N^3LO PDF fits to DIS data in xFitter

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

REF 2025 (Milan, IT)
13/10/2025

Università di Roma Tor Vergata

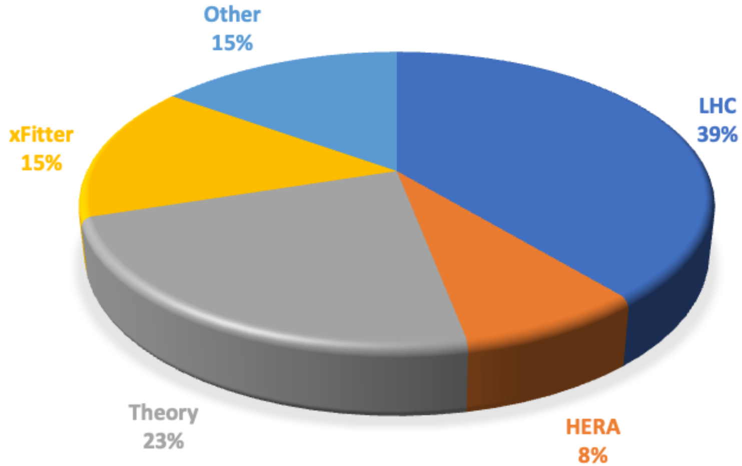
Istituto Nazionale di Fisica Nucleare

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

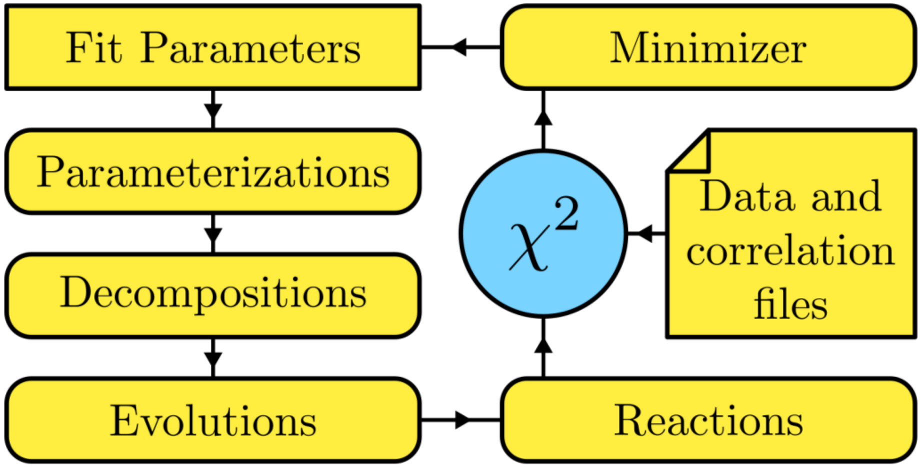
- More than 100 publications obtained using xFitter since the beginning of the project

- List of recent analyses by the xFitter Developers' Team:
  - SMEFT analysis of Z boson couplings using forward-backward DY production at LHC - EPJC 84 (2024) 1277

MORE IN PREPARATION!

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 N^{3}LO

- HERAPDF2.0 parametrization - 1506.06042:

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

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

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

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

- Alternative gluon parametrization (Bonvini-Giuli) - 1902.11125:

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

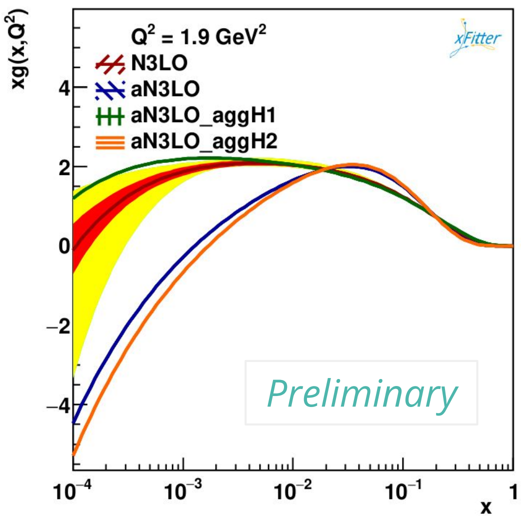
- HERA I+II inclusive and $F_{2,c}$ + $F_{2,b}$ data (1804.01019)

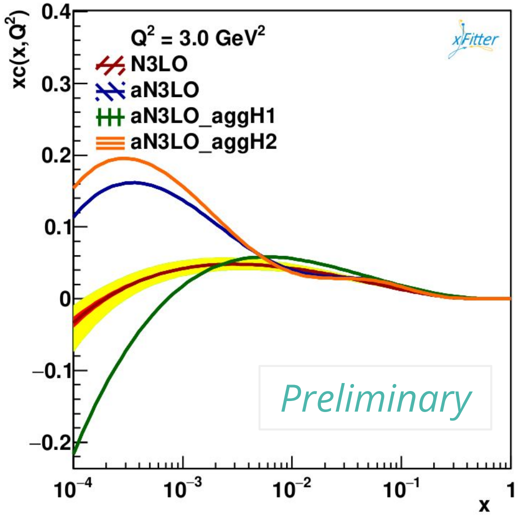
- N^{3}LO evolution implemented in APFEL (1708.00911) – based on HOPPET (0804.3755)

- **Exact** (2311.00644, 2403.00513, 2509.16124, 2510.02175, QCD@LHC talk) and **approximate** N^{3}LO matching conditions implemented in APFEL++ (2404.15711)

- FONLL VFNS implemented in xFitter, checked with fortran APFEL at NNLO

Extact vs approximate N³LO





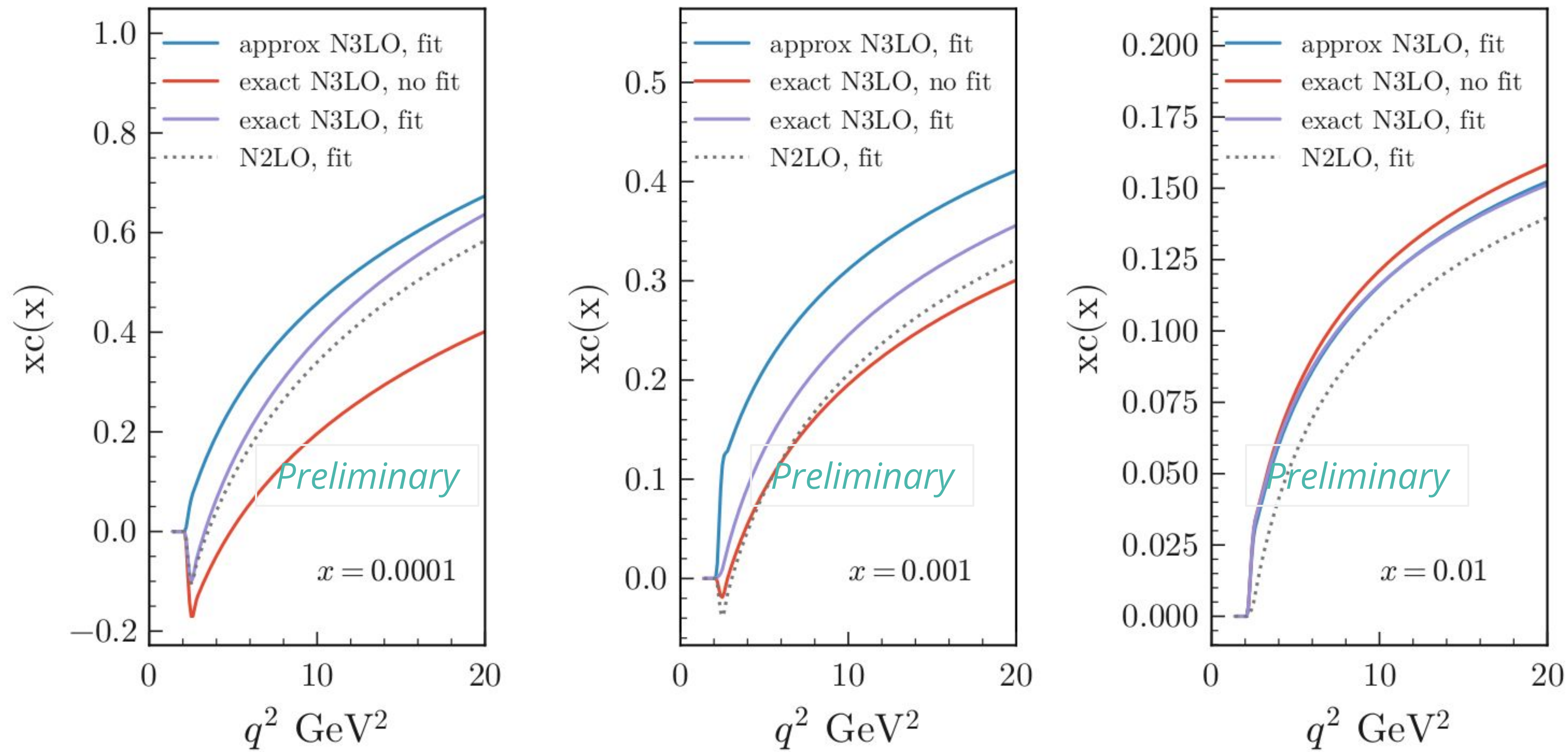
Preliminary

Dataset	N3LO	aN3LO
HERA1+2 NCep 820	66 / 70	68 / 70
HERA1+2 NCep 460	222 / 204	215 / 204
HERA1+2 CCep	48 / 39	48 / 39
HERA1+2 NCem	224 / 159	223 / 159
HERA1+2 CCem	59 / 42	61 / 42
HERA1+2 NCep 575	215 / 254	215 / 254
HERA1+2 NCep 920	471 / 377	476 / 377
Correlated χ^2	106	103
Log penalty χ^2	+9.9	+14
Total χ^2 / dof	1422 / 1131	1422 / 1131

- Fit using **exact N³LO** matching conditions with experimental+model uncertainties
- Large difference wrt aN³LO for xc and xg
- Within uncertainties of aN³LO
- **Fit quality** to the data is **about the same**

Parameter	Variation
Q_0^2	1.9 ± 0.2 GeV²
Q_{min}^2	3.5 ± 1.0 GeV²
m_c	1.47 ± 0.06 GeV
m_b	4.50 ± 0.25 GeV
f_s	0.40 ± 0.08

