MSHT Approximate N3LO PDF Updates

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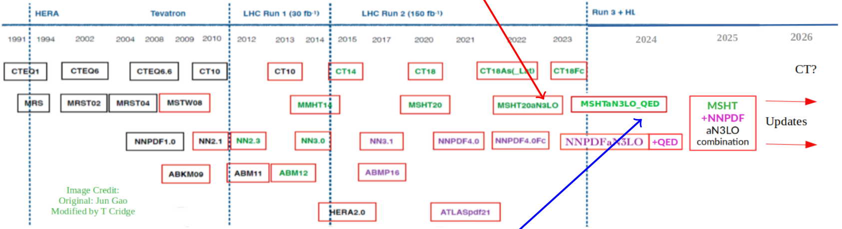
MANCHESTER 1824
The University of Manchester

THE ROYAL SOCIETY

In collaboration with MSHT colleagues: L.A. Harland-Lang, R.S. Thorne.

Approximate N3LO PDFs Available

- World first aN3LO PDF set ⇒ MSHT20aN3LO available for $\gtrsim 3.5$ years.



- Also available for $\gtrsim 2.5$ years: MSHT20an3lo+QED (more later).
- First time at approximate N3LO ("aN3LO") and first inclusion of theory uncertainties in PDFs at highest order.

Basic Idea:

- Include all known N3LO terms into the PDFs (a lot!)
- Include theoretical uncertainty for the missing ingredients

⇒ aN3LO PDFs + theory uncertainty.

What do we need to know for N3LO PDFs?

- Need to know:
  - Splitting functions - at 4-loop to evolve PDFs in (x, Q^2):

$$P(x,\alpha_s) = \alpha_S P^{(0)}(x) + \alpha_S^2 P^{(1)}(x) + \alpha_S^3 P^{(2)}(x) + \alpha_S^4 P^{(3)}(x) + \ldots$$

  - Transition Matrix Elements (TMEs) - at 3-loop to change number of PDF flavours at heavy quark mass (m_h) thresholds.

$$f_\alpha^{n_f+1}(x,Q^2) = [A_{\alpha i}(Q^2/m_h^2) \otimes f_i^{n_f}(Q^2)](x)$$

  - Coefficient Functions for DIS - at 3-loop to determine structure functions.

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

  - Hadronic cross-section k-factors - at N3LO.

$$\sigma = \sigma_0 + \sigma_1 + \sigma_2 + \sigma_3 + \ldots \equiv \sigma_{N3LO} + \ldots$$

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

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    Mellin moments, small x, high x limits
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    Very little known, PDFs need differential with cuts.
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    New moments for $P_{qg,gq,gg}, P_{qq}^{PS}$ (FHRMUVV) (Also now NS via 2604.09534) ⟵ $$P(x,\alpha_s) = \alpha_S P^{(0)}(x) + \alpha_S^2 P^{(1)}(x) + \alpha_S^3 P^{(2)}(x) + \alpha_S^4 P^{(3)}(x) + \ldots$$

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  - Transition Matrix Elements (TMEs) - at 3-loop to change number of PDF flavours at heavy quark mass (m_h) thresholds.

    $A_{Hg}^{(3)}$, $A_{gg,H}$ since determined. (Blümlein et al) ⟵ $$f_\alpha^{n_f+1}(x,Q^2) = [A_{\alpha i}(Q^2/m_h^2) \otimes f_i^{n_f}(Q^2)](x)$$

    Mellin moments, small x, high x limits

  - Coefficient Functions for DIS - at 3-loop to determine structure functions.

    No further info. ⟵ $$F_2(x,Q^2) = \sum_{\alpha\in H,q,g;\beta\in q,H} (C_{\beta,\alpha}^{VF,n_f+1} \otimes A_{\alpha i}(Q^2/m_h^2) \otimes f_i^{n_f}(Q^2))$$

    Light flavour known, heavy flavour high Q^2 known, approx for low Q^2.

