# PDFs @ Approximate N3LO - MSHT Review


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# Overview

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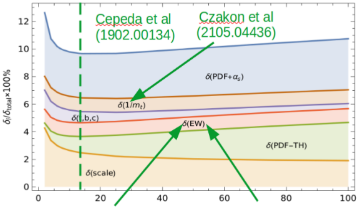


LHC Higgs XSWG 2019

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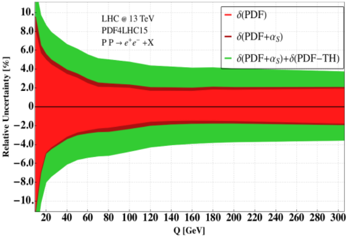


Duhr, Mistelberger 2111.10379

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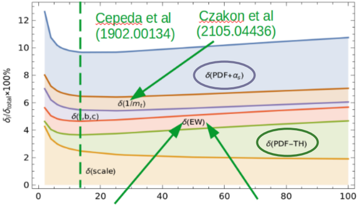


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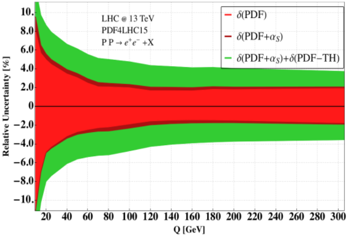


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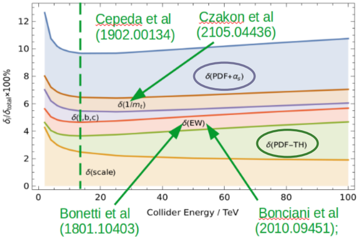


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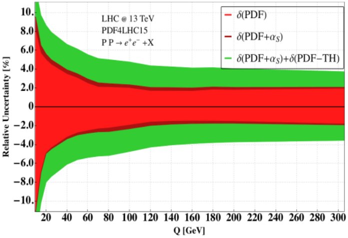


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- PDFs at N3LO with theory uncertainties were becoming a bottleneck.
- Two steps required for *more accurate and precise PDFs*:

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

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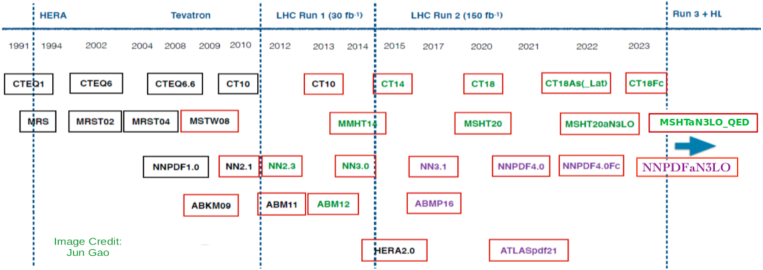

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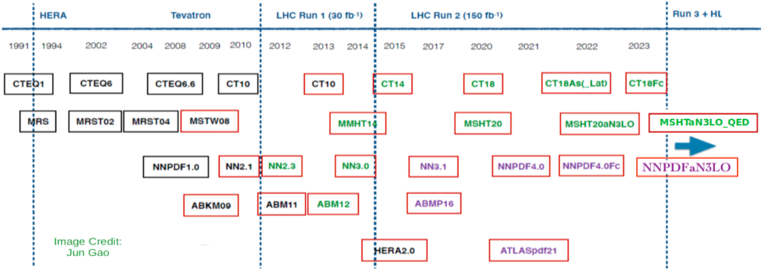


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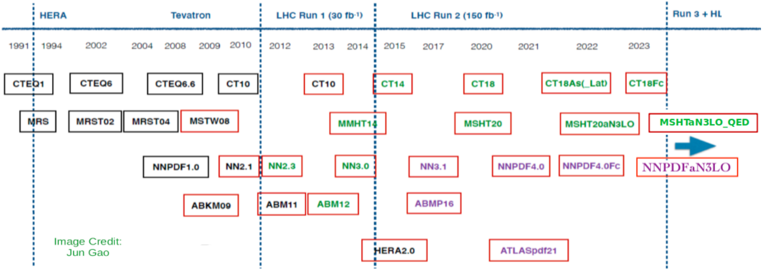


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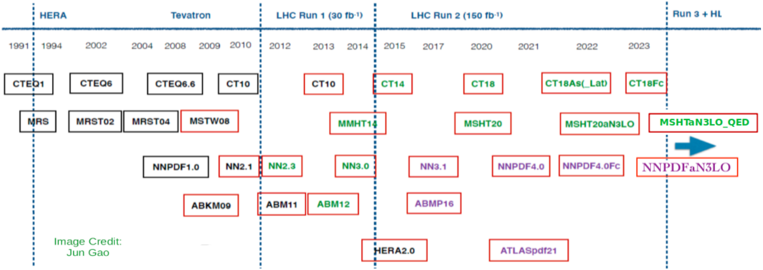


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- Later ⇒ will see similar impacts of aN3LO in both.

# Current Knowledge of N3LO

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  - Coefficient Functions for DIS - at 3-loop to determine structure functions.
    $$F_2(x, Q^2) = \sum_{\alpha \in H,q,g;\beta \in q,H} (C_{\beta,\alpha}^{VF,n_f+1} \otimes A_{\alpha i}(Q^2/m_h^2) \otimes f_i^{n_f}(Q^2))$$

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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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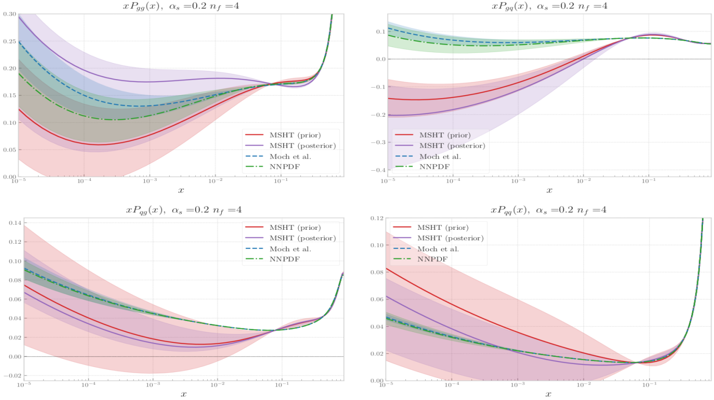
# N3LO PDF Evolution

