PDFs @ N3LO

Standard Model at the LHC 2024, Rome

Thomas Cridge

7th May 2024

Overview

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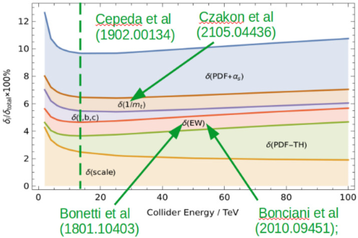

LHC Higgs XSWG 2019

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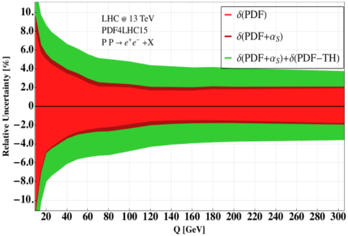

Duhr, Mistelberger 2111.10379

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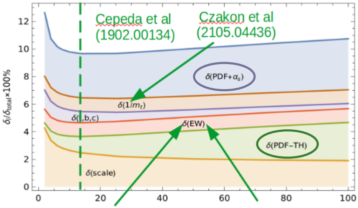

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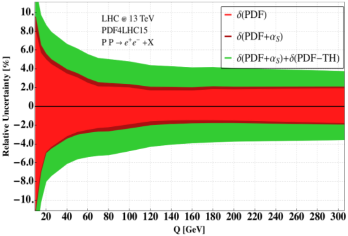

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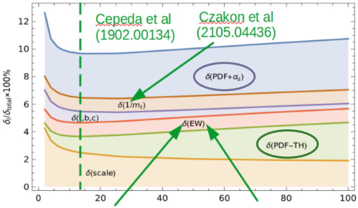

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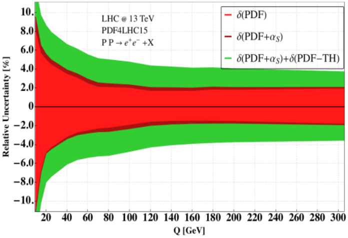

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- PDFs at N3LO with theory uncertainties were becoming a bottleneck.
- Two steps required for *more accurate and precise PDFs*:

1. Higher order PDFs ⇒ aN3LO.
2. Theoretical uncertainties from missing higher orders ⇒ MHOU.

Current Knowledge of N3LO

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

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    Mellin moments, small x, high x limits [11-31].

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    Light flavour known, heavy flavour high Q^2 known, approx for low Q^2 [43-45].

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    Very little known, PDFs need differential with cuts.

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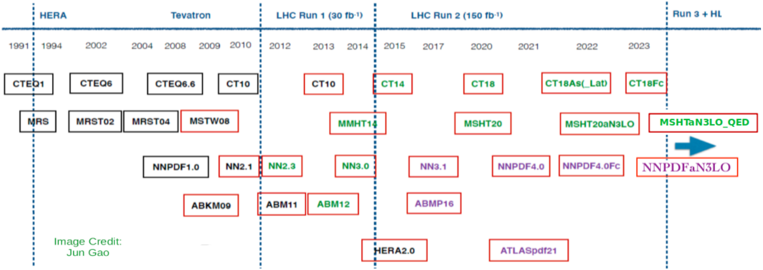

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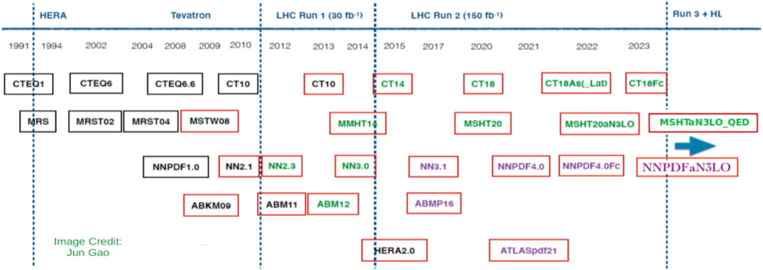

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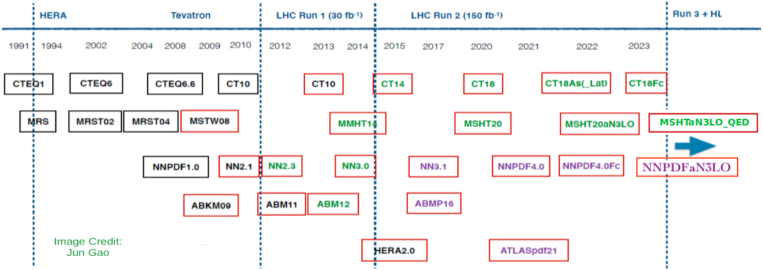

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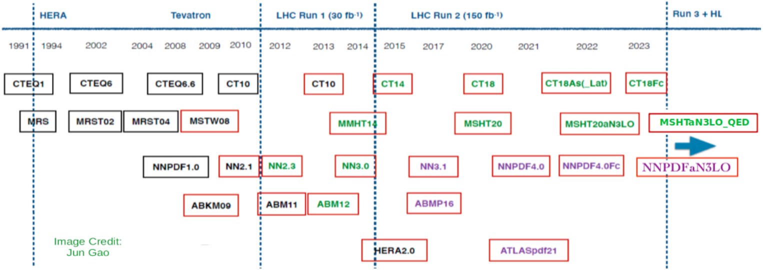

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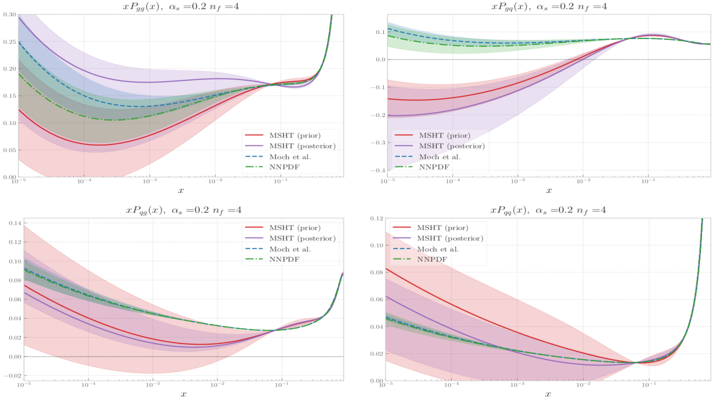
- Later ⇒ will see similar impacts of aN3LO in both.

N3LO PDF Evolution

- Key ingredient is N3LO DGLAP evolution.
- Some more info recently from [26-30] - FHMRUVV (also [31]).
- How do the aN3LO splitting function approximations compare?:



- Validation of methodology - results within uncertainties, exception P_{gq}.

Impact of aN3LO evolution on PDFs:

- N3LO evolution benchmarking - use toy PDFs, no fit or other issues:

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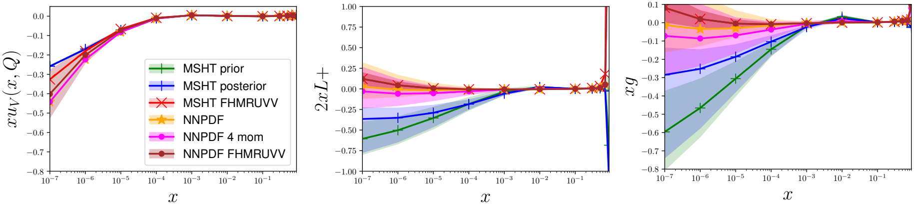

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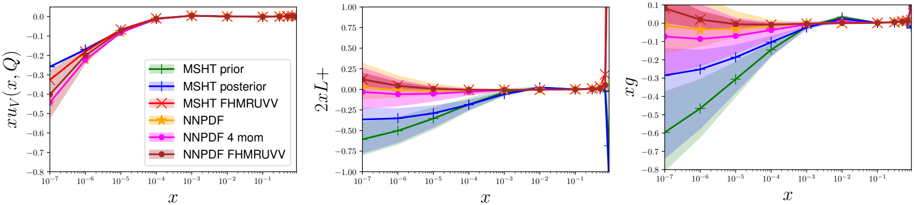

