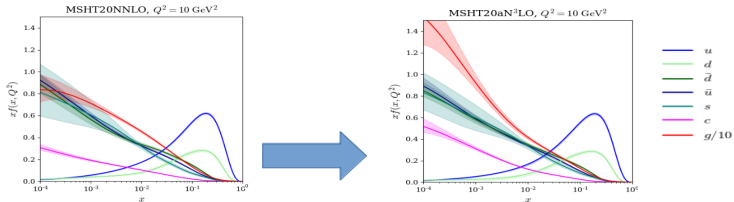
- Over half of fit improvement occurs without N3LO k-factors freedom.
- Average theory nuisance parameter penalty  $0.460 < 1$ . Fit able to describe data well with only small departures around prior.

## aN3LO Fit Quality Breakdown:

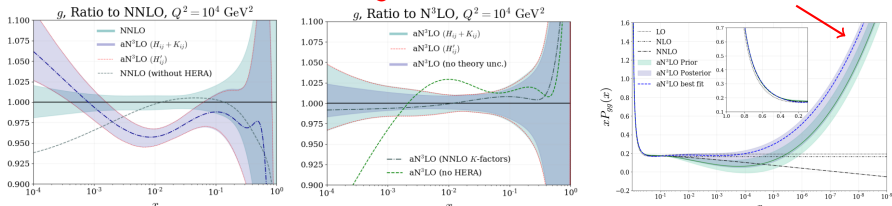
Dataset type	Total $\chi^2/N_{pts}$	$\Delta\chi^2$ from NNLO	$\Delta\chi^2$ from NNLO (but no N3LO k-factors)
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- Biggest improvement in DIS datasets, where most N3LO information known and included.
- Drell-Yan, dimuon, top improvements more from N3LO k-factor freedom; DY and top in approximate agreement with recent results.
- $V p_T / V + \text{jets}$  improves significantly, mostly without N3LO k-factors - ATLAS 8 TeV  $Zp_T$  large improvement from  $\chi^2/N = 1.81$  to 1.04.
- Improvement across whole  $p_T$  range, improvement seems to be related to reduction in tension of small and large  $x$  data in aN3LO fit.
- Inclusive Jets gets worse - does not occur with dijets! (Lucian's talk)

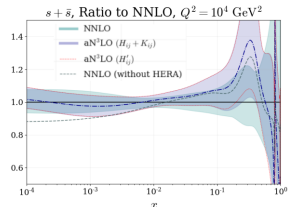
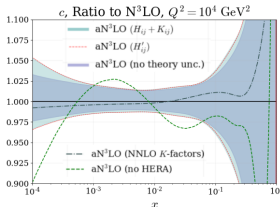
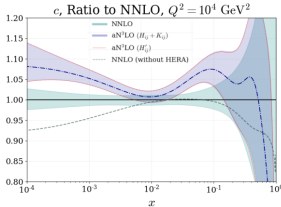
## aN3LO PDFs:



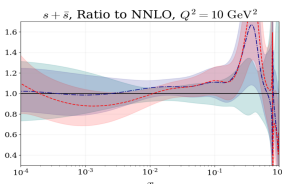
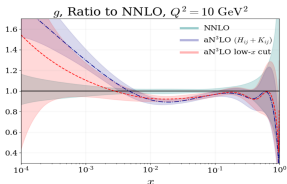
- **Gluon raises significantly at low  $x$**  - from large logs in splitting functions, not present at NNLO. Reduction at  $x \sim 10^{-2}$  due to splitting functions.
- **Gluon uncertainty enlarged at low  $x$**  from splitting functions.
- **Most singular NNLO term at small  $x$  in  $P_{gg}$  ( $\alpha_S^3/x \log^2(1/x)$ ) is 0**, so expect new N3LO piece ( $\alpha_S^4/x \log^3(1/x)$ ) to cause **significant change!**



## aN3LO PDFs:

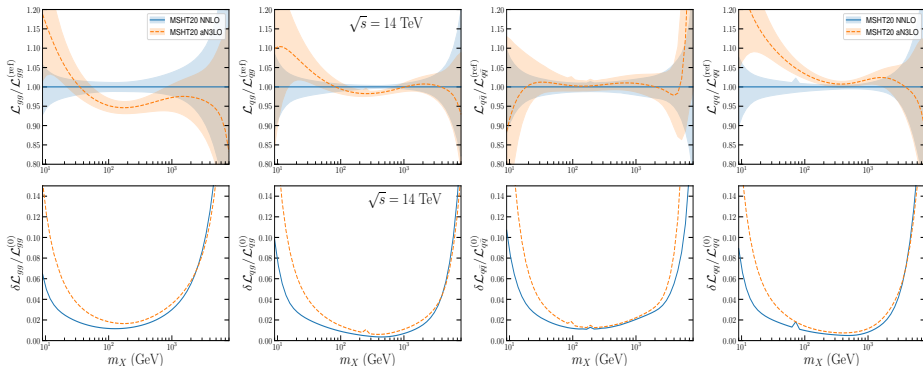


- Heavy quarks - **c and b** (perturbatively generated) **raised** due to increase in gluon at lower  $x$  and raised  $A_{Hg}$  at high  $x$ .
- Charm uncertainty **enlarged**, from both  $A_{Hg}$  at high  $x$  and gluon.
- Fit with no N3LO k-factors gives very similar PDFs to full aN3LO fit.
- Reduced tension of small and large  $x$  data seen at aN3LO:



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

## aN3LO PDF luminosities:



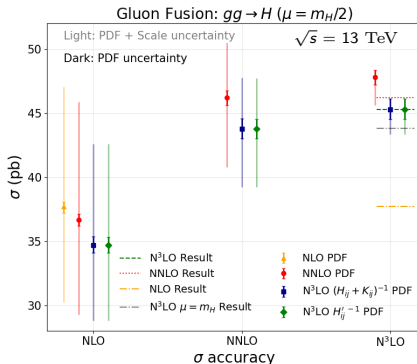
- PDF changes have implications for PDF luminosities for phenomenology.
- $gg$  luminosity reduced around 100 GeV and increased at 10 GeV,  $gg$  uncertainty grows with inclusion of aN3LO and theoretical uncertainties.
- $qq$  luminosity raised at low invariant masses from enhanced charm.
- Luminosity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

# Effect on Cross-sections and Other Results

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

## Impact on Higgs cross-sections - ggF:

- Consider impact of our aN3LO PDFs on known N3LO Higgs production in gluon fusion<sup>24,25</sup> - **shift down due to change in gluon:**



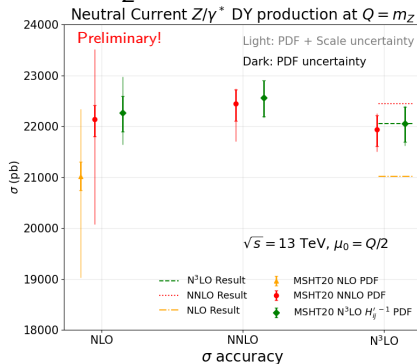
N.B. For scale variations - do  $\mu_R$  and  $\mu_F$  at NNLO but only  $\mu_R$  at aN3LO as PDF uncertainty from MHOs (Missing Higher Orders) already in PDF eigenvectors.

Results obtained using ggHiggs code<sup>36</sup>.

- Increase in cross-section at N3LO compensated by reduction in PDFs at aN3LO  $\Rightarrow$  **important to consider PDF and  $\sigma$  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:

- 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 MHOU.

# Usage

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

## Interpretation and Usage:

- 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

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

LHAPDF6 grid name	Order	$n_f^{\max}$	$N_{\text{mem}}$	$\alpha_S(m_Z^2)$	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 $\gamma$ PDF
MSHT20qed_nnlo_(in)elastic	NNLO	5	77	0.118	NNLO set with QED effects and (in)elastic $\gamma$
MSHT20qed_nnlo_neutron	NNLO	5	77	0.118	NNLO neutron set with QED effects and $\gamma$
MSHT20an3lo_as118	aN3LO	5	105	0.118	Approximate N3LO set with theoretical uncertainties also included
MSHT20an3lo_as118_KCorr	aN3LO	5	105	0.118	Approximate N3LO set with theoretical uncertainties also included, K-factors correlated
PDF4LHC21	NNLO	5	901	0.118	Baseline PDF4LHC21 set
PDF4LHC21_mc	NNLO	5	101	0.118	Replica compressed PDF4LHC21 set
PDF4LHC21_40	NNLO	5	41	0.118	Hessian compressed PDF4LHC21 set

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

Key:

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

- Feel free to contact us with questions about usage.

# Conclusions

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

## Conclusions:

- As demands on PDFs become stronger we must aim for both more precise and more accurate PDF central values and uncertainties.
- We have produced the world **first approximate N3LO PDFs**, including both **higher order effects in PDFs and theoretical uncertainties**.
- Method provides an intuitive and controllable way to include theoretical uncertainties into PDFs. Can be updated as more information becomes available on N3LO.
- Our **aN3LO PDFs are available** and we encourage their use: [MSHT20an3lo\\_as118](#).
- Can be **used if N3LO is known** or where not to **evaluate uncertainty due to missing higher orders in PDFs** and include higher order effects.
- Full information is available in the article [Eur. Phys. J. C 83 \(2023\) 3, 185, arXiv:hep-ph/2207.04739](#).
- Any questions about them/their use  $\Rightarrow$  please ask us!

