PDFs @ Approximate N3LO - MSHT Review

Higgs WG1: aN3LO Meeting, CERN

Thomas Cridge

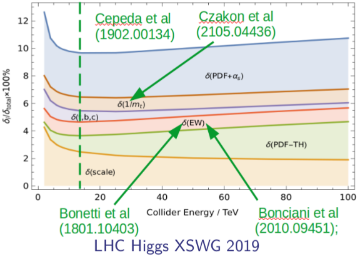
26th June 2024

In collaboration with MSHT colleagues - T.C., L.A. Harland-Lang and R.S. Thorne.

Overview

Context for Gluon Fusion Higgs Production:

- Uncertainties on ggF Higgs production:



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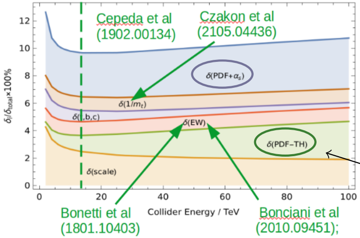

LHC Higgs XSWG 2019

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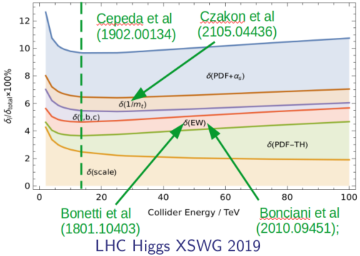

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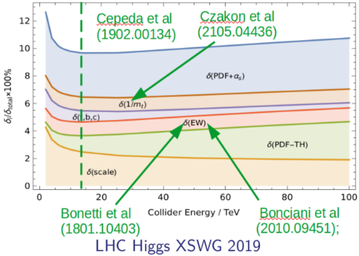

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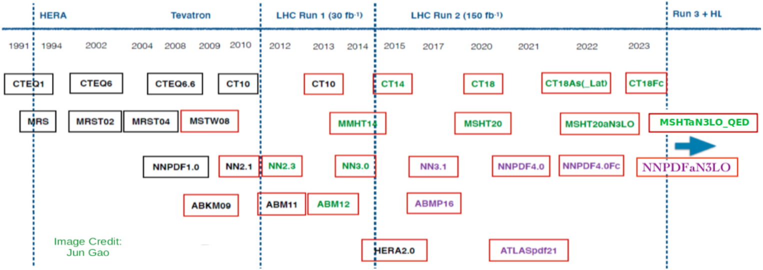

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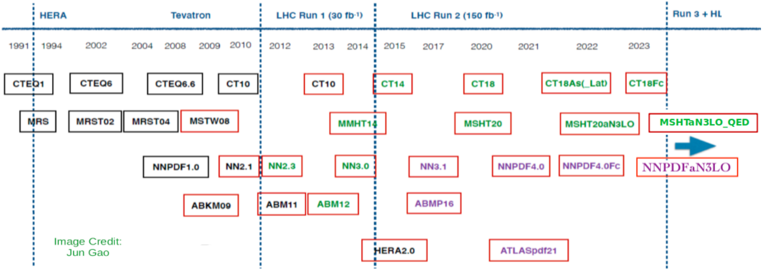

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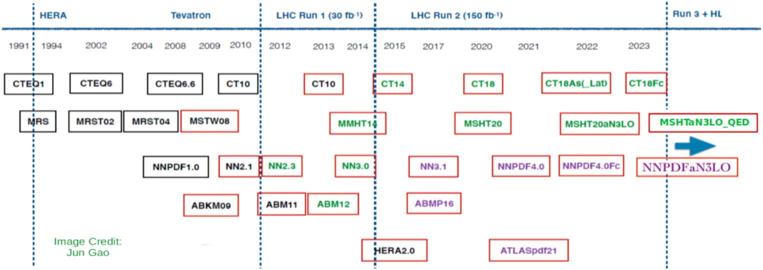

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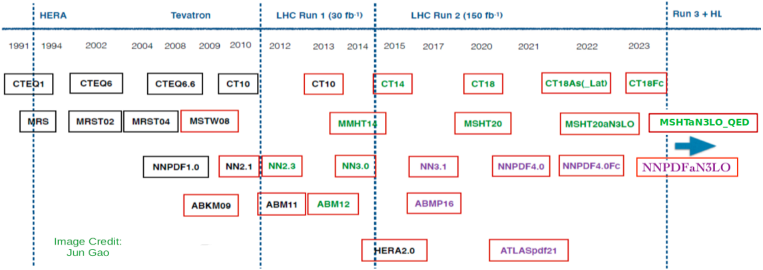

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- Also available for ∼ 6 months:
  MSHT20qed_an3lo, aN3LO QCD + QED PDF set.

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7. Benchmarking of QCD evolution at Approximate N3LO with theory (FHMRUVV), NNPDF and other colleagues (also in Les Houches SM WG Report), 2406.16188.

Current Knowledge of N3LO

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- Much already known, only a few remaining missing pieces.

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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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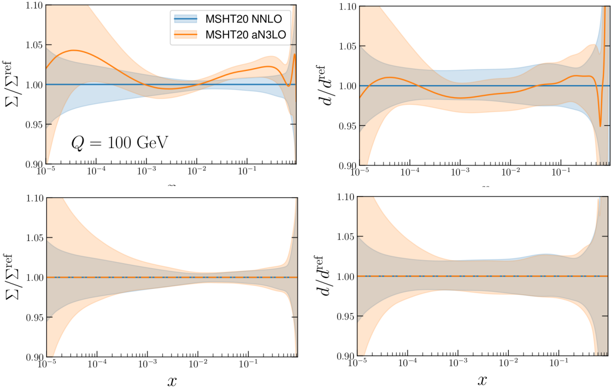
Effect of N3LO on PDFs:

Impacts of aN3LO on MSHT PDFs:

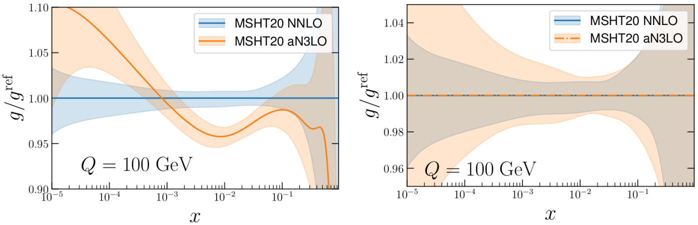
- Mild effects on most PDFs, particularly light quarks:



- Generally percent level impacts of aN3LO in data region and few percent elsewhere. Uncertainty generally similar in data region.
- Inclusion for first time of theoretical uncertainty from MHOUs enlarges PDF uncertainty at small x.

Impacts of aN3LO on MSHT PDFs:

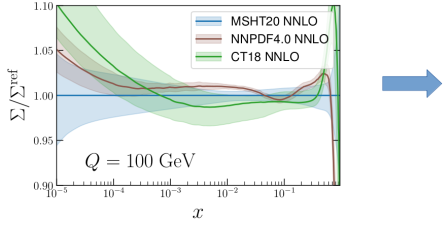
- Larger effect on gluon PDF:

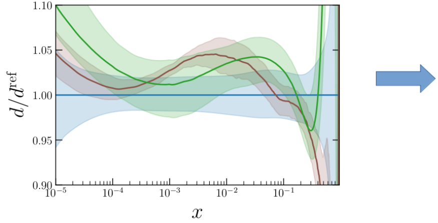


- Observed impact on gluon of aN3LO is larger than for quarks, with $\sim$ 5% dip around 10^{-2}.
- Inclusion of theoretical uncertainty for first time also enlarges gluon uncertainty, including small increase in data (Higgs) region.
- Whilst PDF uncertainty is larger, it's more complete (inclusion of theoretical error), accurate and reliable.