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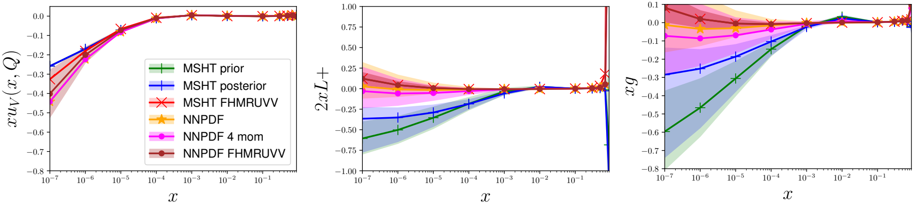

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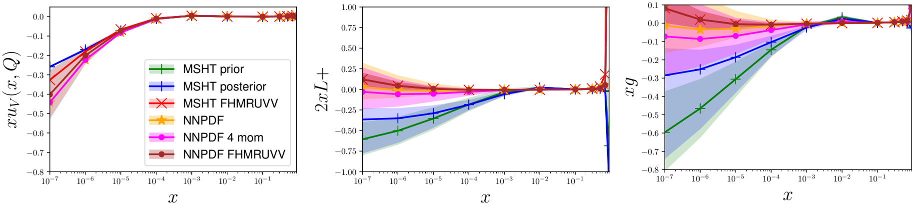

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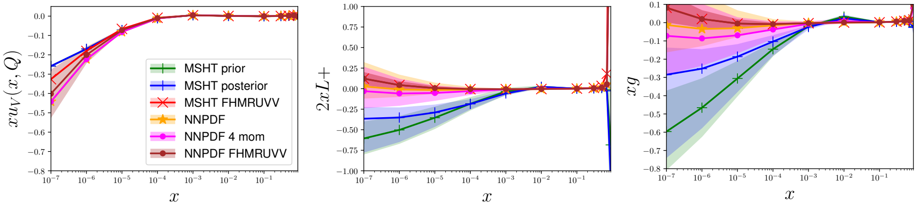

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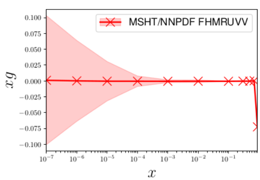

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  - Uncertainty on aN3LO comes through varying functional basis $f_i(x)$ and varying unknown coefficient ("theory nuisance parameter" - TNP).

$\Rightarrow$ aN3LO PDF + theory uncertainty.

How do we incorporate N3LO into PDFs?

- Consider usual PDF fit probability - add N3LO theory and theory uncertainty:

Experimental Nuisance parameters

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

$$\propto \exp\left(-\frac{1}{2}\sum_{k=1}^{N_{pt}} \frac{1}{s_k^2}\left(D'_k - T_k - \sum_{t=1}^{N_{TNPs}} u_{k,t}\theta'_t\right)^2 + \sum_{\alpha=1}^{N_{corr}} {\lambda_\alpha}^2 + \sum_{t=1}^{N_{TNPs}} {\theta'_t}^2\right)$$

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- Upgrade theory, T to now contain known N3LO info (aN3LO) and allow to vary by theory nuisance parameters, θ'.
- Analogous to experimental nuisance parameters, allow fit to shift theory within some prior $\Rightarrow$ theory uncertainty included into PDFs.

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- Analogous to experimental nuisance parameters, allow fit to shift theory within some prior ⇒ theory uncertainty included into PDFs.
- Probes precisely the missing higher order terms.
- Allows inclusion of known N3LO information (a lot) without needing to wait for remaining few pieces.

(Theoretical Nuisance Parameters more generally → F. Tackmann SCET Workshop 2019)

Theory Nuisance Parameter Summary

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

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

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

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

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- Use scale variations (μ_F, μ_R) of current order instead of TNPs to represent MHOU.

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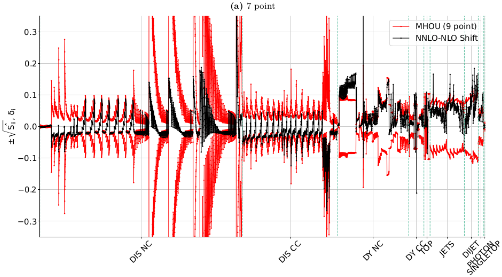
- Use scale variations (μ_F, μ_R) of current order instead of TNPs to represent MHOU.



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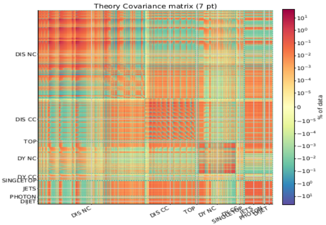
- Construct theory covariance matrix, analogous to TNPs but different estimate of error [8].
- Requires prescription for how to correlate scales in different processes. (As does any approximation in absence of known N3LO K-factors).



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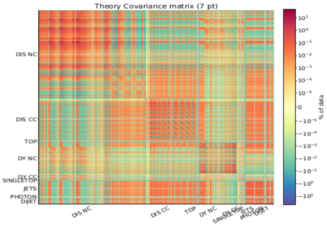
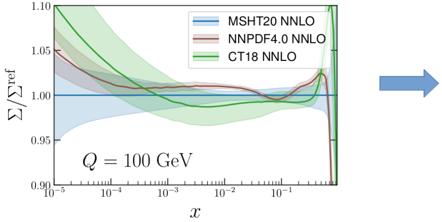


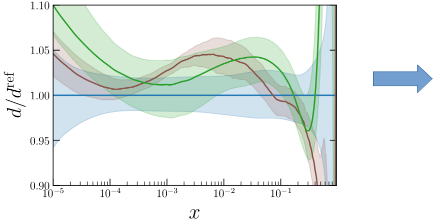
- Overall, like NNLO, at aN3LO MSHT and NNPDF have similar info., formal accuracy, but some differences in approaches.

Effect of N3LO on PDFs:

Impact of aN3LO on PDFs:

- Quarks relatively unaffected:





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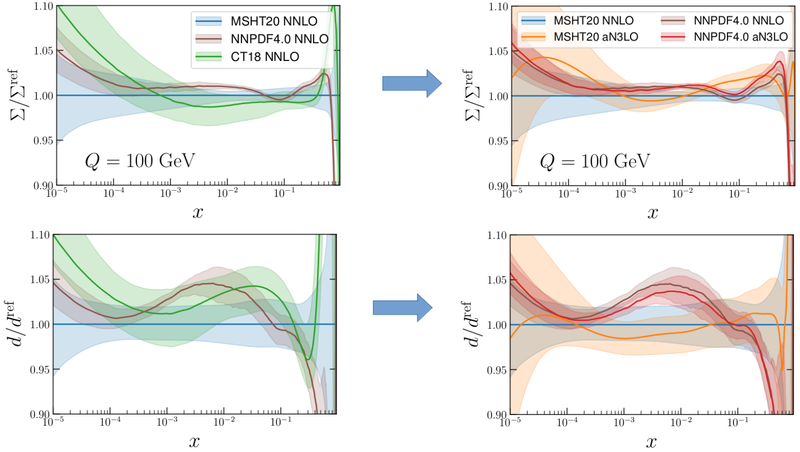