### Selection of some references (others on slides)

- <sup>1</sup> M. Cepeda et al., 1902.00134.
- <sup>2</sup> Duhr, Mistlberger, 2111.10379.
- <sup>3</sup> S. Moch, B. Ruijl, T. Ueda, J. A. M. Vermaseren, and A. Vogt, 1707.08315.
- <sup>4</sup> A. Vogt et al., 1808.08981.
- <sup>5</sup> S. Moch, B. Ruijl, T. Ueda, J. A. M. Vermaseren, and A. Vogt, 2111.15561.
- <sup>6</sup> S. Catani and F. Hautmann, Nucl. Phys. B 427, 475 (1994), hep-ph/9405388.
- <sup>7</sup> L. N. Lipatov, Sov. J. Nucl. Phys. 23, 338 (1976).
- <sup>8</sup> E. A. Kuraev, L. N. Lipatov, and V. S. Fadin, Sov. Phys. JETP 45, 199 (1977).
- <sup>9</sup> I. I. Balitsky and L. N. Lipatov, Sov. J. Nucl. Phys. 28, 822 (1978).
- <sup>10</sup> V. S. Fadin and L. N. Lipatov, hep-ph/9802290.
- <sup>11</sup> M. Ciafaloni and G. Camici, hep-ph/9803389.
- <sup>12</sup> I. Bierenbaum, J. Blumlein, and S. Klein, 0904.3563.
- <sup>13</sup> H. Kawamura, N. A. Lo Presti, S. Moch, and A. Vogt, 1205.5727.
- <sup>14</sup> J. Ablinger et al., 1409.1135.
- <sup>15</sup> J. Ablinger et al., 1402.0359.
- <sup>16</sup> S. Catani, M. Ciafaloni, and F. Hautmann, Nucl. Phys. B 366, 135 (1991).
- <sup>17</sup> E. Laenen and S.-O. Moch, hep-ph/9809550..
- <sup>18</sup> H. Kawamura, N. A. Lo Presti, S. Moch, and A. Vogt, 1205.5727.
- <sup>19</sup> J. Vermaseren, A. Vogt, and S. Moch, hep-ph/0504242.
- <sup>20</sup> W. Van Neervan, A. Vogt, hep-ph/9907472.
- <sup>21</sup> W. Van Neervan, A. Vogt, hep-ph/0006154.
- <sup>22</sup> A. Martin, R.G. Roberts, W.J. Stirling, R.S. Thorne, hep-ph/0006154.
- <sup>23</sup> A. Martin, R.G. Roberts, W.J. Stirling, R.S. Thorne, hep-ph/0201127.
- <sup>24</sup> C. Anastasiou et al., 1602.00695.
- <sup>25</sup> B. Mistlberger, 1802.00833.
- <sup>26</sup> F.A. Dreyer and A. Karlberg, 1606.00840.
- <sup>27</sup> J. Baglio, C. Duhr, B. Mistlberger, R. Szafron, 2209.06138.
- <sup>28</sup> C. Duhr, F. Dulat and B. Mistlberger, 2001.07717.
- <sup>29</sup> C. Duhr, F. Dulat and B. Mistlberger 2007.13313.
- <sup>30</sup> X. Chen et al., 2107.09085.
- <sup>31</sup> C. Duhr and B. Mistlberger, 2111.10379.
- <sup>32</sup> N. Kidonakis, 2203.03698.
- <sup>33</sup> M. Bonvini, 1812.01958.
- <sup>34</sup> R.D. Ball et al, 1710.05935.
- <sup>35</sup> H. Abdolmaleki et al, xFitter, 1802.00064.
- <sup>36</sup> M. Bonvini, arXiv:1805.08785.
- <sup>37</sup> 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).

## MSHT20aN3LO PDFs - Fit quality

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

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

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

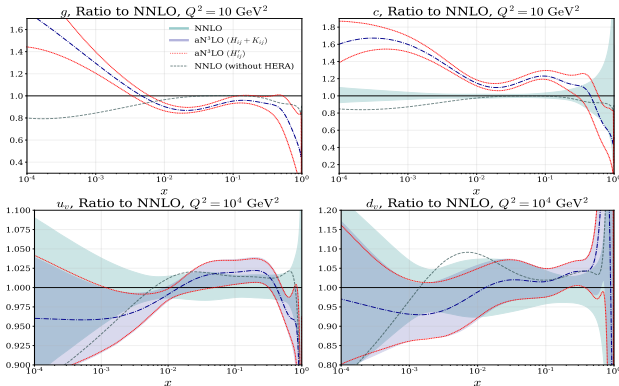
## aN3LO Theory Nuisance Parameters:

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

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

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

## MSHT20aN3LO PDFs - PDF changes



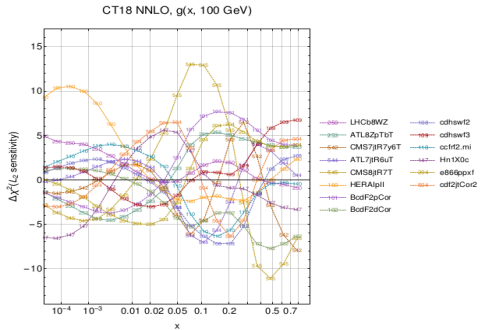
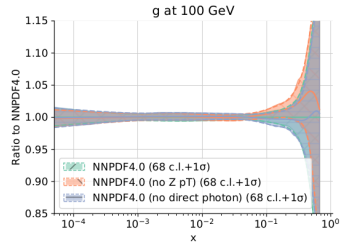
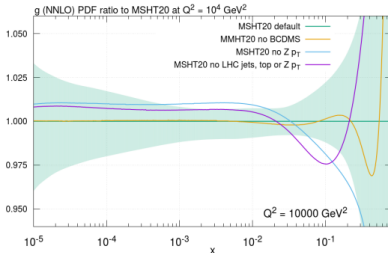
- Small- $x$  low- $Q^2$  gluon enhanced due to large logs included at N3LO.
- Enhanced charm via enlarged  $A_{Hg}^{(3)}$  and increased small- $x$  gluon.
- Reduced quarks at intermediate/small- $x$  accommodate small- $x$  gluon.
- High- $Q^2$ , intermediate/large- $x$  light quarks largely follow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

## ATLAS 8 TeV $Zp_T$ data:

- ATLAS 8 TeV  $Zp_T$  data - **precise data, large NNLO corrections.**
- **Different amounts of data used** and different **uncertainties** applied.
- MSHT20 - Largest amount of data, double differential in  $[p_T^{\parallel}, y_{\parallel}]$  in Z-peak mass bin, others single differential in  $y_{\parallel}$ . 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  $p_T > 150\text{GeV}$  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**  $m_{\parallel} = \{[46, 66], [66, 116], [116, 150]\}\text{GeV}$  bins single differential in  $p_T^{\parallel} < 150\text{GeV}$ . Include a **0.5% uncorrelated uncertainty for k-factor** MC errors + theory uncertainties. Fit quality  $\chi^2/N_{pts} \sim 1.1$  for 27 points, argue other data not so constraining.
- Therefore **different groups see different impacts** and importance.

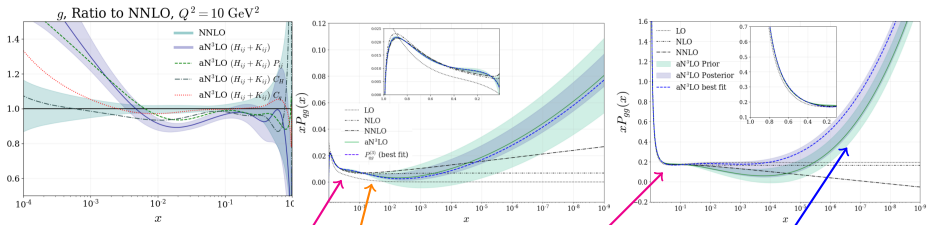
# ATLAS 8 TeV $Zp_T$ data:

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



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

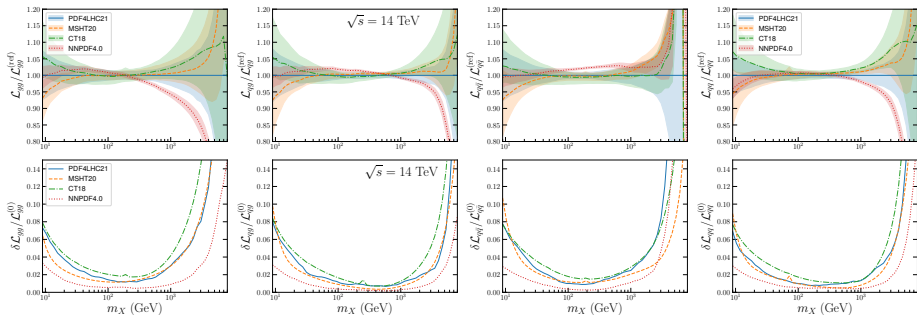
- Around  $10^{-2} \lesssim x \lesssim 10^{-1}$   $P_{ij}$ ,  $C_H$  contribute  $\approx$  equally. Also some  $C_q$ .
- At low  $x$   $P_{ij}$  dominate, this contains much known N3LO information.



- 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. Uncertainty band from leading unknown coefficient (NLL or NNLL).
- Most singular NNLO term at small  $x$  in  $P_{gg}$  ( $\alpha_S^3/x \log^2(1/x)$ ) is 0, so expect new N3LO piece ( $\alpha_S^4/x \log^3(1/x)$ ) to cause significant change!