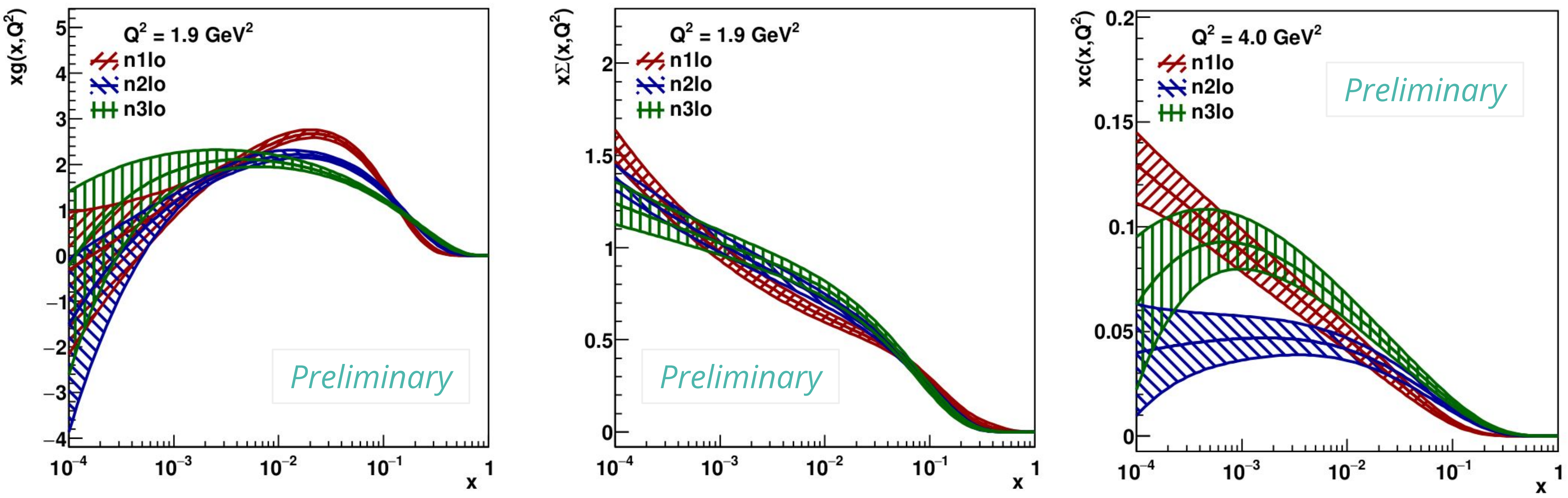
Effect of the matching conditions on charm



- Evaluate xc(x) vs Q^2 at different Bjorken-x values

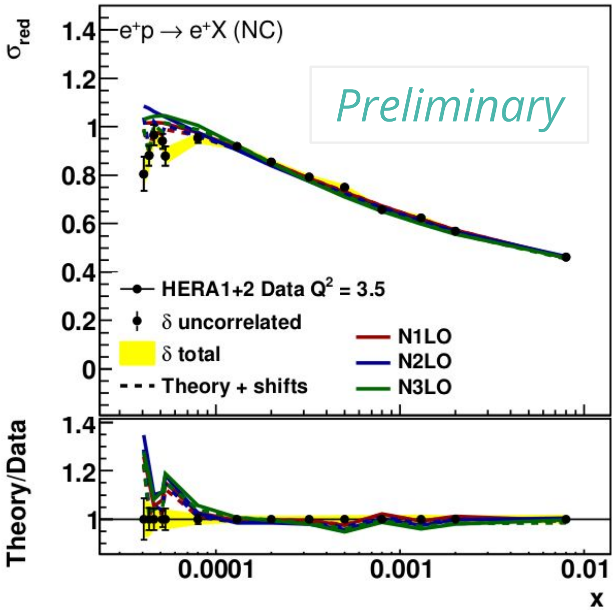
- Compare results from fits using exact N^3LO and aN^3LO matching schemes (and NNLO fits) - **significant differences at low-x visible**

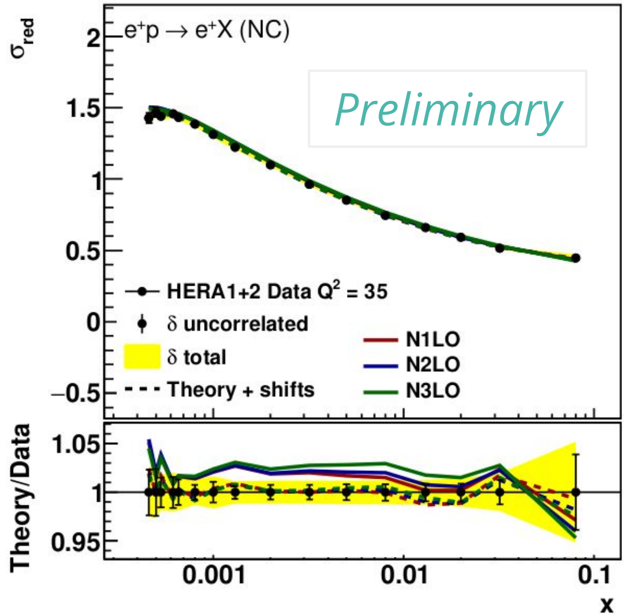
N^3LO vs NNLO vs NLO with exact matching



- Gluon (left), total singlet (middle) and charm (right)
- Fits with alternative gluon parametrisation consistent with HERAPDF style
- N^3LO gluon is the hardest, also largest at small-x
- For $x \geq 0.01$ all orders agree

Comparison to $\sqrt{s}$ = 920 GeV data





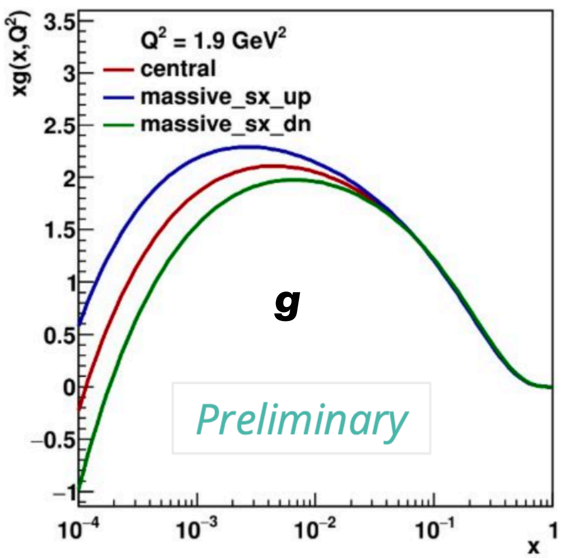
- All fixed-order fits do not described data very well at lowest x/highest inelasticity
- N^{3}LO improving slightly wrt NNLO (low-x)
- Small-x resummation needed - 1802.00064

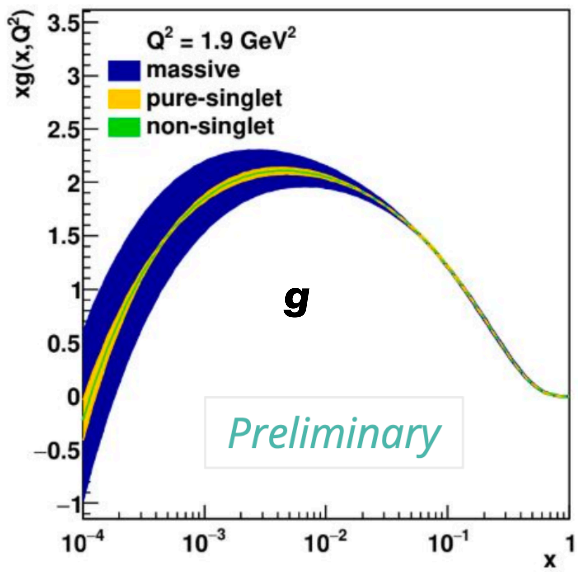
- At intermediate Q^2, N^{3}LO is further above the data
- This drives the increase in χ^2 correlated term

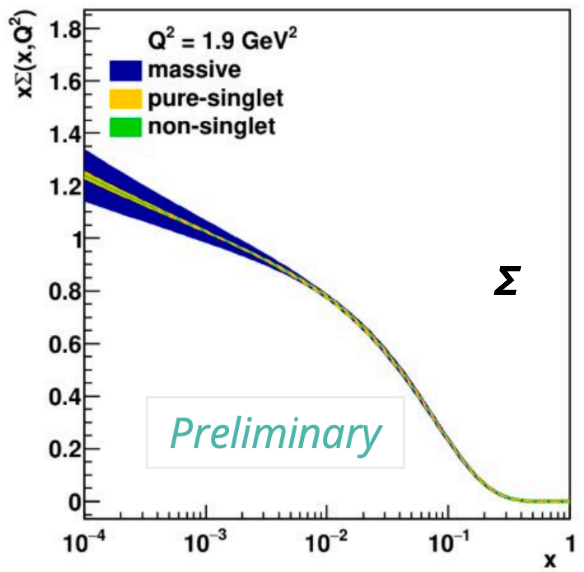
Preliminary

Dataset	N1LO	N2LO	N3LO
HERA1+2 NCep 820	69 / 70	68 / 70	66 / 70
HERA1+2 NCep 460	217 / 204	218 / 204	222 / 204
HERA1+2 CCep	44 / 39	43 / 39	45 / 39
HERA1+2 NCem	213 / 159	217 / 159	226 / 159
HERA1+2 CCem	63 / 42	58 / 42	57 / 42
HERA1+2 NCep 575	215 / 254	221 / 254	216 / 254
HERA1+2 NCep 920	427 / 377	456 / 377	472 / 377
Correlated χ^2	76	95	104
Log penalty χ^2	+8.7	+9.7	+6.2
Total χ^2 / dof	1333 / 1132	1385 / 1132	1414 / 1132