- 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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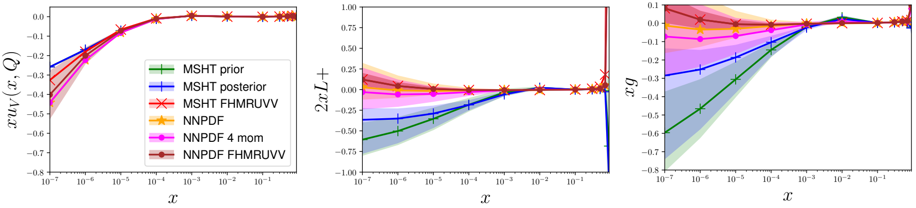


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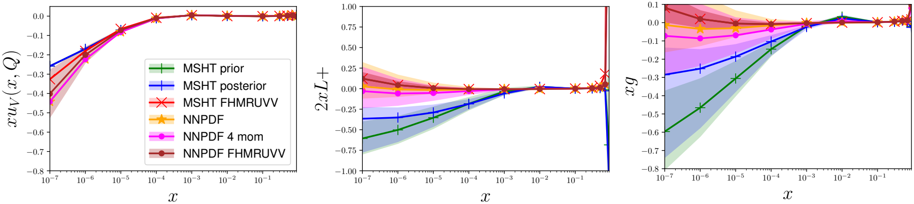


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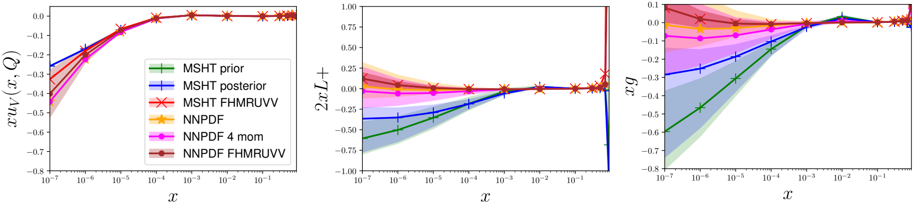


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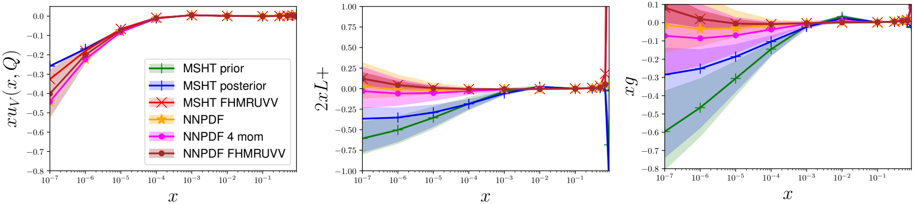


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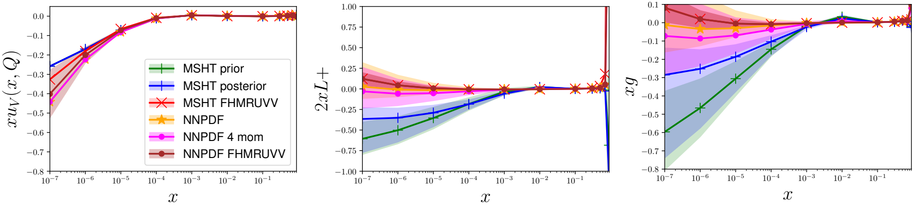


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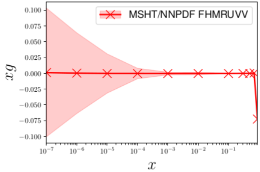


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- 
    - Uncertainty on aN3LO comes through varying functional basis $f_i(x)$ and varying unknown coefficient ("theory nuisance parameter" - TNP).

$\Rightarrow$ 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

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

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

Theory Nuisance Parameters

(See TNP Talks at SCET Workshop 2024)

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

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- Upgrade theory, T to now contain known N3LO info (aN3LO) and allow to vary by theory nuisance parameters, TNPs - $\theta'$.
- 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 $\Rightarrow$ 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.

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# 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 | $Dimuon_{NLO}$, $Dimuon_{NNLO}$ | |

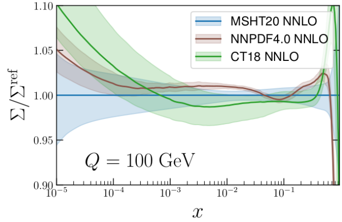
- Using `MSHT20an3lo_as118` eigenvectors as usual naturally incorporates MHOUs at aN3LO into the PDF uncertainties.

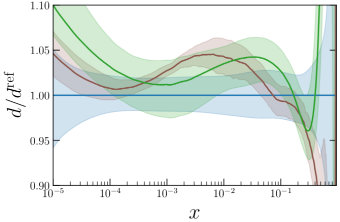
N.B. We find the penalties on these parameters are almost all $< 1 \Rightarrow$ conservative priors set.

# Effect of N3LO on PDFs:

# Impact of aN3LO on PDFs:

- Quarks relatively unaffected:



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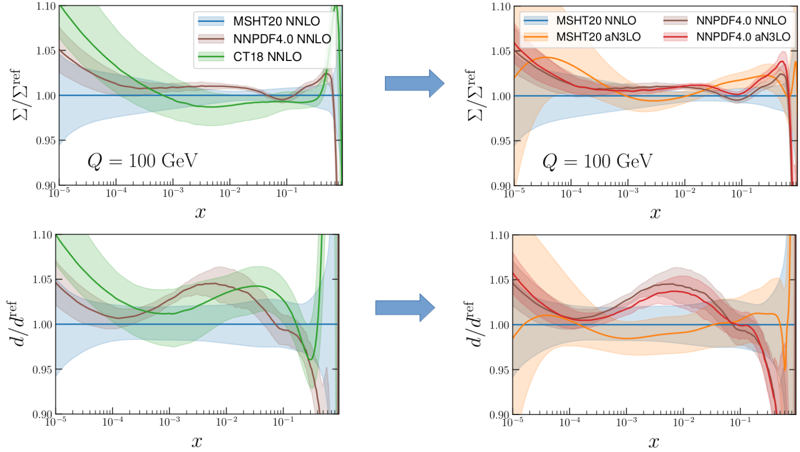