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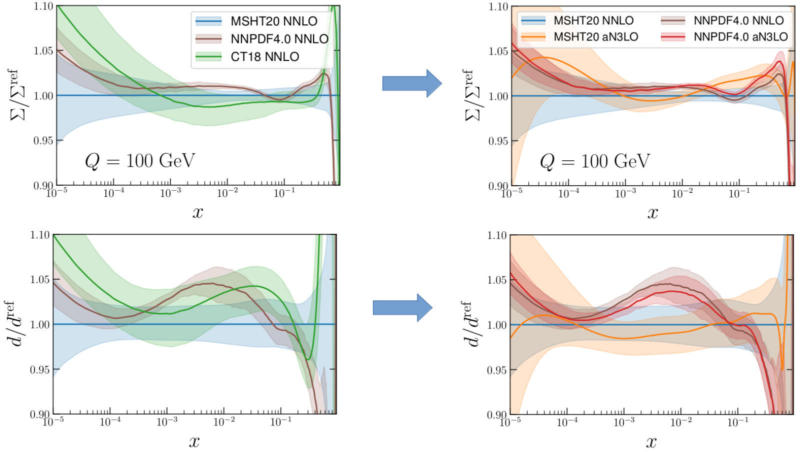
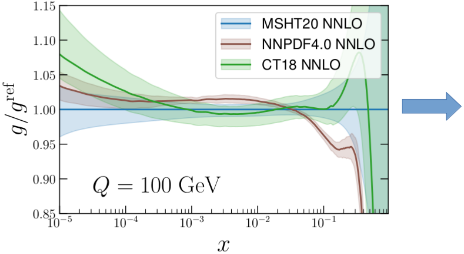


- Singlet PDF - NNLO and aN3LO all show same % level differences.
- Down PDF - as much difference between aN3LO PDFs as NNLO.

Impact of aN3LO on PDFs:

- Largest effect on the gluon PDF,
  as expected from aN3LO splitting functions.



Impact of aN3LO on PDFs:

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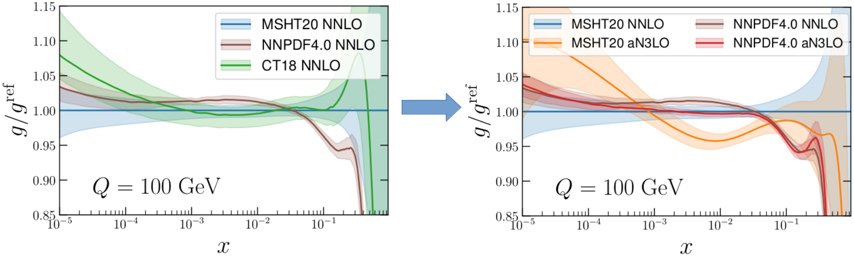

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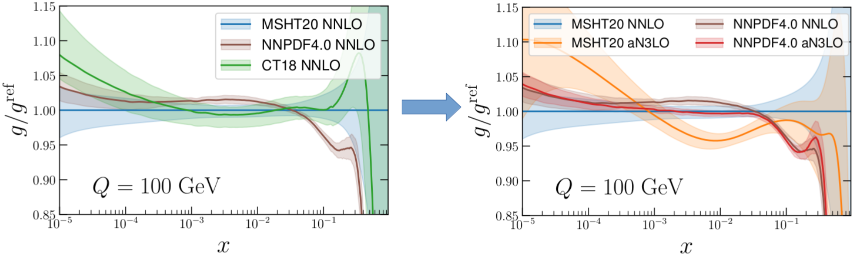

- NNLO - gluon PDFs differ by few % in Higgs region.
- aN3LO - gluon PDFs differ by few % in Higgs region.

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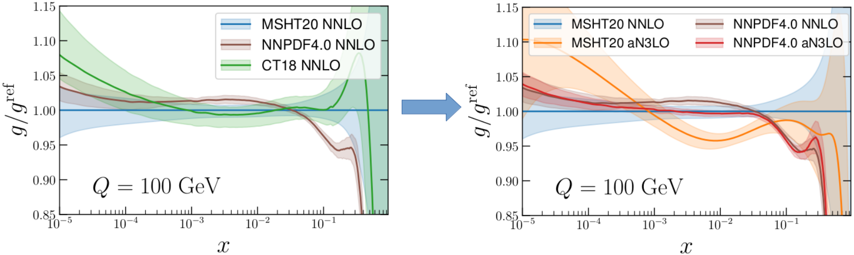

- NNLO - gluon PDFs differ by few % in Higgs region.
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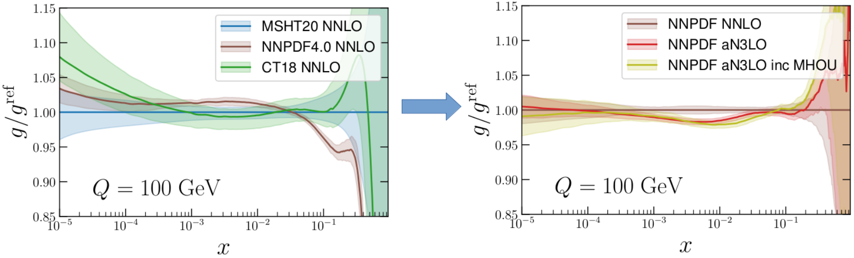

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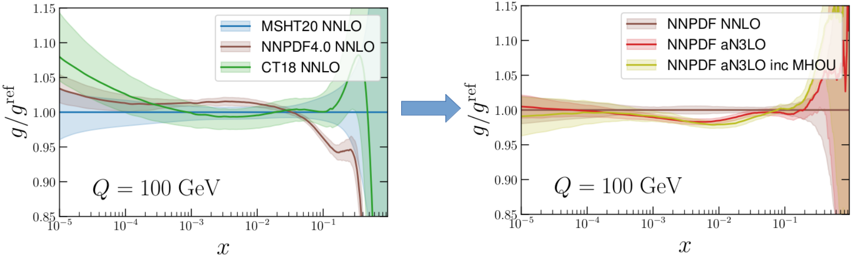

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- NNLO vs aN3LO - MSHT and NNPDF both see dip (2-5%) in gluon at m_H ($x \sim 10^{-2}$) from aN3LO effects.
- Variety of other effects - new FHMV info., other N3LO ingredients, methodology, data can cause 1-2% differences here, (see backup).

Impact of aN3LO + MHOU on PDF uncertainties:

- aN3LO and theory uncertainties from Missing Higher Orders (MHOUs) impact PDF errors.

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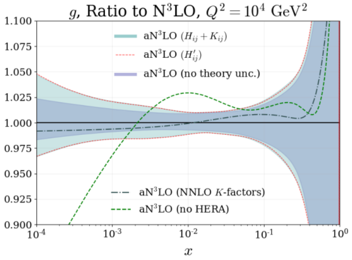
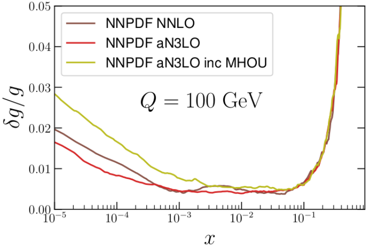
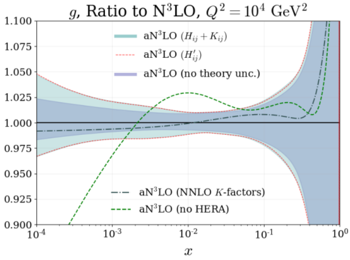
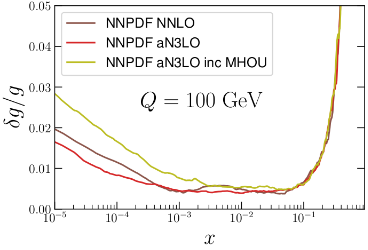




Impact of aN3LO + MHOU on PDF uncertainties:

- aN3LO and theory uncertainties from Missing Higher Orders (MHOUs) impact PDF errors.
- MSHT (left) and NNPDF (right) both see added theory uncertainty increasing PDF uncertainties at low x, e.g. gluon:
- Whilst PDF uncertainty is larger, it's more accurate and reliable.



