Recent progress in global PDF determination and the path to N3LO

Based on 2401.08749 (NNPDF4.0 QED), 2401.10319 (NNPDF4.0 MHOU), and 2402.18635 (NNPDF4.0 aN3LO)

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Joint Northern UK Journal Club

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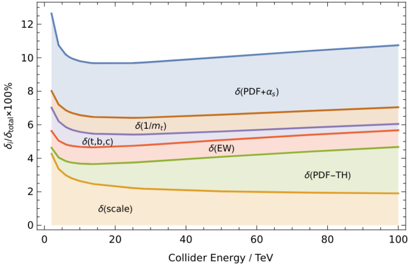
Motivation

$$\sigma(x,Q^2) = \sum_i \int_x^1 \frac{dz}{z} \mathcal{L}_{ij}(z,\mu^2) \hat{\sigma}_{ij}\left(\frac{x}{z}, \frac{Q^2}{\mu^2}, \alpha_s\right)$$

- Predictions for collider processes rely on PDFs and matrix elements
- PDF uncertainties often the dominant source of uncertainty
- Current standard in PDF fits is NNLO in QCD

Progress towards the next generation of PDFs:

- QED effects
- (approximate) N3LO
- Accounting for missing higher order uncertainties



Uncertainties for inclusive Higgs production
[Dulat, Lazopoulos, Mistleberger: 1802.00827]

QED effects in PDFs

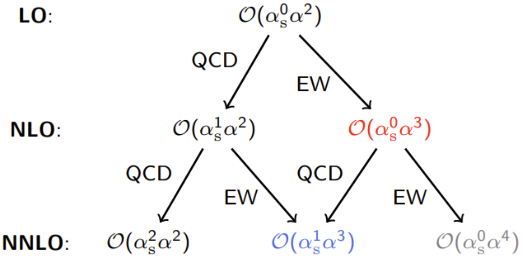
Including QED corrections in a PDF set

The current standard for PDFs determination is at NNLO in QCD, however $\alpha(M_z) \sim \alpha_s^2(M_Z)$

Including QED corrections in PDFs consists of

- QED corrections to DGLAP (at $\mathcal{O}(\alpha)$, $\mathcal{O}(\alpha\alpha_s)$ and $\mathcal{O}(\alpha^2)$):
  $P_{QED} = \alpha P_{ij}^{(0,1)} + \alpha\alpha_s P_{ij}^{(1,1)} + \alpha^2 P_{ij}^{(0,2)} + \dots$
- Adding a photon PDF and including photon initiated contributions to cross-sections
  The momenum sumrule is modified accordingly:

$$\int_0^1 dx\ \left(x\Sigma(x,Q^2) + xg(x,Q^2) + x\gamma(x,Q^2)\right) = 1$$



Example: EW corrections in DY
[C. Schwan DIS 2021]

Determination of the photon PDF

Initially the photon PDF has been determined in different ways:

- physical model: sensitive to underlying model
- fitting: data does not provide strong constraints

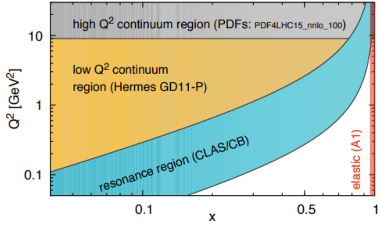
However with the LUXqed approach it can be computed perturbatively
based on the observation that the heavy-lepton production cross-section can be written in two ways:

- in terms of structure functions F_2, F_L
- in terms of PDFs (including the photon)