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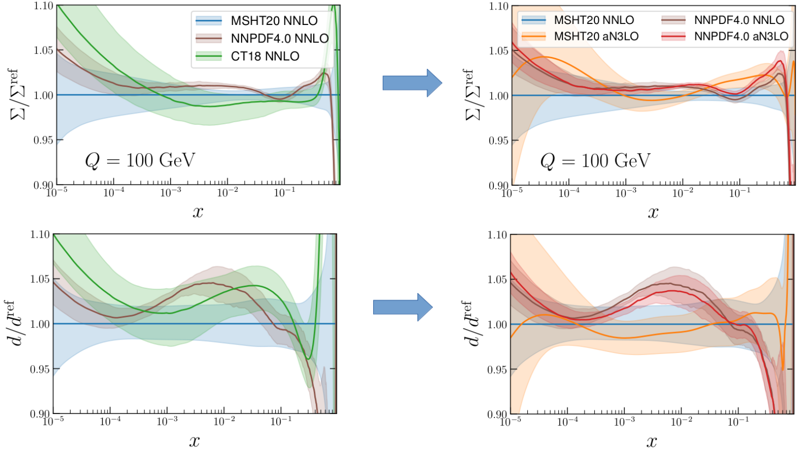
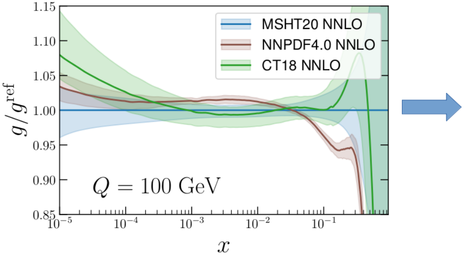



- Singlet PDF - NNLO and aN3LO all show same % level differences.
- Down PDF - as much difference between aN3LO PDFs as NNLO.

# Impact of aN3LO on PDFs:

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



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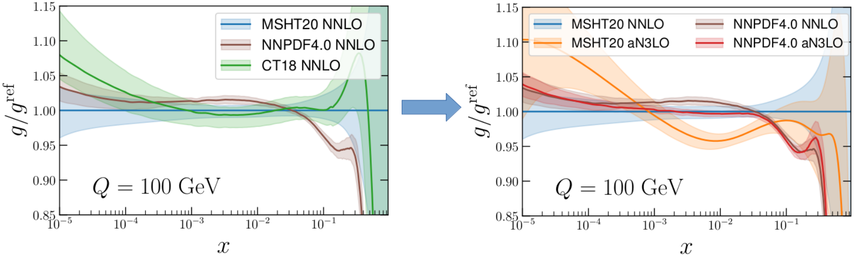

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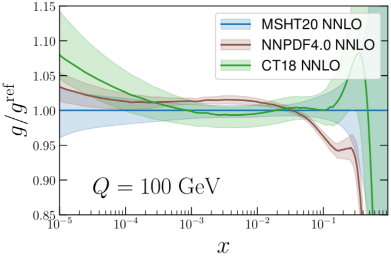


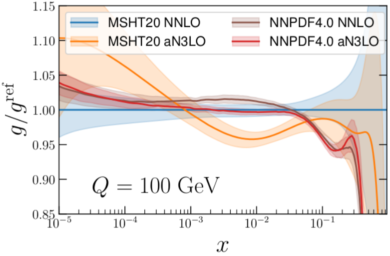


- NNLO - gluon PDFs differ by few % in Higgs region.
- aN3LO - gluon PDFs differ by few % in Higgs region.

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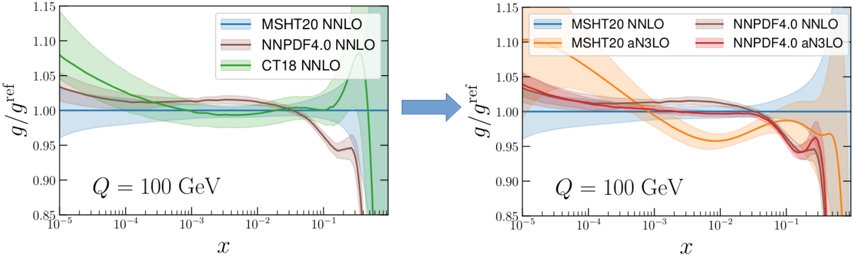


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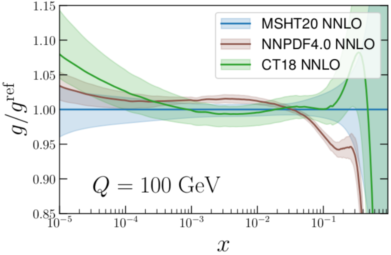


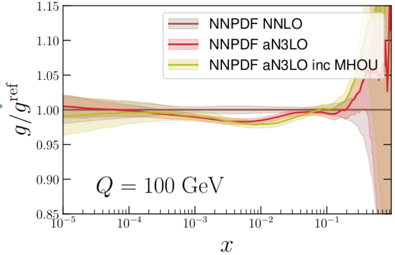


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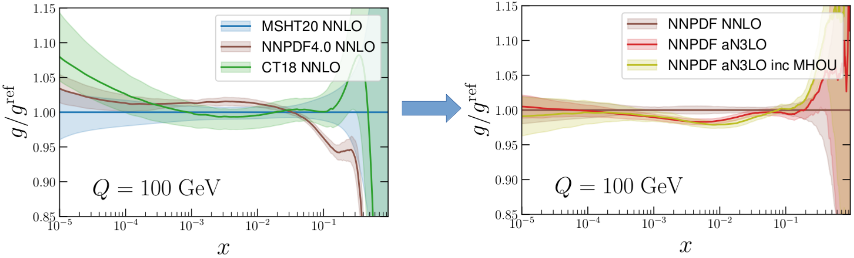


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- NNLO vs aN3LO - MSHT and NNPDF both see dip (2-5%) in gluon at $m_H$ ($x \sim 10^{-2}$) from aN3LO effects.
- Variety of other effects - new FHMV info., other N3LO ingredients, methodology, data can cause 1-2% differences here, (see backup).

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

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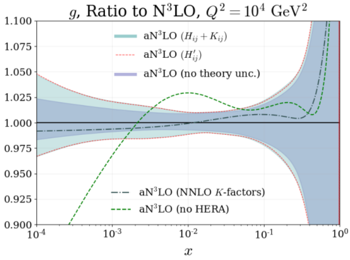


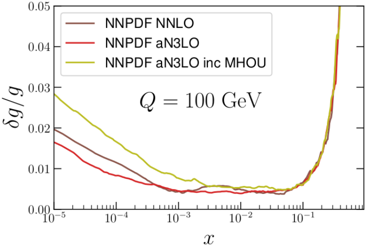

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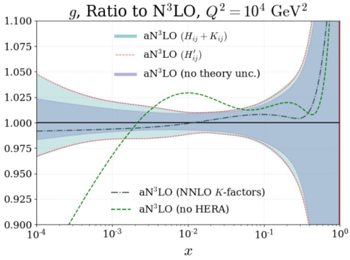
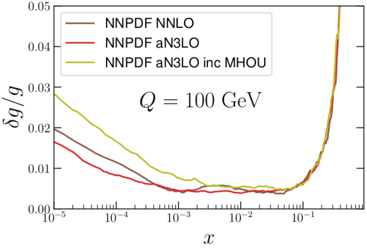
- MSHT (left) and NNPDF (right) both see added theory uncertainty increasing PDF uncertainties at low $x$, e.g. gluon:
- Whilst PDF uncertainty is larger, it's more accurate and reliable.