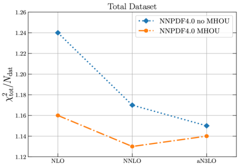


aN3LO effects on the PDF fit:

- aN3LO (and theory uncertainties) have impact on PDF fit.
  - MSHT and NNPDF - Improvement order by order of fit quality:

MSHT χ^2/N_{pts} (4363)	LO	NLO	NNLO	aN3LO
	2.57	1.33	1.17	1.14

$\Delta\chi^2$ improves by ~ -150 at aN3LO.



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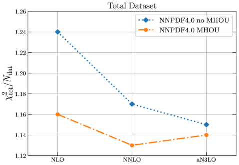
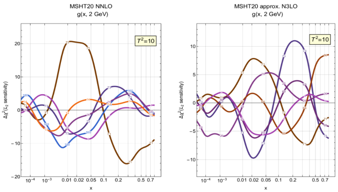
- MSHT - Z p_T data (and DIS data) notably better fit.
- Reduced tensions between data also seen.
- MSHT - Dijet data also better fit at aN3LO than NNLO.

T.C. et al, 2312.12505 [6] .





L2 study 2306.03918

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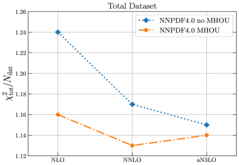
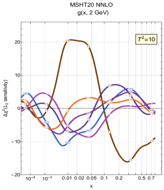
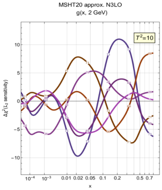
- High precision data requires high precision theory.







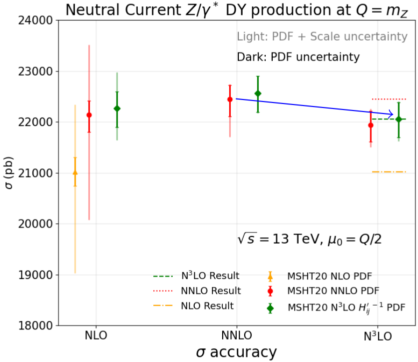
L2 study 2306.03918

Consequences of aN3LO PDFs for Phenomenology

Drell-Yan production:

Produced using the `n3loxs` code[49].

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

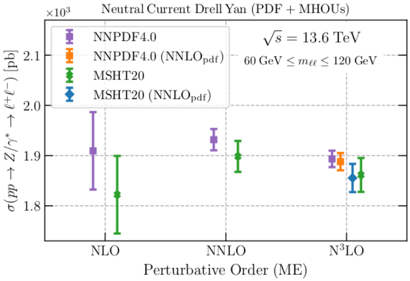


Note greater stability of full NNLO and N3LO xsec + aN3LO PDF results

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

Drell-Yan production:

- Consider impact of our aN3LO PDFs on Drell-Yan production at LHC, e.g. Neutral current at $60\text{GeV} < m_{ll} < 120\text{GeV}$ at 13.6 TeV:



Note greater stability of full NNLO and N3LO xsec + aN3LO PDF results

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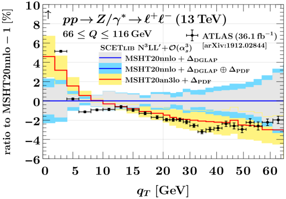
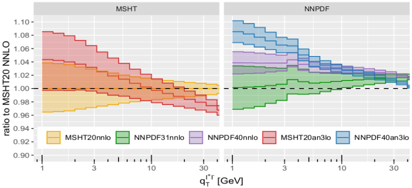
- Predictions with NNLO and aN3LO PDFs are stable.
- NNPDF see similar small impact on DY $\rightarrow$ also see small increase from aN3LO PDFs, also well within uncertainty.

Drell-Yan production - Transverse Momentum:

- $Z\ p_T$ spectrum - wish to use aN3LO PDFs to match resummation accuracy in predictions for Zp_T spectrum at low q_T:
- MSHT20aN3LO and NNPDFaN3LO PDFs have same impact on shape of q_T spectrum:





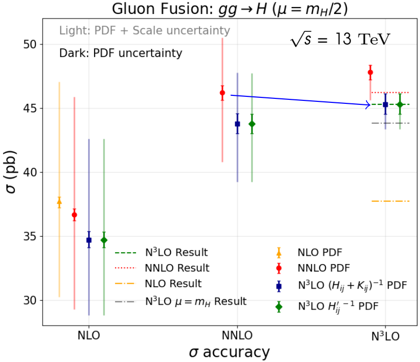
- Substantial aN3LO PDF effect on N3LL'/N4LL q_T spectrum.

Left: `SCETlib` - Johannes Michel LHC EW WG meeting Sep 2022.

Centre: `CuTe-MCFM` - Tobias Neumann Loops and Legs March 2024

Gluon Fusion Higgs Production:

- Consider impact of our aN3LO PDFs on known N3LO Higgs production in gluon fusion[32,33] - shift down due to change in gluon:



Note greater stability of full NNLO and N3LO xsec + aN3LO PDF results

Results obtained using ggHiggs code[50].

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

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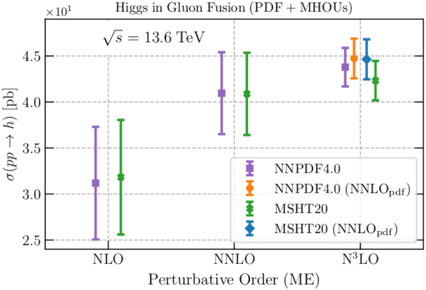

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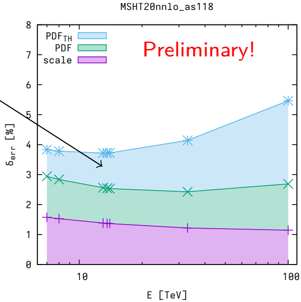
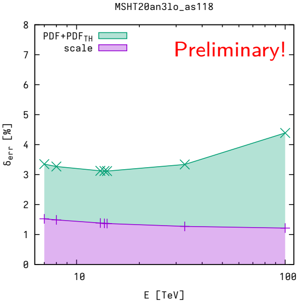
- Increase in cross-section at N3LO compensated by reduction in PDFs at aN3LO ⇒ important to consider PDF and σ changes together.
- aN3LO result lies within uncertainty band of full NNLO.
- NNPDF see similar effects, though slightly reduced due to changes in gluon PDF at aN3LO.

Gluon Fusion Higgs Production Uncertainty:

- Can compare total uncertainty on ggF Higgs production using aN3LO and NNLO PDFs:
- "PDF" uncertainty increased at aN3LO as incorporate "PDF-TH" part into it for first time ⇒ more rigorous determination of theory uncertainty from MHOUs.
- Nonetheless, still observe a net reduction in total uncertainty.

$\delta(PDF - th) = \frac{1}{2}\frac{[\sigma^{(2)}_{NNLO} - \sigma^{(2)}_{NLO}]}{[\sigma^{(2)}_{NNLO}]}$





Les Houches Proceedings (in preparation) - Thanks to A. Huss and S. Jones for plots

Further Devolopments of aNLO PDFs - QED and α_S

More information in articles: T. Cridge, L.A. Harland-Lang, R.S. Thorne, arXiv:hep-ph/2312.07665, 2312.12505, 2404.02964.