Heavy flavour uncertainties

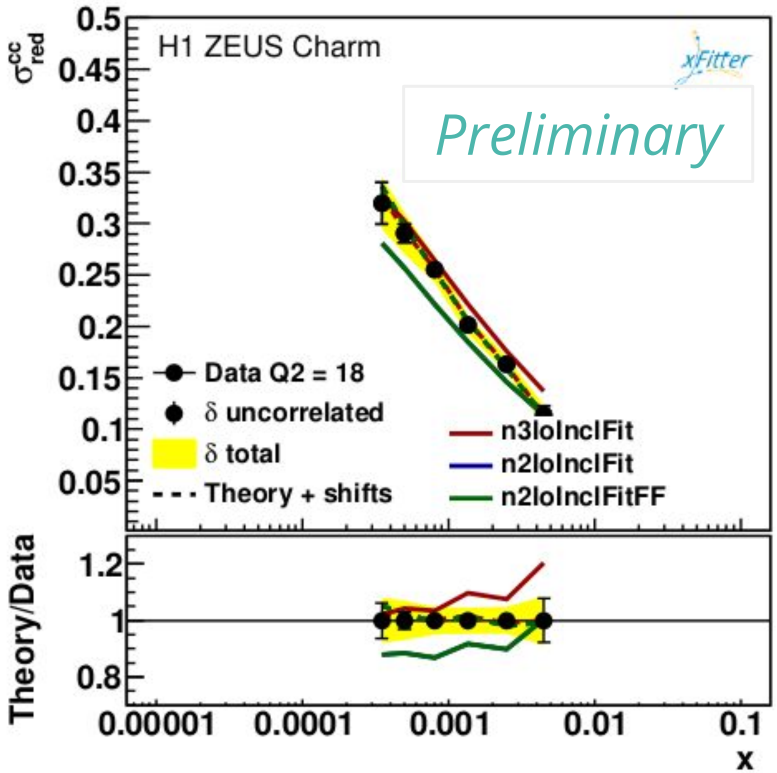






- Use approximation of N^{3}LO DIS massive coefficient function of gluon in heavy quark production (and uncertainties) from 2401.12139
- Dominant uncertainty from NLL small-x approximation of exact coefficient function
- Extra uncertainties from numerical approximation of splitting functions (small)

$F_{2,c}$ predictions



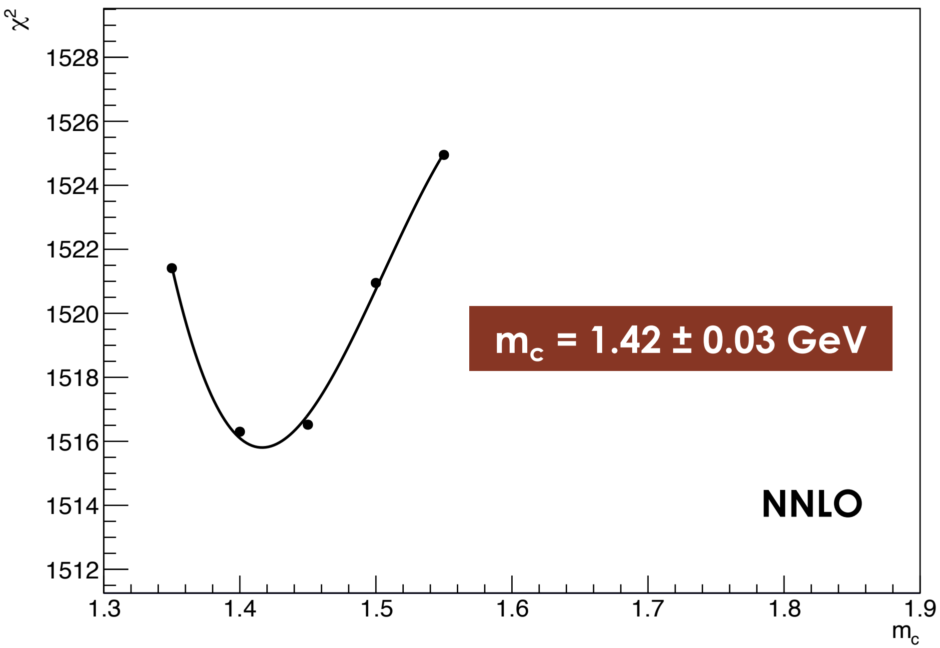
Preliminary

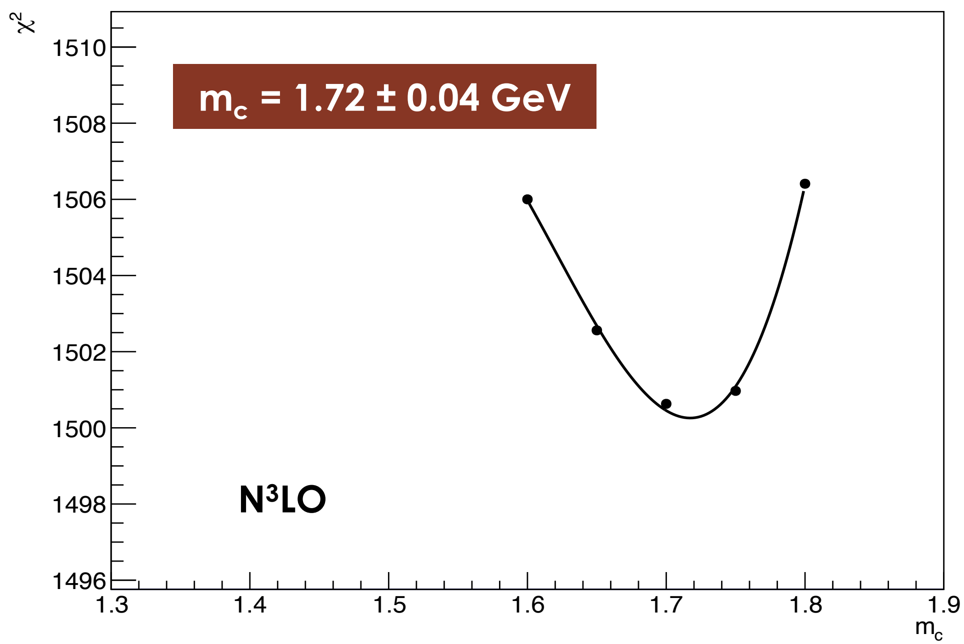
Dataset	N^3LO	N^2LO	N^2LO(fortranAPFEL)
HERA c	41 / 47	50 / 47	50 / 47
HERA b	15 / 26	20 / 26	20 / 26
Correlated χ^2	43	61	61
Log penalty χ^2	+8.6	-5.35	-5.34
Total χ^2 / dof	108 / 59	125 / 59	125 / 59
χ^2 p-value	0.00	0.00	0.00

- Compare predictions of the NNLO and N^3LO fit to the inclusive HERA I+II data only vs charm form combined H1/ZEUS analysis - 1804.01019

- Better χ^2/dof for the N^3LO fit

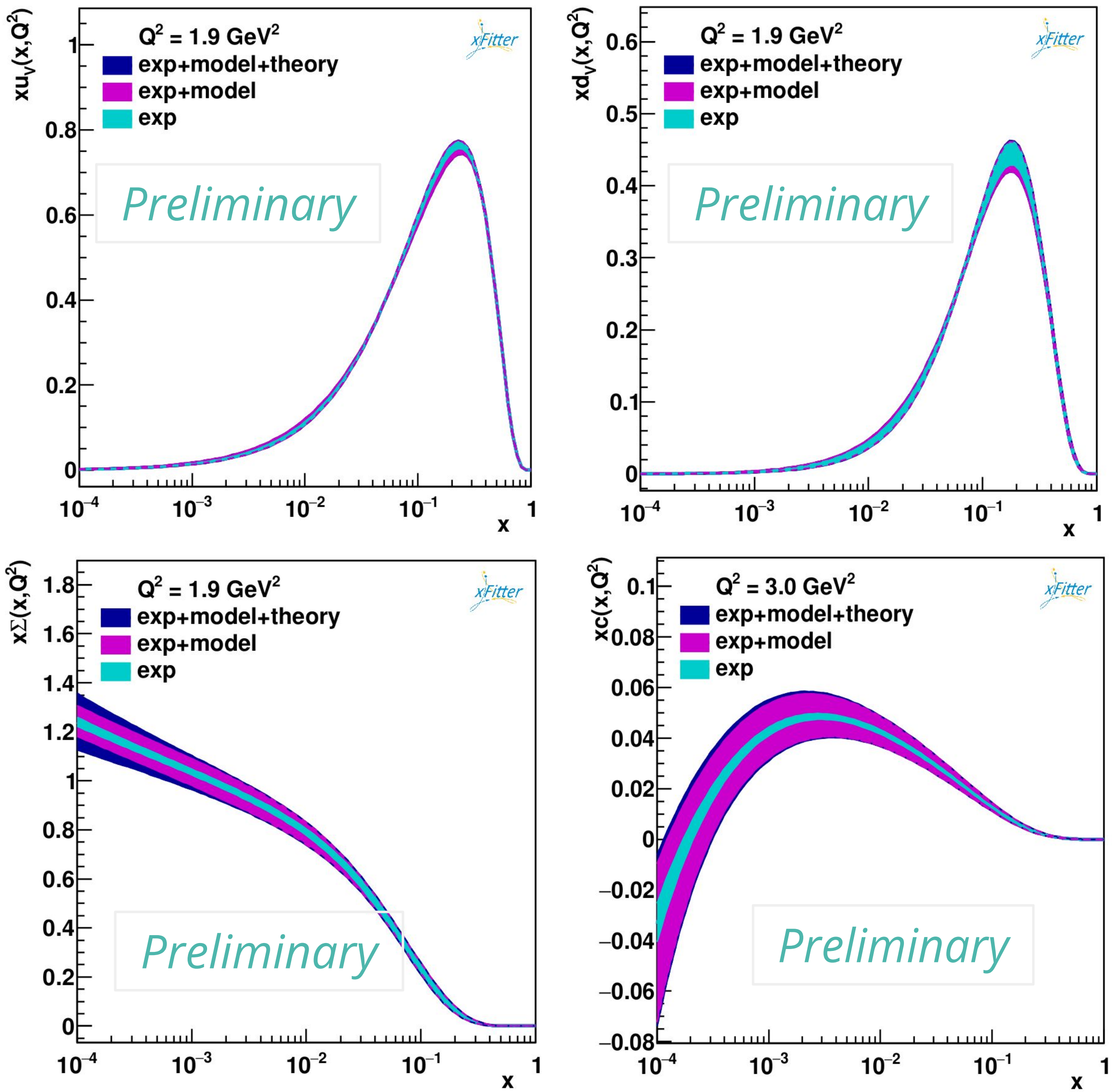
Charm mass scan





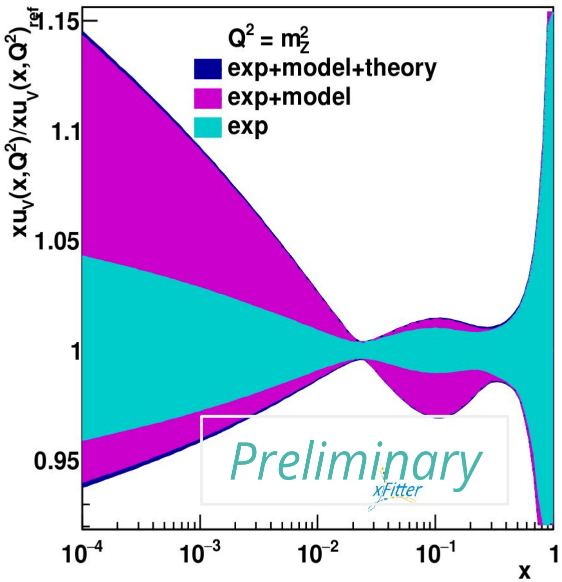
- **Huge dependency on the fit order**
- Pole mass affected by renormalon instability → expected to be larger by 0.22 GeV at N^3LO – 1612.03790
- Larger gluon PDF → splitting in $c\bar{c}$ at higher scale → compensation with a bigger m_c (perturbative charm)
- Corrections to DIS massive coefficient functions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