  - Hadronic cross-section k-factors - at N3LO.

    N3LO DY y distribution, (Chen et al) ⟵ $$\sigma = \sigma_0 + \sigma_1 + \sigma_2 + \sigma_3 + \ldots \equiv \sigma_{N3LO} + \ldots$$

    Very little known, PDFs need differential with cuts.

References in backup

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

Approach in MSHT20aN3LO:

- Include known info (already a lot, even more now) for each ingredient.
- Use Theoretical Nuisance Parameters (TNPs) to include effect of unknown pieces, added to fit a la experimental nuisance parameters.
- Consider PDF fit probability - add N3LO theory and theory uncertainty:

Experimental Nuisance parameters

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

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

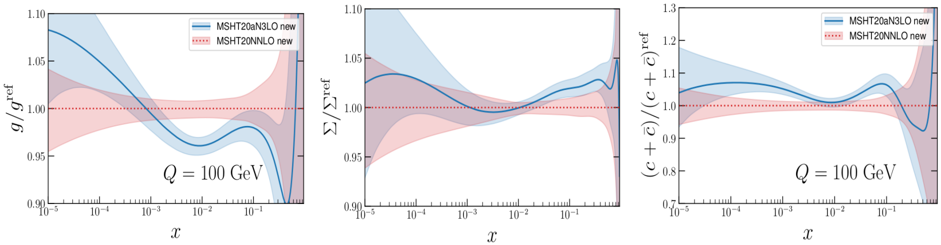
Theory Nuisance Parameters

- Upgrade theory, $T \to \tilde{T}$ to now contain known N3LO info (aN3LO) and allow to vary by theory nuisance parameters, TNPs - θ'.
- Probes precisely the missing higher order terms.

(Applications more widely - e.g. theory uncertainty for Z p_T spectrum and α_S - T.C., G. Marinelli, F. Tackmann 2506.13874.)

Approximate N3LO vs NNLO

- Begin considering our original aN3LO setup, compared to NNLO as a baseline (differs to aN3LO paper due to other updates in PDF fit - see Robert's talk) :



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- Main difference is 4% drop in gluon at $x \approx 10^{-2}$.
- Some increase in heavy quarks.

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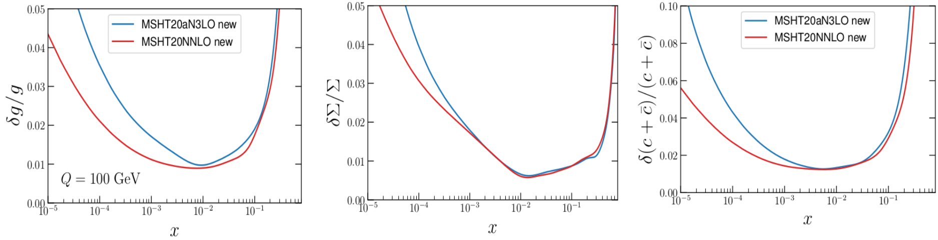


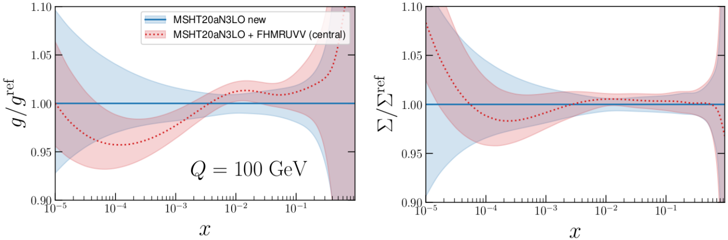
- Most PDFs change within their uncertainties.
- Main difference is 4% drop in gluon at $x \approx 10^{-2}$.
- Some increase in heavy quarks.
- Uncertainties grow due to inclusion of MHOU, particularly at low x.

Approximate N3LO - Update Splitting Functions

- Update to FHMRUVV approximations based on 10 moments (cf 4 in original MSHT20aN3LO) for P_{qq}^{PS}, P_{qg}, P_{gq}, P_{gg}.