Comparison of aN3LO impacts on PDFs:

- Quarks relatively unaffected:





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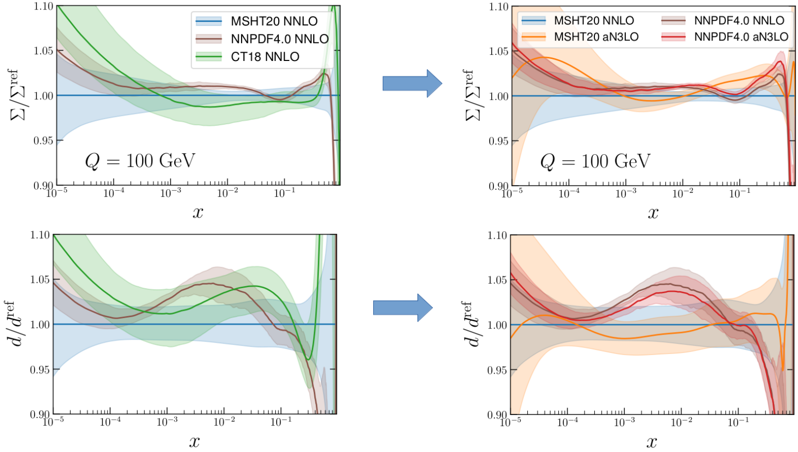

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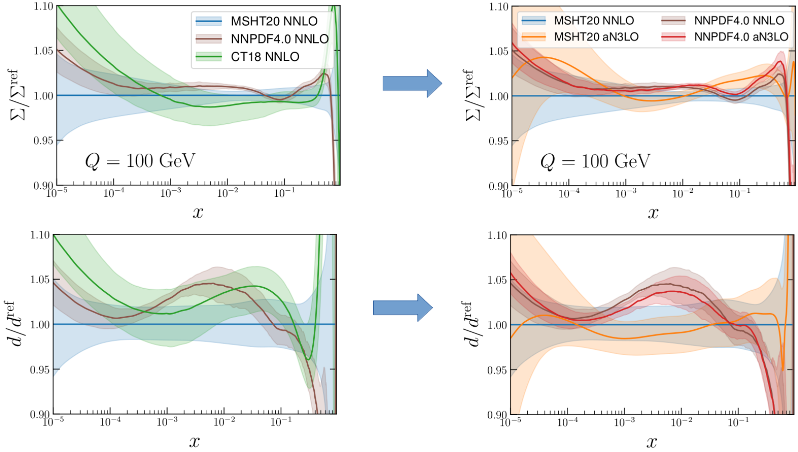
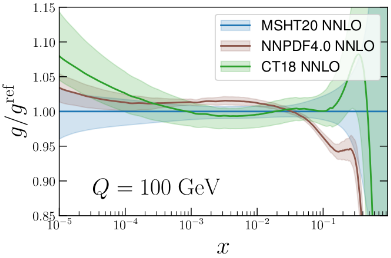


- Singlet PDF - NNLO and aN3LO all show same % level differences.
- Down PDF - as much difference between aN3LO PDFs as NNLO.

Comparison of aN3LO impacts on PDFs:

- Largest effect on the gluon PDF.



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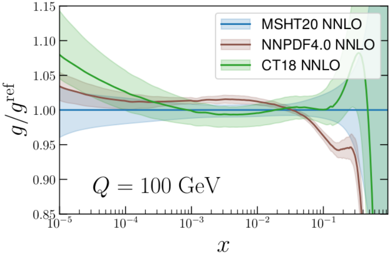

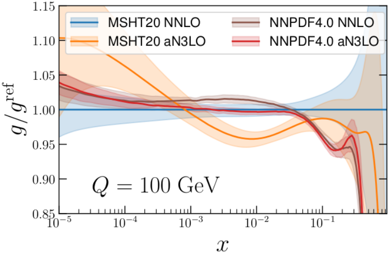

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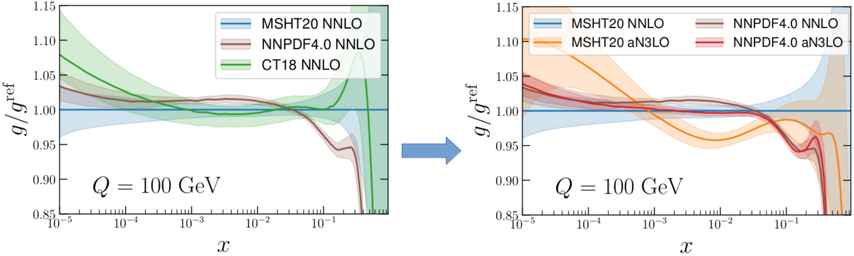

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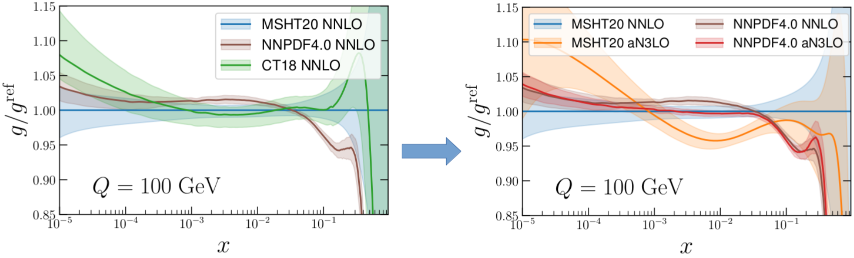

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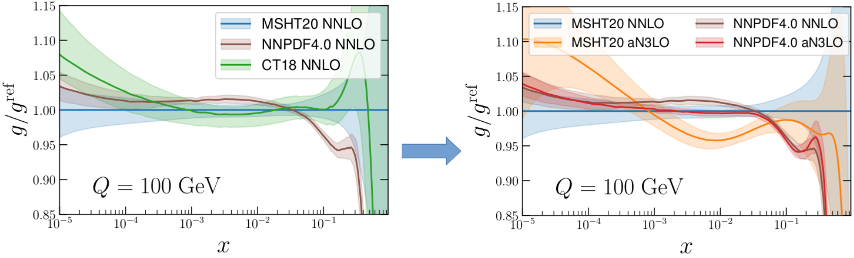

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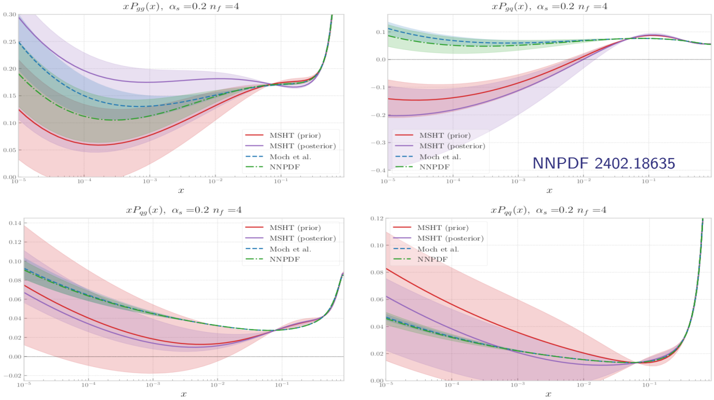
- Uncertainty observed to grow, particularly at small x by both groups.

