

Studies of $N^3\text{LO}$ corrections and resummation scale uncertainties in fits to DIS data using xFitter

F. Giuli (on behalf of the xFitter Developers' team)

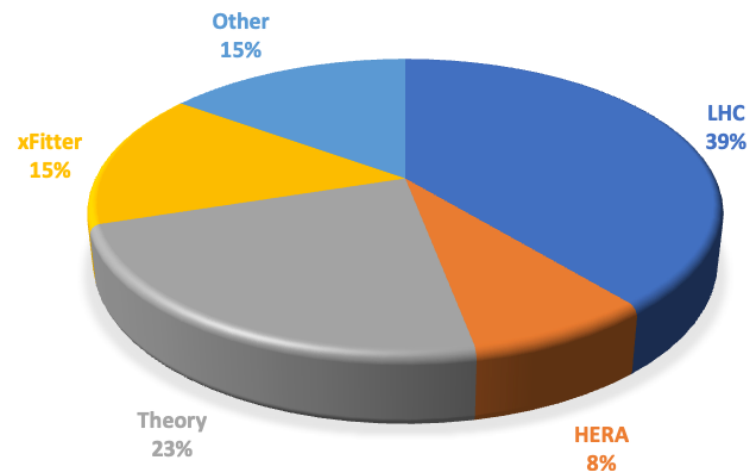
QCD@LHC26 (Oxford, UK)

01/10/2026



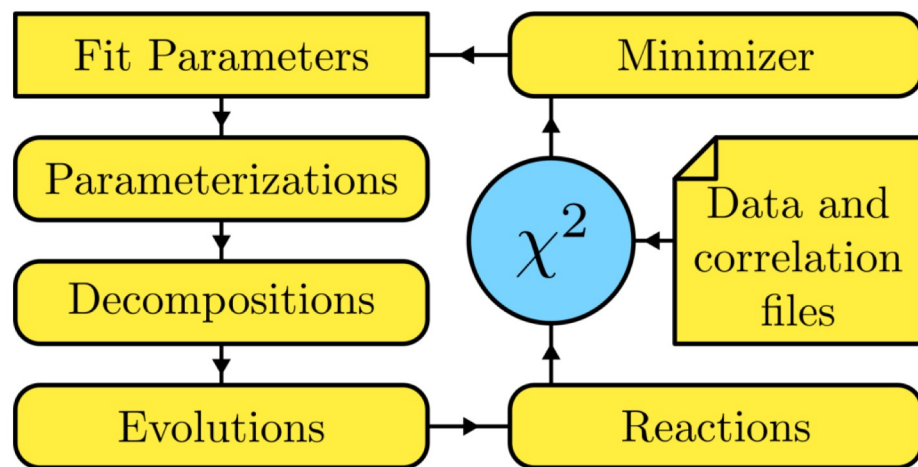
The xFitter Project

- The [xFitter](#) project (former HERAFitter) is a **unique open-source QCD fit framework**
- [GitLab](#) repository ([open access](#))
- This code allows users to:
 - **extract PDFs** from a large variety of data
 - assess the **impact** of **new data on PDFs**
 - check the **consistency** of experimental data
 - test different **theoretical assumptions**
- Several active developers between experimentalists and theorists
- More than [500 publications](#) obtained using xFitter since the beginning of the project
- Next xFitter External meeting in Bilbao at the end of May - [indico](#)



Flexibility of xFitter

- xFitter is **UNIQUE** and **so VERSATILE**
- PDF parametrization at the starting scale → enough to type your favourite formulas
- PDF decomposition: construct gluon, valence and sea, apply sum rules (automatic numerical integration)
- PDF evolution: interfaced with various codes i.e. QCDNUM, APFEL(++), LHAPDF etc. - TMD PDF evolution available in a branch)
- Various heavy-quarks schemes for ep DIS
- Interfaces to fast interpolation tables allows us to get recent higher-order calculations
- Flexible χ^2 implementation (treatment of experimental uncertainties)
- χ^2 minimization: MINUIT, CERES



Analysis of DIS data at N³LO

- HERAPDF2.0 parametrization - [1506.06042](#):

$$xu_v(x, \mu_0^2) = A_{u_v} x^{B_{u_v}} (1-x)^{C_{u_v}} [1 + E_{u_v} x^2]$$

$$xd_v(x, \mu_0^2) = A_{d_v} x^{B_{d_v}} (1-x)^{C_{d_v}}$$

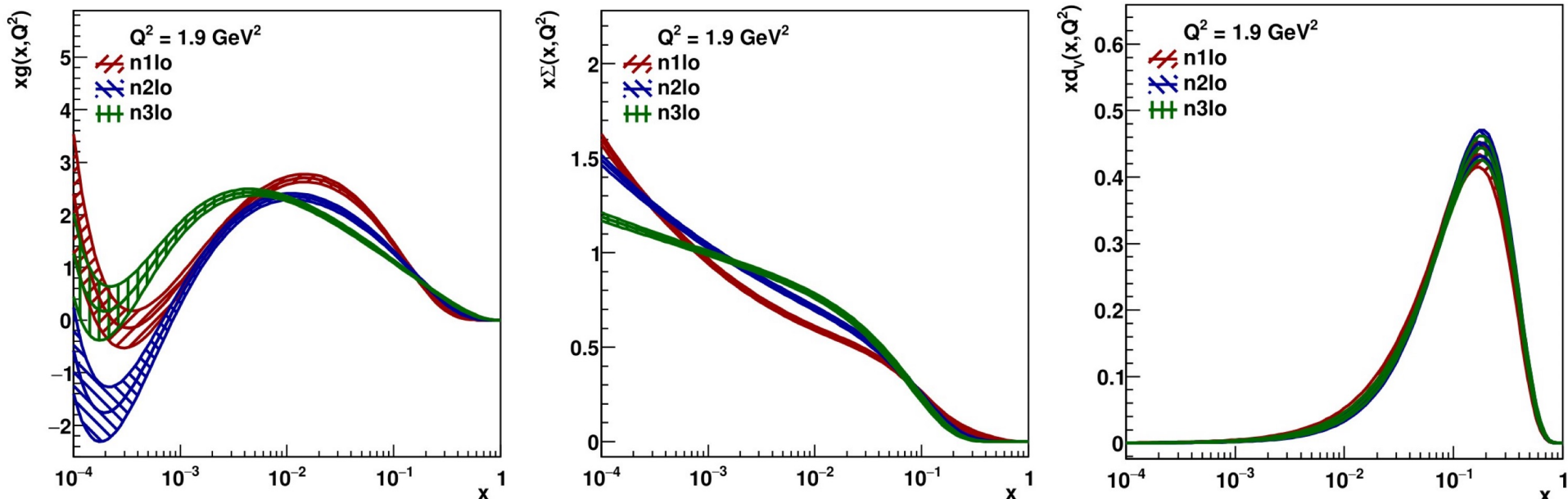
$$x\bar{u}(x, \mu_0^2) = A_{\bar{u}} x^{B_{\bar{u}}} (1-x)^{C_{\bar{u}}} [1 + D_{\bar{u}} x]$$

$$x\bar{d}(x, \mu_0^2) = A_{\bar{d}} x^{B_{\bar{d}}} (1-x)^{C_{\bar{d}}}, \quad xs(x, \mu_0^2) = x\bar{s}(x, \mu_0^2) = r_s x\bar{d}(x, \mu_0^2) \quad \text{with} \quad r_s = \frac{f_s}{1-f_s}$$

$$xg(x, \mu_0^2) = A_g x^{B_g} (1-x)^{C_g} [1 + F \log x] - [1902.11125](#)$$

- HERA I+II inclusive and $F_{2,c} + F_{2,b}$ data ([1804.01019](#))
- N³LO evolution implemented in APFEL++ ([1708.00911](#)) – benchmarked with HOPPET ([2404.15711](#))
- **Exact** ([2311.00644](#), [2403.00513](#), [2509.16124](#), [2510.02175](#), [QCD@LHC talk](#), [2602.10334](#), [2604.09534](#), [2609.37563](#)) N³LO matching conditions implemented in APFEL++
- FONLL VFNS implemented in xFitter, checked with fortran APFEL at NNLO