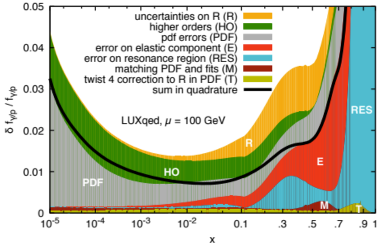
luxQED result [Manohar, Nason, Salam, Zanderighi: 1607.04266, 1708.01256]:

$$x\gamma(x,\mu^2) = \frac{2}{\alpha(\mu^2)} \int_x^1 \frac{dz}{z} \left\{ \int_{\frac{m_p^2 x^2}{1-z}}^{\frac{\mu^2}{1-z}} \frac{dQ^2}{Q^2} \alpha^2(Q^2) \left[-z^2 F_L(x/z, Q^2) \right. \right.$$

$$\left. \left. + \left(z P_{\gamma q}(z) + \frac{2x^2 m_p^2}{Q^2} \right) F_2(x/z, Q^2) \right] - \alpha^2(\mu^2) z^2 F_2(x/z, \mu^2) \right\}$$



Input to construct F_2 and F_L



Sources of uncertainty

LUXqed PDF determinations

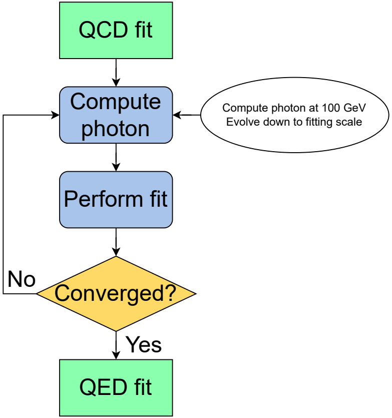
LUXqed has been used in all of the most recent QED PDFs:

- LUXqed_plus_PDF4LHC15 [1607.04266]
- LUXqed17_plus_PDF4LHC15 [1708.01256]
- MMHT2015qed [1907.02750]
- NNPDF3.1luxQED [1712.07053]
- CT18lux and CT18qed [2106.10299]
- MSHT20QED [2111.05357]
- MSHT20qed_an3lo [2312.07665]
- NNPDF4.0QED [2401.08749]

The photon PDF

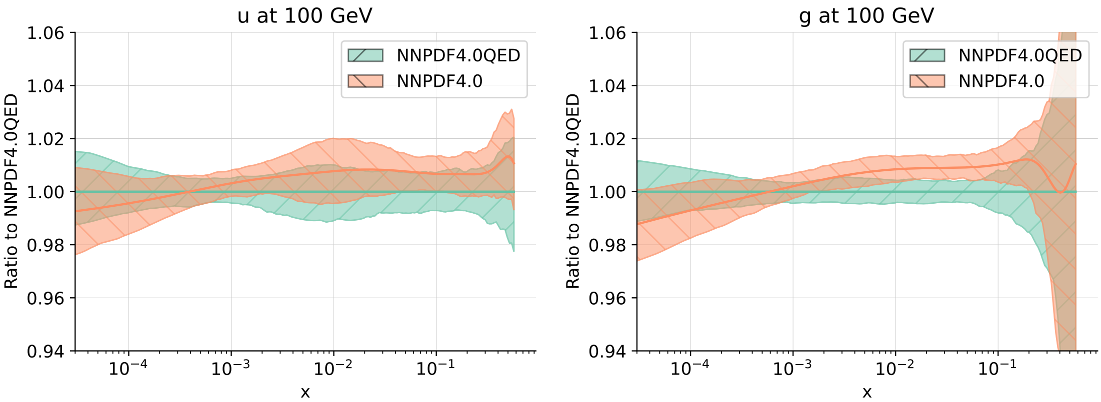
An iterative procedure is used to address the interplay between the photon and other PDFs due to the momentum sumrule

$$\int_0^1 dx\ \left(x\Sigma(x,Q^2) + xg(x,Q^2) + x\gamma(x,Q^2)\right) = 1$$



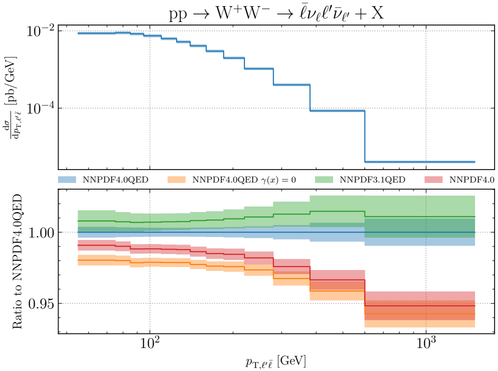
[NNPDF3.1QED: 1712.07053]