N3LO PDF Evolution

- One key ingredient is the 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:

Les Houches Proceedings (2406.00708) and recent (yesterday) article - (2406.16188).

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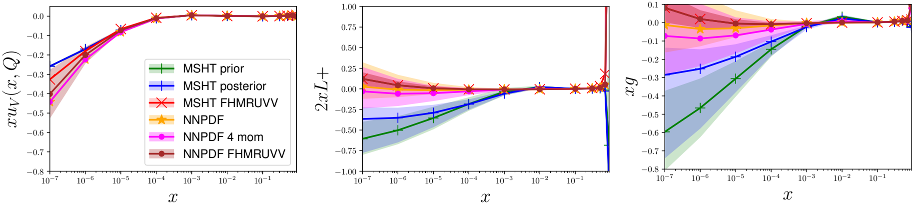

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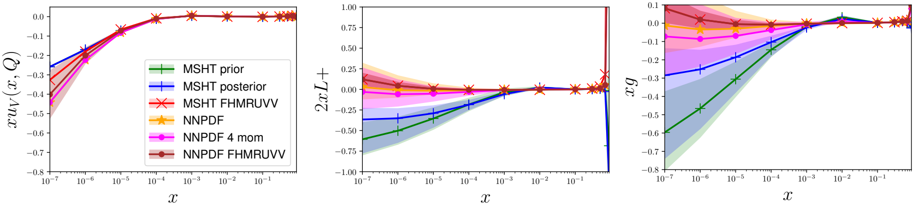

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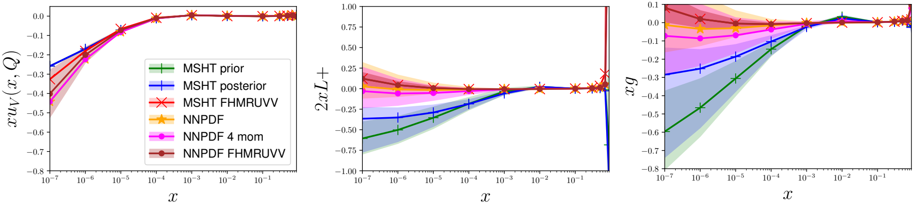

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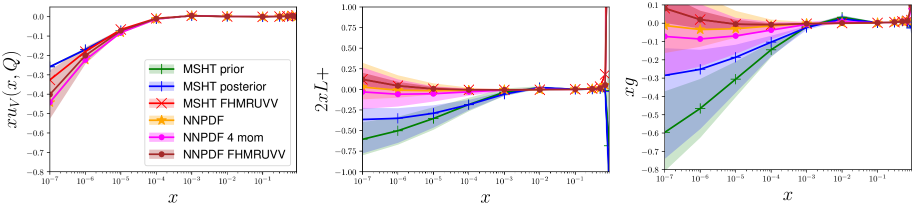

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- Per mille agreement when using the same splitting functions (right).

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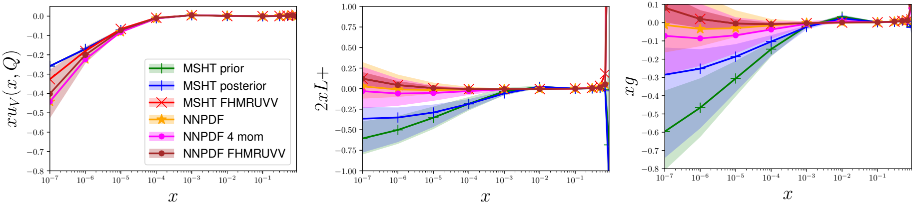

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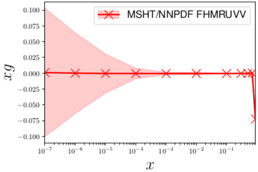

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aN3LO QCD + QED:

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

- MSHT now for first time provide aN3LO QCD + QED PDFs!

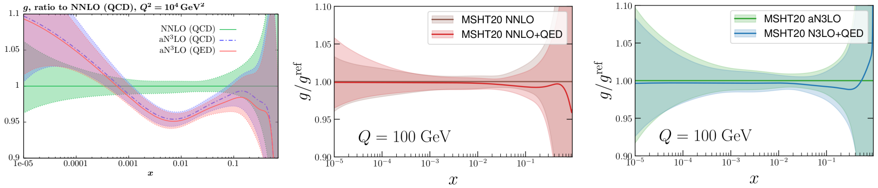
QED $$P_{ij} = \frac{\alpha}{2\pi} P_{ij}^{(0,1)} + \frac{\alpha\alpha_S}{(2\pi)^2} P_{ij}^{(1,1)} + \left(\frac{\alpha}{2\pi}\right)^2 P_{ij}^{(0,2)}$$

NNLO QCD $$+ \frac{\alpha_S}{2\pi} P_{ij}^{(1,0)} + \left(\frac{\alpha_S}{2\pi}\right)^2 P_{ij}^{(2,0)} + \left(\frac{\alpha_S}{2\pi}\right)^3 P_{ij}^{(3,0)}$$

aN3LO QCD $$+ \left(\frac{\alpha_S}{2\pi}\right)^4 P_{ij}^{(4,0)} .$$

	$\chi^2/N_{\rm pt}$ 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)

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

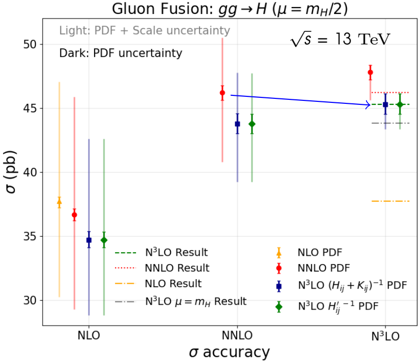


- Impact small relative to aN3LO QCD corrections in most regions.
- Same effect at NNLO (centre) and aN3LO (right), slight reduction in gluon due to momentum sum rule.

Consequences of aN3LO PDFs for Phenomenology

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

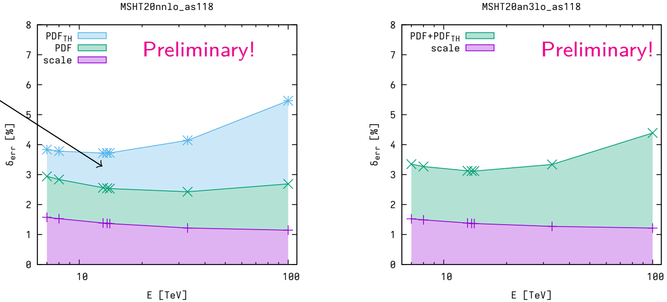
Results obtained using ggHiggs code[50].

- 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.

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.

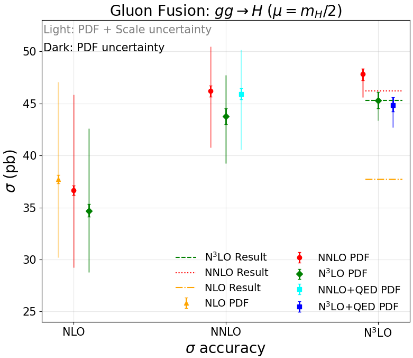
$\delta(PDF - th) = \frac{1}{2}\frac{[\sigma^{(2)}_{NNLO} - \sigma^{(2)}_{NLO}]}{[\sigma^{(2)}_{NNLO}]}$



Les Houches Proceedings (2406.00708) - Thanks to A. Huss and S. Jones for plots

Gluon Fusion Higgs Production - PDFs:

- What is the effect of including QED on top of aN3LO QCD?:
  - Net effect is a further ∼ 1% reduction in ggF Higgs production:



Impact of addition of QED ≈ factorises from PDF QCD order.