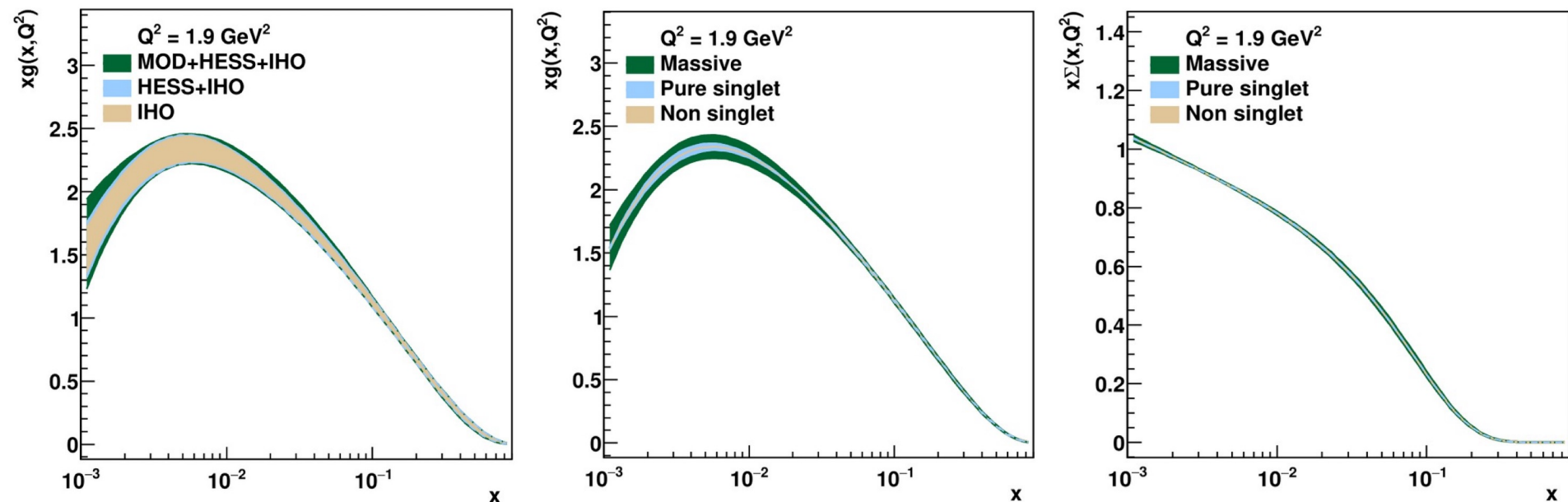
N³LO vs NNLO vs NLO



- Gluon (left), total singlet (middle) and d-valence (right)
- N³LO gluon is harder and larger than NNLO at small-x
- For $x \geq 0.01$ all orders agree
- **Slightly better χ^2 wrt NNLO fit**

Dataset	n1lo	n2lo	n3lo
HERA1+2 NCep 820	72 / 70	75 / 70	68 / 70
HERA1+2 NCep 460	217 / 204	220 / 204	221 / 204
HERA1+2 CCep	49 / 39	46 / 39	46 / 39
HERA1+2 NCem	214 / 159	218 / 159	222 / 159
HERA1+2 CCem	65 / 42	62 / 42	58 / 42
HERA1+2 NCep 575	215 / 254	220 / 254	217 / 254
HERA1+2 NCep 920	426 / 377	433 / 377	437 / 377
Correlated χ^2	69	78	80
Log penalty χ^2	-0.51	+0.51	-3.41
Total χ^2 / dof	1327 / 1131	1353 / 1131	1345 / 1131

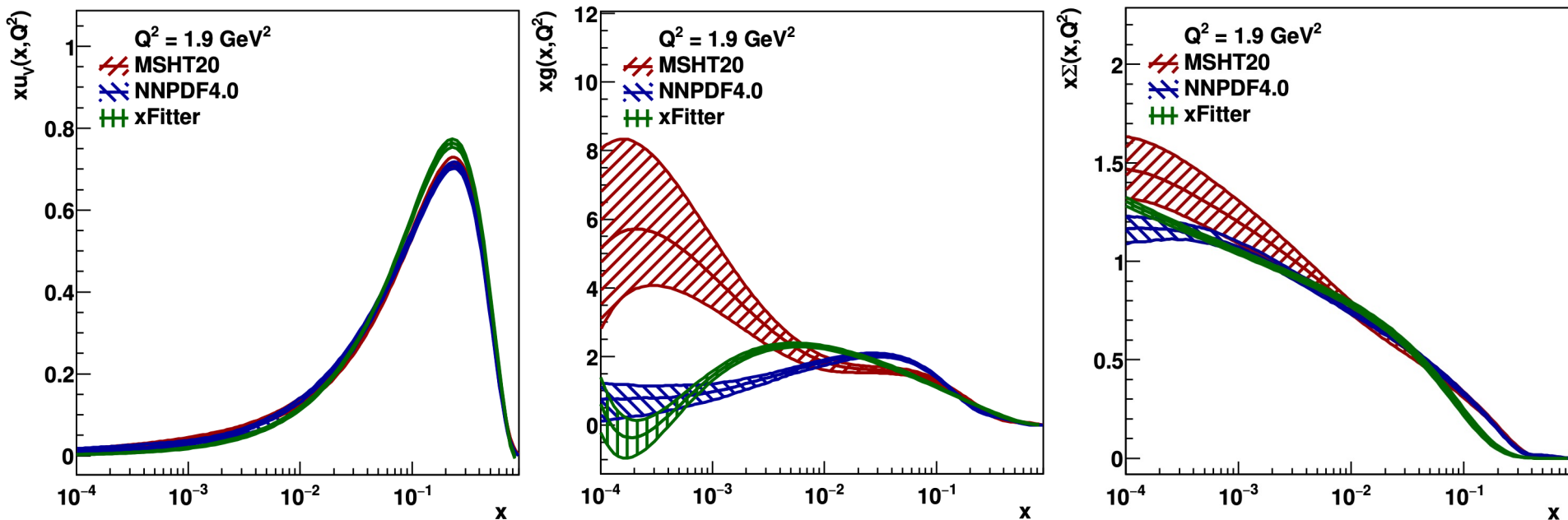
Heavy flavour uncertainties



- Use approximation of N³LO DIS massive coefficient function of gluon in heavy quark production (and uncertainties) from [2401.12139](#)
- Dominant uncertainty from NLL small- x approximation of exact coefficient function
- Extra uncertainties from numerical approximation of splitting functions (small)

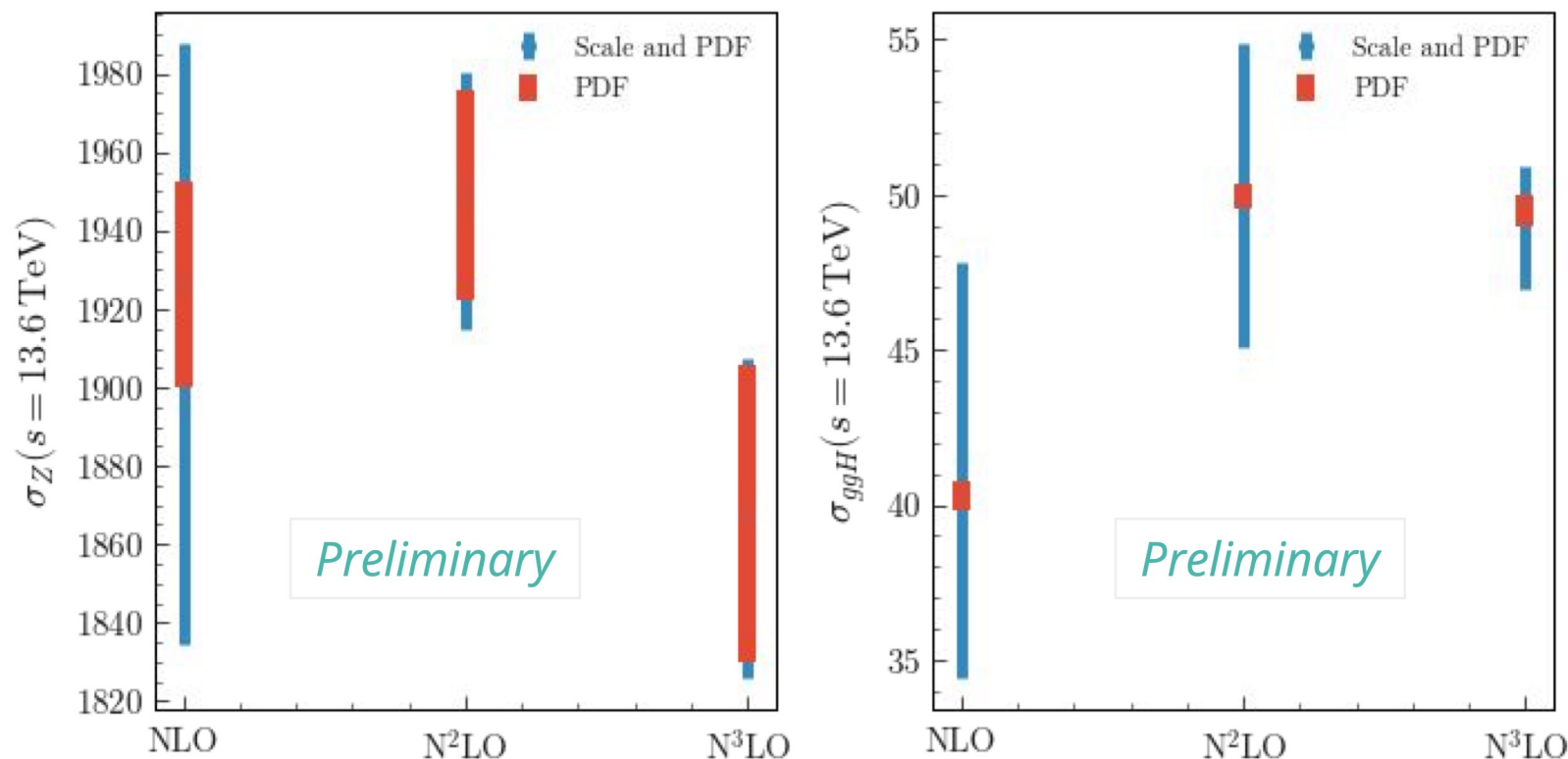
Parameter	Variation
Q_0^2	$1.9 \pm 0.2 \text{ GeV}^2$
Q_{min}^2	$3.5 \pm 1.0 \text{ GeV}^2$
m_c	$1.65 \pm 0.06 \text{ GeV}$
m_b	$4.50 \pm 0.25 \text{ GeV}$
f_s	0.40 ± 0.08