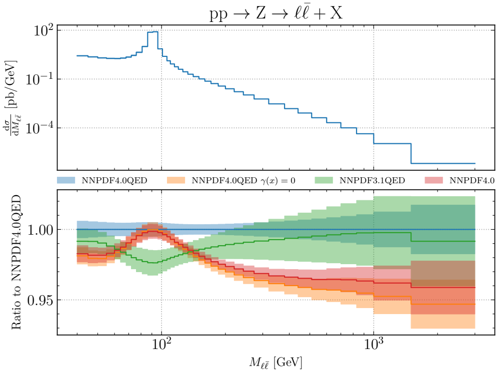
Results: Impact of the photon on other PDFs



- Non-negligible impact, but PDFs are in agreement within uncertainty
- Gluon reduced due to momentum sum rule with photon carrying additional momentum

Results: phenomenological impact





- NLO in both QCD and QED, only PDF uncertainties are shown
- Non-negligable QED corrections (up to 5%) in the large invariant mass and large-p_T regions relevant for new physics searches
- In most other cases studied, QED corrections are at the percent level

Theory in puts for approximate N3LO PDFs

Theory requirements for PDFs at N3LO

Several theory inputs are needed in a PDF fit:

- Splitting functions for DGLAP evolution
- Matching conditions for heavy-quark mass schemes
  $f_i^{(n_f+1)}\left(x,Q^2\right) = A_{ij}\left(x,\alpha_s\right) f_j^{(n_f)}\left(x,Q^2\right)$
- DIS coefficient functions
- Hadronic cross sections,

Not all available at N3LO, but information is available for all. What is the best we can do?

- Use N3LO calculations where known
- Construct approximate results where possible
- Account for theory uncertainties of the missing or incomplete higher order

No need to wait for complete N3LO results and more information can be included as it becomes available

Splitting functions

Complete results for the N3LO splitting functions are not yet available, but a lot of information exists (with important contributions from Liverpool and Edinburgh):

- Small-x limits (BFKL resummation) [Bonvini and Marzani: 1805.06460] [Davies, Kom, Moch, Vogt: 2202.10362]
- Large-x limits (threshold resummation) [Soar, Moch, Vermaseren, Vogt: 0912.0369], [Henn, Korchemsky, Mistlberger: 1911.10174], [Duhr, Mistlberger, Vita 2205.04493]
- Large-n_f limit [Davies, Ruijl, Ueda, Vermaseren, Vogt: 1610.0744], [Gehrmann, Manteuffel, Sotnikov, Yan: 2308.07958]
- Mellin moments [Falcioni, Herzog, Moch, Ruijl, Ueda, Vermaseren, Vogt: 1707.08315, 2111.15561, 2302.07593, 2307.04158]

How can we use this information to construct approximate splitting functions?

Splitting functions

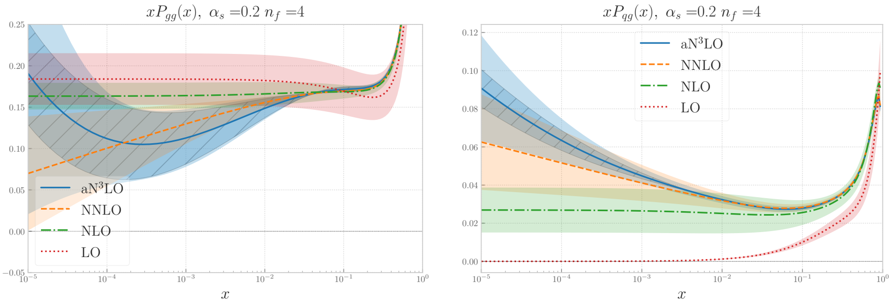
1. The approximation is performed in Mellin space as an expansion in n_f, where any double counting terms present in the resummed small-x and large-x expressions are removed

$$\gamma_{ij}^{(3)} = \gamma_{ij,n_f}^{(3)} + \gamma_{ij,N\to\infty}^{(3)} + \gamma_{ij,N\to 0}^{(3)} + \gamma_{ij,N\to 1}^{(3)} + \widetilde{\gamma}_{ij}^{(3)}$$