  - Impact comes through effect on gluon PDF.
  - Recommend to use aN3LO QCD + QED PDF, it's the highest accuracy we have.
  - Similar effects seen in NNPDF, though slightly larger in NNPDF.

Gluon Fusion Higgs Production - PDFs:

- ggF Higgs total inclusive σ (pb) at N3LO at $\sqrt{s} = 14\mathrm{TeV}$
  rough numbers with different PDFs, central values only:

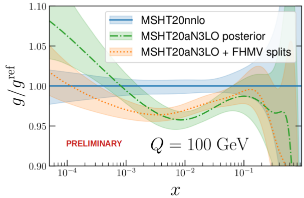
NNLO PDFs		aN3LO PDFs		aN3LO + QED PDFs	
MSHT20 NNLO	53.759	MSHT20 aN3LO	50.932	MSHT20 aN3LO + QED	50.500
"	"	MSHT20 aN3LO + FHMRUVV	50.954	"	"
NNPDF4.0 NNLO	54.134	NNPDF4.0 aN3LO	52.978	NNPDF4.0 aN3LO + QED	52.106

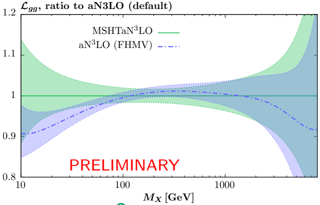
Produced using the `n3loxs` code[49].

- Observe: (not at all "official" numbers, for comparison only)
  - $\sim$ 2% difference using NNLO (without QED) PDFs.
  - $\sim$ 3% difference using aN3LO + QED PDFs.
  - MSHT/NNPDF see $\sim 5/2\%$ reduction in NNLO $\rightarrow$ aN3LO PDFs.
  - MSHT/NNPDF see $\sim 1/2\%$ further reduction in aN3LO $\rightarrow$ aN3LO+QED PDFs.
  - So net reduction MSHT/NNPDF see is $\sim 6/4\%$ in NNLO $\rightarrow$ aN3LO+QED.
  - PDF uncertainty (inc. th) $\sim 1-2\%$, PDF+scale uncertainty $\sim$ few %.
- Overall consistent picture qualitatively of net reduction of ggF Higgs from aN3LO QCD + QED gluon relative to NNLO QCD only.

Examination of aN3LO on gluon and ggF:

- Overall consistent trends observed, but some differences in sizes of effects, though similar to usual PDF differences! Can we explain them?
- New moments available for some splitting functions [26-30] since MSHT20an3lo (and further [31] since even NNPDFan3lo).
- Benchmarking is just evolution, what about effect in PDF fit?:

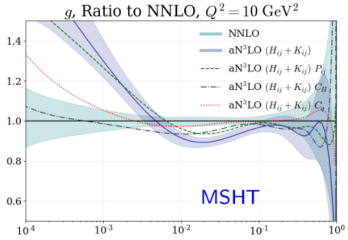


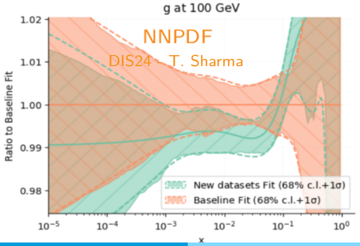


- Slight $\sim 1.5\%$ increase in gluon at $x \approx 10^{-2}$, though still consistent with MSHT20an3lo uncertainties.
- However, gg luminosity (and $\sigma_{gg\to H}$) almost unchanged at m_H.
- Occurs as luminosity integrates over rapidity so increase at $x \approx 10^{-2}$ is compensated by reduction in neighbouring regions of x.

Examination of aN3LO on gluon and ggF:

- Other potential sources of difference in the gluon PDF?
  - Other N3LO ingredients also important (lower left) - e.g. heavy flavour transition matrix elements, more info. now available [40-42].
  - Different implementation of theoretical uncertainties - theory nuisance parameters and scale variations.
- Plus we have the usual sources of PDF changes/differences:
  - Methodology, e.g. perturbative vs fitted charm, positivity can cause $\sim$ 1% differences in the gluon.
  - Data, e.g. new 13TeV jet data lower NNPDF gluon (lower right).
  - Interplay of aN3LO effects with rest of PDF fit is non-trivial.





Initial Thoughts for YR5:

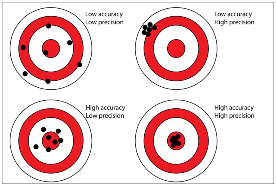
- MSHT recommend to use highest order PDFs available, aN3LO QCD effects should be included. In fact we see evidence of greater perturbative stability of “whole orders” rather than “partial orders”.
- Trend of reduced gluon PDF and ggF Higgs xsec for aN3LO PDFs seen by both groups, difference in details.
- Incorporation of theoretical uncertainty into PDFs important at this level of precision, impacts PDF central values and uncertainty.
- aN3LO PDFs include this directly in PDF eigenvectors (or replicas), output PDF uncertainty includes this out-of-the box ⇒ no need for artificial proxy used previously of extra $\delta(PDF - TH) \approx \frac{1}{2}\frac{[\sigma^{(2)}_{NNLO} - \sigma^{(2)}_{NLO}]}{[\sigma^{(2)}_{NNLO}]}$.
- Important to also consider QED effects on PDF ⇒ MSHT recommend using the aN3LO QCD + QED PDFs as highest accuracy: `MSHT20qed_an3lo`.
- We observe impact of QED on the fit approximately factorises, therefore potential to consider effect on top of PDF4LHC21?

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.
- N3LO evolution benchmarking almost complete and shows consistency.
- Generally consistent results seen by both groups in terms of PDF impacts and consequences for phenomenology.
- Also aN3LO QCD + QED PDFs produced and publicly available.
- Important to consider aN3LO QCD and QED effects for ggF Higgs.
- Many developments, 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)	$n_f^{\max}$	$N_{\rm mem}$	$\alpha_S(m_Z^2)$	Description
MSHT20nnlo_as118	NNLO	5	65	0.118	Default NNLO set
MSHT20nlo_as120	NNLO	5	65	0.118	Default NLO set
MSHT20lo_as130	NNLO	5	65	0.118	Default LO set
MSHT20nnlo_as_largerange	NNLO	5	23	0.108-0.130	$\alpha_S(M_Z^2)$ variation NNLO set
MSHT20nlo_as_largerange	NLO	5	23	0.108-0.130	$\alpha_S(M_Z^2)$ variation NLO set
MSHT20nnlo_mcrange_nf5	NNLO	5	9	0.118	Charm mass variation (1.2-1.6 GeV) NNLO set
MSHT20nnlo_mbrange_nf5	NNLO	5	7	0.118	Bottom mass variation (4.0-5.5 GeV) NNLO set
MSHT20nnlo_nf3,4	NNLO	3, 4	65	0.118	NNLO set with max. 3 or 4 flavours
MSHT20qed_nnlo	NNLO	5	77	0.118	NNLO set with QED effects and γ PDF
MSHT20qed_nnlo_(in)elastic	NNLO	5	77	0.118	NNLO set with QED effects and (in)elastic γ
MSHT20qed_nnlo_neutron	NNLO	5	77	0.118	NNLO neutron set with QED effects and γ
MSHT20an3lo_as118	aN3LO	5	105 (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):