Comparison to other $\alpha\text{N}^3\text{LO}$ PDF



- Based on grids publicly available on LHAPDF
- Only Hessian uncertainty for xFitter
- The sets agree for $x u_v$
- $x g \rightarrow$ very different! MSHT outlier at low- x
- $x \Sigma \rightarrow$ much closer, xFitter below MSHT and NNPDF for $x > 0.1$

Impact on LHC predictions



- Predictions at NLO, NNLO and N³LO for **Z** (left) and **ggH** (right) production computed using **n3loxs** – [2209.06138](https://arxiv.org/abs/2209.06138)
- PDF uncertainties from N³LO include theory uncertainties
- Good convergence for H, not so good for Z

Emergence of resummation scale

- Applications of QCD to collider physics involve solution of Renormalisation Group Equations (RGEs) for α_s , PDF, etc.:

$$\frac{d \ln R}{d \ln \mu} = \Gamma(\alpha_s(\mu))$$

$$\Gamma(\alpha_s(\mu)) = \sum_{n=0}^k \Gamma_n \alpha_s^{n+1}(\mu)$$

- Difference between solutions which are formally equivalent at the nominal logarithmic accuracy but differ by sub-leading terms
 - **RGE theory uncertainties**
- RGEs can be solved either analytically or numerically
 - RGE theory uncertainties emerge in both cases
- Parametrized by changing $\mu \rightarrow \xi \mu$ in numerical solution
 - Varying ξ by factor 2, analogously to μ_R and μ_F uncertainties
- This is different from μ_R and μ_F dependence:
 - μ_R and μ_F dependence takes into account MHO in the hard scattering part
 - $\xi \mu$ takes into account MHO in RGE kernels for α_s and PDF evolutions

2202.03380

2407.20842

PDF fit with resummation scale

- PDF parametrisation and fit settings follow BG paper - [1902.11125](#)

Differences in the fit setup	Setup of Sect. 3 , same as [10]	New setup, same as [22]
heavy flavour scheme	TR	FONLL
initial scale μ_0	1.38 GeV	1.6 GeV
charm matching scale μ_c	m_c	1.12 m_c
charm mass m_c	1.43 GeV	1.46 GeV

[2609.35344](#)

- Inclusive HERA data, virtuality $Q_{\min}^2 > 3.5$ (10) GeV^2 , $Q_0 = 1.6$ (3.2) GeV
- NNLO, FONLL-C, $\alpha_s(m_Z) = 0.118$, $m_c = 1.46$ GeV , $m_b = 4.5$ GeV

$$xg(x) = A_g x^{B_g} (1-x)^{C_g} (1 + F_g \log(x) + G_g \log^2(x))$$

$$xu_v(x) = A_{u_v} x^{B_{u_v}} (1-x)^{C_{u_v}} (1 + E_{u_v} x^2 + F_{u_v} \log(x) + G_{u_v} \log^2(x))$$

$$xd_v(x) = A_{d_v} x^{B_{d_v}} (1-x)^{C_{d_v}}$$

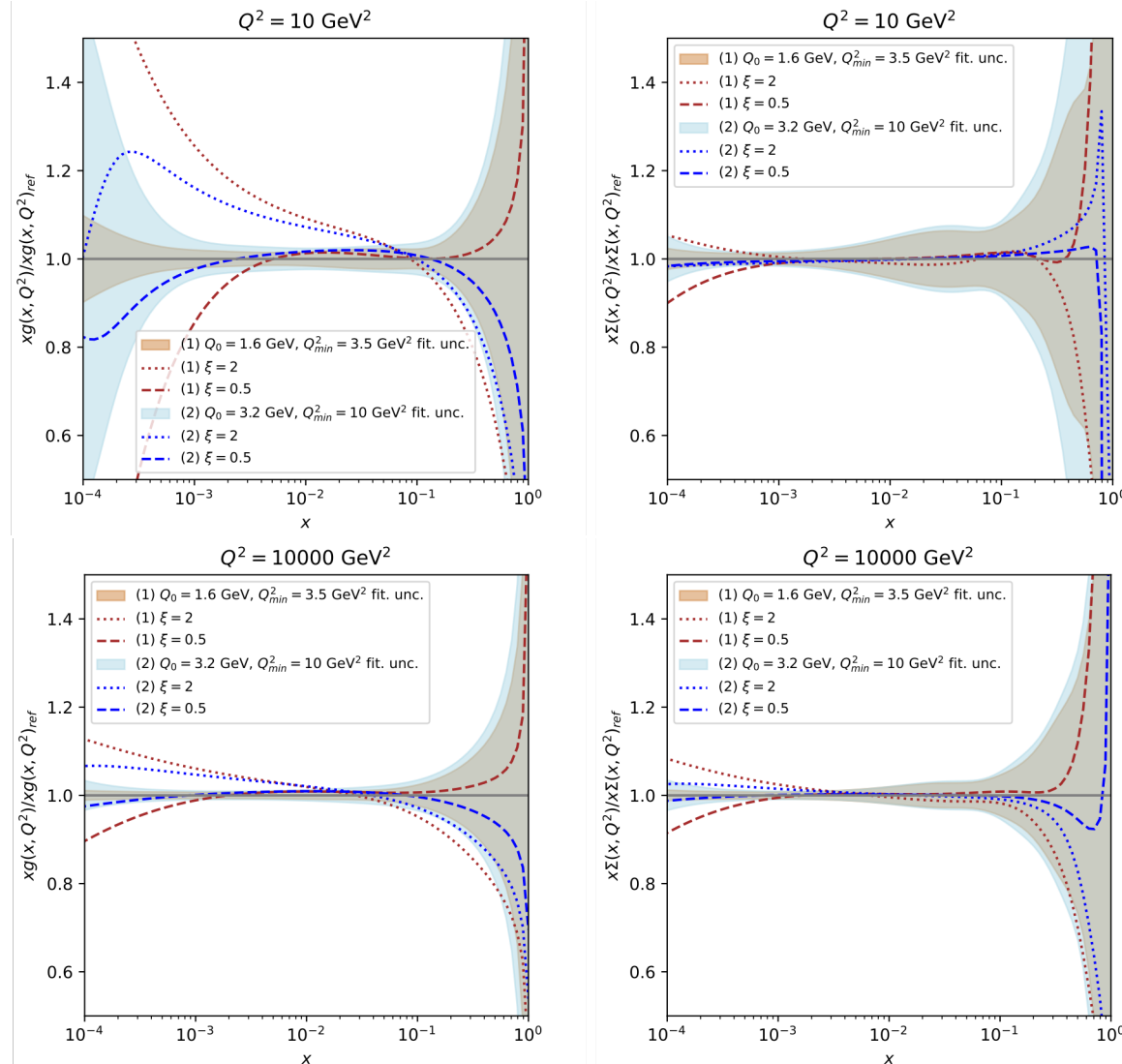
$$x\bar{U}(x) = A_{\bar{U}} x^{B_{\bar{U}}} (1-x)^{C_{\bar{U}}} (1 + D_{\bar{U}} x)$$

$$x\bar{D}(x) = A_{\bar{D}} x^{B_{\bar{D}}} (1-x)^{C_{\bar{D}}} (1 + D_{\bar{D}} x + F_{\bar{D}} \log(x))$$

- Provides **best description of HERA data at NNLO** ($\chi^2/\text{dof} = 1312/1127$ wrt $\chi^2/\text{dof} = 1388/1131$ using HERAPDF parametrisation)

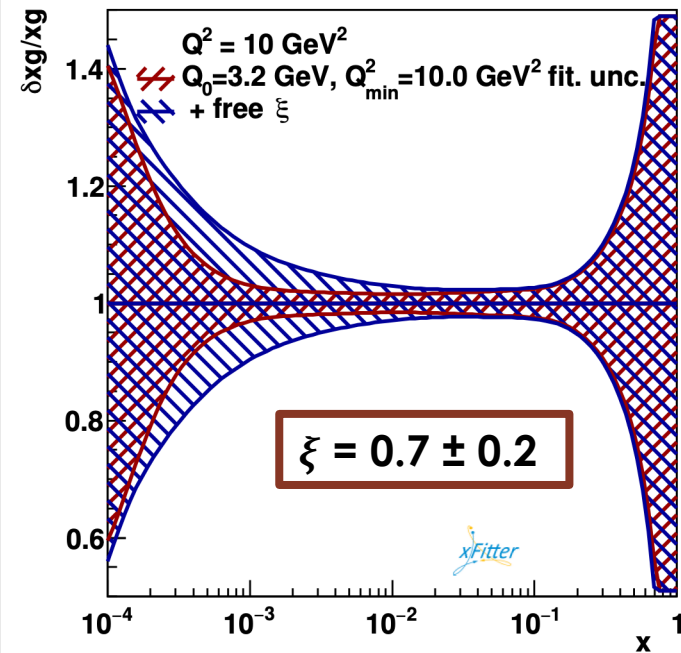
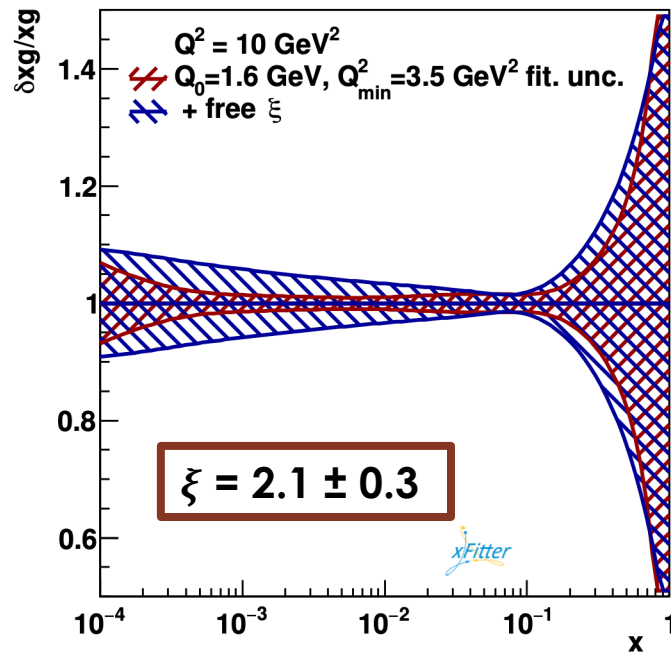
PDF fit with resummation scale