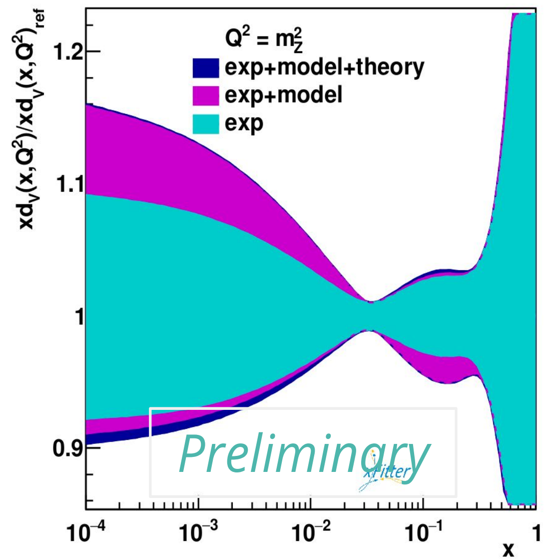
N^{3}LO PDF with full uncertainties

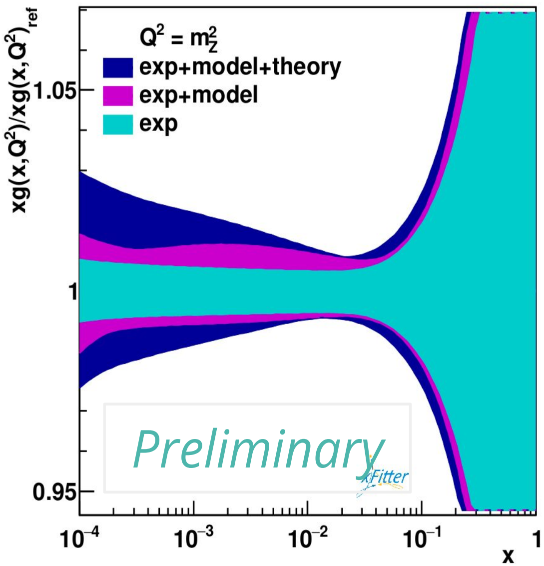


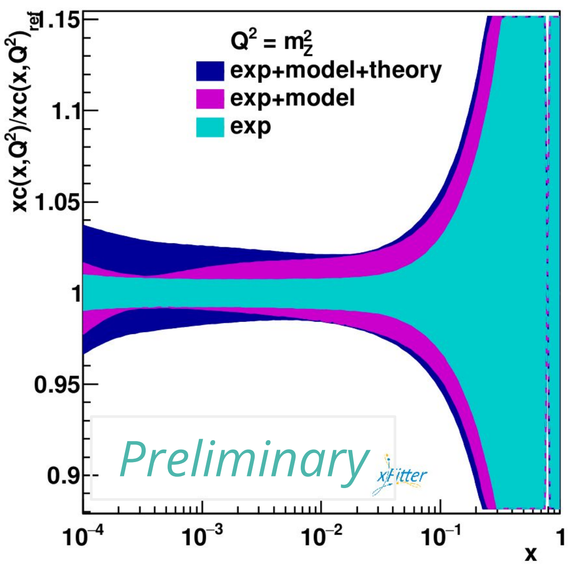
- PDF obtained for N^{3}LO fit, including model + theory uncertainties
- Leading model uncertainty: m_c variation

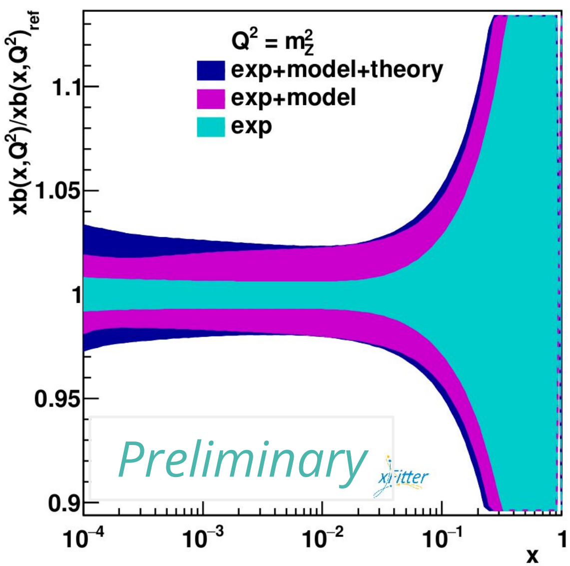
N³LO PDF with full uncertainties





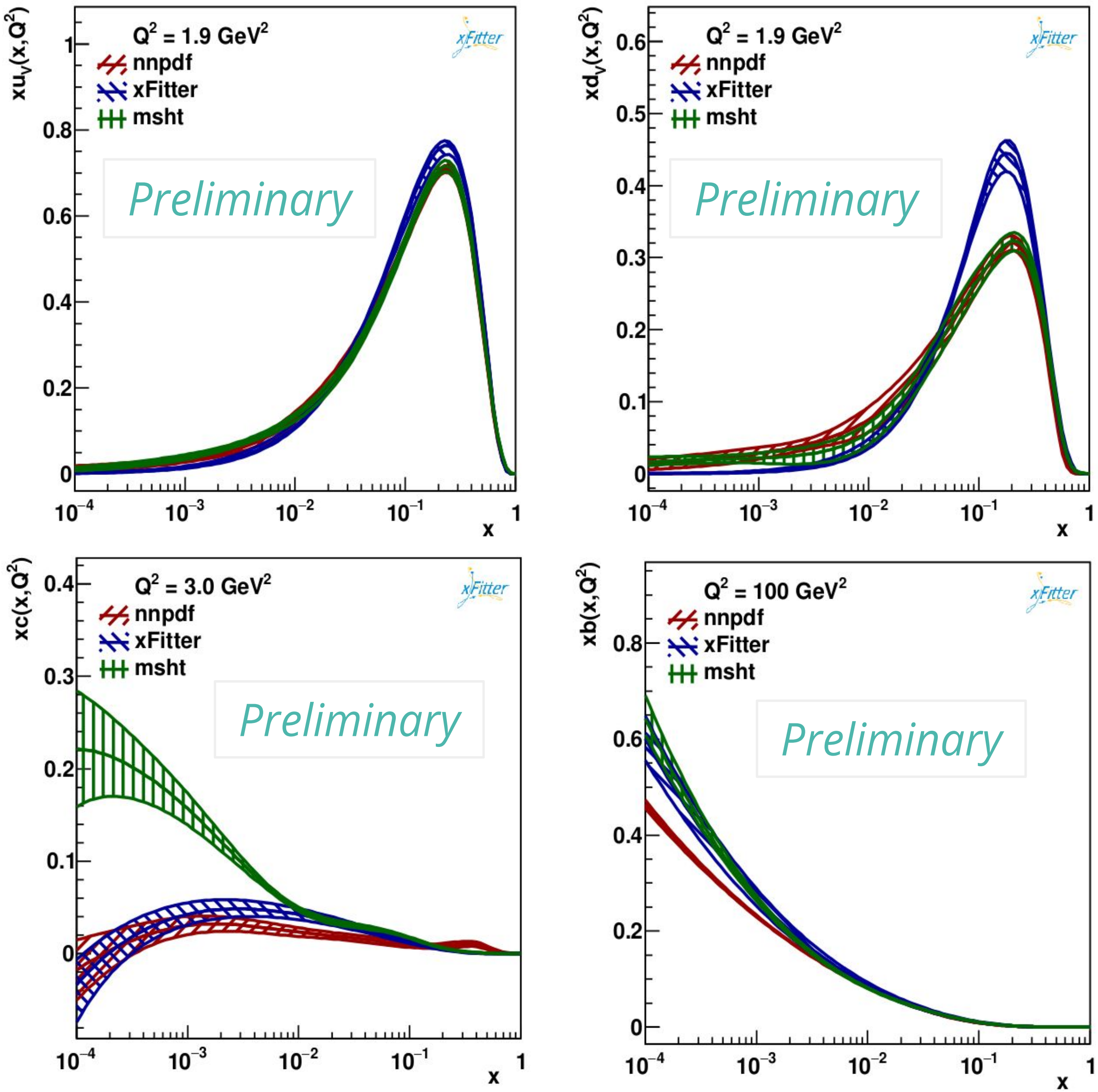






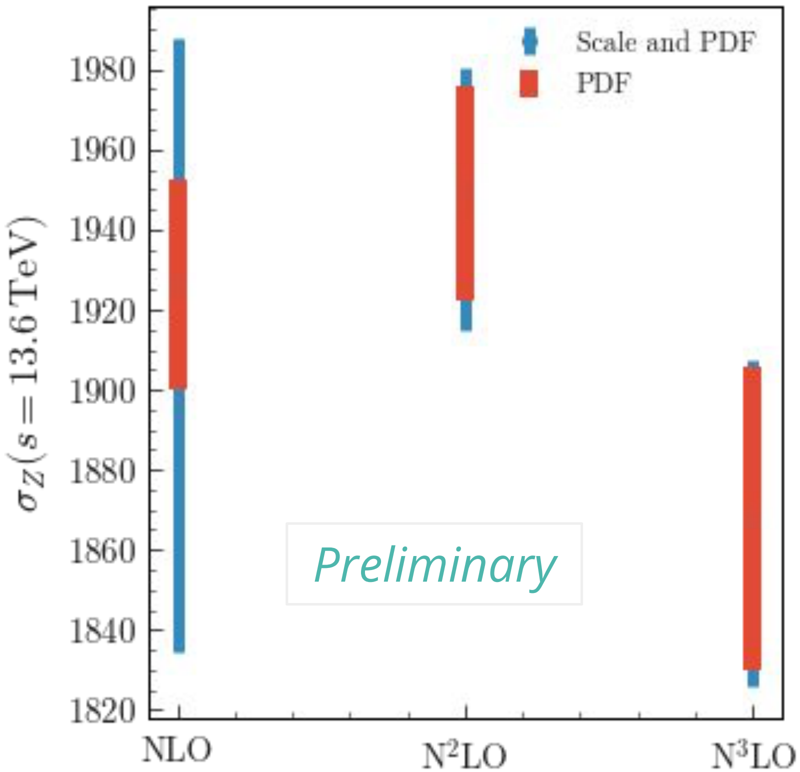
- At higher scales, large uncertainties for valence quarks (low-x)
- Significant theory uncertainty for xg at x < 0.01
- Charm/bottom uncertainties from m_c/m_b variations