1 M. Cepeda et al., 1902.00134.
2 Duhr, Mistelberger, 2111.10379.
3 J. McGowan et al. (inc. TC), 2207.04739.
4 R. D. Ball et al, 2402.18635.
5 T. Cridge et al., 2312.07665.
6 T. Cridge et al., 2312.12505.
7 T. Cridge et al., 2404.02964
8 R. D. Ball et al, 2401.10319.
9 L.A. Harland-Lang and R.S. Thorne, 1811.08434.
10 X. Jing et al (inc. TC), 2306.03918.
11 S. Moch, et al. 1707.08315.
12 J. Davies et al., 1610.07477.
13 J. M. Henn et al., 1911.10174.
14 C. Duhr et al, 2205.04493.
15 Y. L. Dokshitzer et al., hep-ph/0511302.
16 A. A. Almasy et al., 1012.3352.
17 V. S. Fadin et al., Phys. Lett. B 60, 50 (1975).
18 E. A. Kuraev et al., Sov. Phys. JETP 44, 443.
19 L. N. Lipatov, Sov. J. Nucl. Phys. 23, 338 (1976).
20 E. A. Kuraev et al., Sov. Phys. JETP 45, 199.
21 V. S. Fadin and L. N. Lipatov, hep-ph/9802290.
22 T. Jaroszewicz, Phys. Lett. B 116, 291 (1982).
23 M. Ciafaloni and G. Camici, hep-ph/9803389.
24 S. Catani and F. Hautmann, hep-ph/9405388.
25 J. Davies et al., 2202.10362.
26 G. Falcioni et al., 2302.07593.
27 G. Falcioni et al., 2307.04158.
28 G. Falcioni et al., 2310.01245.
29 S. Moch et al., 2310.05744.
30 G. Falcioni et al., 2404.09701.
31 T. Gehrmann et al., 2308.07958.
32 H. Kawamura et al., 1205.5727.
33 I. Bierenbaum et al., 0904.3563.
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.
38 J. Ablinger et al., 1409.1435.
39 J. Ablinger et al., 1402.0359.
40 J. Ablinger et al., 2211.05462.
41 J. Ablinger et al., 2311.00644.
42 J. Ablinger et al., 2403.00513.
43 S. Catani et al., Phys. B 366, 135 (1991).
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.
55 X. Chen et al., 2102.07607.
56 N. Kidonakis, 2203.03698.
57 M. Cacciari et al, 1506.02660.
58 NNPDF, 2406.01779.

Backup Slides

aN3LO effects on the PDF fit:

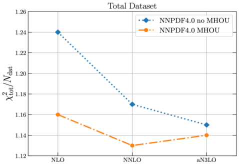
- aN3LO (and theory uncertainties) have impact on PDF fit.
  - MSHT and NNPDF - Improvement order by order of fit quality:

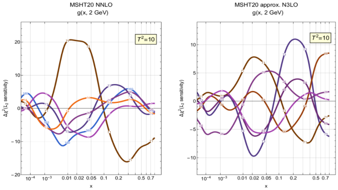
MSHT χ^2/N_{pts} (4363)	LO	NLO	NNLO	aN3LO
	2.57	1.33	1.17	1.14

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

- 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] .
- High precision data requires high precision theory.





L2 study 2306.03918

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.

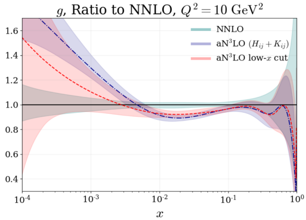
- Improvement in fit quality from NNLO to aN3LO is $\Delta\chi^2 = -154.4$.
  - Much larger than number of parameters (20) introduced.

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.

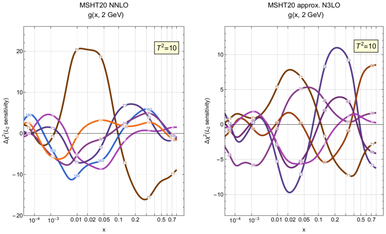
Perform aN3LO fit - Reduced Tensions:

- 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 χ^2/N_{pts}.

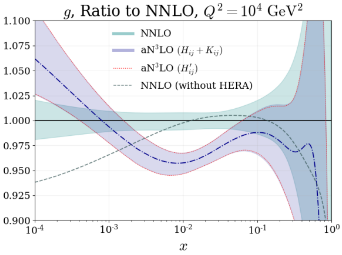


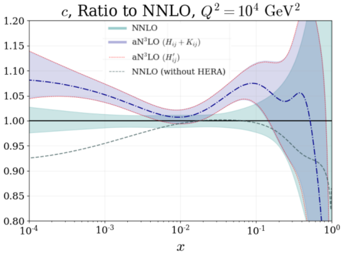
X. Jing et al. (inc. TC) 2306.03918 [10]

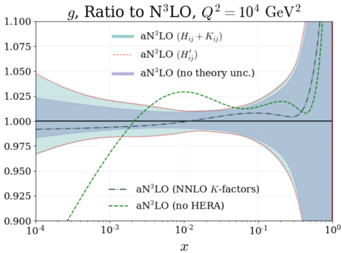
- Tensions between ATLAS 8TeV Zp_T and other data reduced at aN3LO.
- High precision data requires high precision theory.

Perform aN3LO fit - PDF impacts:

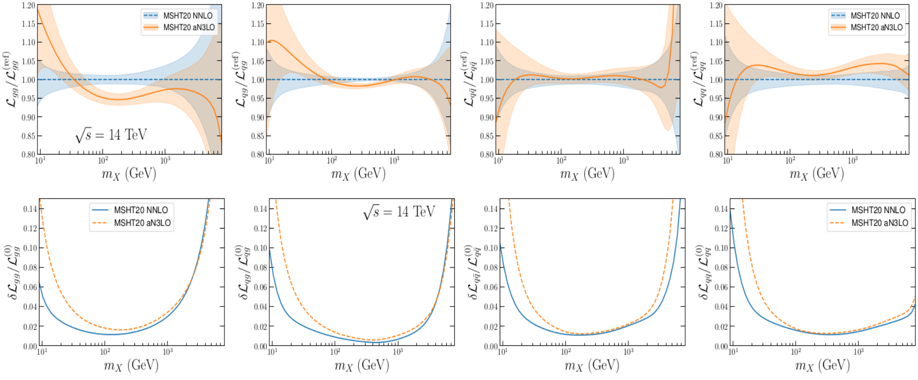
- Gluon enhanced at small x - due to higher power large logs that appear.
- Gluon uncertainty increased at small x due to theory uncertainty, largely on splitting functions.
- Heavy quarks - c and b (perturbatively generated) raised due to increase in gluon at lower x and raised A_{Hg} at high x.