- Study the impact of resummation scale variations in a PDF fit using inclusive HERA data - $Q^2_{\min} = 3.5 \text{ GeV}^2$, $Q_0 = 1.6 \text{ GeV}$



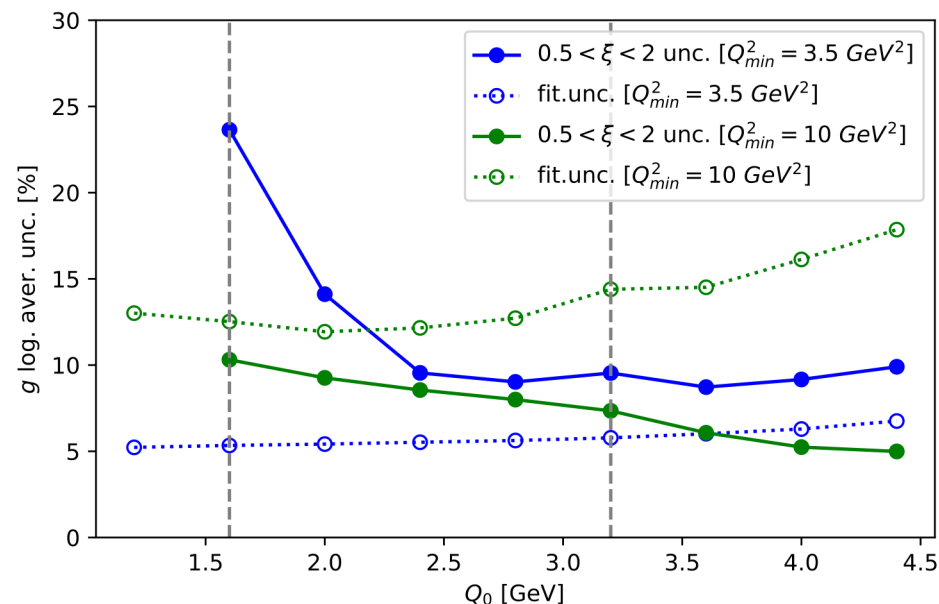
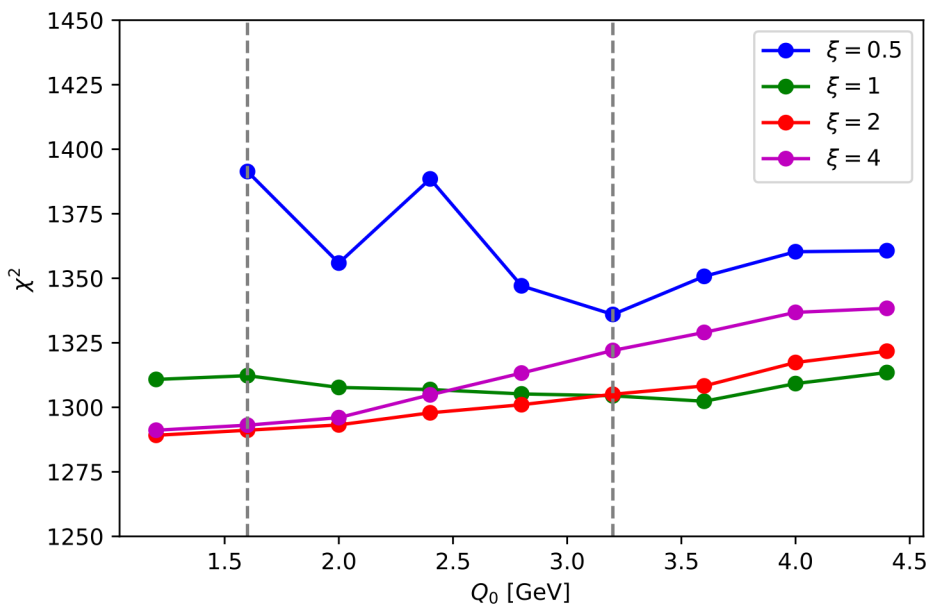
- Significant impact of ξ variations which exceeds experimental uncertainties
- Impact of ξ variations significantly reduced when increasing $Q^2_{\min} = 10 \text{ GeV}^2$
- Corresponding uncertainties are still there even when evolved to large scale $Q \sim 100 \text{ GeV}$
- Study with changing Q_0 and $Q^2_{\min}$ separately (backup)

Resummation scale as a free parameter



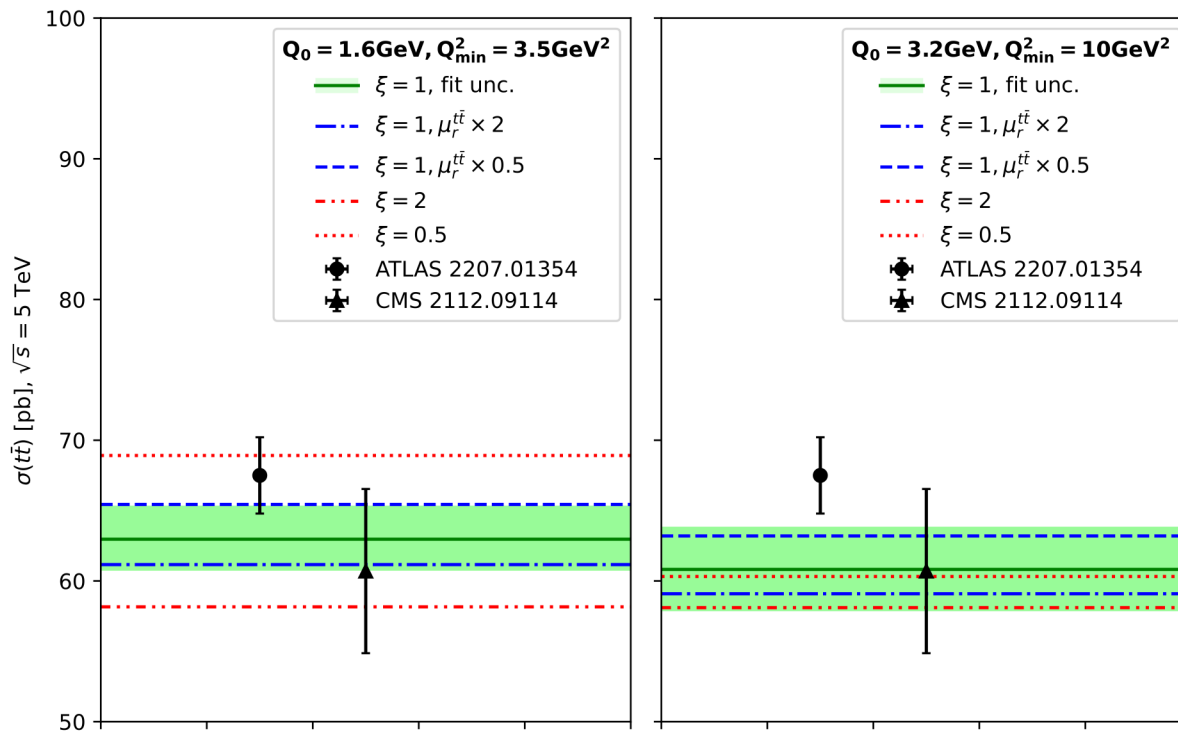
- ξ as a free parameter in the PDF fit - noticeable increase of PDF uncertainties
- The ranges of ξ constrained by the data appear to be much narrower than the conventional $0.5 < \xi < 2$ variation range
- The increase of the PDF uncertainties is generally smaller than the ones coming from the ξ variation
- Same qualitative effect is observed

PDF fit with resummation scale



- Varied starting scale $1.2 \leq Q_0 \leq 4.4 \text{ GeV}$
- The impact of ξ variation reduced for $Q_0 \gtrsim 3.0 \text{ GeV}$
- Choose **$Q_0 = 3.2 \text{ GeV}$** as **optimal starting scale**
- **$Q_{\min}^2 = 10 \text{ GeV}^2$** to avoid low-momentum-transfer data
- With higher cut on virtuality, uncertainties due to ξ variation reduced