What about QED corrections? aN3LO+QED:

- All groups now provide NNLO + QED PDF sets. Important as naively $\alpha_{\rm QED}(M_Z) \sim \alpha_S^2(M_Z)$. Now combine with aN3LO QCD for highest possible precision!
- Need to combine aN3LO QCD evolution and $\mathcal{O}(\alpha, \alpha\alpha_S, \alpha^2)$:

$$\begin{aligned} \textbf{QED} \qquad & P_{ij} = \frac{\alpha}{2\pi}P_{ij}^{(0,1)} + \frac{\alpha\alpha_S}{(2\pi)^2}P_{ij}^{(1,1)} + \left(\frac{\alpha}{2\pi}\right)^2 P_{ij}^{(0,2)} \\ \textbf{NNLO QCD} \qquad & + \frac{\alpha_S}{2\pi}P_{ij}^{(1,0)} + \left(\frac{\alpha_S}{2\pi}\right)^2 P_{ij}^{(2,0)} + \left(\frac{\alpha_S}{2\pi}\right)^3 P_{ij}^{(3,0)} \\ \textbf{aN3LO QCD} \qquad & + \left(\frac{\alpha_S}{2\pi}\right)^4 P_{ij}^{(4,0)} \, . \end{aligned}$$

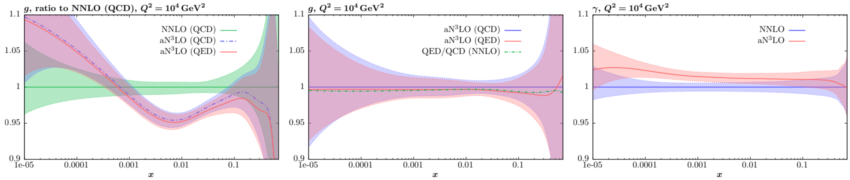
- Impact on fit at NNLO and aN3LO, substantial fit quality improvement remains true after adding QED:

	$\chi^2/N_{\rm pt}$ aN^{3}LO (QED)	$\Delta\chi^2_{\rm aN^3LO}$ QED-QCD	$\Delta\chi^2_{\rm NNLO}$ QED-QCD	$\Delta\chi^2_{\rm QCD,QED}$ aN^{3}LO-NNLO
Total	5323.6/4534	(+3.6)	(+17.3)	(-209.3, -223.1)

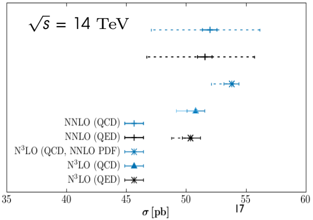
T.C., L.A. Harland Lang, R.S. Thorne 2312.07665 [5]

What about QED corrections? aN3LO+QED:

- Impact small relative to aN3LO QCD corrections in most regions.
- Effect of adding QED similar when applied to NNLO and aN3LO.



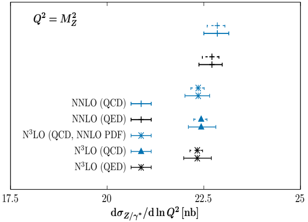
- Knock-on impact on cross-sections, ggF Higgs (left), Z (right):



N3LO QCD + NNLO PDFS

N3LO QCD + aN3LO PDFS

N3LO QCD + aN3LO/QED PDFS



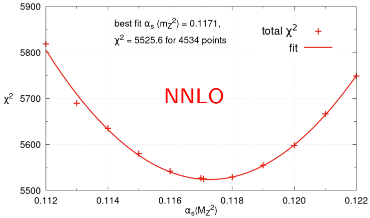
T.C., L.A. Harland Lang, R.S. Thorne 2312.07665 [5]

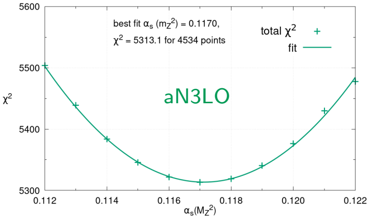
MSHT20 α_S dependence - NNLO and aN3LO

(first ever!)

- First PDF $\alpha_S(M_Z^2)$ determination at aN3LO.
- Consistent with NNLO determination within uncertainties.
- Good perturbative convergence of α_S determination.

$$\alpha_{S,\mathrm{NNLO}}^{new}(M_Z^2) = 0.1171 \qquad \alpha_{S,\mathrm{aN3LO}}^{new}(M_Z^2) = 0.1170$$





Nice Quadratic χ^2 profile ✓

- Can also determine bounds (next slide).

T.C., L.A. Harland-Lang, R.S. Thorne 2404.02964 [7].

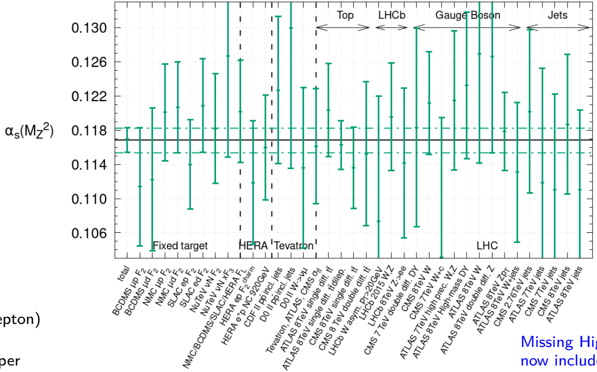
MSHT20 α_S bounds - aN3LO

Consistent with α_S bounds seen in previous studies, and between orders (NNLO and aN3LO).

BCDMSp data strongest constraint upwards: $\Delta\alpha_S(M_Z^2) = +0.0013$.

F_2^C provides upwards bound of: $\Delta\alpha_S(M_Z^2) = +0.0020$.

CMS and ATLAS (dilepton) $t\bar{t}$ single diff. would give slightly higher upper α_S bounds, but not used.



SLAC deuteron data gives lower bound: $\Delta\alpha_S(M_Z^2) = -0.0016$.

NMC deuteron, ATLAS 8 TeV Z both give lower bounds of $\Delta\alpha_S(M_Z^2) = -0.0017$.

Missing Higher Order Uncertainties now included, in particular causes some LHC bounds to weaken as unknown N3LO K-factors.

- Therefore upper/lower bounds are $+0.0013$/-0.0016 at aN3LO.

$$\alpha_{S,\mathrm{aN3LO}}(M_Z^2) = 0.1170 \pm 0.0016$$

Consistent with (NNLO) World Average of 0.1180 ± 0.0009.

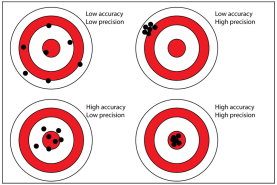
T.C., L.A. Harland-Lang, R.S. Thorne 2404.02964 [7].

Conclusions

Conclusions:

MSHT20aN3LO 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.
- MSHT produced the world first approximate N3LO PDFs, including both higher order effects in PDFs and also theoretical uncertainties. NNPDFaN3LO recently also available.
- N3LO evolution benchmarking almost complete and shows consistency.
- Consistent results seen by both groups in terms of PDF impacts and consequences for phenomenology.
- MSHT20aN3LO and NNPDFaN3LO both publicly available and we encourage their use!
- All part of ongoing work to increase PDF precision and accuracy.
- Any questions about them/their use $\Rightarrow$ please ask us!



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(QCD)	$n_f^{\max}$	N_{mem}	$\alpha_S(m_Z^2)$	Description
MSHT20nnlo_as118	NNLO	5	65	0.118	Default NNLO set
MSHT20nlo_as120	NNLO	5	65	0.118	Default NLO set
MSHT20lo_as130	NNLO	5	65	0.118	Default LO set
MSHT20nnlo_as_largerange	NNLO	5	23	0.108-0.130	$\alpha_S(M_Z^2)$ variation NNLO set
MSHT20nlo_as_largerange	NLO	5	23	0.108-0.130	$\alpha_S(M_Z^2)$ variation NLO set
MSHT20nnlo_mcrange_nf5	NNLO	5	9	0.118	Charm mass variation (1.2-1.6 GeV) NNLO set
MSHT20nnlo_mbrange_nf5	NNLO	5	7	0.118	Bottom mass variation (4.0-5.5 GeV) NNLO set
MSHT20nnlo_nf3,4	NNLO	3, 4	65	0.118	NNLO set with max. 3 or 4 flavours
MSHT20qed_nnlo	NNLO	5	77	0.118	NNLO set with QED effects and γ PDF
MSHT20qed_nnlo_(in)elastic	NNLO	5	77	0.118	NNLO set with QED effects and (in)elastic γ
MSHT20qed_nnlo_neutron	NNLO	5	77	0.118	NNLO neutron set with QED effects and γ
MSHT20an3lo_as118	aN3LO	5	105 (85)	0.118	Approximate N3LO set with theoretical uncertainties also included
MSHT20qed_an3lo	aN3LO	5	97	0.118	Approximate N3LO set with theoretical uncertainties also included and QED effects and γ PDF

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

Key:

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

- Feel free to contact us with questions about usage.