Preliminary!

- First take central values (no uncertainty): As in TC et al (MSHT): 2510.09321



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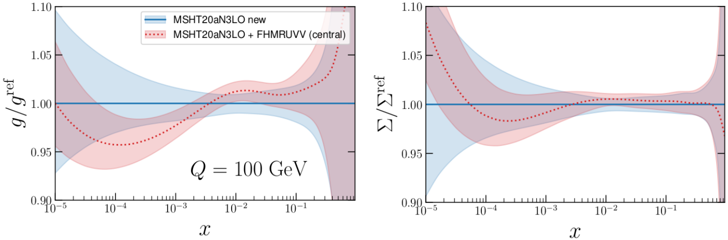

- 1% increase in gluon at $x \sim 10^{-2}$.
- How to account for uncertainty? Apply TNP with penalty $\Delta\chi^2 = 1$:

$$P_{ij} = P_{ij}^{\mathrm{FHMRUVV}}[\mathrm{central}] + \theta_{ij}(\mathrm{P}_{ij}^{\mathrm{FHMRUVV}}[\mathrm{up}] - \mathrm{P}_{ij}^{\mathrm{FHMRUVV}}[\mathrm{down}])$$

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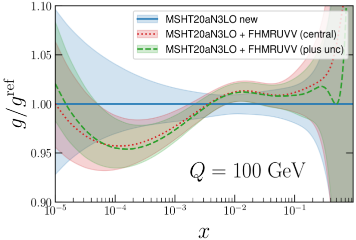
- First take central values (no uncertainty), now add uncertainty:



- 1% increase in gluon at $x \sim 10^{-2}$. Reduced uncertainty at low x.
- How to account for uncertainty? Apply TNP with penalty $\Delta\chi^2 = 1$:

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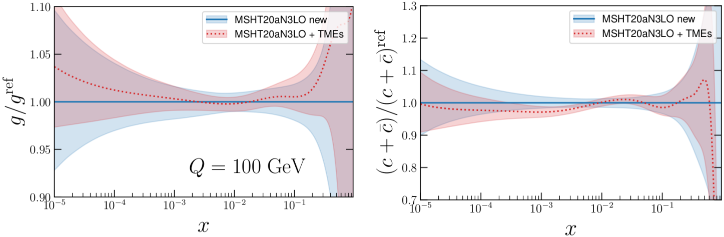
- Very little change in PDFs, but some fit quality improvement (later).

Approximate N3LO - Update TMEs

- Update Transition Matrix Elements (TMEs) to exact $A_{gg,H}$, A_{Hg}, $A_{qq,H}$, $A_{qg,H}$.

Via grids, as in TC et al (MSHT): 2510.09321



- Limited effects on PDF central values, within uncertainties.
- Effects on heavy quarks larger near threshold, though still consistent.

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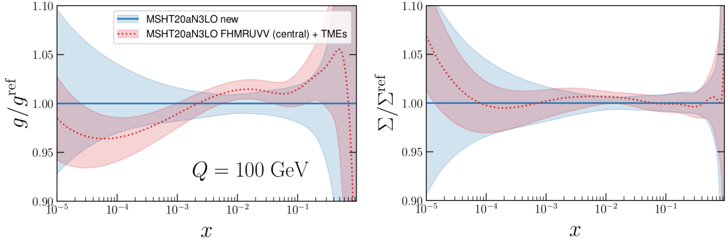

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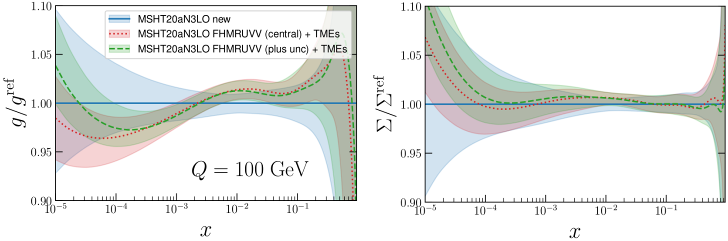