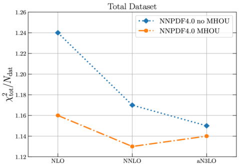



# aN3LO effects on the PDF fit:

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

| MSHT $\chi^2/N_{pts}$ (4363) | LO | NLO | NNLO | aN3LO |
|---|---|---|---|---|
| | 2.57 | 1.33 | 1.17 | 1.14 |

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



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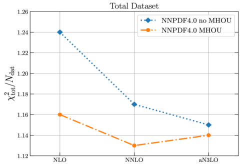
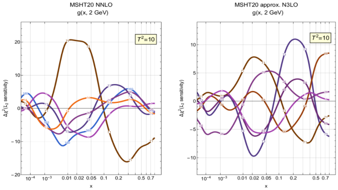
- MSHT - $Z\ p_T$ data (and DIS data) notably better fit.
- Reduced tensions between data also seen.
- MSHT - Dijet data also better fit at aN3LO than NNLO.

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




L2 study 2306.03918

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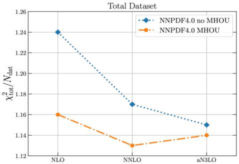
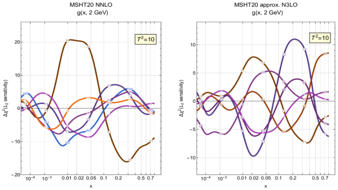
- High precision data requires high precision theory.



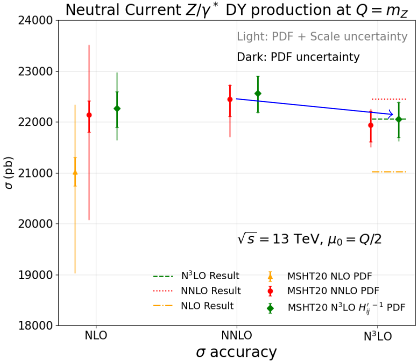

L2 study 2306.03918

# 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:

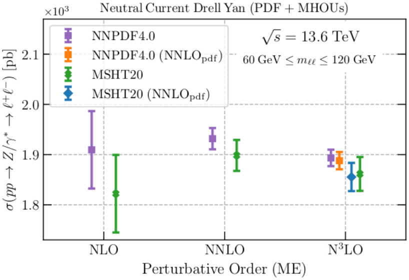



Note greater stability of full NNLO and N3LO xsec + aN3LO PDF results

- 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:

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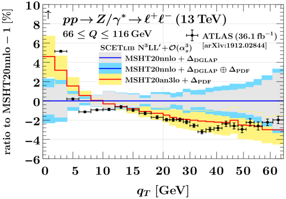
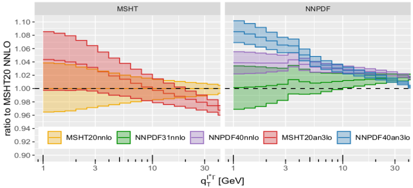
- Only small change in using aN3LO PDFs relative to NNLO PDFs.
- Predictions with NNLO and aN3LO PDFs are stable.
- NNPDF see similar small impact on DY $\rightarrow$ also see small increase from aN3LO PDFs, also well within uncertainty.

# 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:



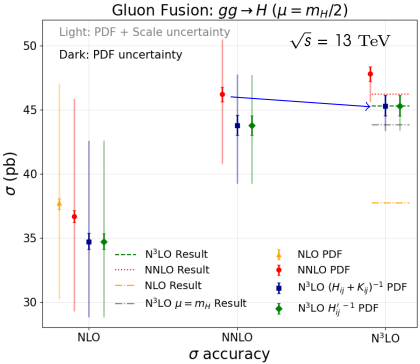

- Substantial aN3LO PDF effect on N3LL'/N4LL $q_T$ spectrum.

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

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

# 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 $\sigma$ changes together.
- aN3LO result lies within uncertainty band of full NNLO.
- aN3LO PDF uncertainty bands enlarged - inclusion of MHOUs.

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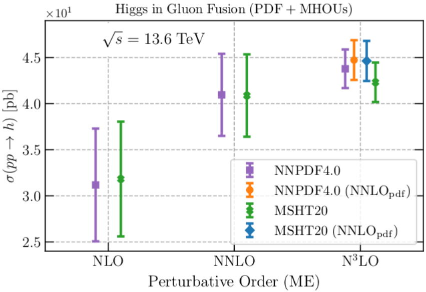


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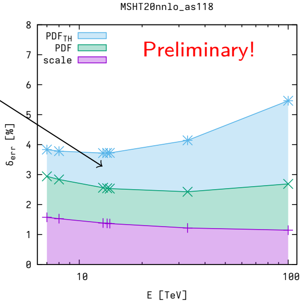
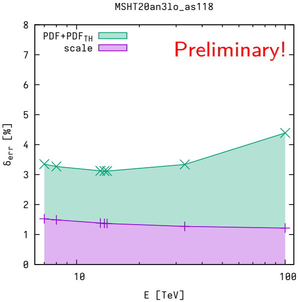
- Increase in cross-section at N3LO compensated by reduction in PDFs at aN3LO ⇒ important to consider PDF and $\sigma$ changes together.
- aN3LO result lies within uncertainty band of full NNLO.
- NNPDF see similar effects, though slightly reduced due to changes in gluon PDF at aN3LO.

# 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 aN3LO PDFs - QED and $\alpha_S$

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

# aN3LO QCD + QED:

- All groups now provide NNLO + QED PDF sets.

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

# aN3LO QCD + QED:

- All groups now provide NNLO + QED PDF sets. MSHT now for first time combine with aN3LO QCD for highest possible precision!