Selection of some references (others on slides):

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2. Duhr, Mistelberger, 2111.10379.
3. J. McGowan et al. (inc. TC), 2207.04739.
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34. J. Ablinger et al., 1406.4654.
35. J. Ablinger et al., 1409.1135.
36. J. Blümlein et al, 2107.06267.
37. J. Ablinger et al., 1405.4259.
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39. J. Ablinger et al., 1402.0359.
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44. E. Laenen and S.-O. Moch, hep-ph/9809550.
45. J. A. M. Vermaseren et al. hep-ph/0504242.
46. C. Anastasiou et al., 1602.00695.
47. B. Mistlberger, 1802.00833.
48. F.A. Dreyer and A. Karlberg, 1606.00840.
49. J. Baglio et al., 2209.06138.
50. M. Bonvini, arXiv:1805.08785. 34
51. C. Duhr et al., 2001.07717.
52. C. Duhr et al., 2007.13313.
53. X. Chen et al., 2107.09085.
54. C. Duhr and B. Mistlberger, 2111.10379.
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56. N. Kidonakis, 2203.03698.
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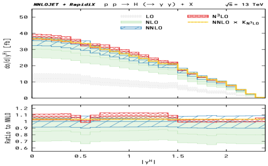
Backup Slides

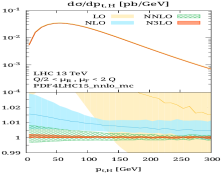
Particle Physics and N3LO Progress

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

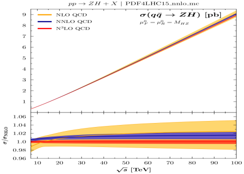
1. Higgs - Differential for ggF (y_H, etc) and VBF (p_T^H, y_H), inclusive VH:



Chen et al 2102.07607

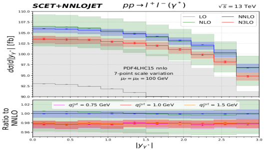


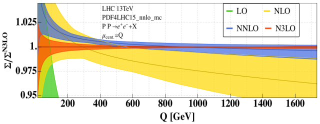
Dreyer et al 1606.00840

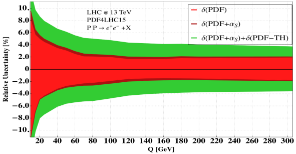


Baglio et al 2209.06138

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 . . .

Theory Uncertainty via TNPs

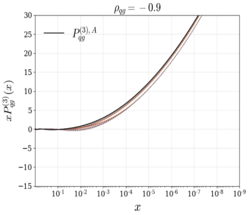
Advantages of TNP method:

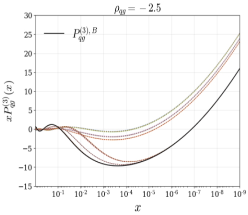
- Probes precisely the missing higher order terms.
- Allows inclusion of known N3LO information (a lot) without needing to wait for remaining few pieces.
- Can be included in PDF fit in same way experimental data are.
- No requirement for scale variations - can underestimate MHOU, issue of correlation between PDF fit and use [11].
- Exactly same data can be included at all orders - no need to raise Q^2 cut on data to enable downwards scale variations.
- Output eigenvectors include theory uncertainty from missing higher orders out-of-the-box ⇒ using `MSHT20aN3LO` PDF set exactly as previous sets includes theory uncertainty for no extra user effort.

- Applications also more widely - e.g. theory uncertainty for Z p_T spectrum and α_S. F. Tackmann SCET 2019; and T.C., G. Marinelli, F. Tackmann (work in progress).

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 $\Rightarrow$ prior set conservatively.

Transition Matrix Elements

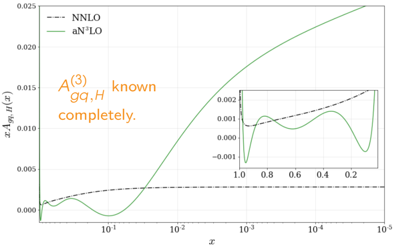
Ingredient 2

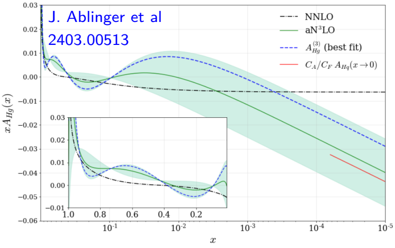
- Several transition matrix elements known completely - $A_{Hq}^{PS,(3)}$, $A_{gq,H}^{(3)}$.
- For others we know:
  - Even low-integer N Mellin Moments (4-8)
    - constrain intermediate and high x via $\int_0^1 dx\, x^{N-1} P(x)$.
  - Form at low x, in some case low and high x limits.
- Deal with as 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 $a_{Hg}, a_{qq,H}^{NS}, a_{gg,H}$.

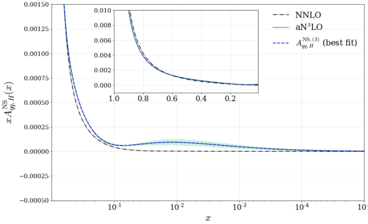
J. Ablinger et al 2311.00644.

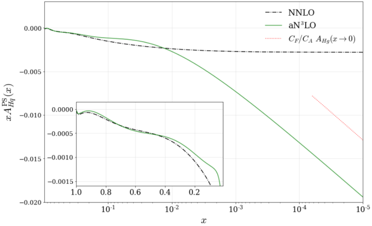
J. Ablinger et al 2211.05462.

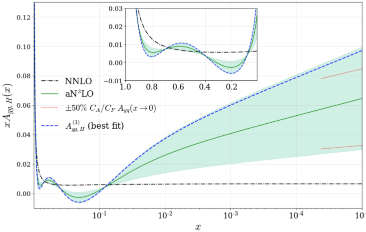




Transition Matrix Elements:







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

DIS Coefficient Functions

Ingredient 3

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

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

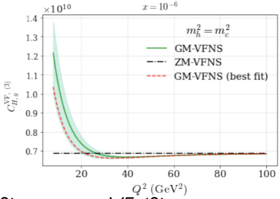
DIS Coefficient Functions

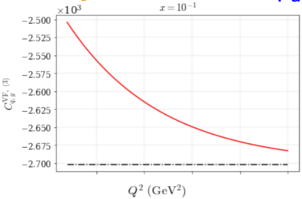
$$C^{VF,(3)}_{H,g} = C^{FF,(3)}_{H,g} - C^{VF,(2)}_{H,g} \otimes A^{(1)}_{gg,H} - C^{VF,NS+PS,(2)}_{H,H} \otimes A^{(1)}_{Hg}$$
$$- C^{VF,(1)}_{H,g} \otimes A^{(2)}_{gg,H} - C^{VF,(1)}_{H,H} \otimes A^{(2)}_{Hg} - C^{VF,(0)}_{H,H} \otimes A^{(3)}_{Hg}$$

- 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 ⇒ introduce theory nuisance parameters c_q^{NLL} and c_g^{NLL}:

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

⇒ 2 Theory Nuisance Parameters from here.