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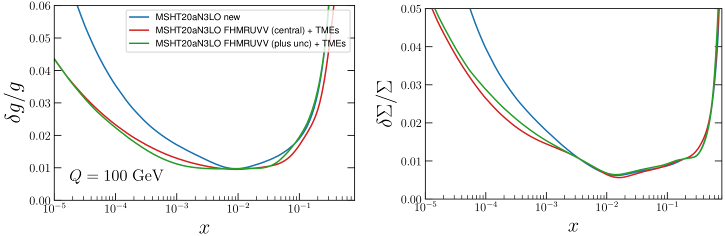

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- Effects on heavy quarks larger near threshold, though still consistent.
- Combine TME + FHMRUVV updates: first central, then + uncertainty.
- Limited effects on PDFs within uncertainties, some increase in small x gluon.
- Overall updates result in reduced PDF uncertainties, mainly at low x.

Approximate N3LO - Update FHMRUVV + TMEs

- When you include a theory uncertainty in fit you allow the central theory to move (whether via TNPs or theory cov matrix*). *in Gaussian, linear limit
- How do post-fit splitting functions look?

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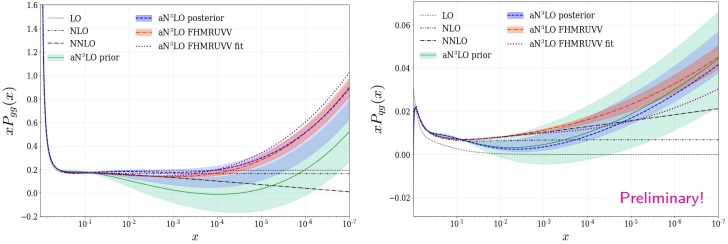
- How do post-fit splitting functions look? First without TME update:



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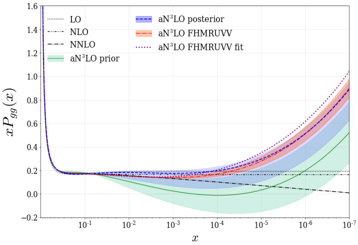

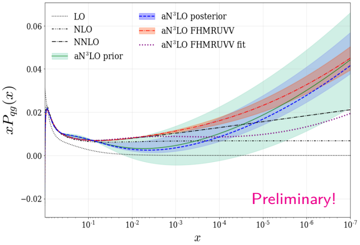

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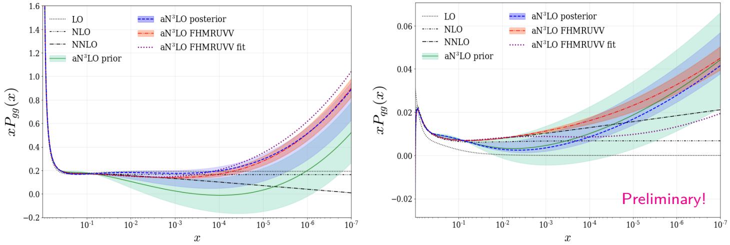

- Splitting Functions follow FHMRUVV central down to $x \sim 10^{-3}$, slight shifts at lower x.
- P_{qg} most pulled, particularly after adding TME updates, still at low x.
- Work ongoing to investigate more general approach via TNPs for splitting functions.

Approximate N3LO - Update FHMRUVV + TMEs

- Fit qualities, $\Delta\chi^2$ compared to new baseline NNLO fit: Preliminary!