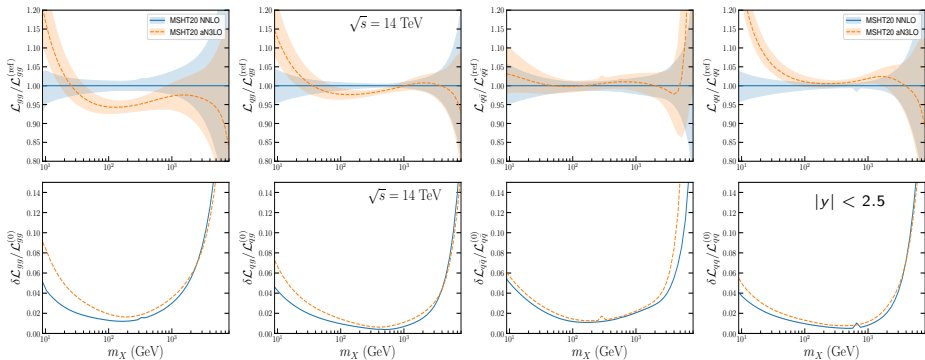
# Global Fits Luminosities Comparison (NNLO):

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



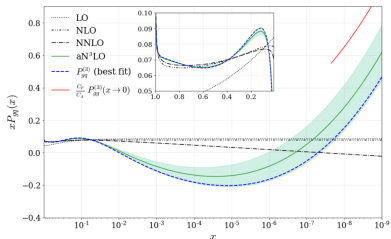
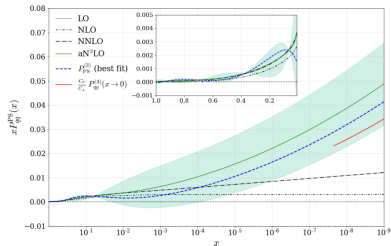
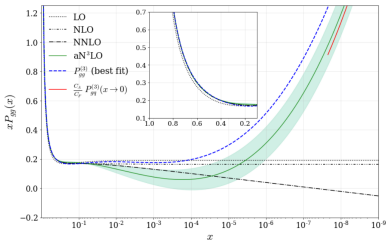
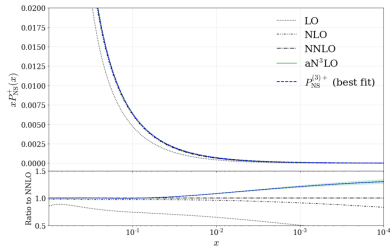
- Generally good agreement for central  $m_X$ , at least for  $qq$ ,  $qg$ ,  $gg$  luminosities. Exception is NNPDF4.0 higher for  $q\bar{q}$ .
- More marked differences at high  $m_X$ , largely unconstrained so more extrapolation driven.
- Significant differences in uncertainties reflect differences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

## aN3LO PDF luminosities with rapidity cut:



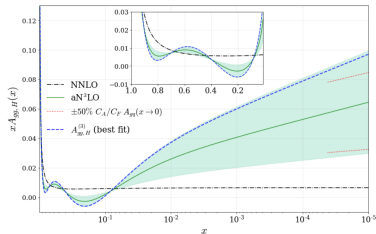
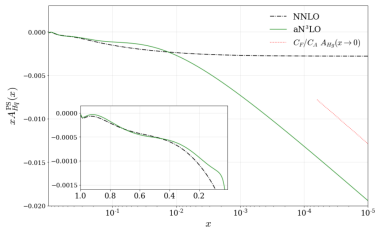
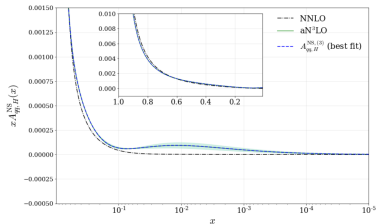
- **gg luminosity reduced around 100GeV** and increased at 10GeV, **gg uncertainty grows** with inclusion of aN3LO and theoretical uncertainties.
- **qq luminosity raised at low invariant masses** from enhanced charm.
- **Luminosity uncertainties enlarged** (and more so at lower invariant masses) due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

# Splitting Functions:



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

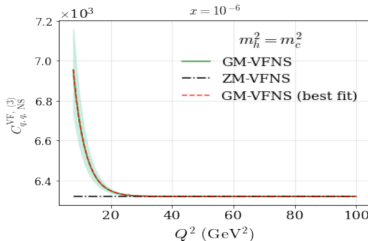
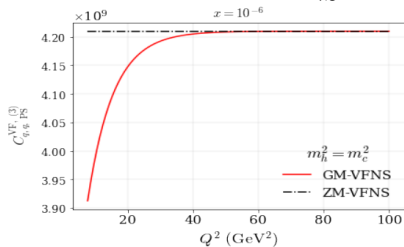
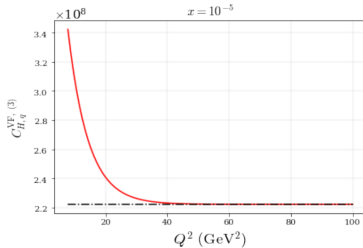
# Transition Matrix Elements:



- $A_{Hq}^{PS,(3)}$ ,  $A_{gq,H}^{(3)}$  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:

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

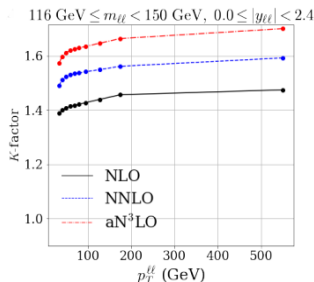
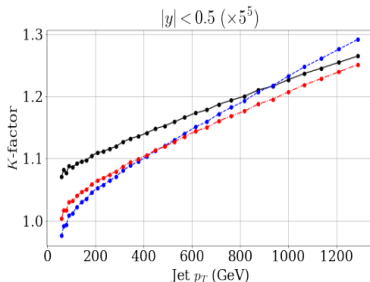


- $C_{Hq}^{VF,(3)}$  and  $C_{Hg}^{VF,(3)}$  have uncertainties from  $c_q^{NLL}$  and  $c_g^{NLL}$  parameters,  
 $C_{Hg}^{VF,(3)}$  and  $C_{qq,NS}^{VF,(3)}$  inherit uncertainty from  $A_{Hg}^{(3)}$  and  $A_{qq,NS}^{(3)}$ .

# Hadronic K-factors

## 4 Jets (lower left plot)

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



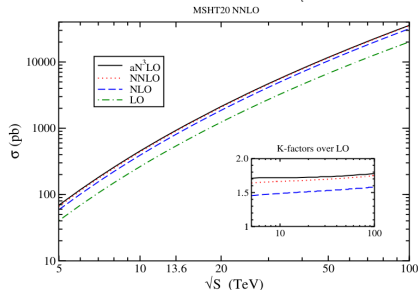
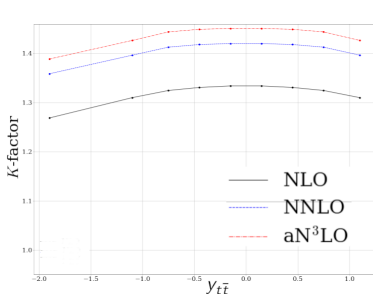
## 5 Vector boson + jets, $Zp_T$ (upper right plot)

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

## Hadronic K-factors - Top and Dimuon

### 2 Top

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



### 3 Dimuon - Semi-inclusive DIS

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

## How can we incorporate N3LO knowledge into PDFs?

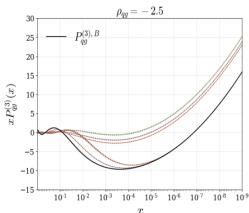
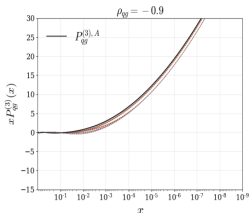
- After subbing in and rewriting obtain:

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

- First term is **posterior penalty** when the **theory strays from the best fit**.
- Second term is  **$\chi^2$  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:

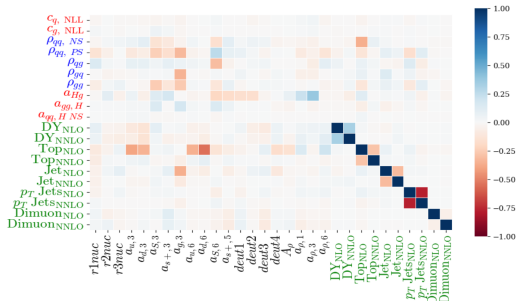
- Key part of the theoretical nuisance parameter framework for missing N3LO pieces is **setting up the priors and penalties** on their variations.
- Q. How do we do this? A. **Conservatively!**
- Set  $\rho_{ab}$  prior variation by requiring:
  - 1 At low  $x$  bound set once exact expression  $f_e(x,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

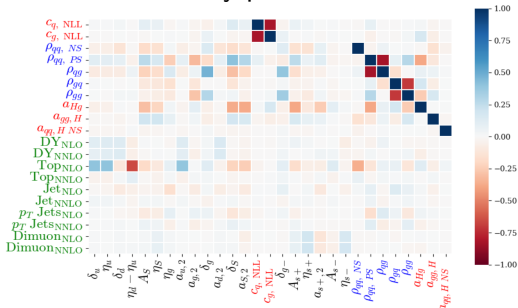
$$H_{ij}'^{-1} \rightarrow H_{ij}^{-1} + \sum_{p=1}^{N_p} K_{ij,p}^{-1}$$

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!**

## 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:

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

- Produce two PDF uncertainty sets - MSHT20an3lo\_as118\_Kcorr and MSHT20an3lo\_as118, default is latter. **Very little difference in PDF uncertainties!**

## New data - Dijets - Introduction

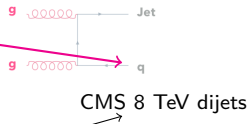
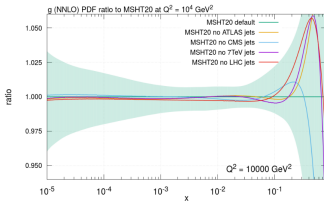
- High  $x$  gluon is of interest in PDFs, with tensions between datasets.
- MSHT20 - data on inclusive jets from ATLAS, CMS at 7 and 8 TeV, sensitive to high- $x$  gluon. Different pulls.
- Known issues with systematic correlations in ATLAS 7, 8 TeV inclusive jets (latter therefore not included in MSHT20).
- Theoretical issues: scale choice, non-unitary nature of inclusive jets.
- Dijets also allow triple differential measurement, cf double differential for single inclusive jets. Schematically at LO:

$$x = \frac{p_T}{\sqrt{s}} (e^{y_j} + e^{y_{j'}})$$

Integrated over in inclusive jet case

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

Dijets when triple differential more sensitive to  $x$ -dependence.