2. The remainder term $\widetilde{\gamma}_{ij}^{(3)}$ is constructed as a linear combination of interpolating functions:
   - A function for the leading unknown large-N contribution
   - A function for the two leading unknown small-N contribution
   - Functions for the subleading small-N and large-N contributions
3. The weights of these interpolating functions are determined by equating to the known moments
4. Then, vary the subleading contributions included in the basis of interpolating functions to estimate incomplete higher order uncertainties (IHOU) on the splitting functions

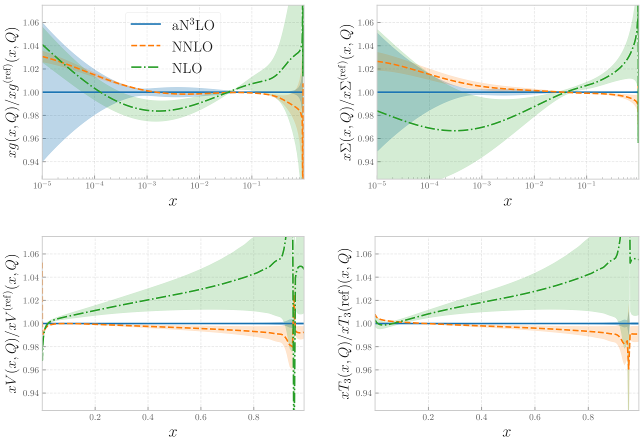
More details on how to account for IHOUs in a fit follows later

Splitting functions



- Dark blue band is IHOU only, light blue is sum in quadrature of MHOU and IHOU
- Good perturbative agreement at large-x
- IHOU are not negligible

NNPDF4.0 evolved from $Q = 1.65$ GeV to $Q = 100$ GeV



- Effects of N3LO corrections to DGLAP evolution at most percent level, except at small-x and large-x
- Good perturbative convergence

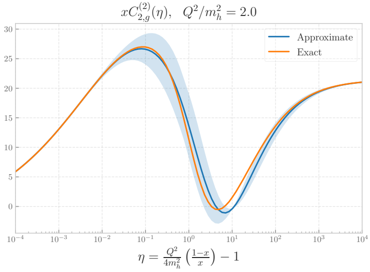
DIS coefficient functions

- DIS coefficient functions are known up to N3LO in the massless limit (again with contributions from Liverpool) [Larin, Nogueira, Van Ritbergen, Vermaseren: 9605317], [Moch Vermaseren Vogt: 0411112, 0504242], [Davies, Moch, Vermaseren, Vogt: 0812.4168, 1606.08907]
- Massive coefficient functions can be constructed by smoothly joining the known limits from high energy and threshold resummations and the massless limit ($Q^2 \to m_h^2$, $x \to 0$, and $Q^2 \gg m_h^2$) [Barontini, Bonvini, Laurenti: in preparation]

$$C^{(3)}(x, m_h^2/Q^2) = C^{(3),\mathrm{thr}}(x, m_h^2/Q^2) f_1(x) + C^{(3),\mathrm{asy}}(x, m_h^2/Q^2) f_2(x)$$

$$f_1(x) \xrightarrow[x\to 0]{} 0, \quad f_1(x) \xrightarrow[x\to x_{\max}]{} 1\,,$$