MSHT new fits Δ^2 cf NNLO	aN3LO	aN3LO + FHMRUVV central	aN3LO + FHMRUVV plus unc	aN3LO + TMEs	aN3LO + FHMRUVV central + TMEs	aN3LO + FHMRUVV plus unc + TMEs
DIS	-41.0	17.1	-4.5	44.6	96.2	37.2
DY	-133.0	-99.2	-130.0	-105.1	-110.1	-121.5
Jets	-24.4	-25.7	-26.4	-23.8	-23.8	-21.8
Top	-4.8	-4.3	-4.9	-4.2	-4.2	-4.0
Theory penalties (none at NNLO)	13.8	10.7	11.5	23.1	9.0	17.3
Total (N_{pts} = 4892)	-189.5	-101.5	-154.3	-65.3	-32.9	-92.8

- In all cases aN3LO fit quality notably better than NNLO.
- Reduces as less uncertainty on aN3LO ingredients.
- Slight worsening of DIS (F_2^c) at aN3LO offset by improvement of DY data (mainly ATLAS 8TeV Zp_T, ATLAS 7TeV W, Z and CMS 7TeV Z).

Approximate N3LO - Coefficient Functions

- In original MSHT20aN3LO MHOU on DIS coefficient functions came from unknown heavy flavour contributions + MHOU on TMEs:
- E.g. $C_{H,g}^{VF,(3)}$ from $C_{H,g}^{FF,(3)}$ and $A_{Hg}^{(3)}$:

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

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  - Low-Q^2 FFNS CFs $C_{H,\{q,g\}}^{FF,(3)}$ - known LL small x, but unknown NLL small x $\Rightarrow$ introduce TNPs c_q^{NLL} and c_g^{NLL}.

$$C_{H,i}^{(3)}(Q^2 \to 0) \propto c_i^{LL}(m_H^2/Q^2)\frac{1}{x}[\ln 1/x - (c_i^{NLL} - 4)](1-x)^{20}, \text{ for } i = q, g.$$

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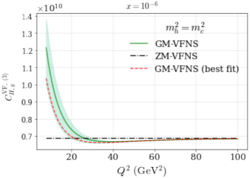
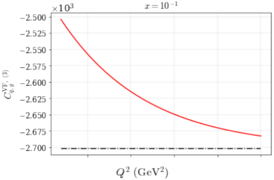
  - High-Q^2 FFNS CFs $C^{FF,(3)}_{H,\{q,g\}}$ - tend to known ZM-VFNS results.

Approximate N3LO - Coefficient Functions

- Then interpolate to connect low-Q^2 approximate and known ZM-VFNS result at high Q^2, guided by lower orders.
  - Used regression model to investigate interpolations (form in backup).
- Note no approximation for heavy flavour contributions to light quark F_2^q at low-Q^2, however very small and weakly-Q^2 dependent.





Preliminary!

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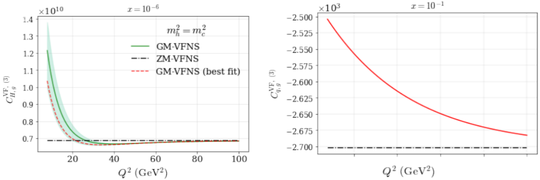

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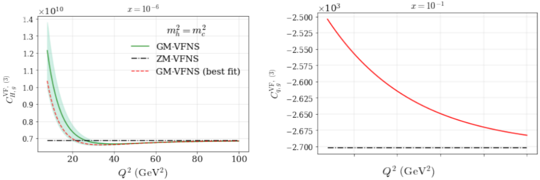

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- Work ongoing on adding TNPs to account for this, e.g. more general x-dependence and Q^2 dependence, e.g.:

Preliminary!

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Approximate N3LO - m_c dependence

- With updated TMEs dependence on m_c may change, compare MSHT20aN3LO original (left) with updated (right):

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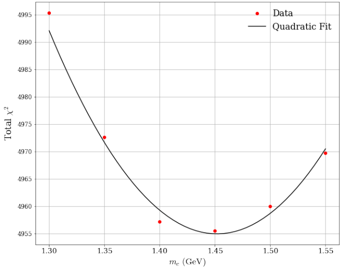

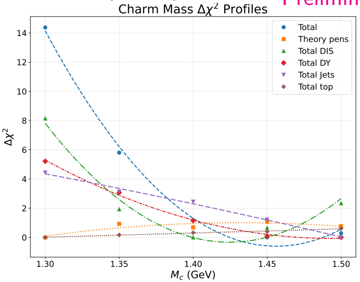

- Similar overall m_c dependence with minimum around 1.45 GeV.
- Dependence almost completely from DIS, mainly for F_2^C data as expected, magnitude slightly reduced.
- Ongoing work to improve parameterisation of DIS Coefficient Functions may affect this.