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- Need to combine aN3LO QCD evolution and $\mathcal{O}(\alpha, \alpha\alpha_S, \alpha^2)$:

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

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

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

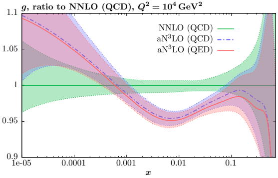
- Impact on fit at NNLO and aN3LO, substantial fit quality improvement remains true after adding QED:

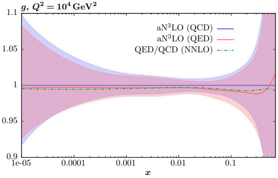
| | $\chi^2/N_{\rm pt}$ aN$^3$LO (QED) | $\Delta\chi^2_{\rm aN^3LO}$ QED-QCD | $\Delta\chi^2_{\rm NNLO}$ QED-QCD | $\Delta\chi^2_{\rm QCD,QED}$ aN$^3$LO-NNLO |
|---|---|---|---|---|
| Total | 5323.6/4534 | (+3.6) | (+17.3) | (-209.3, -223.1) |

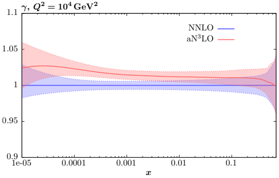
T.C., L.A. Harland Lang, R.S. Thorne 2312.07665 [5]

# aN3LO QCD + QED:

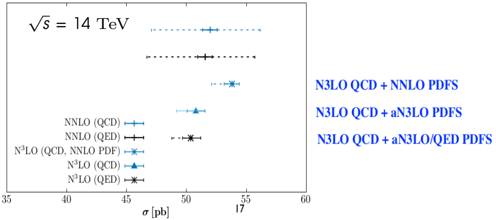
- Impact small relative to aN3LO QCD corrections in most regions.
- Effect of adding QED similar when applied to NNLO and aN3LO.

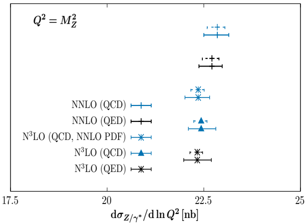



- Knock-on impact on cross-sections, ggF Higgs (left), Z (right):



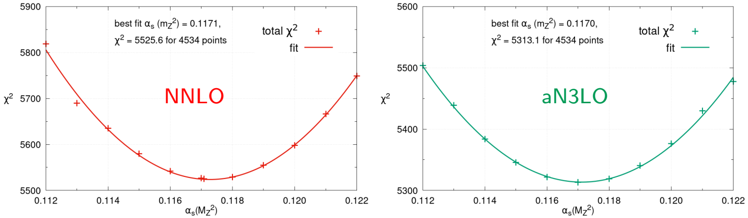

T.C., L.A. Harland Lang, R.S. Thorne 2312.07665 [5]

# MSHT20 $\alpha_S$ 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 $\alpha_S$ determination.

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




Nice Quadratic $\chi^2$ profile ✓

- Can also determine bounds (next slide).

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

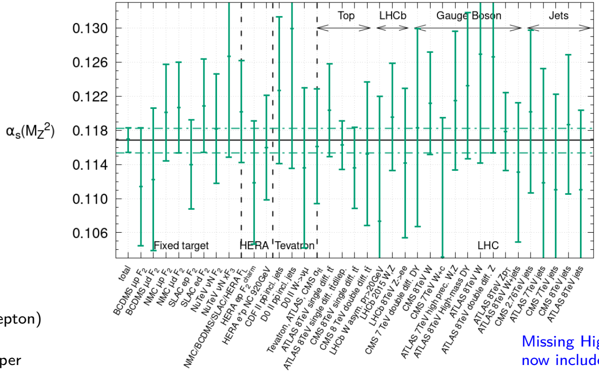
# MSHT20 $\alpha_S$ bounds - aN3LO

Consistent with $\alpha_S$ 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:

$\Delta\alpha_S(M_Z^2) = +0.0020$.




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 $\Delta\alpha_S(M_Z^2) = -0.0017$.

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

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 $0.1180 \pm 0.0009$.

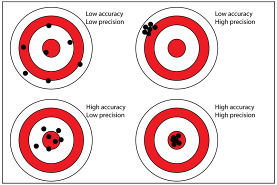
T.C., L.A. Harland-Lang, R.S. Thorne 2404.02964 [7].

# 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. aN3LO PDFs publicly available!
- N3LO evolution benchmarking almost complete and shows consistency.
- Consistent results seen by both groups in terms of PDF impacts and consequences for phenomenology.
- Further developments - aN3LO QCD + NLO QED/EW, aN3LO $\alpha_S$ determination.
- 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 $\gamma$ PDF |
| MSHT20qed_nnlo_(in)elastic | NNLO | 5 | 77 | 0.118 | NNLO set with QED effects and (in)elastic $\gamma$ |
| MSHT20qed_nnlo_neutron | NNLO | 5 | 77 | 0.118 | NNLO neutron set with QED effects and $\gamma$ |
| MSHT20an3lo_as118 | aN3LO | 5 | 105 (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 $\gamma$ 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.
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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.
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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.
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28. G. Falcioni et al., 2310.01245.
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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.
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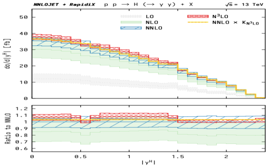
44. E. Laenen and S.-O. Moch, hep-ph/9809550.
45. J. A. M. Vermaseren et al. hep-ph/0504242.
46. C. Anastasiou et al., 1602.00695.
47. B. Mistlberger, 1802.00833.
48. F.A. Dreyer and A. Karlberg, 1606.00840.
49. J. Baglio et al., 2209.06138.
50. M. Bonvini, arXiv:1805.08785. 34
51. C. Duhr et al., 2001.07717.
52. C. Duhr et al., 2007.13313.
53. X. Chen et al., 2107.09085.
54. C. Duhr and B. Mistlberger, 2111.10379.
55. X. Chen et al., 2102.07607.
56. N. Kidonakis, 2203.03698.
57. M. Cacciari et al, 1506.02660.

# Backup Slides

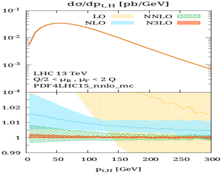
# Particle Physics and N3LO Progress

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

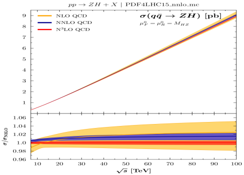
1. Higgs - Differential for ggF ($y_H$, etc) and VBF ($p_T^H$, $y_H$), inclusive VH:




Chen et al 2102.07607

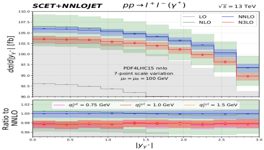



Dreyer et al 1606.00840

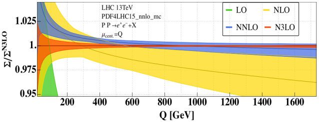


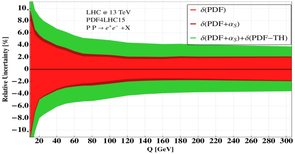

Baglio et al 2209.06138

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:

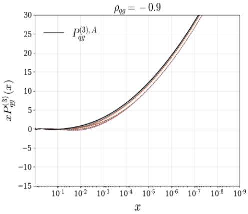
- Probes precisely the missing higher order terms.
- Allows inclusion of known N3LO information (a lot) without needing to wait for remaining few pieces.
- Can be included in PDF fit in same way experimental data are.
- No requirement for scale variations - can underestimate MHOU, issue of correlation 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 $\Rightarrow$ using `MSHT20aN3LO` PDF set exactly as previous sets includes theory uncertainty for no extra user effort.