PDF fit with resummation scale



- $t\bar{t}$ cross section at 13 TeV computed at NNLO using [Hathor](#)
- **~5% effect:** comparable to experimental uncertainties and $t\bar{t}$ scale variations
- **Reduced to < 1%** if $Q_0 = 3.2 \text{ GeV}, Q_{\min}^2 = 10 \text{ GeV}^2$ is used
- Very similar observation for $t\bar{t}$ cross section at 5 and 100 TeV (backup)

Summary and outlook

- **DIS-only analysis** with **consistent N³LO** for the PDF evolution and coefficient functions
- **First analysis including exact matching conditions**
- **Visible impact on PDF** (i.e. largest gluon at small-x) and predictions for the LHC phenomenology
- Further studies including small-x resummation ongoing! ☺
- First study about the **inclusion of resummation scale variations in a PDF fit**
- **Large impact on the gluon PDF** in the low-x region
- **Visible effect** on observables i.e. $t\bar{t}$ cross section
- These uncertainties can be reduced by avoiding low momentum transfer region → **requires increasing both Q_0 and $Q^2_{\min}$ cut**



Backup Slides



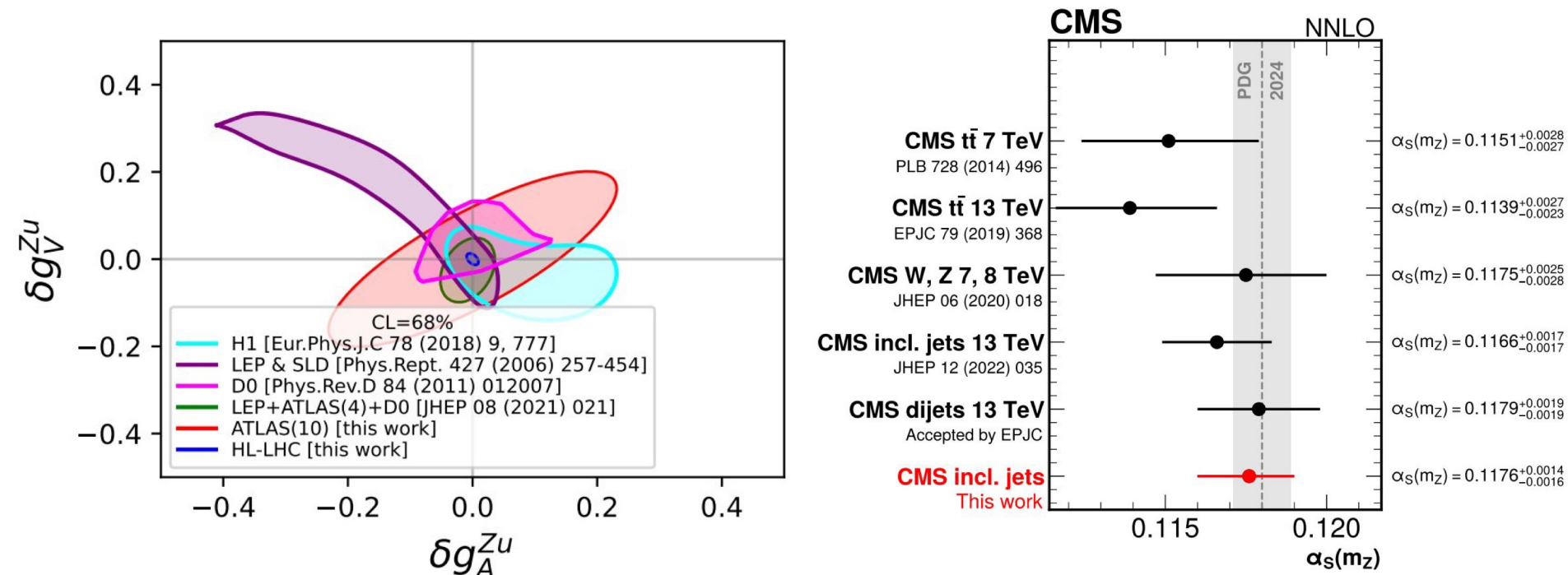
Status of the xFitter project

- Project is in active development on [Gitlab](#)
- Stable release 2.2.0 ("Future freeze") – extensive Wiki [here](#)
- Nightly master branch built and validated vs several public results
- Nightly docker image

```
docker run -it gitlab-registry.cern.ch/fitters/xfitter:master bash
```

- Many updates of the functionality and productivity
- Added interfaces to **Ploughshare**, **Hoppet**, **PineAPPL**, **CIJET**
- Added **N³LO FONLL for APFEL++**, updates of DYTurbo interface
- Numerical improvements: parallel derivatives in CERES, parallel profiling, parallel asymmetric Hessian uncertainties evaluation (based on J. Pumplin [hep-ph:0101032](#))

Results using xFitter from the last year

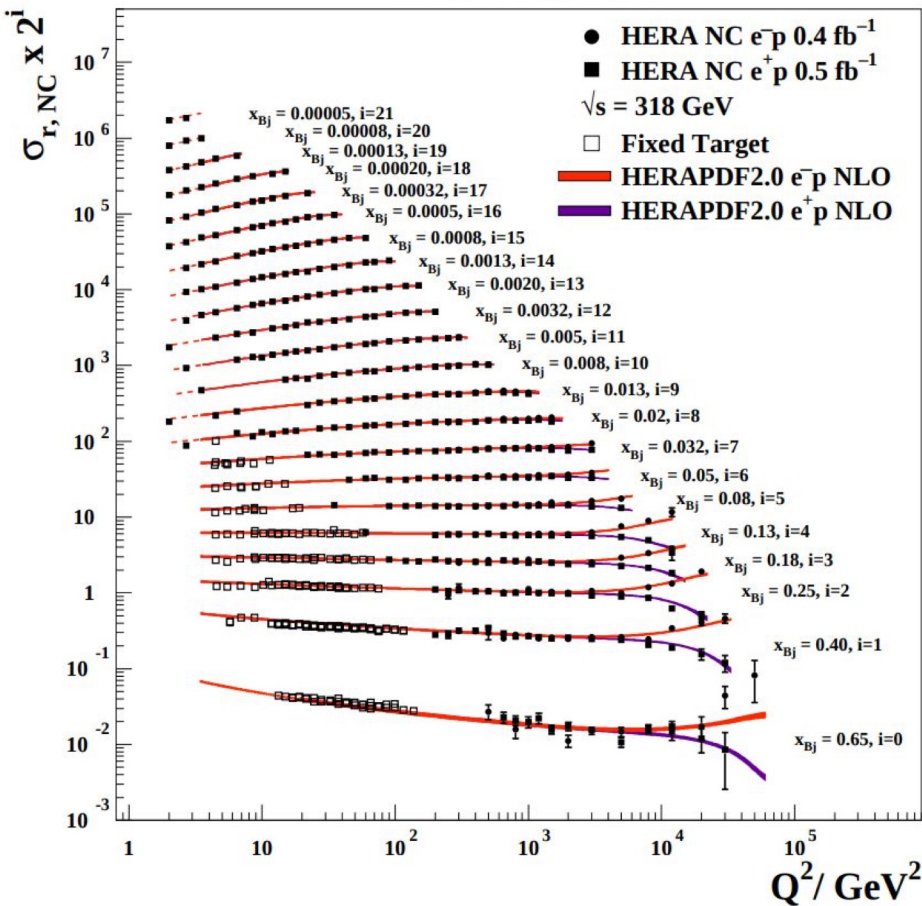


- Many analyses using xFitter last year
- SMEFT analysis of Z boson couplings using forward-backward DY production at LHC - [2310.19638](#)
- CMS analysis of inclusive jet production cross section to extract α_s - [2412.16665](#)

PDF determination using HERA data

1506.06042

H1 and ZEUS



$$\frac{d^2\sigma_{e^\mp p}^{NC}}{dx dQ^2} = \frac{2\pi\alpha^2 Y_+}{xQ^4} \left(F_2 - \frac{y^2}{Y_+} F_L \pm \frac{Y_-}{Y_+} x F_3 \right)$$