Conclusions

- Approximate N3LO PDFs vital for precision targets for Higgs, DY, etc.
- In MSHT, we have updated our PDFs based on FHMRUVV splitting functions and new exact Transition Matrix Elements.
- See limited effect on PDF central values, small increase in gluon by $\approx 1\%$ at $x \sim 10^{-2}$. Brings results closer to elsewhere.
- Updates result in reduction in PDF uncertainties at low x.
- Overall PDFs stable within uncertainties upon updating with new theory info.
- Ongoing work on DIS Coefficient Function uncertainties given TME updates.

More information in: MSHT: 2207.04739, 2312.07665, 2510.09321.

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Thankyou!

Any Questions?

More information in: MSHT: 2207.04739, 2312.07665, 2510.09321.

Backup Slides

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aN3LO Splitting Functions:

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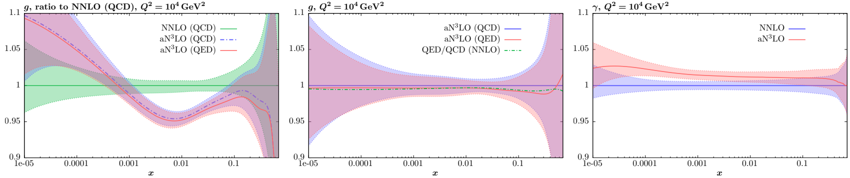
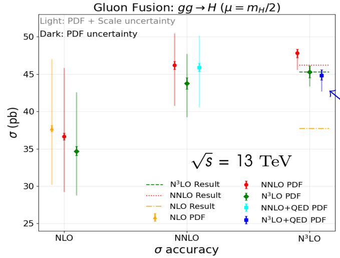
aN3LO QCD + QED:

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

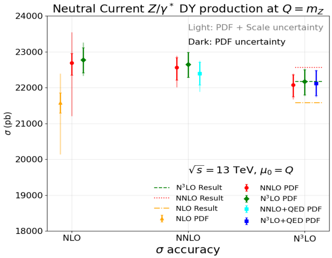
- Impact small relative to aN3LO QCD corrections in most regions.
- Effect of adding QED similar when applied to NNLO and aN3LO.



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



ggH xsec reduced by $\approx$ 1% by QED effects.



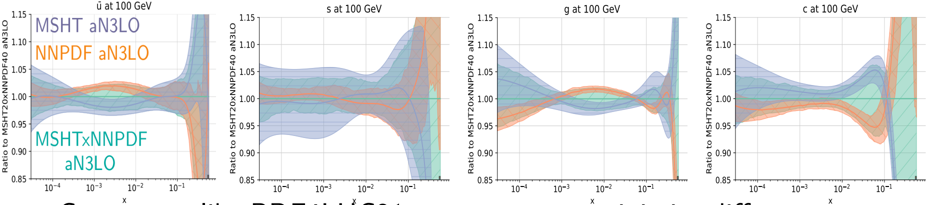
Combination of the aN3LO PDFs:

- Given the different aN3LO PDFs, a conservative approach to estimate the total aN3LO PDF uncertainty is to combine them.

> **Central value:** unweighted average of two sets
> **Uncertainty:** accounts for both individual PDF sets' uncertainties and any differences in their central values.

- À la PDF4LHC21, constructed by combining 100 replicas of MSHT and NNPDF aN3LO sets.