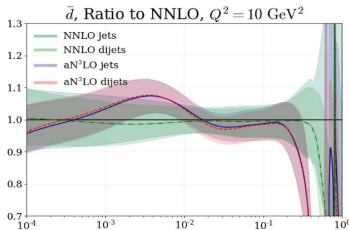
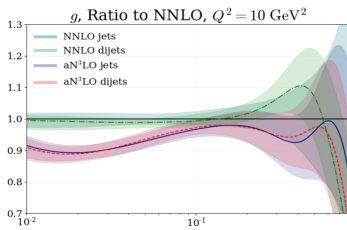
## Dijet data aN3LO vs NNLO:

Preliminary!

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

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

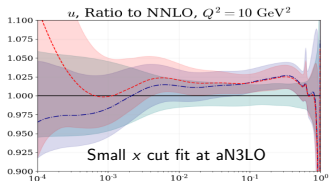
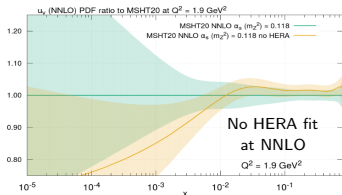
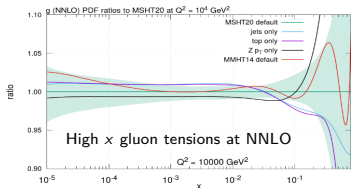
- Effect of jets vs dijets on PDFs and rest of data similar at NNLO and aN3LO, and no significant change in uncertainty.



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

## Dataset tensions at NNLO:

Fit qualities of fits excluding HERA data:

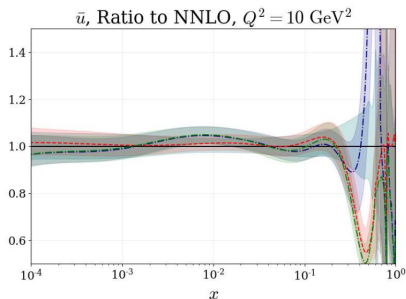
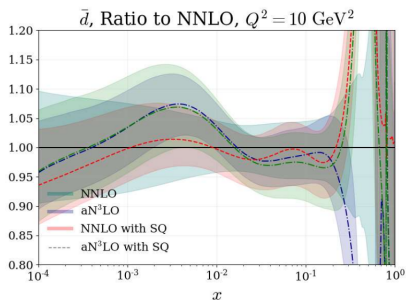


Dataset	$N_{\text{pts}}$	$\Delta\chi^2_{\text{aN3LO}}$	$\Delta\chi^2_{\text{NNLO}}$
BCDMS $\mu p F_2$	163	+1.4	-5.5
BCDMS $\mu d F_2$	151	-0.0	-2.1
NMC $\mu p F_2$	123	-7.8	-4.5
NMC $\mu d F_2$	123	-16.6	-16.1
E665 $\mu d F_2$	53	+1.3	+3.9
E665 $\mu p F_2$	53	+1.5	+4.3
E866 / NuSea $pp$ DY	184	+2.3	+2.9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

## MSHT20aN3LO PDFs - Seaquest

Preliminary!

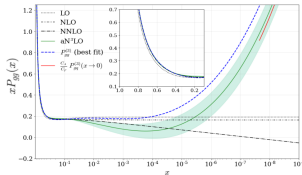
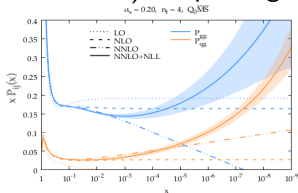
- At aN3LO, the  $\bar{d}$  become negative above  $x \sim 0.5$  with a minimum at  $x \sim 0.6$ . Nonetheless remains positive within uncertainties.
- Like at NNLO, adding the Seaquest data raises the  $\bar{d}/\bar{u}$ .