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

Hadronic K-factors

Ingredient 4

- N3LO calculations becoming available but not yet for PDF fits:
  - Drell-Yan - Inclusive and some differential calculations [51–55] - not yet for relevant fiducial cross-sections or in form usable for PDFs.
  - Higgs - ggF, VBF and VH [46–50] - doesn't go in PDFs.
  - Top (aN3LO) - soft gluon resummation approximation[56].
- Overall, much less known than for other N3LO PDF fit ingredients.
- Parameterise N3LO k-factor as combination of NLO and NNLO k-factors, a_1, a_2 coeffs incorporating MHOUs into PDF uncertainties:

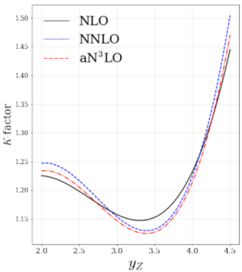
$$K^{N3LO/LO} = K^{NNLO/LO}(1 + a_1 \mathcal{N}^2 \alpha_S^2 (K^{NLO/LO} - 1) + a_2 \mathcal{N} \alpha_S (K^{NNLO/LO} - 1))$$

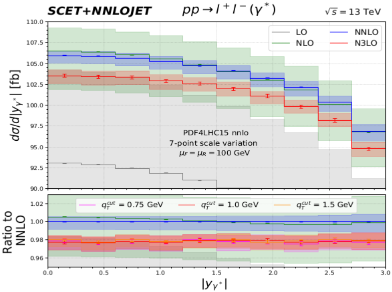
- Default prior is $a_1, a_2 = 0$, i.e. no N3LO correction.
- Categorise all hadronic processes into 5 types - jets (or dijets), Drell-Yan, top, vector boson p_T/jets, and dimuon.
- 2 theory nuisance parameters each ⇒ 10 theoretical parameters added.

Hadronic K-factors - Drell-Yan

1. **Drell-Yan (DY)**

- Fit prefers a ≈ 1% decrease in the N3LO k-factors relative to NNLO.
- Improved perturbative convergence with aN3LO PDFs.
- In qualitative agreement with recent N3LO results for NC DY[53].

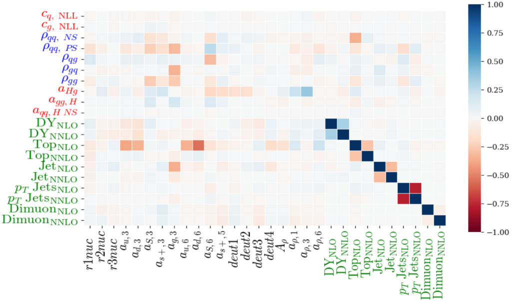




- Key point: Method allows N3LO info. on any piece to be incorporated as it becomes available, rather than needing to wait for all info. - e.g. can include N3LO k-factors as they become available for PDFs.

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!

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.

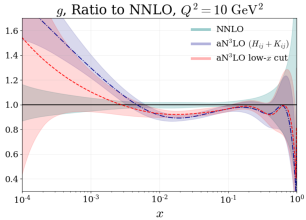
- Improvement in fit quality from NNLO to aN3LO is $\Delta\chi^2 = -154.4$.
  - Much larger than number of parameters (20) introduced.

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

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

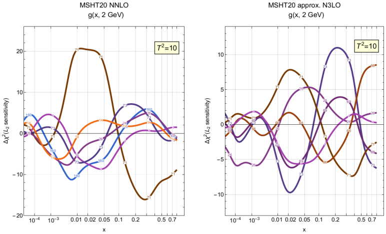
Perform aN3LO fit - Reduced Tensions:

- Reduced tensions between some datasets seen at aN3LO.
- Small x - high x data tension reduced.
- Precise ATLAS 8 TeV Zp_T data fit quality at NNLO is poor, but at aN3LO is good:



Order	NNLO	aN3LO
ATLAS 8 TeV Zp_T	1.87	1.04
Total	1.22	1.17

Fit qualities $\chi^2/N_{\rm pts}$.

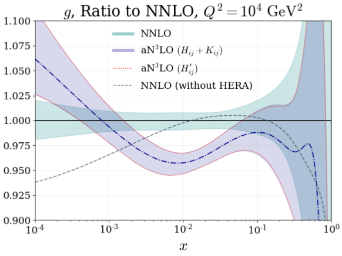


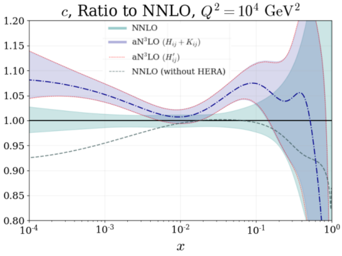
X. Jing et al. (inc. TC) 2306.03918 [10]

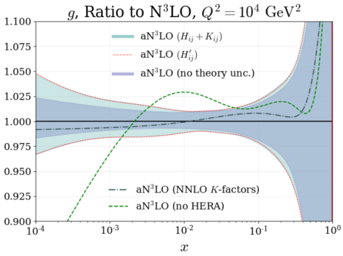
- Tensions between ATLAS 8TeV Zp_T and other data reduced at aN3LO.
- High precision data requires high precision theory.

Perform aN3LO fit - PDF impacts:

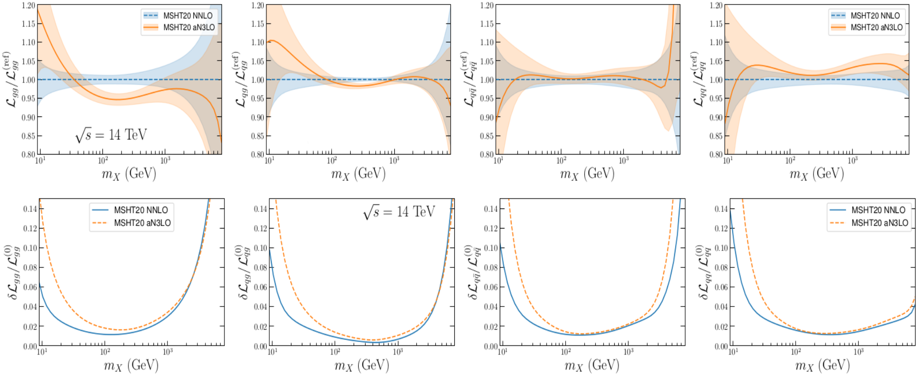
- Gluon enhanced at small x - due to higher power large logs that appear.
- Gluon uncertainty increased at small x due to theory uncertainty, largely on splitting functions.
- Heavy quarks - c and b (perturbatively generated) raised due to increase in gluon at lower x and raised A_{Hg} at high x.





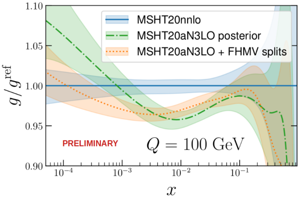


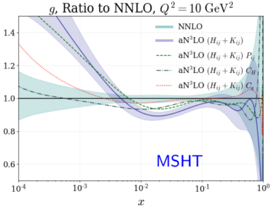
aN3LO PDF luminosities:

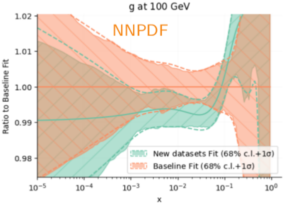


- PDF changes have implications for PDF luminosities for phenomenology.
- *gg* luminosity reduced around 100GeV and increased at 10GeV.
- Luminosity uncertainties enlarged (and more so at lower invariant masses) due to inclusion of aN3LO and PDF theory uncertainties.

Further Considerations and PDF impacts:

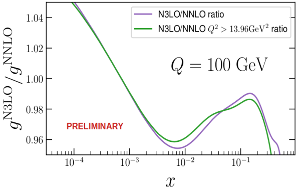






- New moments cause small increase, though consistent with before.
- Other aN3LO effects important, e.g. DIS coefficient functions.
- New data also changes gluon, e.g. new 13TeV jet data lower NNPDF gluon *closer to MSHT*.