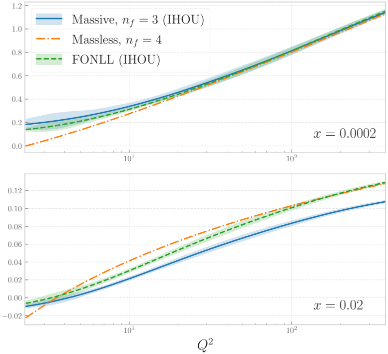
$$f_2(x) \xrightarrow[x\to 0]{} 1, \quad f_1(x) \xrightarrow[x\to x_{\max}]{} 0\,,$$



We can validate the procedure at NNLO

DIS variable flavor number scheme (VFNS)

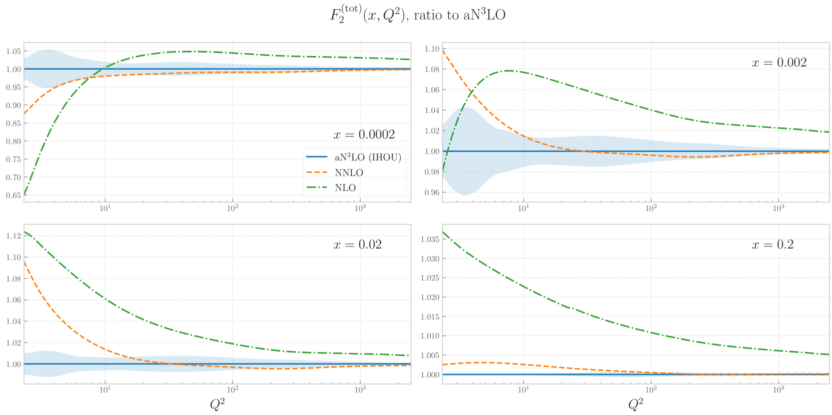
- In a PDF fit different flavour number schemes are joined in a variable flavour number scheme (VFNS) to ensure reliable results from $Q^2 \sim m_h^2$ up to $Q^2 \gg m_h^2$
- The matching conditions encoding the transition between schemes have almost completely been computed up to N3LO
- The VFNS used in NNPDF is the FONLL scheme below
- FONLL extended for arbitrary number of mass scales in the recent `EKO` (DGLAP) and `yadism` (DIS) codes



$F_2^{(c)}$

$$F_{\mathrm{FONLL}}(Q^2, m_c) = F^{(n_f+1)}(Q^2, m_h = 0) + F^{(n_f)}(Q^2, m_c) - \lim_{m_c \to 0} F^{(n_f)}(Q^2, m_h)$$

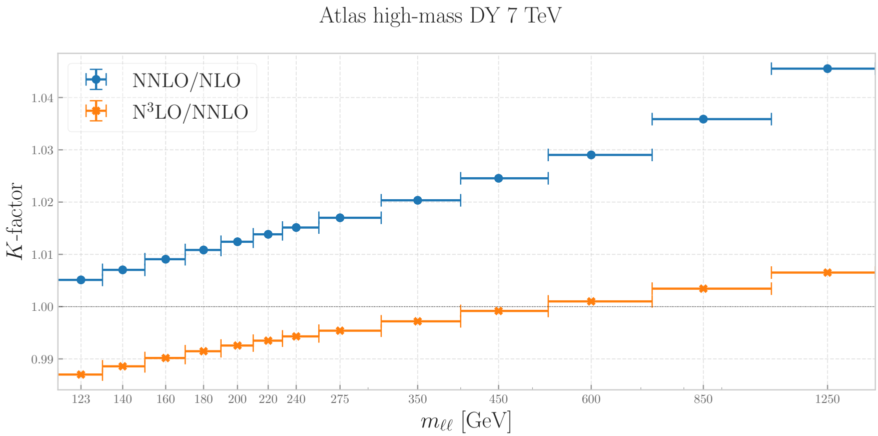
DIS structure functions



- The uncertainty band corresponds to IHOU of the massive coefficient functions
- N3LO corrections are significant at low-Q