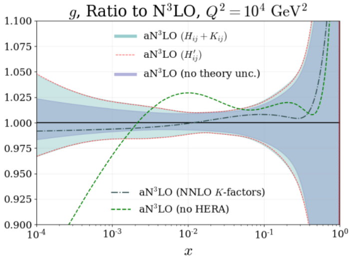
aN3LO PDF luminosities:

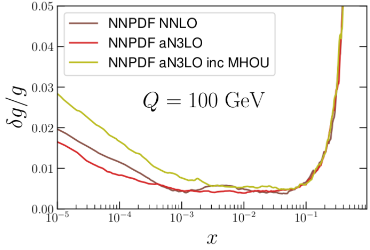


- PDF changes have implications for PDF luminosities for phenomenology.
- *gg* luminosity reduced around 100GeV and increased at 10GeV.
- Luminosity uncertainties enlarged (and more so at lower invariant masses) due to inclusion of aN3LO and PDF theory uncertainties.

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.





How do we incorporate N3LO into PDFs?

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

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

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

Experimental Nuisance parameters

Theory Nuisance Parameters

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

(See TNP Talks at SCET Workshop 2024)

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

Theoretical Uncertainties - Splitting Functions:

- aN3LO PDF sets also first at highest order in QCD to include theory uncertainty from missing higher orders.
- MSHT and NNPDF take different approaches.
- Consider MSHT (first implementation of MHOUs at aN3LO):
  - Add varying parameter for missing piece of each N3LO ingredient. E.g. for P^3_{qg}:

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

Construct from known Mellin moments.

Variational parameter as unknown coefficient.

Contains exact small (and high) x info e.g. from resummation.

where

Known structure

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

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

$\Rightarrow$ aN3LO PDF + theory uncertainty.

Transition Matrix Elements

Ingredient 2

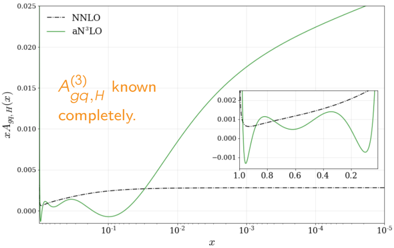
- Several transition matrix elements known completely - $A_{Hq}^{PS,(3)}$, $A_{gq,H}^{(3)}$.
- For others we know:
  - Even low-integer N Mellin Moments (4-8) - constrain intermediate and high x via $\int_0^1 dx\, x^{N-1} P(x)$.
  - Form at low x, in some case low and high x limits.
- Deal with as for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

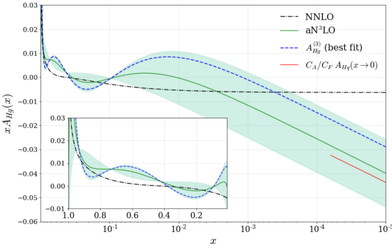
$\Rightarrow$ 1 nuisance parameter each - 3 in total from here $a_{Hg}, a_{qq,H}^{NS}, a_{gg,H}$.

J. Ablinger et al 2311.00644, 2403.00513

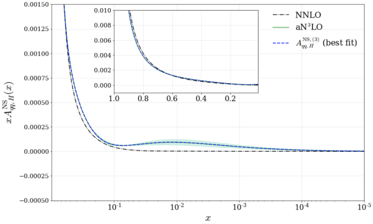
J. Ablinger et al 2211.05462.

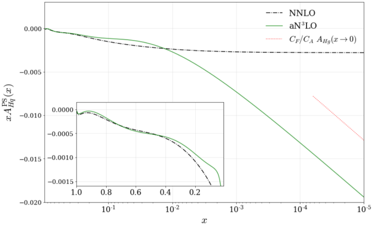
Known via [33,34,36].

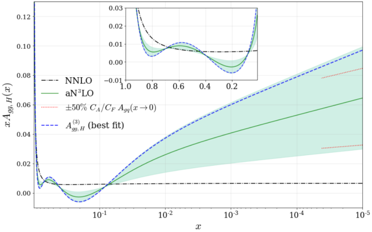




Transition Matrix Elements:







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

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

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

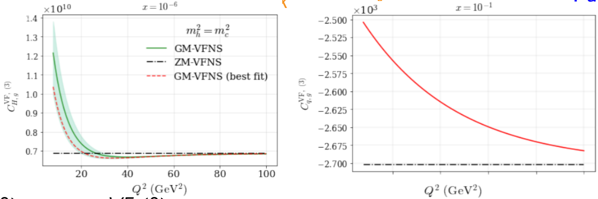
DIS Coefficient Functions

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

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

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

$\Rightarrow$ 2 Theory Nuisance Parameters from here.



- $C_{Hq}^{VF,(3)}$ 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

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:

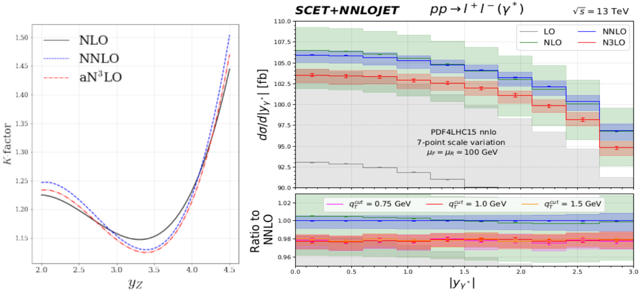
$$K^{N3LO/LO} = K^{NNLO/LO}(1 + a_1 \mathcal{N}^2 \alpha_S^2 (K^{NLO/LO} - 1) + a_2 \mathcal{N} \alpha_S (K^{NNLO/LO} - 1))$$

- 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 $\Rightarrow$ 10 theoretical parameters added.

Hadronic K-factors - Drell-Yan

1 Drell-Yan (DY)

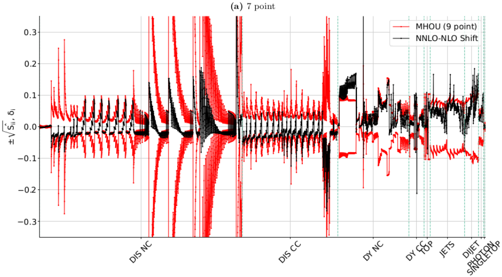
- Fit prefers a ≈ 1% decrease in the N3LO k-factors relative to NNLO.
- Improved perturbative convergence with aN3LO PDFs.
- In qualitative agreement with recent N3LO results for NC DY[53].



- 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.

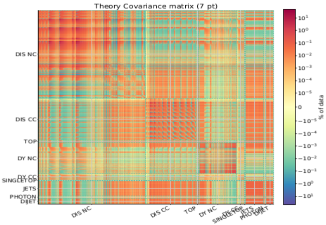
Alternative: Theory Uncertainty via Scale Vars

- New NNPDF aN3LO also include known N3LO pieces with uncertainty from missing info.
- Also vary functions for approximations of aN3LO splitting functions etc.
- Use scale variations (μ_F, μ_R) of current order instead of TNPs to represent MHOU.



Alternative: Theory Uncertainty via Scale Vars

- New NNPDF aN3LO also include known N3LO pieces with uncertainty from missing info.
- Also vary functions for approximations of aN3LO splitting functions etc.
- Use scale variations (μ_F, μ_R) of current order instead of TNPs to represent MHOU. (C.f. MSHT also use TNPs for N3LO K-factors).
- 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).



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

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.