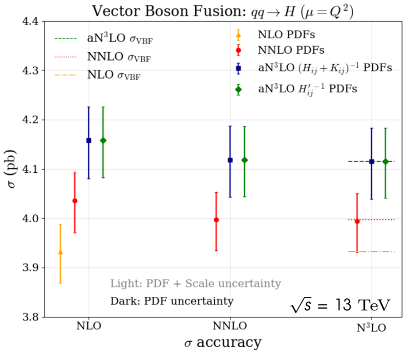
- If cut low Q^2 data as can be required for scale variation approach, impacts gluon.
- Several different aspects contribute to any differences. *Consistent picture emerging...*



Impact on Higgs cross-sections - VBF:

Preliminary!

- 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.

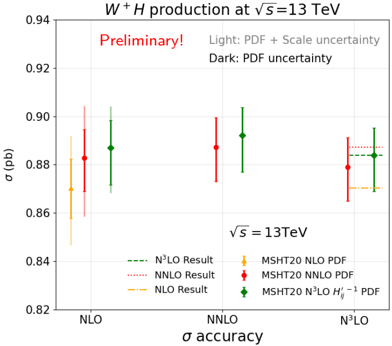
Results obtained using `proVBFH` code[48,57].

- 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[49].

- 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.

NLO and NNLO Cross-section Scale Variations

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

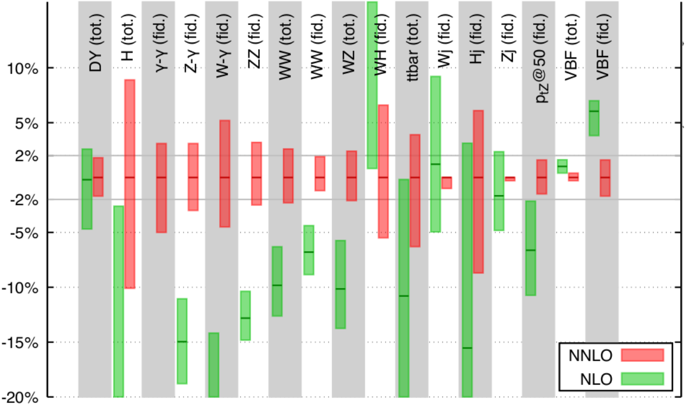
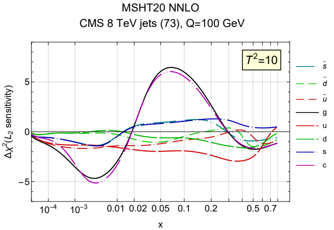
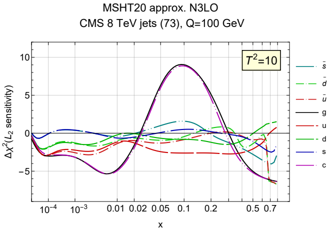


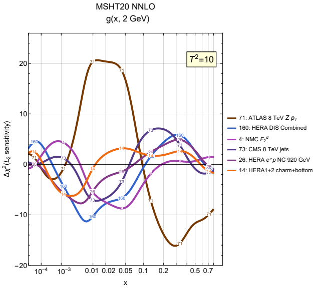
Image Credit: G. Salam

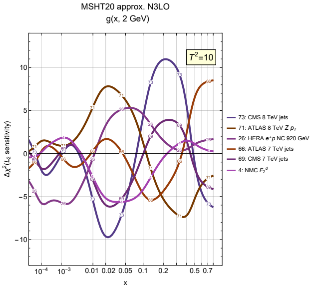
- Is there a better way to do this?

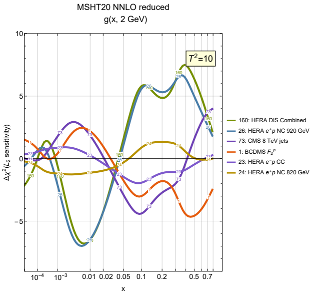
NNLO and aN3LO Data "Pulls" - L_2 Sensitivities - g





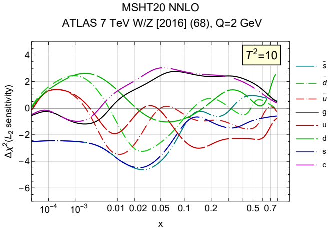


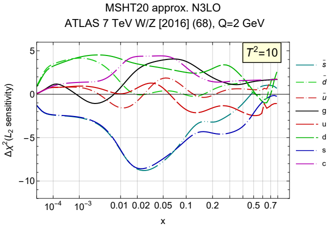


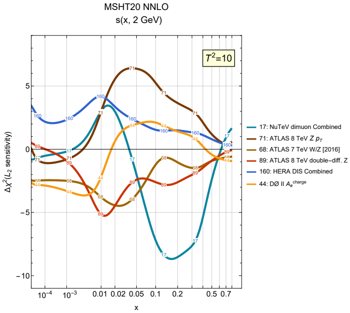


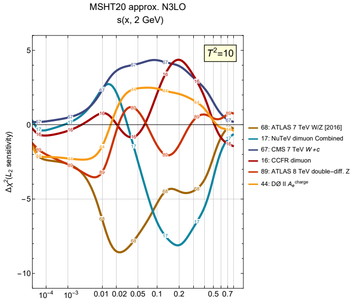
See X. Jing et al. (inc. TC) 2306.03918 [10]

NNLO and aN3LO Data “Pulls” - L_2 Sensitivities - s^+





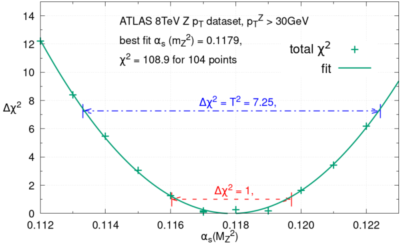




See X.Jing et al. (inc. TC) 2306.03918 [10]

MSHT20 ATLAS 8 TeV Z p_T α_S dependence

- ATLAS 8 TeV Z p_T data with $p_T^Z > 30$ GeV is in the MSHT PDF fit.
- What bounds does it offer within the global PDF fit on $\alpha_S(M_Z^2)$?

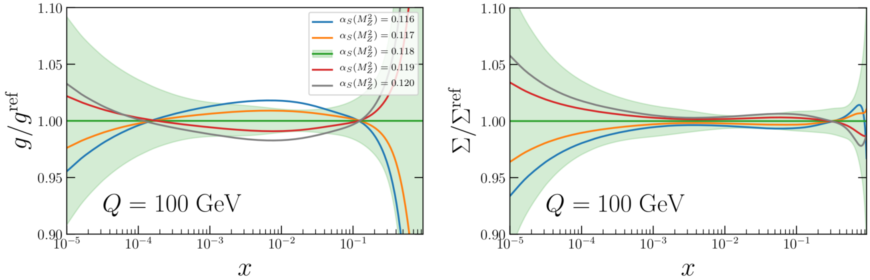


- If you do individual dataset extraction you use $\Delta\chi^2 = 1$ for bounds.
- If you do do in a global fit, factoring in tensions with other data you use $\Delta\chi^2 = T^2 = 7.25$ for bounds.
- $p_T^Z > 30$ GeV not very constraining on $\alpha_S(M_Z^2)$ in global PDF fit.
- ATLAS Z p_T α_S result used $p_T^Z < 29$GeV part of spectrum. Used MSHT20 aN3LO PDFs to correspond to accuracy used in resummation.

MSHT20 PDF α_S dependence

Forte, Kassabov: 2001.04986

- Correlations between PDFs and $\alpha_S \Rightarrow$ necessity of global fit.



- Changes generally within PDF uncertainties for $\Delta\alpha_S(M_Z) \approx \pm 0.001$.
- Gluon anti-correlated with $\alpha_S(M_Z^2)$ for $x \lesssim 0.1$ as maintains $dF_2/dQ^2 \sim \alpha_S g$. Implies correlated at high $x \gtrsim 0.1$ by momentum sum rule.
- Larger effect at low Q^2 as less evolution distance.
- Smaller effects on quarks, reduced/increased at high/low x by splitting. s less impacted, at high x may absorb some of change.

Acknowledgments

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