Hadronic processes

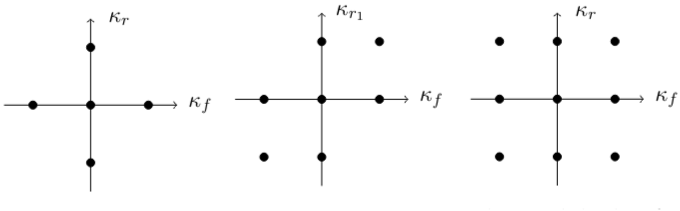
- Corrections to collider DY and W production can be included through k-factors
- N3LO effects around 1 to 2% for LHC observables
- For many processes N3LO corrections are not available, for those we introduce account for MHOU through μ_r variations



Inclusion of theory uncertainties

Theory errors from scale variations

- Missing higher order uncertainties are estimated through variations of the nonphysical factorization (μ_f) and renormalization (μ_r) scales
- μ_r and μ_f are varied sumultaneously following the 7-point prescription



5,7,9 point prescription

- Factorization scale variations estimate MHOUs in DGLAP evolution
- Renormalization scale variations estimate MHOUs in matrix elements

Missing higher order uncertainties covmat

How can we account for theory uncertainties in a PDF fit?

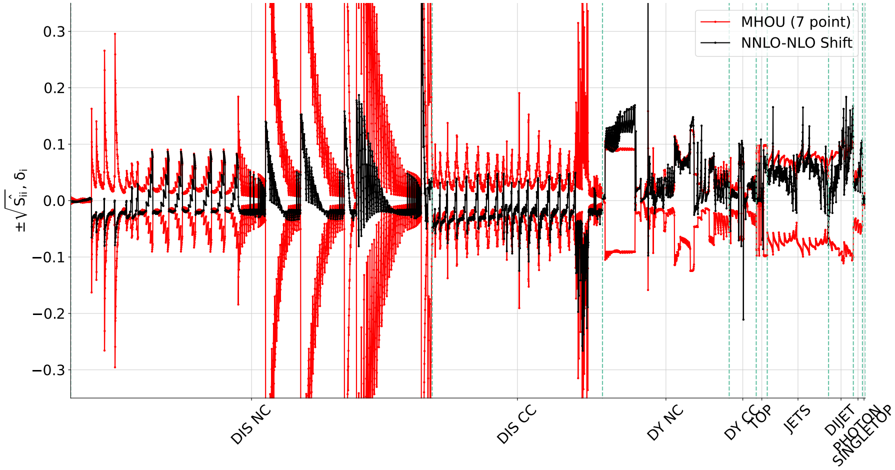
- In a fit we minimize the χ^2:
  $P(T|D) \propto \exp\left[-\frac{1}{2}(T-D)\,C_{\rm exp}^{-1}\,(T-D)\right] \propto \exp\left[-\frac{1}{2}\chi^2\right]$
- Include theory covmat $C_{\rm MHOU}$ at same footing as exp covmat $C_{\rm exp}$: $C_{\rm exp} \to C_{\rm exp} + C_{\rm MHOU}$

$$C_{{\rm MHOU},ij} = n_m \sum_{V_m} \left(T_i(\rho_f,\rho_r) - T_i(0,0)\right)\left(T_j(\rho_f,\rho_r) - T_j(0,0)\right)$$

Can we trust the faithfulness of these uncertainties on the unknown order?