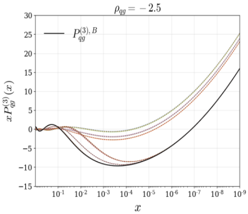
---

- Applications also more widely - e.g. theory uncertainty for $Z$ $p_T$ spectrum and $\alpha_S$. 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 $\rho_{ab}$ prior variation by requiring:
  1. At low $x$ bound set once exact expression $f_e(x, \rho_{ab})$ exits range of results from different (larger) $x$ functional forms, e.g. see lower plots.
  2. At high $x$ bound set if N3LO correction becomes too large (rare).
  3. Once functional form fixed, check range of prior and extend as necessary to incorporate different functional form variation.




- Find penalties on theory nuisance parameters after fit are small and posterior errorbands reduced relative to prior $\Rightarrow$ prior set conservatively.

# Transition Matrix Elements

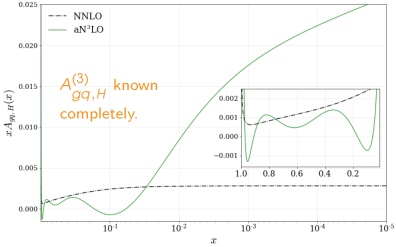
**Ingredient 2**

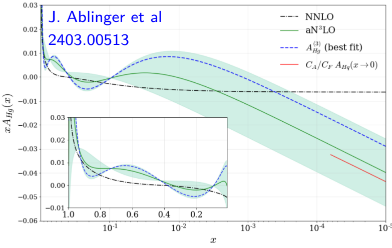
- Several transition matrix elements known completely - $A_{Hq}^{PS,(3)}$, $A_{gq,H}^{(3)}$.
- For others we know:
  - Even low-integer $N$ Mellin Moments (4-8) - constrain intermediate and high $x$ via $\int_0^1 dx\, x^{N-1} P(x)$.
  - Form at low $x$, in some case low and high $x$ limits.
- Deal with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

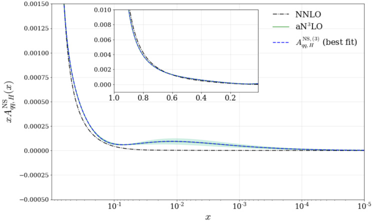
J. Ablinger et al 2311.00644.

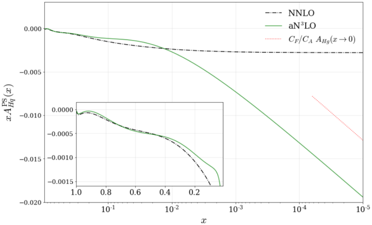
J. Ablinger et al 2211.05462.

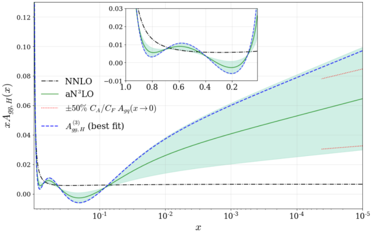


# Transition Matrix Elements:




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

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

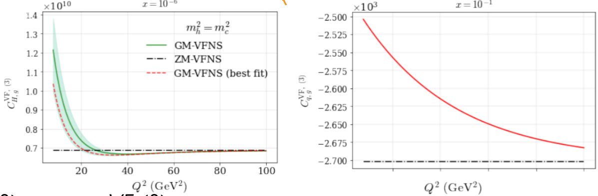
# DIS Coefficient Functions

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

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

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

$\Rightarrow$ 2 Theory Nuisance Parameters from here.




- $C^{VF,(3)}_{Hq}$ 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:

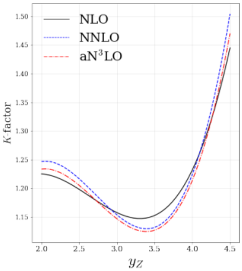
$$K^{N3LO/LO} = K^{NNLO/LO}\left(1 + a_1 \mathcal{N}^2 \alpha_S^2 (K^{NLO/LO} - 1) + a_2 \mathcal{N} \alpha_S (K^{NNLO/LO} - 1)\right)$$

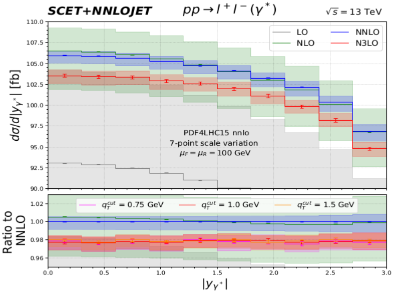
- Default prior is $a_1, a_2 = 0$, i.e. no N3LO correction.
- Categorise all hadronic processes into 5 types - jets (or dijets), Drell-Yan, top, vector boson $p_T$/jets, and dimuon.
- 2 theory nuisance parameters each ⇒ 10 theoretical parameters added.

# Hadronic K-factors - Drell-Yan

## 1 Drell-Yan (DY)

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

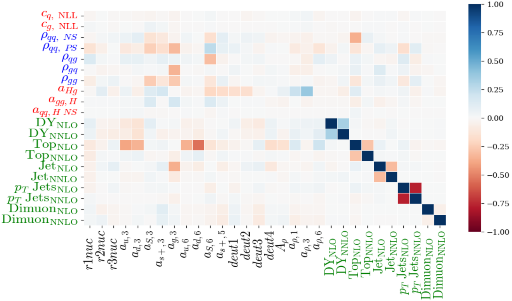



- Key point: Method allows N3LO info. on any piece to be incorporated as it becomes available, rather than needing to wait for all info. - e.g. can include N3LO k-factors as they become available for PDFs.