(See TC et al - MSHT and NNPDF - 2411.05373)



- Caveat - unlike PDF4LHC21 no attempt to minimise differences, e.g. different heavy quark masses ⇒ use only at sufficiently large Q^2.

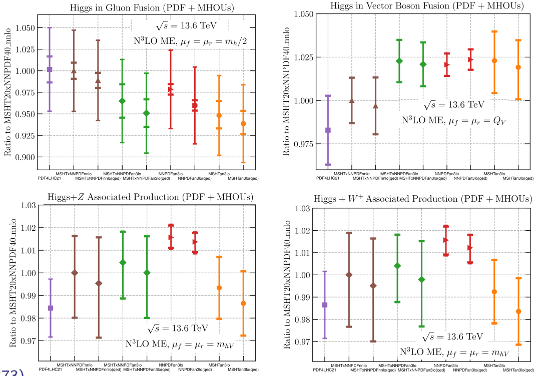
aN3LO PDF effects on Cross-sections: Higgs

- Largest aN^{3}LO effect is on Higgs production in gluon-gluon fusion.

PDF		MSHT	NNPDF	MSHTxNNPDF
ggF xsec shift relative to NNLO	aN3LO	-5%	-2%	-4%
	aN3LO+QED	-6%	-4%	-5%

- Smaller aN^{3}LO effects for quarks and hence for VBF, ZH, $W^{\pm}H$.

- VBF: aN^{3}LO+QED result in +2.5%.
- ZH and $W^{\pm}H$: all observe $\approx$ +0.5% from aN^{3}LO+QED.
- Consistent trends in all cases between MSHT and NNPDF aN^{3}LO PDFs.



(See TC et al - MSHT and NNPDF - 2411.05373)

aN3LO PDF effects on Xsecs:

- aN3LO PDFs can be used:
  1. With N3LO matrix elements to compute cross-sections more precisely.
  2. To evaluate the PDF uncertainty from using NNLO PDFs with N3LO cross-sections (previous “highest order” available).

- Before aN3LO PDFs, often N3LO cross-section with NNLO PDFs taken as “highest order” result + $\Delta^{\text{approx}}_{\text{NNLO}}$ for PDF MHOU uncertainty.

$$\Delta^{\text{approx}}_{\text{NNLO}} = \frac{1}{2}\left|\frac{\sigma^{\text{NNLO-xsec}}_{\text{NNLO-PDF}} - \sigma^{\text{NNLO-xsec}}_{\text{NLO-PDF}}}{\sigma^{\text{NNLO-xsec}}_{\text{NNLO-PDF}}}\right|$$

2. Compare with $\Delta^{\text{exact}}_{\text{NNLO}}$:

$$\Delta^{\text{exact}}_{\text{NNLO}} = \left|\frac{\sigma^{\text{N3LO-xsec}}_{\text{N3LO-PDF}} - \sigma^{\text{N3LO-xsec}}_{\text{NNLO-PDF}}}{\sigma^{\text{N3LO-xsec}}_{\text{N3LO-PDF}}}\right|$$

PDF set	Δ	$\sigma(gg \to H)$	$\sigma(H\ VBF)$
MSHT20	$\Delta^{\text{exact}}_{\text{NNLO}}$	5.3%	2.3%
	$\Delta^{\text{approx}}_{\text{NNLO}}$	1.4%	1.3%
NNPDF4.0	$\Delta^{\text{exact}}_{\text{NNLO}}$	2.2%	1.3%
	$\Delta^{\text{approx}}_{\text{NNLO}}$	0.2%	0.2%
MSHT20xNNPDF4.0	$\Delta^{\text{exact}}_{\text{NNLO}}$	3.3%	2.3%
	$\Delta^{\text{approx}}_{\text{NNLO}}$	1.6%	0.5%

- $\Delta^{\text{approx}}_{\text{NNLO}}$ is very unreliable, underestimating $\Delta^{\text{exact}}_{\text{NNLO}}$ for ggF and VBF.