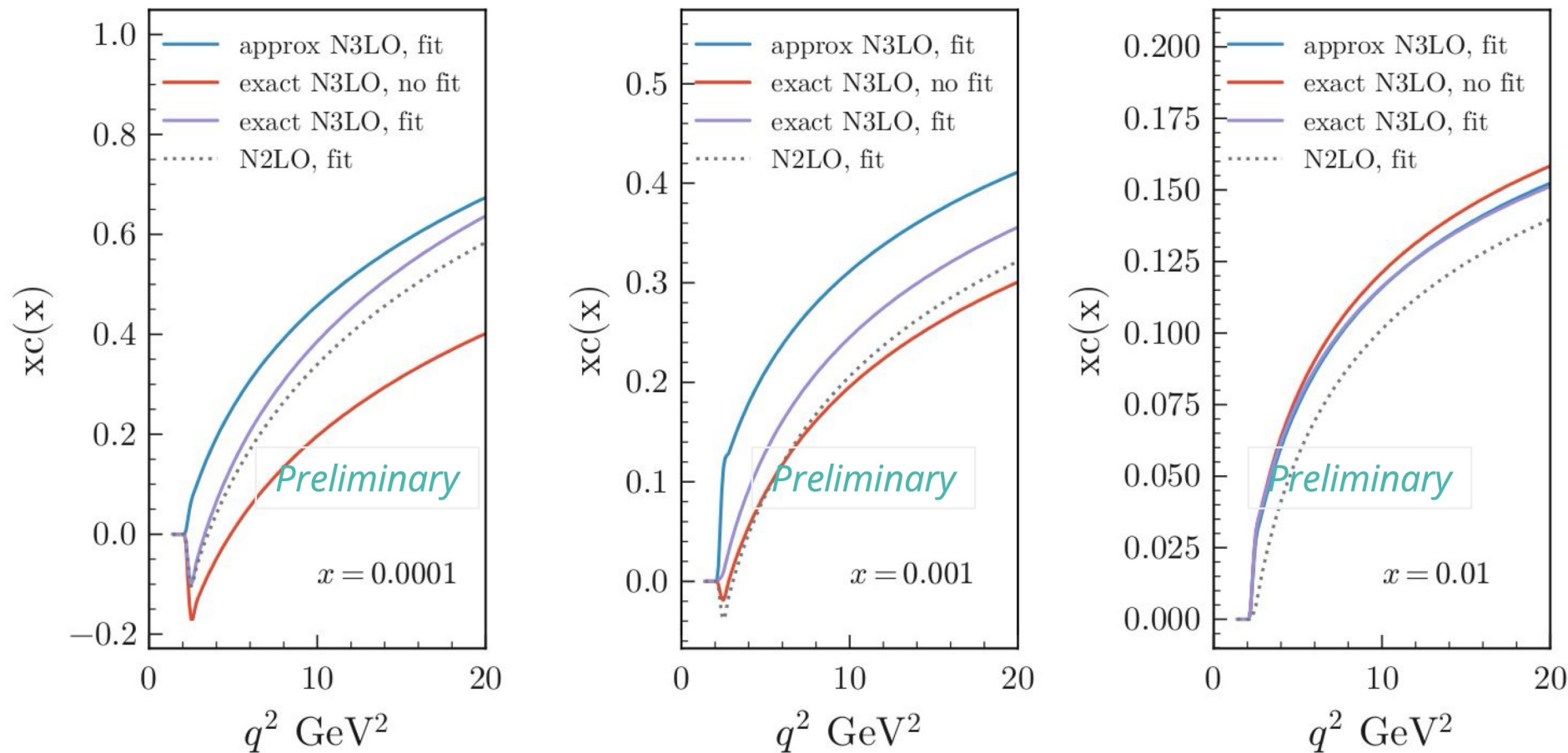
$$Y_{\pm} = 1 \pm (1-y)^2$$

$$F_2 = x \sum e_q^2 (q(x) + \bar{q}(x))$$

$$xF_3 = x \sum 2e_q a_q (q(x) - \bar{q}(x))$$

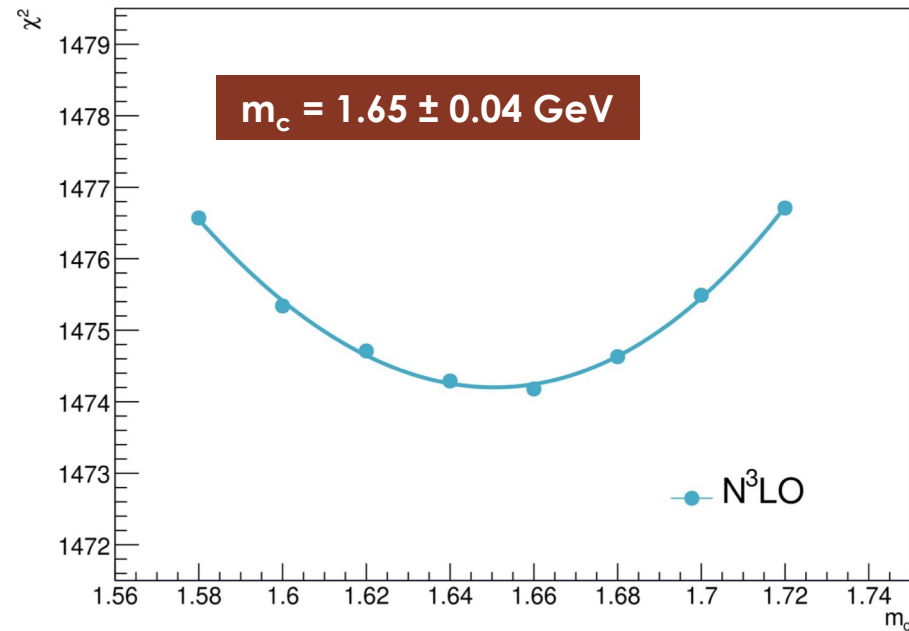
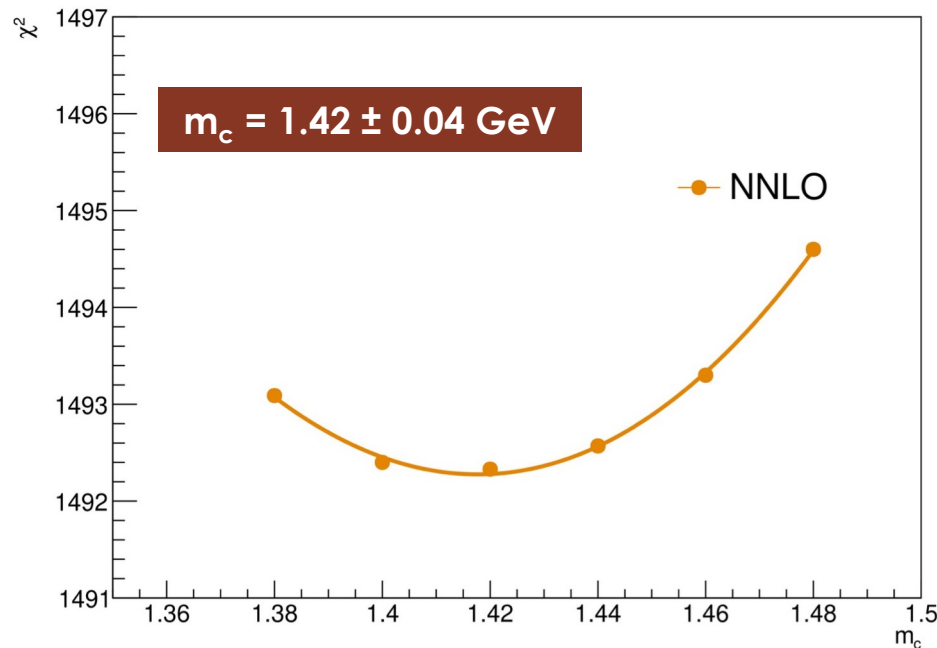
- At HERA γ exchange dominates, the best PDF determined is xu_v
- At low- x , contribution of xc is sizeable too (up to 30% of F_2)
- Gluon is measured from q^2 dependence of the structure function F_2
- Lower accuracy at high- x , xu_v and xd_v , separated using charged-current data

Effect of the matching conditions on charm



- Evaluate $\sigma_C(x)$ vs Q^2 at different Bjorken- x values
- Compare results from fits using exact N³LO and aN³LO matching schemes (and NNLO fits) - **significant differences at low- x visible**

Charm mass scan



- **Huge dependency on the fit order**
- Pole mass affected by renormalon instability → expected to be larger by 0.22 GeV at N^3 LO – [1612.03790](#)
- Larger gluon PDF → splitting in $c\bar{c}$ at higher scale → compensation with a bigger m_c (perturbative charm)
- Corrections to DIS massive coefficient functions still approximate – work in progress by Barontini, Bonvini and Laurenti

Resummation uncertainties scaling

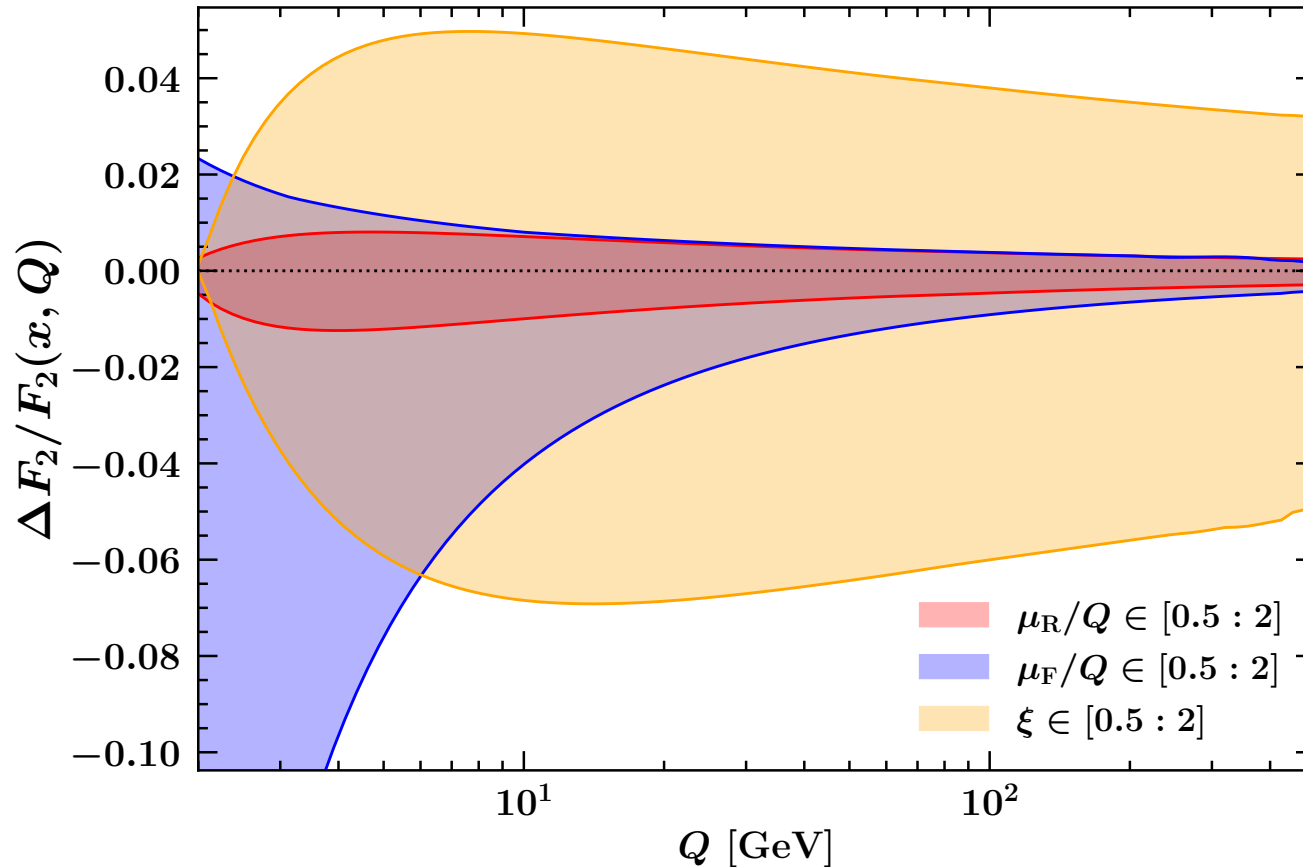
- How do resummation-scale uncertainties scale? At NLL for PDF:

$$\Delta f(\mu, \xi) = f(\mu, \xi) - f(\mu, 1) = [\alpha_s^2(\mu) - \alpha_s^2(\mu_0)] \ln \xi \left(\gamma_1 + \gamma_0 \frac{\beta_1}{2\beta_0} - \frac{1}{2} \beta_0 \gamma_0 \ln \xi \right) f(\mu) + \mathcal{O}(\alpha_s^3)$$

- Very distinctive behaviour
- Δf is $\mathcal{O}(\alpha_s^2)$ without any large logs i.e. it is a purely NNLO effect → **subleading**
- Proportional to **$\ln \xi$**
- For $\mu \sim \mu_0$, Δf is small **no matter the value ξ** (proportional to $\alpha_s^2(\mu) - \alpha_s^2(\mu_0)$)
- General scaling at N^kLL: $\alpha_s^{k+1}(\mu) - \alpha_s^{k+1}(\mu_0)$
- For $\mu \gg \mu_0$, Δf is **dominated by $\alpha_s(\mu_0)$**
- Resummation scale uncertainties scale fundamentally **differently from $\mu_{R,F}$ uncertainties** that at N^kLO scale as $\alpha_s^{k+1}(\mu_{R,F})$

F_2 uncertainty scaling

NLO, $x = 0.01$

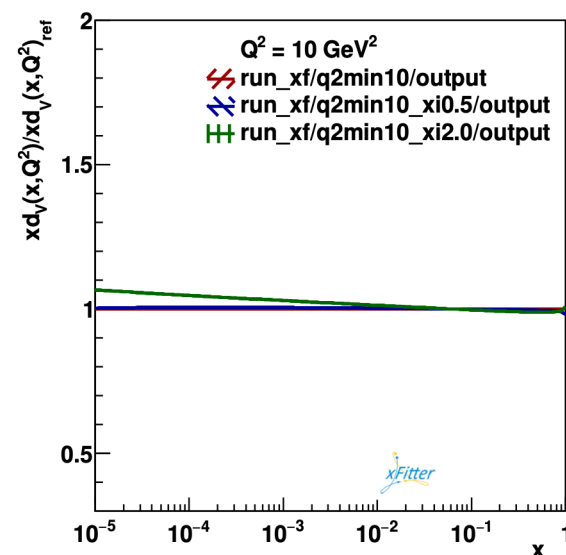
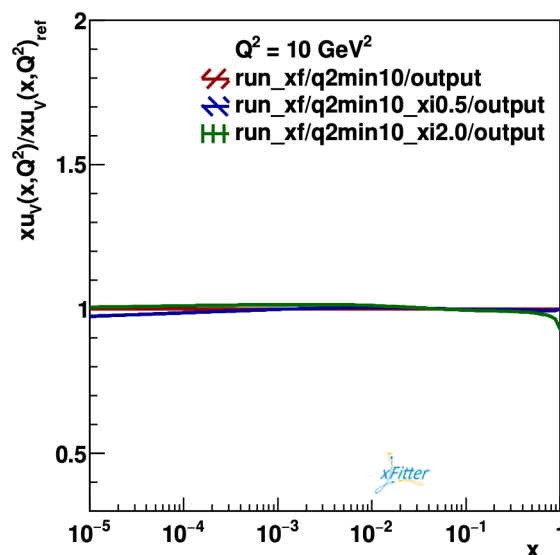
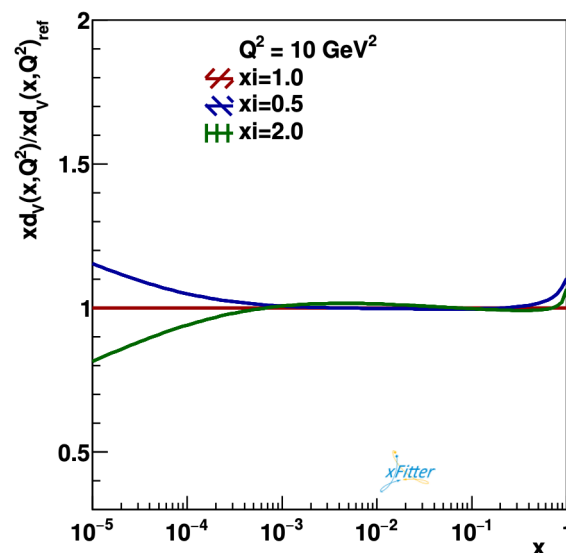
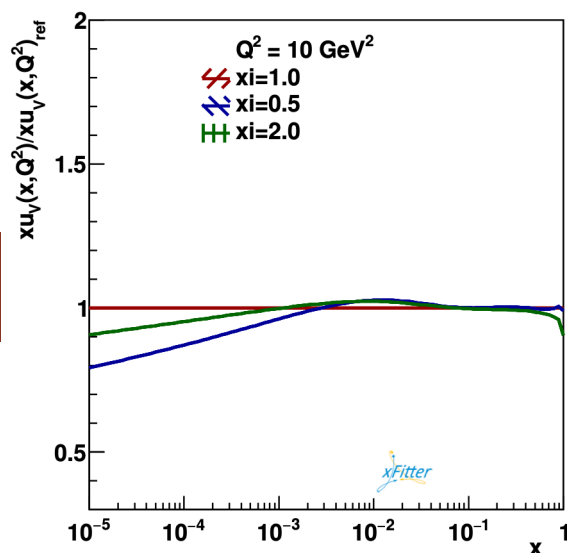


- μ_R and μ_F uncertainties decrease as the scale grows
- Resummation scale uncertainties tends to grow at large scales
- Important to account for resummation scale uncertainties in PDF fits