# 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!

# 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.

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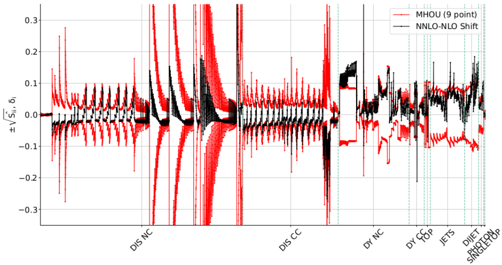
(a) 7 point



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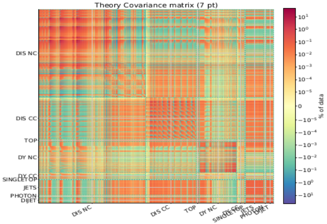
- Construct theory covariance matrix, analogous to TNPs but different estimate of error [8].
- Requires prescription for how to correlate scales in different processes. (As does any approximation in absence of known N3LO K-factors).



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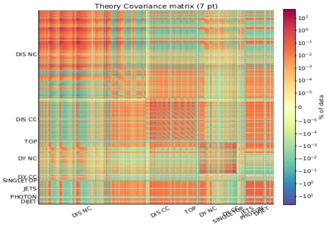



- Overall, like NNLO, at aN3LO MSHT and NNPDF have similar info., formal accuracy, but some differences in approaches.

# Perform aN3LO fit - fit quality:

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

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

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

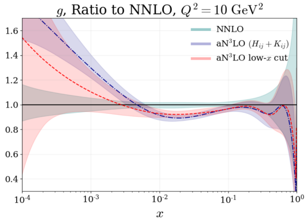
- Improvement in fit quality from NNLO to aN3LO is $\Delta\chi^2 = -154.4$.
  - Much larger than number of parameters (20) introduced.

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

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

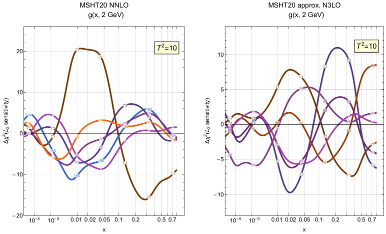
# Perform aN3LO fit - Reduced Tensions:

- 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 $\chi^2/N_{\mathrm{pts}}$.

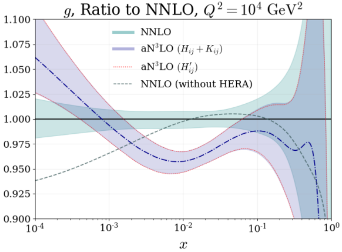


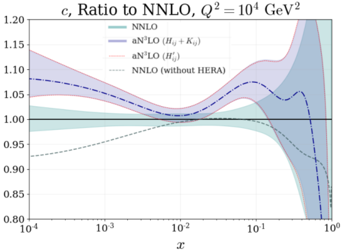

X. Jing et al. (inc. TC) 2306.03918 [10]

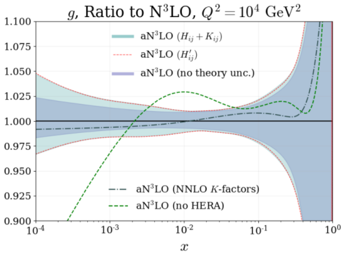
- Tensions between ATLAS 8TeV $Zp_T$ and other data reduced at aN3LO.
- High precision data requires high precision theory.

# Perform aN3LO fit - PDF impacts:

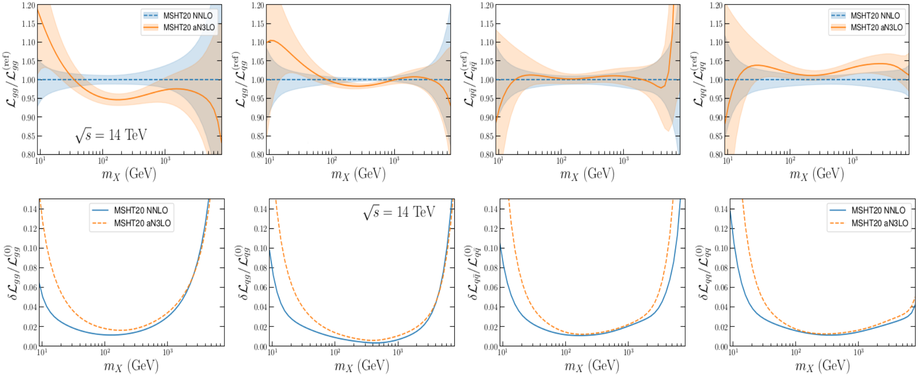
- Gluon enhanced at small $x$ - due to higher power large logs that appear.
- Gluon uncertainty increased at small $x$ due to theory uncertainty, largely on splitting functions.
- Heavy quarks - c and b (perturbatively generated) raised due to increase in gluon at lower $x$ and raised $A_{Hg}$ at high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



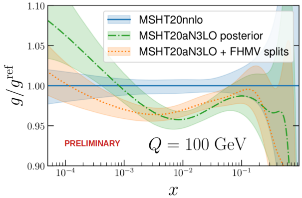



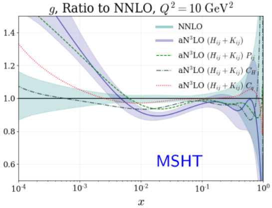
# aN3LO PDF luminosities:

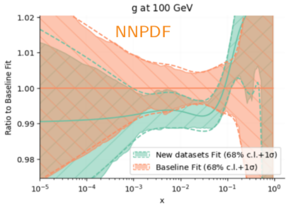



- PDF changes have implications for PDF luminosities for phenomenology.
- $gg$ luminosity reduced around 100GeV and increased at 10GeV.
- Luminosity uncertainties enlarged (and more so at lower invariant masses) due to inclusion of aN3LO and PDF theory uncertainties.

# Further Considerations and PDF impacts:

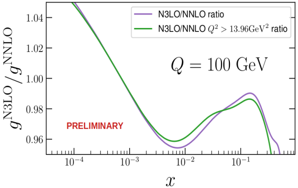



- New moments cause small increase, though consistent with before.
- Other aN3LO effects important, e.g. DIS coefficient functions.
- New data also changes gluon, e.g. new 13TeV jet data lower NNPDF gluon *closer to MSHT*.

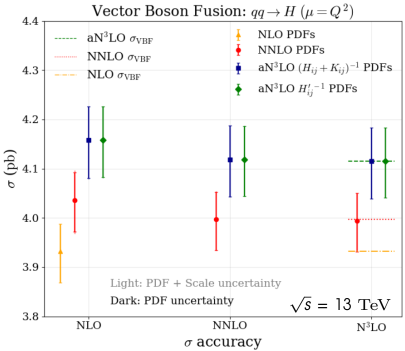
- If cut low $Q^2$ data as can be required for scale variation approach, impacts gluon.
- Several different aspects contribute to any differences. *Consistent picture emerging...*



# 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 $\mu_R$ and $\mu_F$ at NNLO but only $\mu_R$ at aN3LO as PDF uncertainty from MHOs already in PDF eigenvectors.