Missing higher order uncertainties covmat

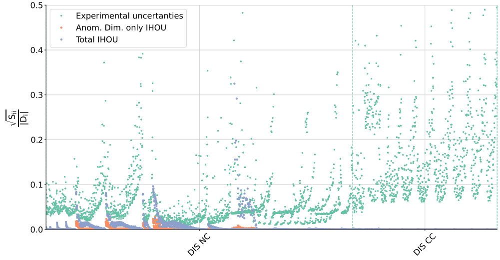
Validate the MHOU procedure by testing the NLO MHOU covmat



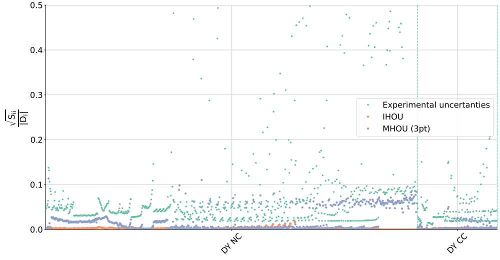
Incomplete higher order uncertainties covmat

- We construct an IHOU matrix following a similar approach by varying the subleading functions
- IHOU are independent of MHOU so the uncertainties are added in quadrature

$$C = C_{\text{exp}} + C_{\text{MHOU}} + C_{\text{IHOU}}$$



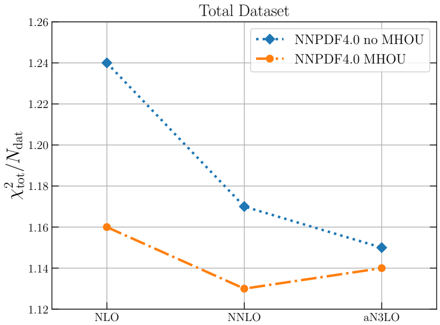
IHOU have a large effect on small-x, low-Q DIS data



NNLO MHOU included where N3LO not available
MHOU can similar magnitude as the experimental uncertainty

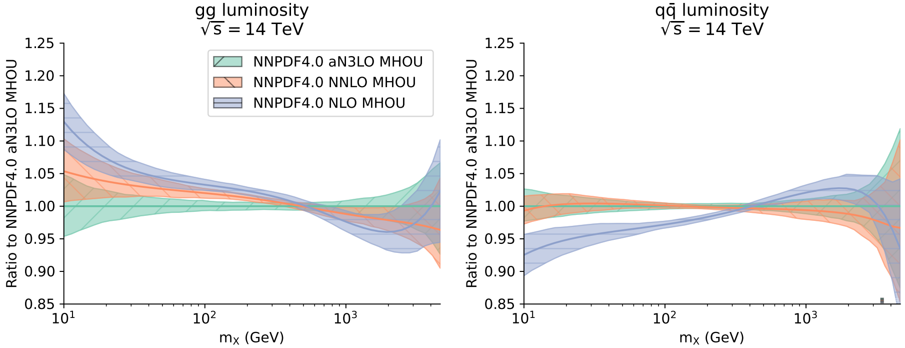
Results

Fit quality



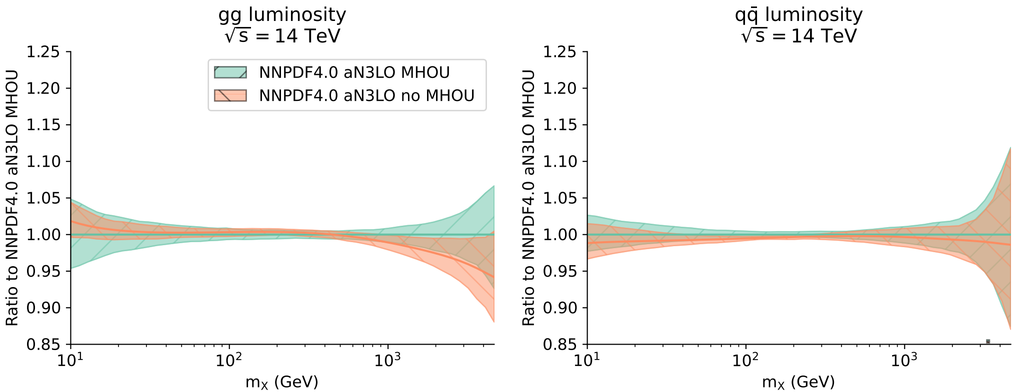
- Without MHOUs the χ^2 improves with the perturbative accuracy
- With MHOUs the χ^2 stabilizes significantly
- At N3LO MHOUs have a small impact