(See TC et al - MSHT and NNPDF - 2411.05373)

Approximate N3LO - Coeff Funcs Interpolation

- Obtain desired VFNS Coefficient Function $C_{ij}^{VF,(3)}$ by equating F_2 in FFNS and VFNS, then VFNS coefficient function at N3LO can be written as sum of terms involving FFNS coefficient function $C_{ij}^{FF,(3)}$ at N3LO, TMEs at N3LO $A_{ij}^{(3)}$ and lower order cross-terms, e.g.:

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

- Now $A_{ij}^{(3)}$ are known, remaining aspect is $C_{ij}^{FF,(3)}(x, Q^2/mu^2, Q^2/m_H^2)$.
- $Q^2 \to \infty$ becomes known ZM-VFNS results $C_{ij}^{FF,(3)}(x, Q^2 \to \infty)$.
- $Q^2 \sim m_H^2$ for heavy quark structure function, use known approximations based on exact LL small-x logs, known mass threshold terms $\tilde{f}(m_H^2/Q^2)$ and we known NLL small-x structure $\Rightarrow$ use TNP for this.
- $Q^2 \sim m_H^2$ for light quark structure function contribution from heavy quarks is both very small and only weakly Q^2 independent.

Approximate N3LO - Coeff Funcs Interpolation

- Obtain desired VFNS Coefficient Function $C_{ij}^{VF,(3)}$ by equating F_2 in FFNS and VFNS, then VFNS coefficient function at N3LO can be written as sum of terms involving FFNS coefficient function $C_{ij}^{FF,(3)}$ at N3LO, TMEs at N3LO $A_{ij}^{(3)}$ and lower order cross-terms, e.g.:

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- We used regression model to investigate interpolations, ultimately used function $\exp[0.3(1 - Q^2/m_H^2)]$ for heavy quark structure function and $\exp[-AQ^2/m_H^2 + B]$ for light quarks with A, B channel-dependent. Both based on guidance from lower orders.
- Now no uncertainty from TME, more complex x dependence at low Q^2 and Q^2/m_H^2 dependence of interpolation + TNPs for this under investigation.

Approximate N3LO - Coeff Funcs Interpolation

- I.e. for the interpolations for the heavy and light quark structure functions for the FFNS part we used:

$$C^{\mathrm{FF},\ (3)}_{H,\ \{q,g\}} = \begin{cases} C^{\mathrm{FF},\ (3)}_{H,\ \{q,g\},\ \text{low-}Q^2}(x, Q^2 = m_h^2)\ e^{0.3\ (1-Q^2/m_h^2)} \\ \qquad + C^{\mathrm{FF},\ (3)}_{H,\ \{q,g\}}(x, Q^2 \to \infty)\left(1 - e^{0.3\ (1-Q^2/m_h^2)}\right) & ,\ \text{if } Q^2 \geq m_h^2, \\ C^{\mathrm{FF},\ (3)}_{H,\ \{q,g\},\ \text{low-}Q^2}(x, Q^2) & ,\ \text{if } Q^2 < m_h^2. \end{cases}$$

$$C^{\mathrm{FF},\ (3)}_{q,\ \{q,g\}} = \begin{cases} C^{\mathrm{FF},\ \mathrm{NS},\ (3)}_{q,\ q}(x, Q^2 \to \infty)\left(1 + e^{-0.5\ (Q^2/m_h^2)-3.5}\right), \\ C^{\mathrm{FF},\ \mathrm{PS},\ (3)}_{q,\ q}(x, Q^2 \to \infty)\left(1 - e^{-0.25\ (Q^2/m_h^2)-0.3}\right), \\ C^{\mathrm{FF},\ (3)}_{q,\ g}(x, Q^2 \to \infty)\left(1 - e^{-0.05\ (Q^2/m_h^2)+0.35}\right), \end{cases}$$

- Now no uncertainty from TME, more complex x dependence at low Q^2 and Q^2/m_H^2 dependence of interpolation + TNPs for this under investigation.