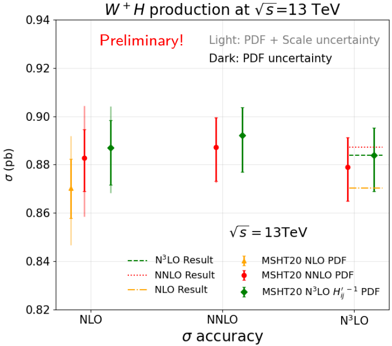
Results obtained using `proVBFH` code[48,57].

- Increase in $\sigma$ 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 $\mu_R$ and $\mu_F$ at NNLO but only $\mu_R$ 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 $\sigma$ + aN3LO PDF result very close to NNLO $\sigma$ + 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.

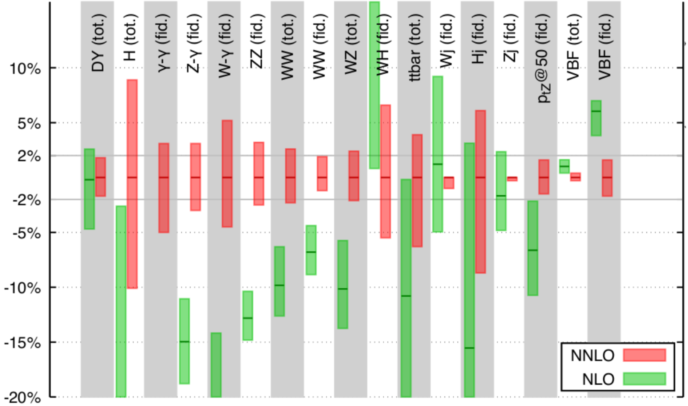
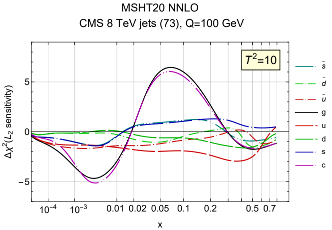
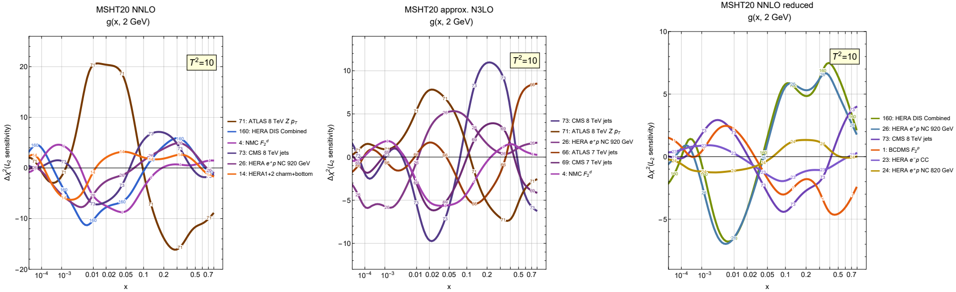



Image Credit: G. Salam

- Is there a better way to do this?

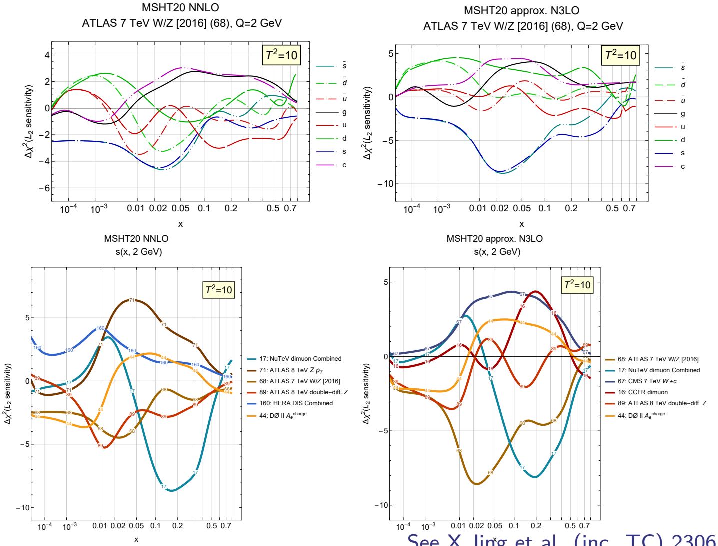
# NNLO and aN3LO Data "Pulls" - $L_2$ Sensitivities - $g$




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

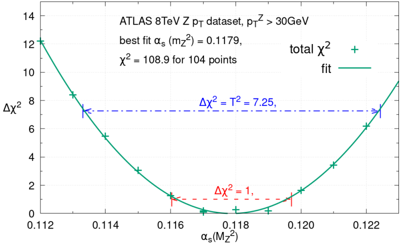
# NNLO and aN3LO Data “Pulls” - $L_2$ Sensitivities - $s^+$




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

# MSHT20 ATLAS 8 TeV $Z$ $p_T$ $\alpha_S$ dependence

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

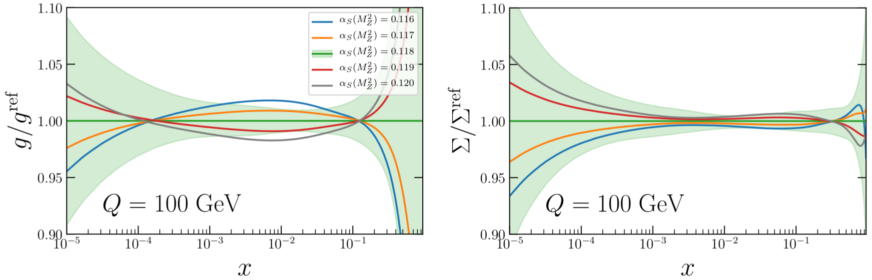



- If you do individual dataset extraction you use $\Delta\chi^2 = 1$ for bounds.
- If you do do in a global fit, factoring in tensions with other data you use $\Delta\chi^2 = T^2 = 7.25$ for bounds.
- $p_T^Z > 30\ \mathrm{GeV}$ not very constraining on $\alpha_S(M_Z^2)$ in global PDF fit.
- ATLAS $Z$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

# MSHT20 PDF $\alpha_S$ 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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