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

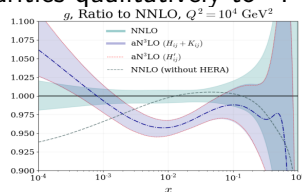
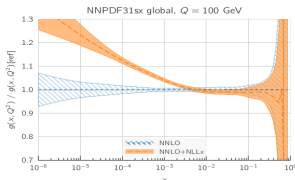
## aN3LO at low $x$ vs resummed:

- We include up to (N)LL low  $x$  resummed terms (and (N)NLL with variable coefficient) in splitting functions - compare with resummed<sup>33</sup>:



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

- Similar effects qualitatively (note scheme difference!) on  $P_{ij}$ .
- Impact on gluon also shows similarities qualitatively to<sup>34</sup>:



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

# Other approaches for theoretical uncertainties in PDFs?

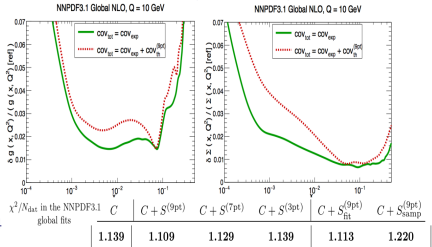
- Alternative is **through scale variations**.
- Vary renormalisation and factorisation scales in fit data to give a “**theory covariance matrix**” to incorporate into PDF uncertainties.
- Can also instead do a joint fit of PDF and scale uncertainties.

- So far both **only NLO** by NNPDF3.1, marginally increased PDF uncertainties and improved  $\chi^2/N_{pts}$ .

NNPDF  
2207.07616

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

NNPDF, 1905.04311, 1906.10698, 2105.05114



- Specific issues include:

- Need to **correlate PDF scale variations** with theoretical predictions.
- Only **varies terms appearing at lower order, not new terms**.
- Does **not incorporate already-known higher order information**.

# NLO and NNLO Cross-section Scale Variations

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

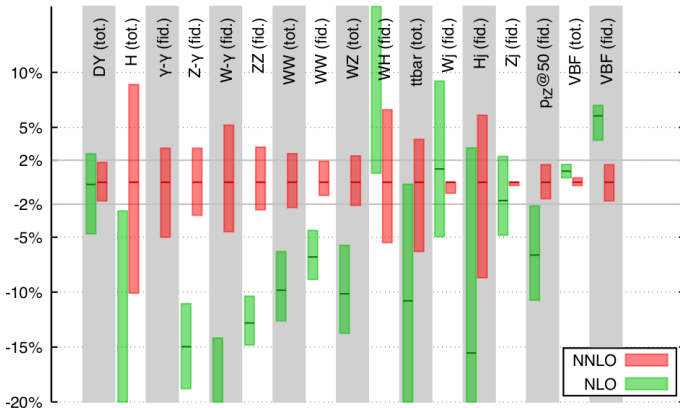


Image Credit:  
G. Salam

- 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:

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

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

$\sigma$ order	PDF order	$\sigma + \Delta\sigma_+ - \Delta\sigma_-$ (pb)	$\sigma$ (pb) $+ \Delta\sigma_+ - \Delta\sigma_-$ (%)
PDF uncertainties			
N <sup>3</sup> LO	aN <sup>3</sup> LO (no theory unc.)	4.1150 + 0.0638 - 0.0724	4.1150 + 1.55% - 1.76%
	aN <sup>3</sup> LO ( $H_{ij} + K_{ij}$ )	4.1150 + 0.0682 - 0.0755	4.1150 + 1.66% - 1.83%
	aN <sup>3</sup> LO ( $H'_{ij}$ )	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 <sup>3</sup> LO	aN <sup>3</sup> LO (no theory unc.)	4.1150 + 0.0638 - 0.0724	4.1150 + 1.55% - 1.76%
	aN <sup>3</sup> LO ( $H_{ij} + K_{ij}$ )	4.1150 + 0.0683 - 0.0755	4.1150 + 1.66% - 1.83%
	aN <sup>3</sup> LO ( $H'_{ij}$ )	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.

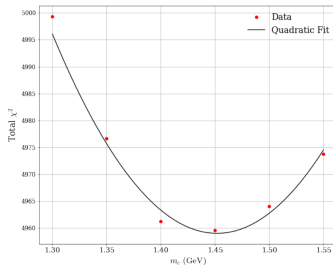
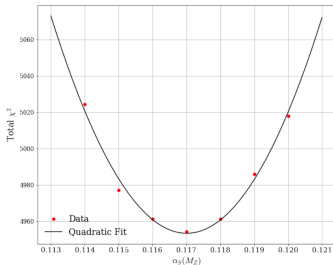
$\sigma$ order	PDF order	$\sigma + \Delta\sigma_+ - \Delta\sigma_-$ (pb)	$\sigma$ (pb) $+ \Delta\sigma_+ - \Delta\sigma_-$ (%)
N <sup>3</sup> LO	aN <sup>3</sup> LO $n_f = 5$	4.1150 + 0.0683 - 0.0755	4.1150 + 1.66% - 1.83%
	aN <sup>3</sup> LO $n_f = 4$	4.0270 + 0.0685 - 0.0765	4.0270 + 1.70% - 1.90%
	aN <sup>3</sup> LO $n_f = 3$	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.

## 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  $m_c^{\text{pole}} = 1.5 \pm 0.2 \text{ GeV}$ .
- Lower  $\alpha_S(M_Z^2)$  and raised  $m_c$  suggest fit favouring slight suppression of gluon and charm.