PDF fit with resummation scale

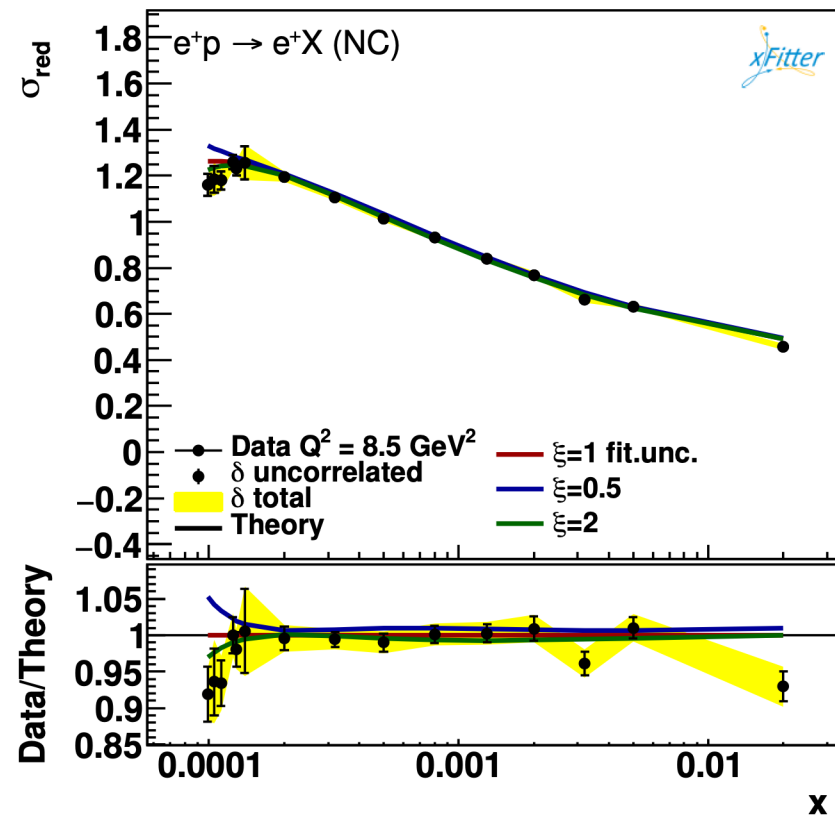
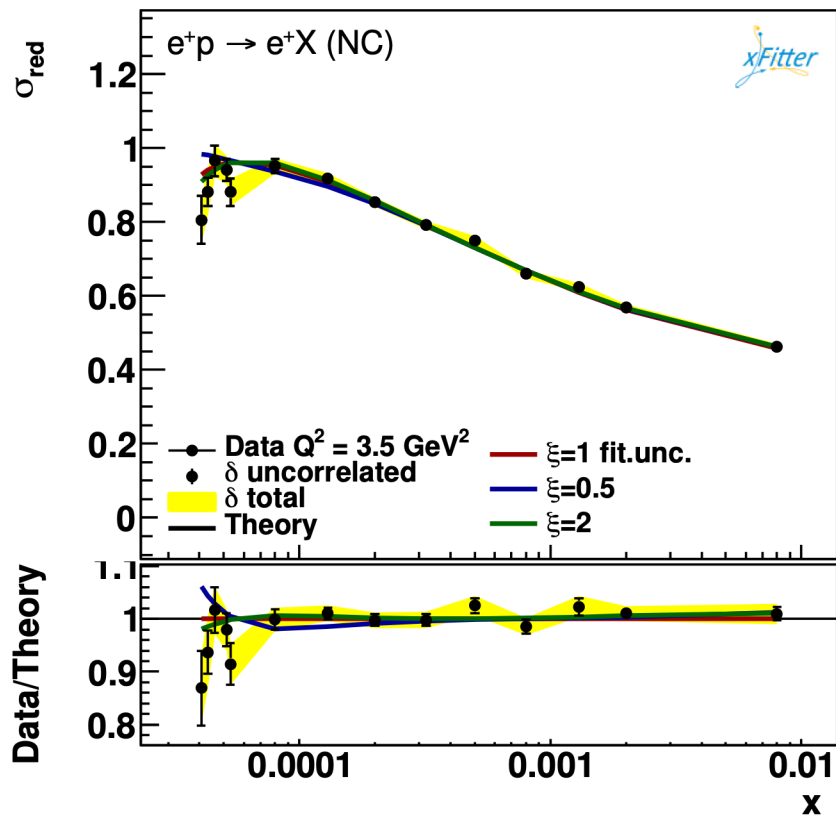
- The impact of resummation scale variations in a PDF fit on valence is tiny

$$Q_0 = 1.6 \text{ GeV},$$

$$Q_{\min}^2 = 10 \text{ GeV}^2$$

$$Q_0 = 3.2 \text{ GeV},$$

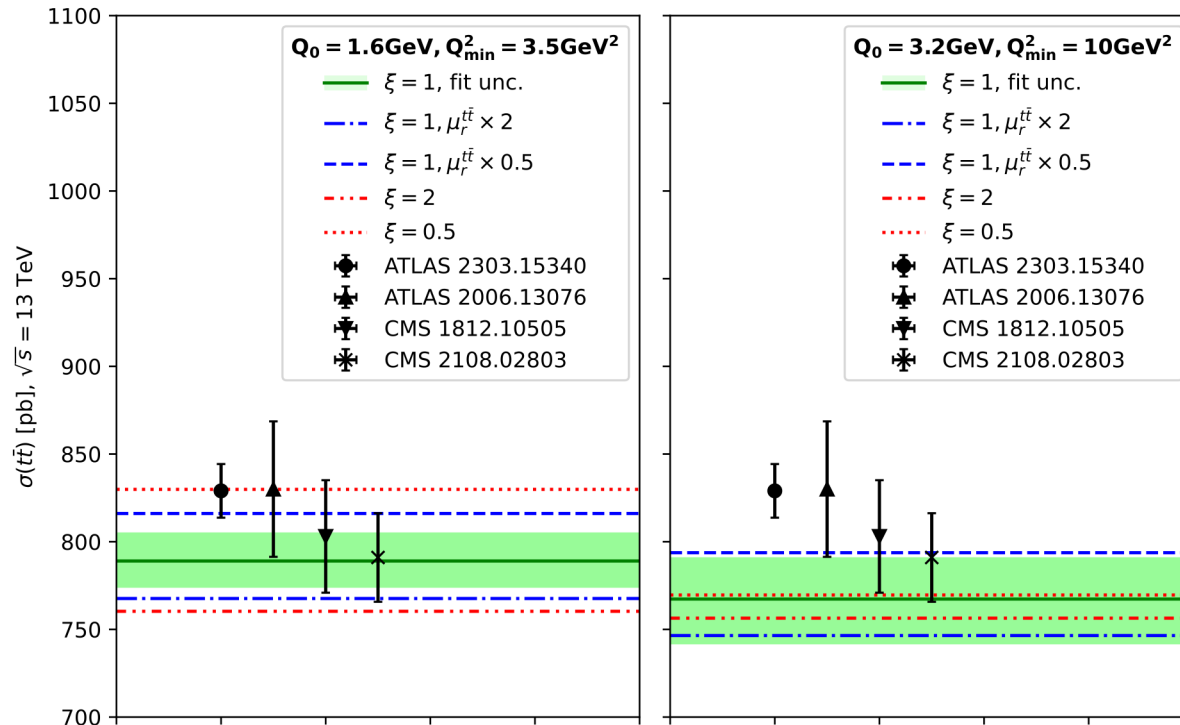
$$Q_{\min}^2 = 10 \text{ GeV}^2$$

PDF fit with resummation scale



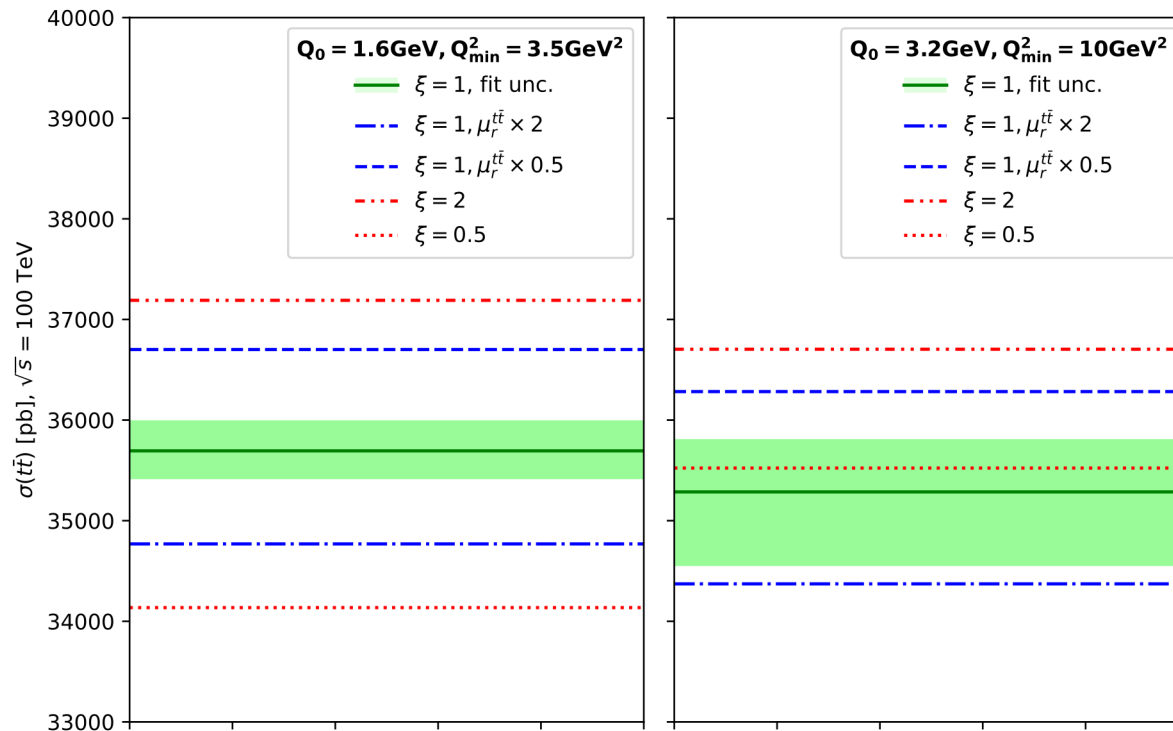
- $Q_0 = 1.6 \text{ GeV}$, $Q^2_{\text{min}} = 3.5 \text{ GeV}^2$
- Largest differences at lowest Q^2 , x

PDF fit with resummation scale



- $t\bar{t}$ cross section at 5 TeV computed at NNLO using [Hathor](#)
- Reduction in the resummation scale uncertainty is more pronounced
- At lower $\sqrt{s}$, top-quark pair production sensitive to higher Bjorken x
- Region non directly constrained by HERA, but by PDF extrapolation i.e. momentum sum rules

PDF fit with resummation scale



- $t\bar{t}$ cross section at 100 TeV computed at NNLO using [Hathor](#)
- Uncertainty associated with the resummation procedure constitutes an additional source of theoretical uncertainty even at FCC
- In the improved PDF fit setup with $Q_0 = 3.2 \text{ GeV}$, $Q_{\min}^2 = 10 \text{ GeV}^2$, uncertainty reduced to $\sim 1\%$ $\rightarrow$ sensitivity suppressed, while preserving the benefits of threshold resummation