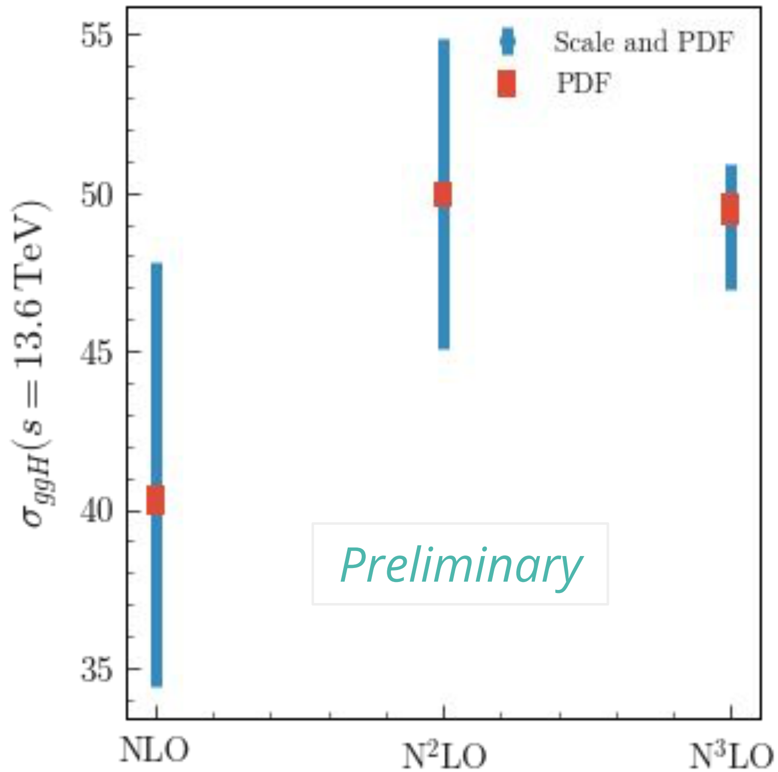
Comparison to other aN^{3}LO PDF



- **Based on grids publicly available on LHAPDF**
- The sets agree for xu_v
- xd_v → xFitter outlier
- xg, xc → MSHT20 outlier
- xb → NNPDF4.0 outlier

Impact on LHC predictions





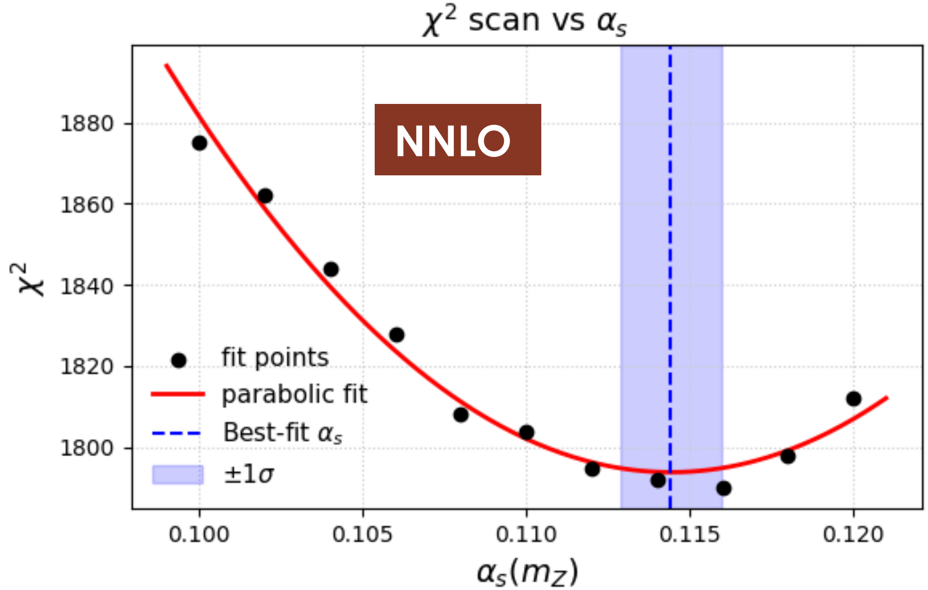
- Predictions at NLO, NNLO and N³LO for **Z** (left) and **ggH** (right) production computed using **n3loxs** – [2209.06138]
- PDF uncertainties from N³LO include theory uncertainties
- <u>Good convergence for H, not so good for Z</u>

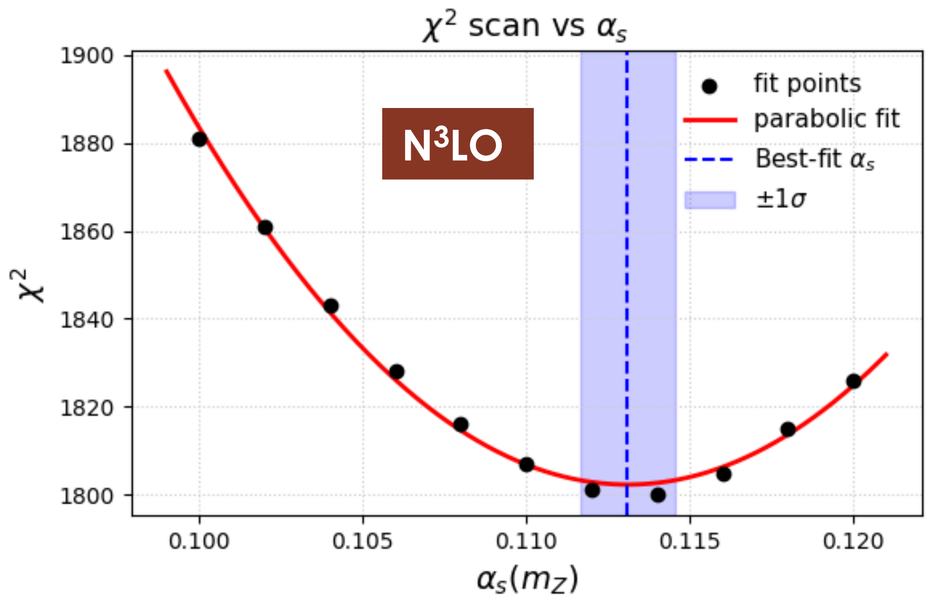
α_s scan

- Fixed target data from BCDMS, NMC and SLAC as well
- χ^2 scan at NNLO and N^{3}LO
- HERA-only, NNLO: $\boldsymbol{\alpha_s} = \mathbf{0.1065 \pm 0.0029}$
- HERA+fixed target, NNLO: $\boldsymbol{\alpha_s} = \mathbf{0.1144 \pm 0.0015}$
- HERA+fixed target, N^{3}LO: $\boldsymbol{\alpha_s} = \mathbf{0.1131 \pm 0.0015}$

Just PDF uncertainties (no model/parametrisation) with $\Delta\chi^2 = 1$ criterion

Not claiming this is the preferred α_s value at N^{3}LO





PDF fit with resummation scale

- Study of the solution of a generic renormalization group equation (RGE):

$$\frac{d}{d\ln\mu}\ln R(\mu) = \gamma(\alpha_s(\mu)) \qquad \gamma(\alpha_s(\mu)) = \frac{\alpha_s(\mu)}{4\pi}\sum_{n=0}^{\infty}\left(\frac{\alpha_s(\mu)}{4\pi}\right)^n \gamma_n$$

- Defined the Green's function (evolution operator) such that:

$$R(\mu_1) = G(\mu_1, \mu_2) \otimes R(\mu_2)$$

with R = $\boldsymbol{\alpha_s}$, **PDF, TMD**, running masses, etc

- We consider effects due to solving the RGE **analytically**, as opposed to a **numerical** solution, by means of expansions in α_s that cause the inequality:

$$G(\mu_1, \mu_0) \otimes G(\mu_0, \mu_2) \neq G(\mu_1, \mu_2)$$

- This identity is violated by *subleading* terms

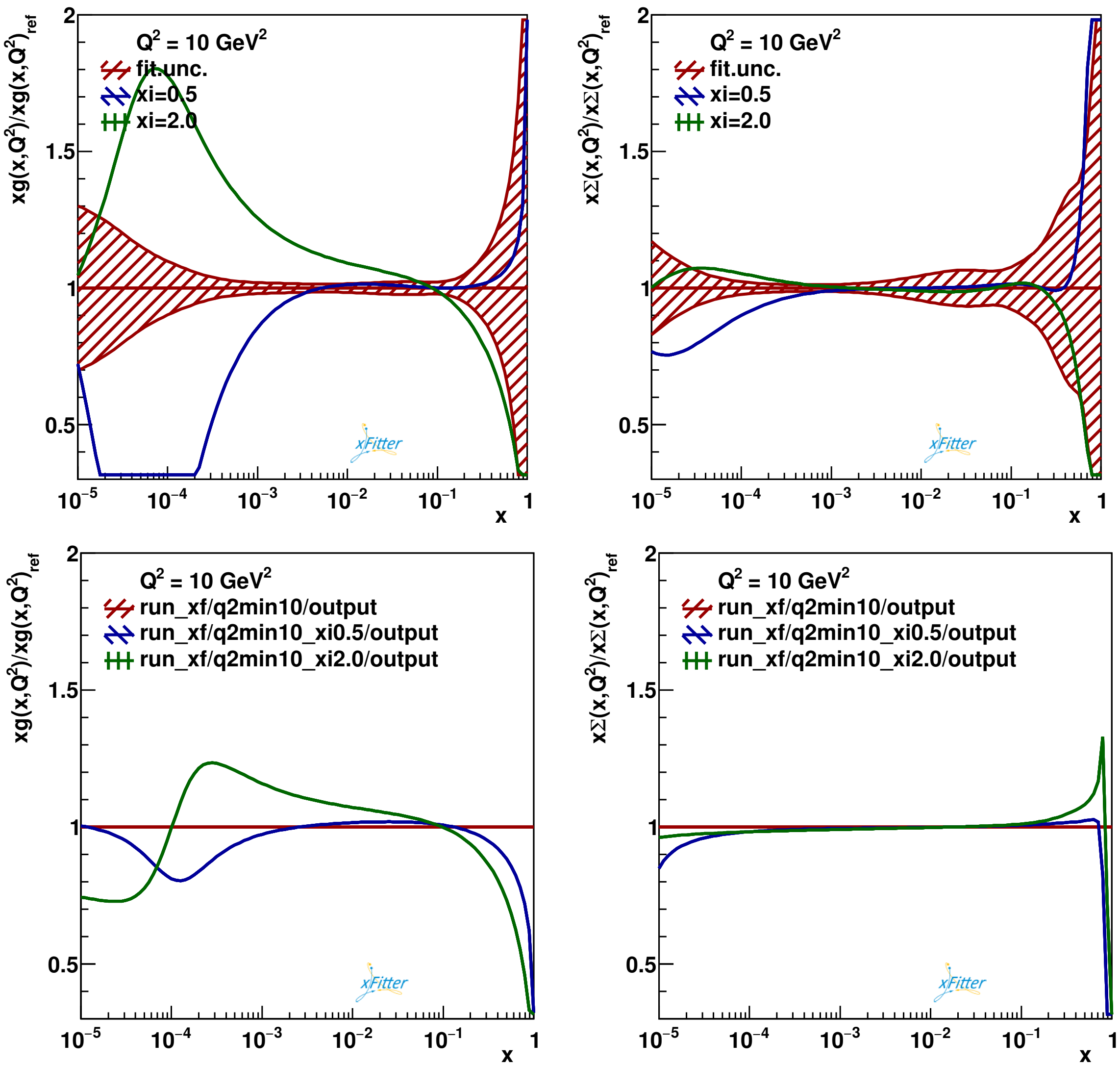
- Introduction of the **resummation scale $\boldsymbol{\mu_{res}}$** at the level of the solution of the RGE - 2407.20842, Giuseppe's talk

- Variations of μ_{res} around μ provide an estimate of subleading (higher-order) corrections

- Bottom line: **the evolution of $\boldsymbol{\alpha_s}$ has an uncertainty** (which is often neglected)

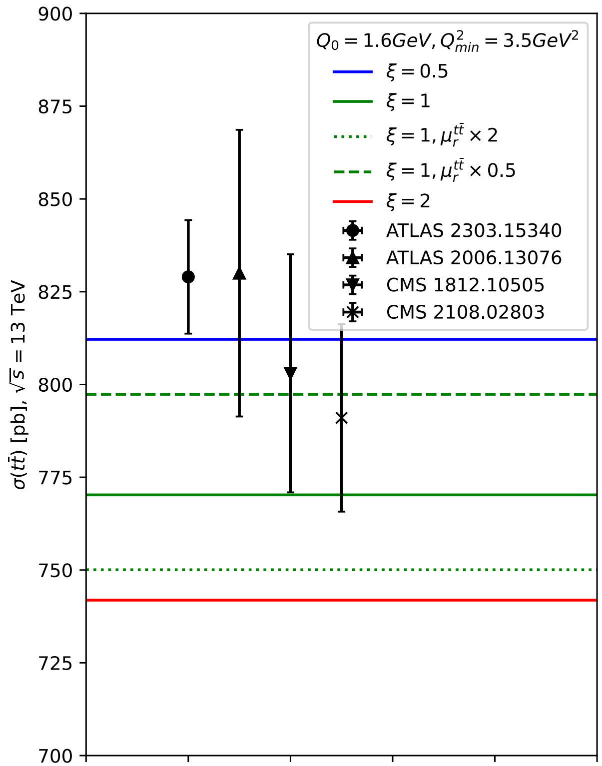
PDF fit with resummation scale

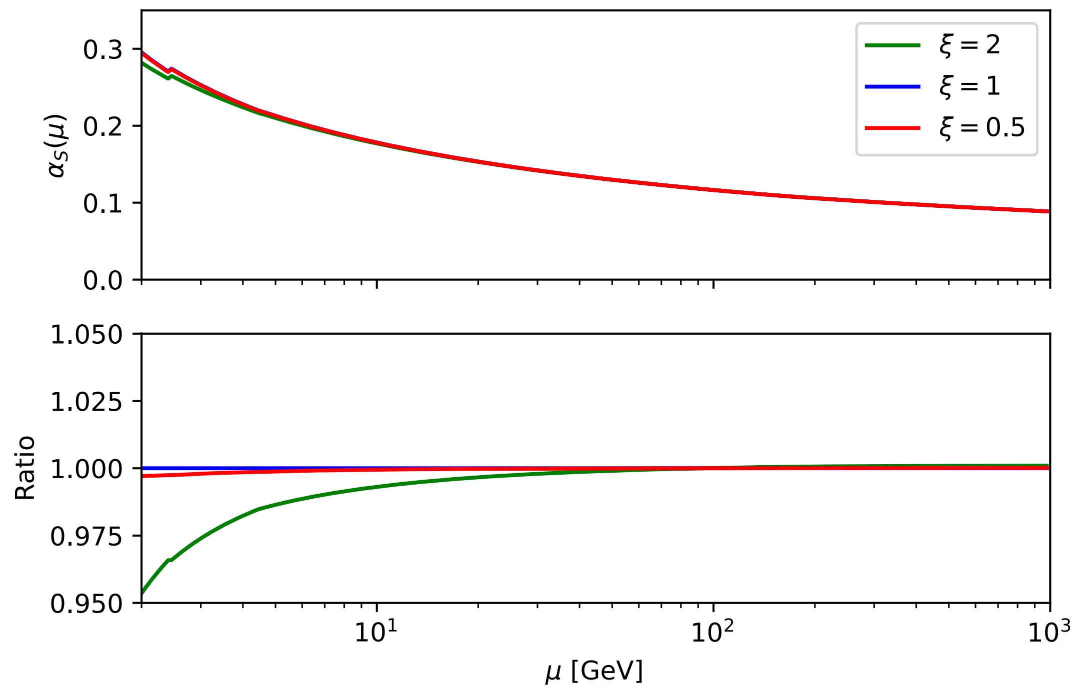
- Study the impact of resummation scale variations in a PDF fit using inclusive HERA data



- PDF parametrization and fit setting follow the Bonvini-Giuli paper
- Q_0 = 1.6 GeV, Q^2_{min} = 3.5 GeV² (top)
- Q_0 = 3.2 GeV, Q^2_{min} = 10 GeV² (bottom)
- Significant dependence on the resummation scale
- Ignored in global fits so far
- Impact of μ_{res} reduced if Q_0 is higher i.e. ~2-3 GeV

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 GeV, Q^2_{min} = 10 GeV^2 is used (backup)
- Study on the α_s running - **huge impact at low scales**, but **~negligible at Q^2 = m_Z^2 GeV^2**

Summary and outlook

- **DIS-only analysis** with **consistent N^{3}LO** 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 or α_s