Theory Uncertainty via TNPs

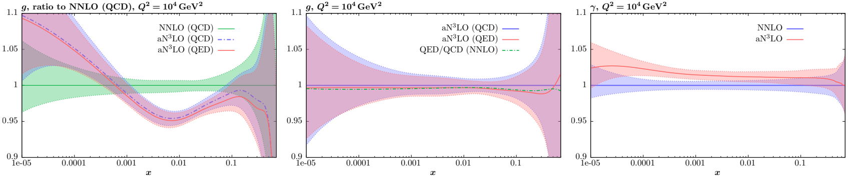
Advantages of TNP method:

- 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 $\Rightarrow$ using `MSHT20aN3LO` PDF set exactly as previous sets includes theory uncertainty for no extra user effort.

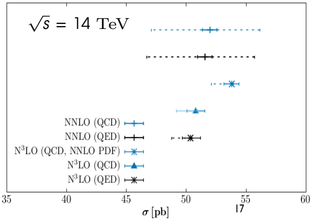
- Applications also more widely - e.g. theory uncertainty for Z p_T spectrum and α_S. F. Tackmann SCET 2019; and T.C., G. Marinelli, F. Tackmann (work in progress).

aN3LO QCD + QED:

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



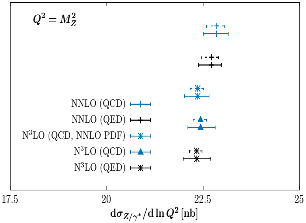
- Knock-on impact on cross-sections, ggF Higgs (left), Z (right):



N3LO QCD + NNLO PDFS

N3LO QCD + aN3LO PDFS

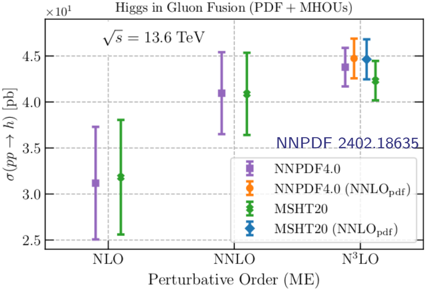
N3LO QCD + aN3LO/QED PDFS



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

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:

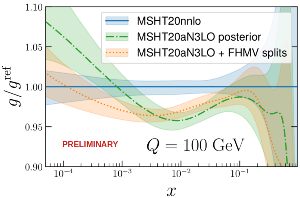


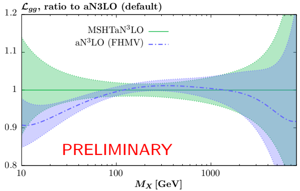
Note greater stability of full NNLO and N3LO xsec + aN3LO PDF results

- 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.

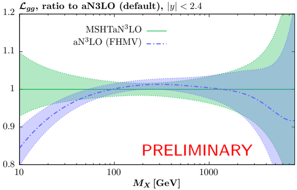
gg Luminosity with FHMV and rapidity cuts:

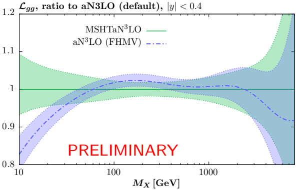
- Despite rise in gluon PDF with FHMV splitting functions[26-30], very little change in gg luminosity as integrating over rapidity (x).



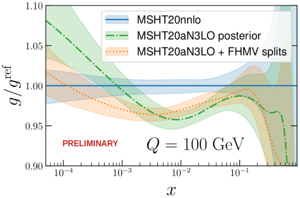


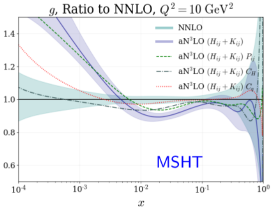
- Adding rapidity cuts - no change with $|y| < 2.4$ (lower left), only with stricter cuts (e.g. $|y| < 0.4$, lower right) do we see the lumi rise.

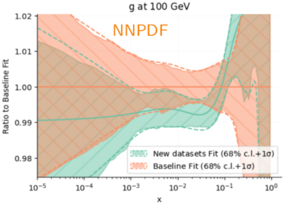




Further Considerations and PDF impacts:

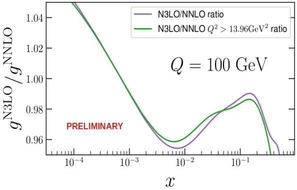






- New moments cause small increase, though consistent with before.
- Other aN3LO effects important, e.g. DIS coefficient functions.
- New data also changes gluon, e.g. new 13TeV jet data lower NNPDF gluon *closer to MSHT*.

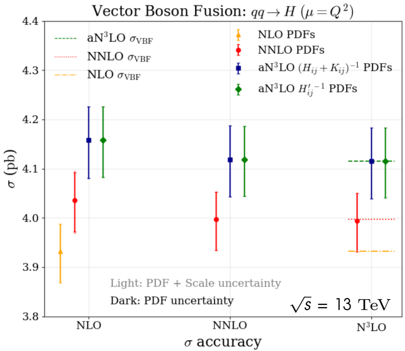
- If cut low Q^2 data as can be required for scale variation approach, impacts gluon.
- Several different aspects contribute to any differences. *Consistent picture emerging...*



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.

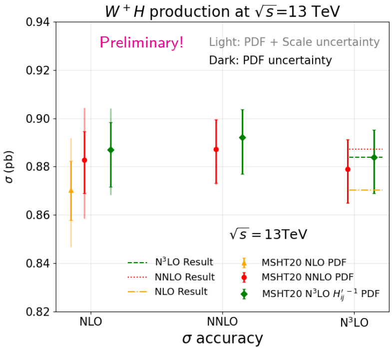
Results obtained using `proVBFH` code[48,57].

- 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.

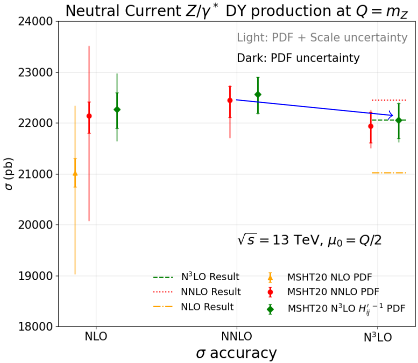
Results obtained using the `n3loxs` code[49].

- 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.

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:

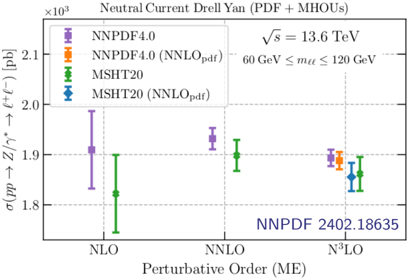


Note greater stability of full NNLO and N3LO xsec + aN3LO PDF results

- 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 $60\mathrm{GeV} < m_{ll} < 120\mathrm{GeV}$ at 13.6 TeV:

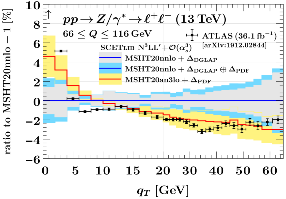


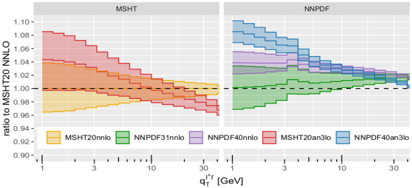
Note greater stability of full NNLO and N3LO xsec + aN3LO PDF results

- Only small change in using aN3LO PDFs relative to NNLO PDFs.
- Predictions with NNLO and aN3LO PDFs are stable.
- 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.