Perturbative convergence



- Good perturbative convergence
- Moderate impact of N3LO corrections, especially for the quark luminosities
- $\sim 2\%$ suppression of gg luminosity around the Higgs mass

Impact of MHOUs at N3LO

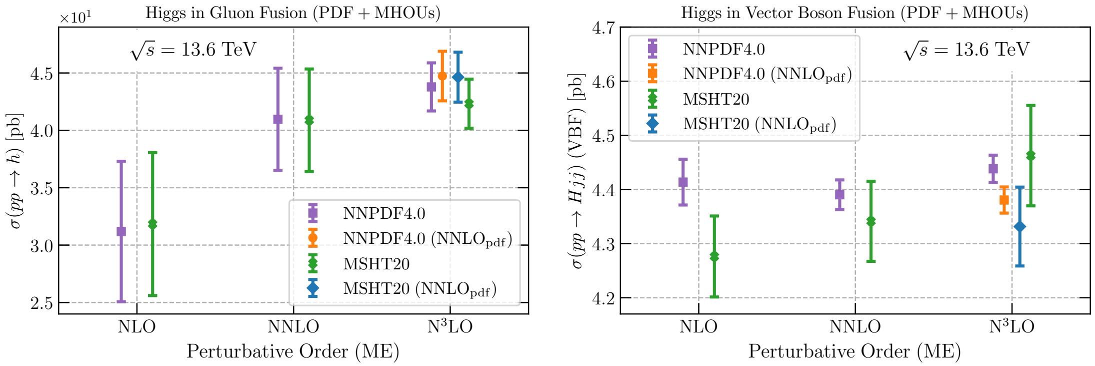


- Non-negligible impact of MHOUs even at N3LO

$\Rightarrow$ reason to include exact N3LO calculations for hadronic processes

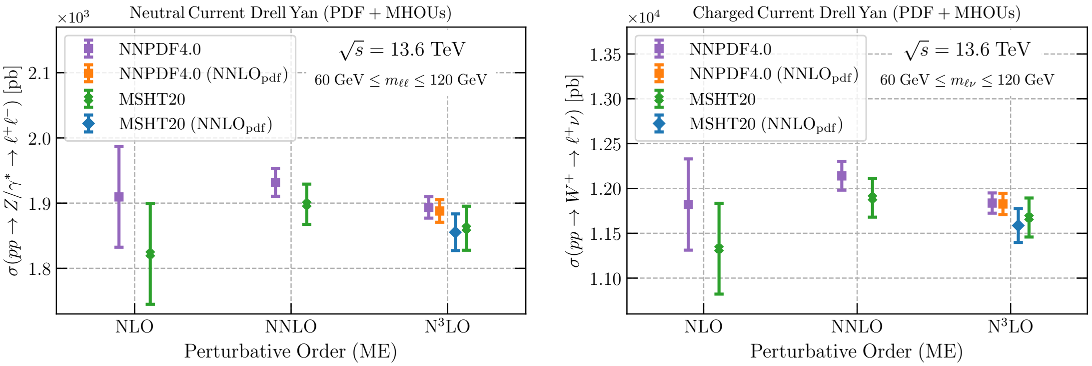
LHC phenomenology

Higgs production



- Matrix elements for both Higgs in gluon fusiona and VBF available at N3LO
- N3LO correction to Higgs in gluon fusion, small suppression compared to NNLO
- Higgs in VBF perturbatively stable

Drell-Yan



- Good convergence also for quark initiated processes

Summary and outlook

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- N3LO PDFs and QED corrections are a requirement for LHC predictions at 1% accuracy
- All sources of theory uncertainty should be accounted for
- NNPDF4.0 aN3LO allows for consistent N3LO calculations. Initial results for Higgs and DY production suggest good perturbative convergence
- Work towards combining N3LO, MHOU and QED is ongoing

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Thank you for your attention!