Backup Slides

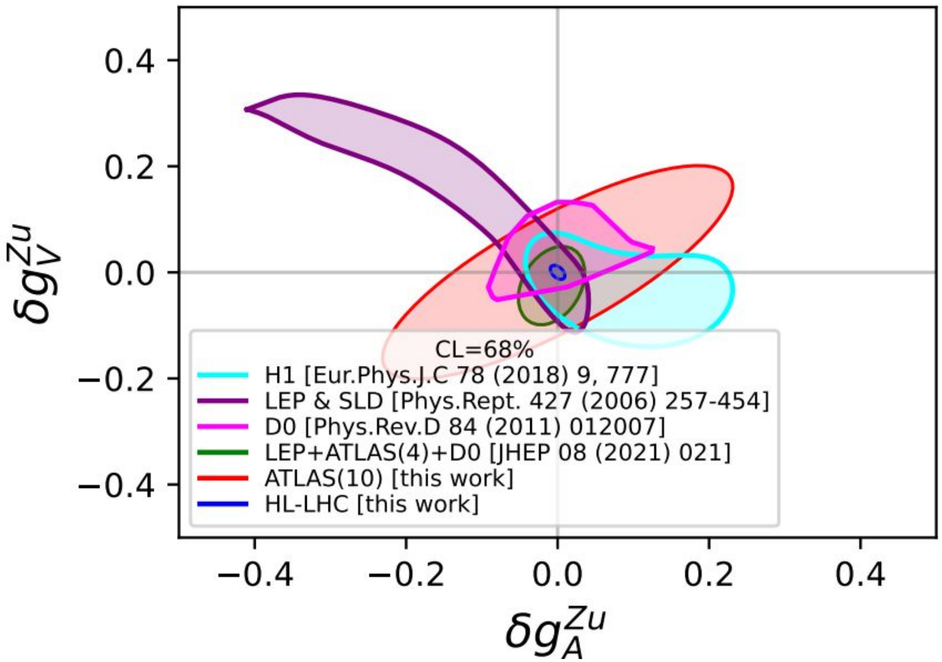
Status of the xFitter project

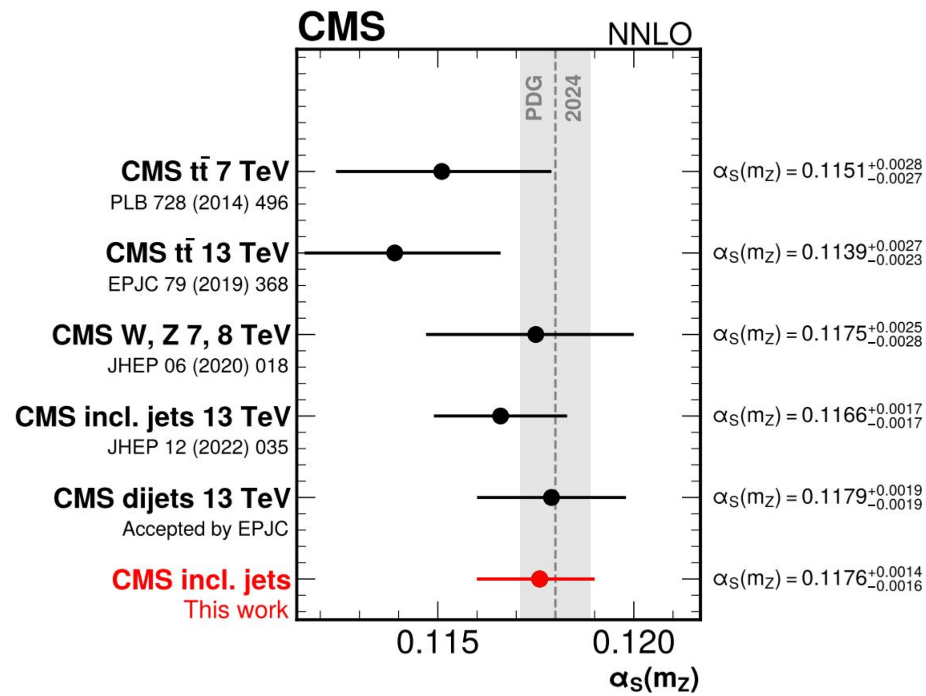
- Project is in active development on Gitlab
- Stable release 2.2.0 ("Future freeze") – extensive Wiki here
- Nightly master branch built and validated vs several public results
- Nightly docker image

```
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 **N^3LO 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

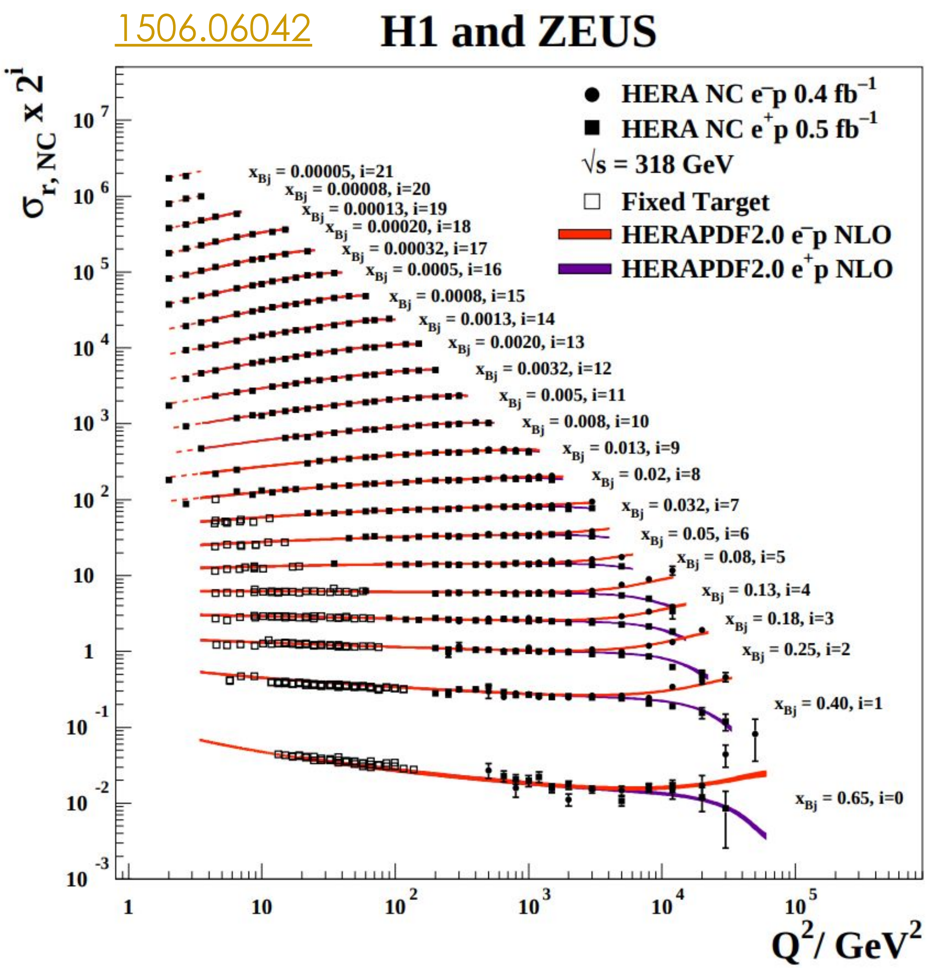




- Many analyses using xFitter last year
- SMEFT analysis of Z boson couplings using forward-backward DY production at LHC - 2310.19638
- CMS analysis of inclusive jet production cross section to extract α_s - 2412.16665

PDF determination using HERA data

1506.06042



$$\frac{d^2\sigma^{NC}_{e^\mp p}}{dxdQ^2} = \frac{2\pi\alpha^2 Y_+}{xQ^4}\left(F_2 - \frac{y^2}{Y_+}F_L \pm \frac{Y_-}{Y_+}xF_3\right)$$

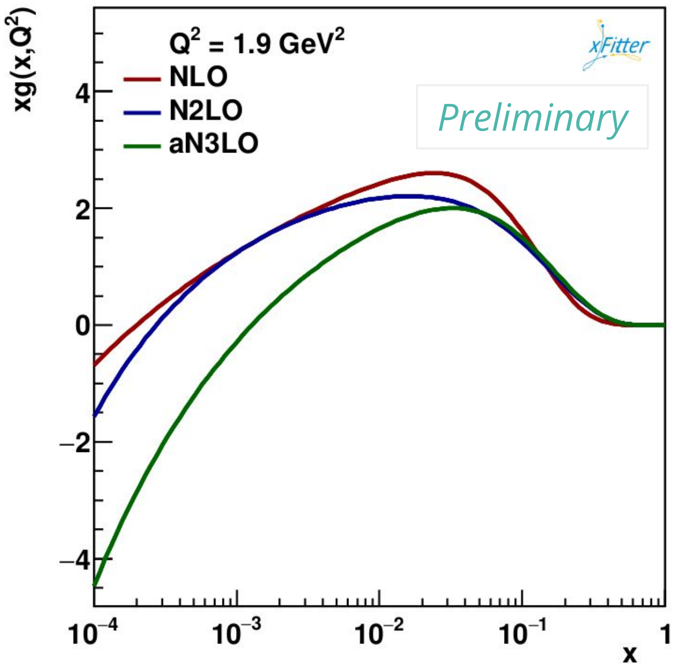
$$Y_\pm = 1 \pm (1-y)^2$$

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

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

- At HERA γ exchange dominates, the best PDF determined is $\boldsymbol{xu_v}$
- At low-x, contribution of $\boldsymbol{xc}$ 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, $\boldsymbol{xu_v}$ and $\boldsymbol{xd_v}$ separated using charged-current data

aN^{3}LO vs NNLO vs NLO

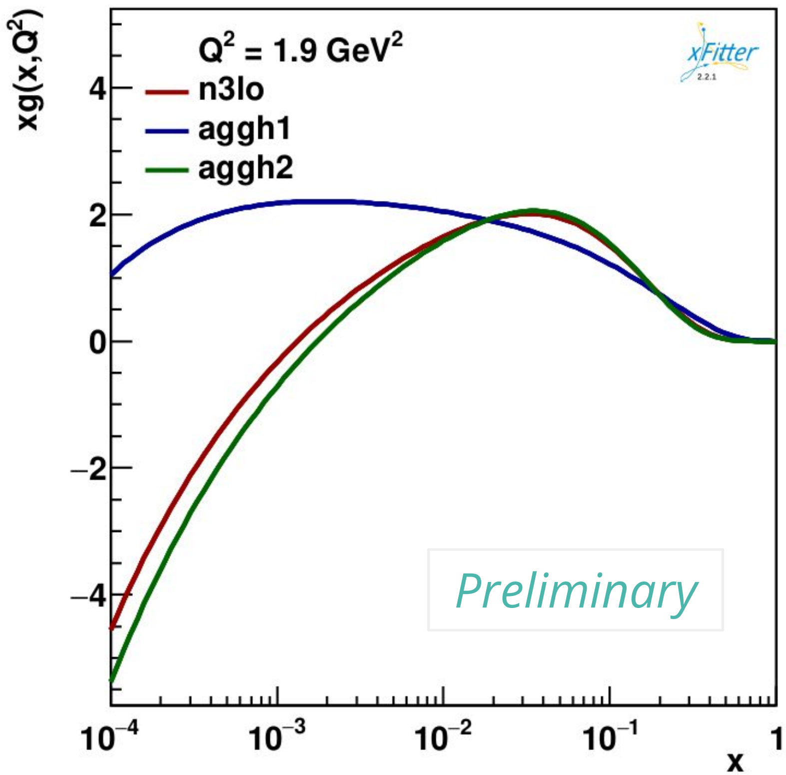


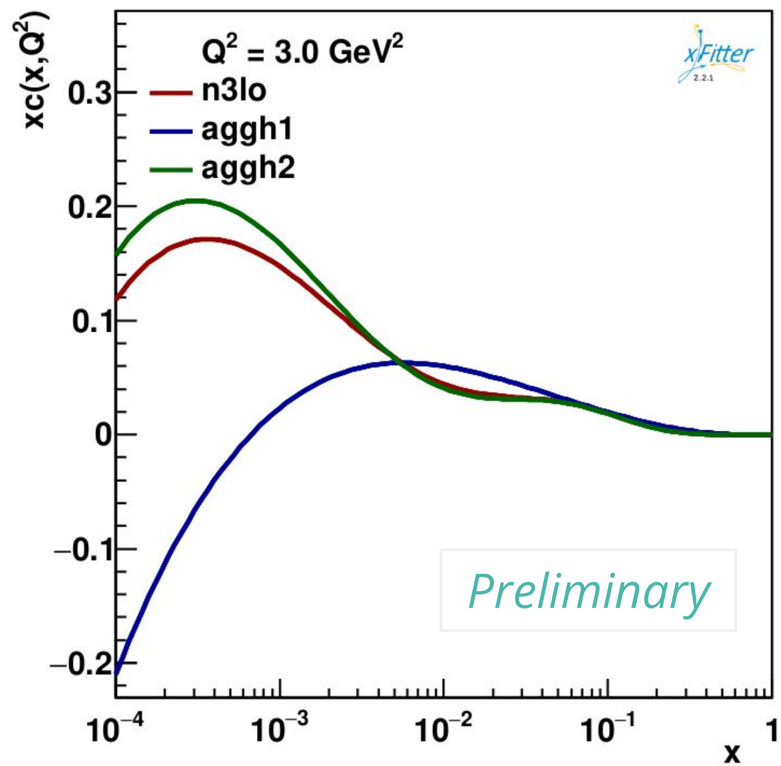
Preliminary

Dataset	NLO	N2LO	aN3LO