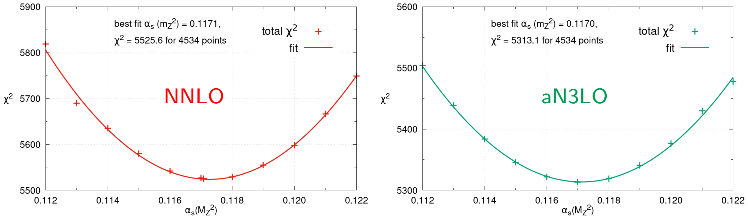
Centre: `CuTe-MCFM` - Tobias Neumann Loops and Legs March 2024

MSHT20 α_S dependence - NNLO and aN3LO

(first ever!)

- First global 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].

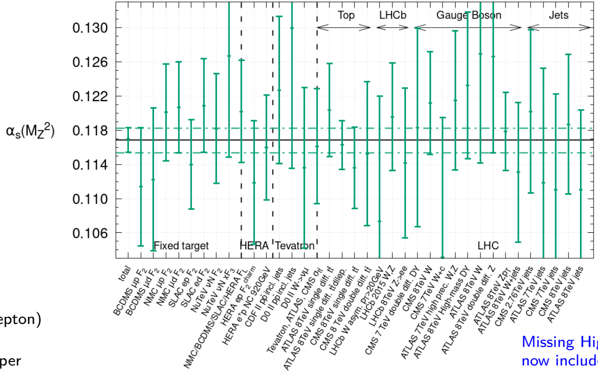
MSHT20 α_S bounds - aN3LO

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.

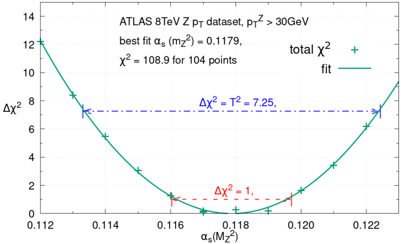
$$\alpha_{S,\mathrm{aN3LO}}(M_Z^2) = 0.1170 \pm 0.0016$$

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

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

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 $\alpha_S(M_Z^2)$?

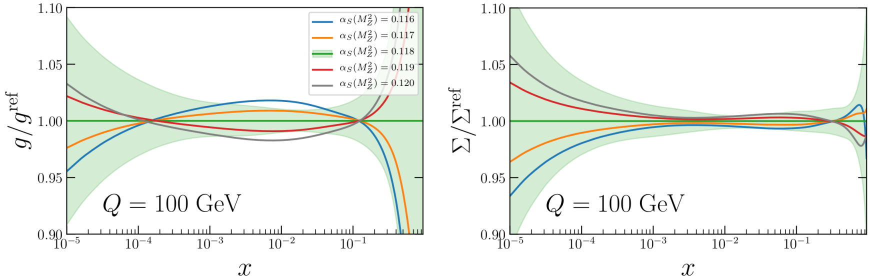


- If you do individual dataset extraction you use $\Delta\chi^2 = 1$ for bounds.
- If you do do in a global fit, factoring in tensions with other data you use $\Delta\chi^2 = T^2 = 7.25$ for bounds.
- $p_T^Z > 30$ GeV not very constraining on $\alpha_S(M_Z^2)$ in global PDF fit.
- ATLAS Z p_T α_S result 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.

NLO and NNLO Cross-section Scale Variations

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

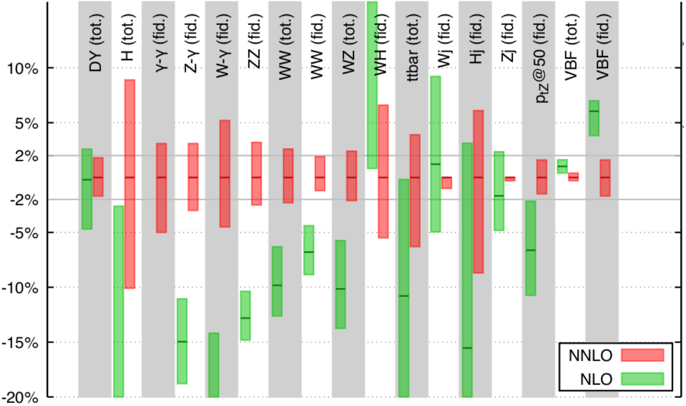
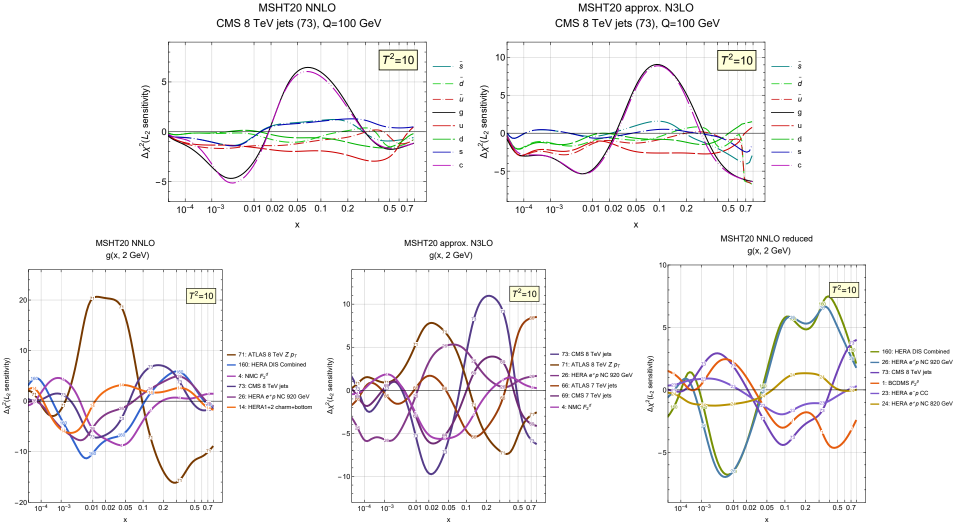


Image Credit: G. Salam

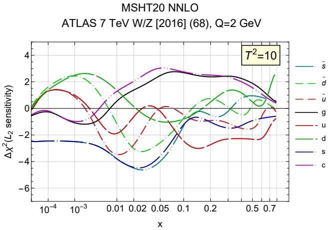
- Is there a better way to do this?

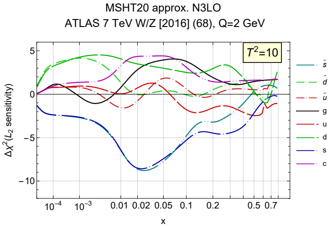
NNLO and aN3LO Data “Pulls” - L_2 Sensitivities - g

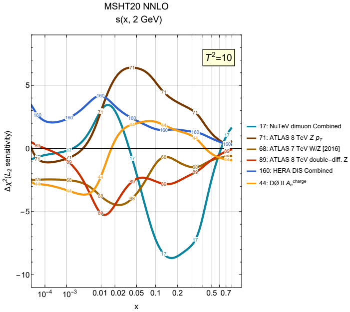


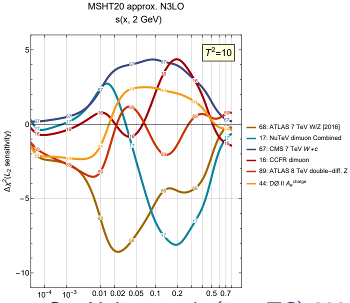
See X. Jing et al. (inc. TC) 2306.03918 [10]

NNLO and aN3LO Data "Pulls" - L_2 Sensitivities - s^+









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

Acknowledgments

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).