HERA1+2 NCep 820	68 / 70	67 / 70	68 / 70
HERA1+2 NCep 460	217 / 204	218 / 204	215 / 204
HERA1+2 CCep	43 / 39	44 / 39	48 / 39
HERA1+2 NCem	218 / 159	216 / 159	223 / 159
HERA1+2 CCem	53 / 42	56 / 42	61 / 42
HERA1+2 NCep 575	216 / 254	220 / 254	215 / 254
HERA1+2 NCep 920	424 / 377	452 / 377	476 / 377
Correlated χ^2	77	98	103
Log penalty χ^2	+7.7	+14	+14
Total χ^2 / dof	1325 / 1131	1385 / 1131	1422 / 1131

- Approximate N^{3}LO based on 2207.04739 (MSHT20 approximation)
- Similar pattern as observed in the past
- N^{3}LO gluon is more negative at low-x at the starting scale
- χ^2/dof is the worst

aN³LO matching conditions



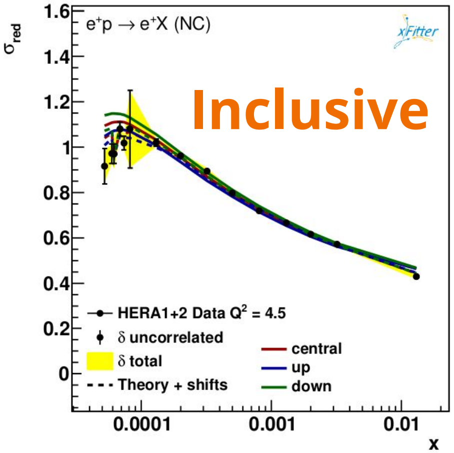


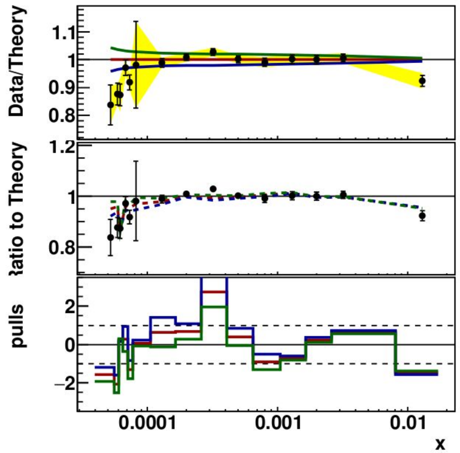
- Approximate matching conditions have uncertainties for transition matrix elements

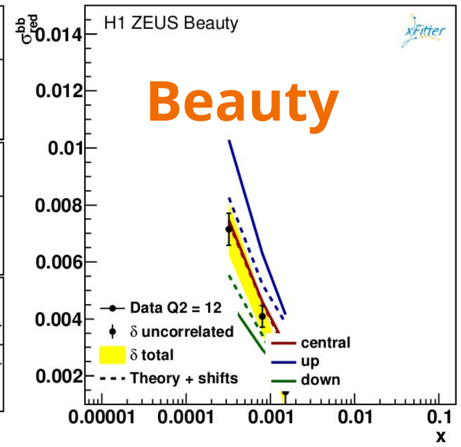
- Large impact on xc and xg due to **– 2000 < $a_{gg,H}$ < - 700**

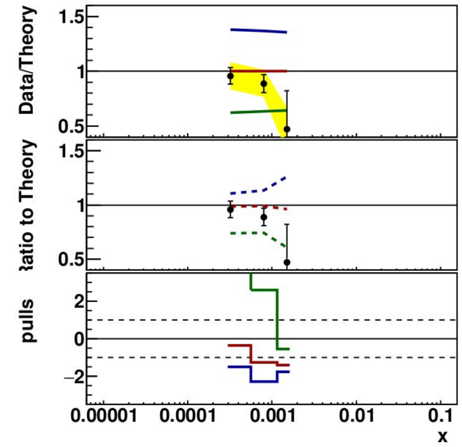
$$A_{gg,H}^{(3)} = A_1 \ln^2(1-x) + A_2 \ln(1-x) + A_3 x^2 + A_4 \ln x + A_5 x + \boxed{a_{gg,H} \frac{\ln x}{x}}$$

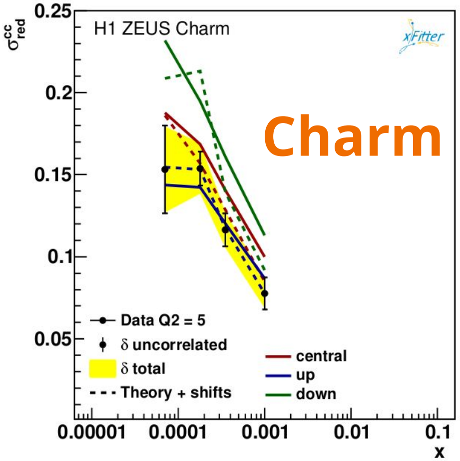
Uncertainties on massive coefficient functions

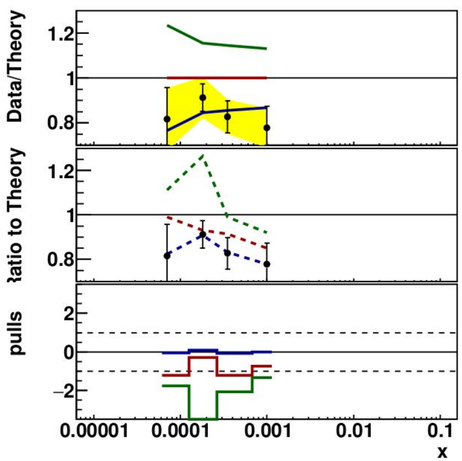








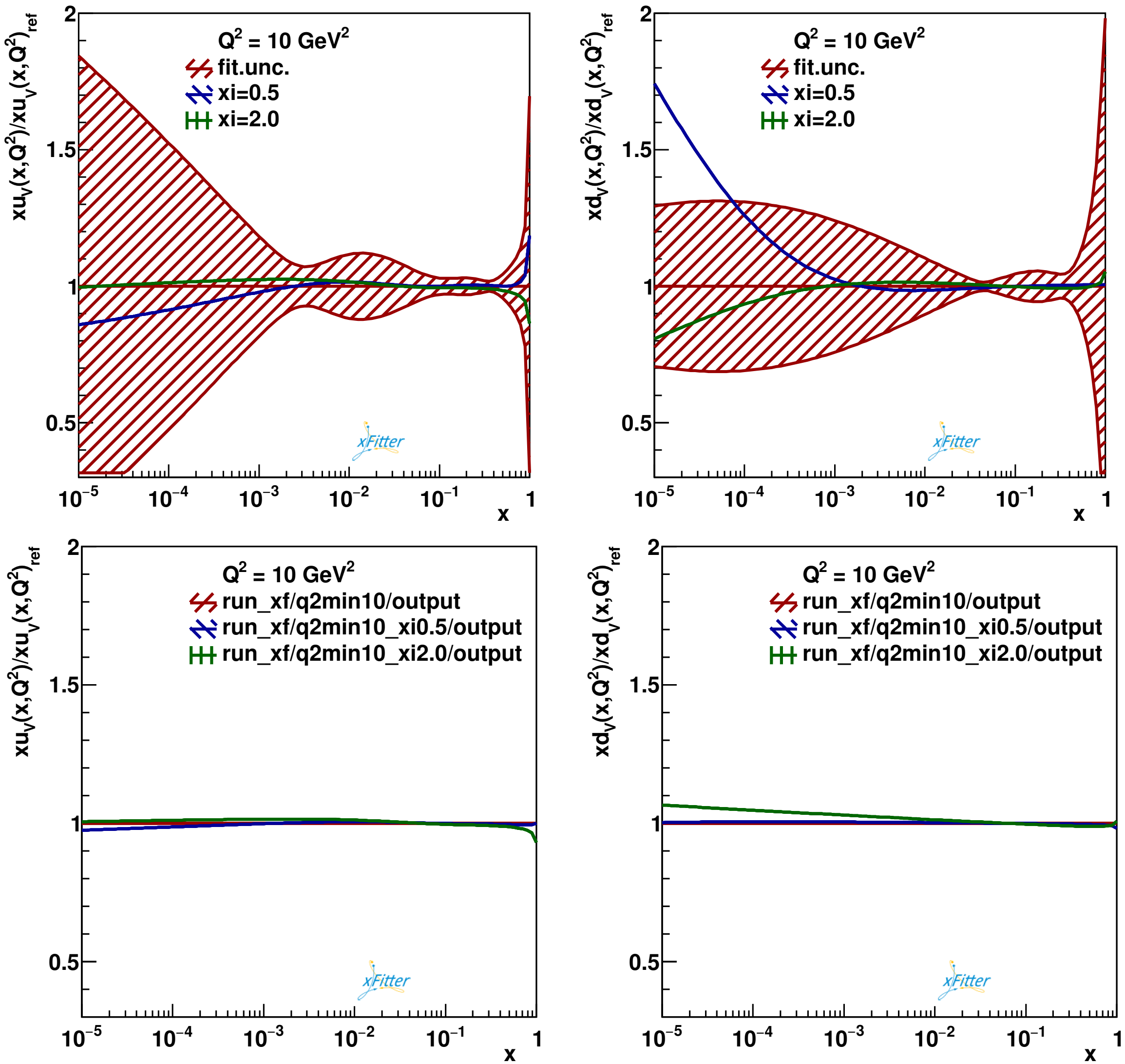




- Reduced impact on inclusive data at low-x
- Low-x uncertainties in massive coefficient functions lead to sizable variation of $F_{2,c}$ and $F_{2,b}$
- In the FONLL prescription, important for sub-threshold regions

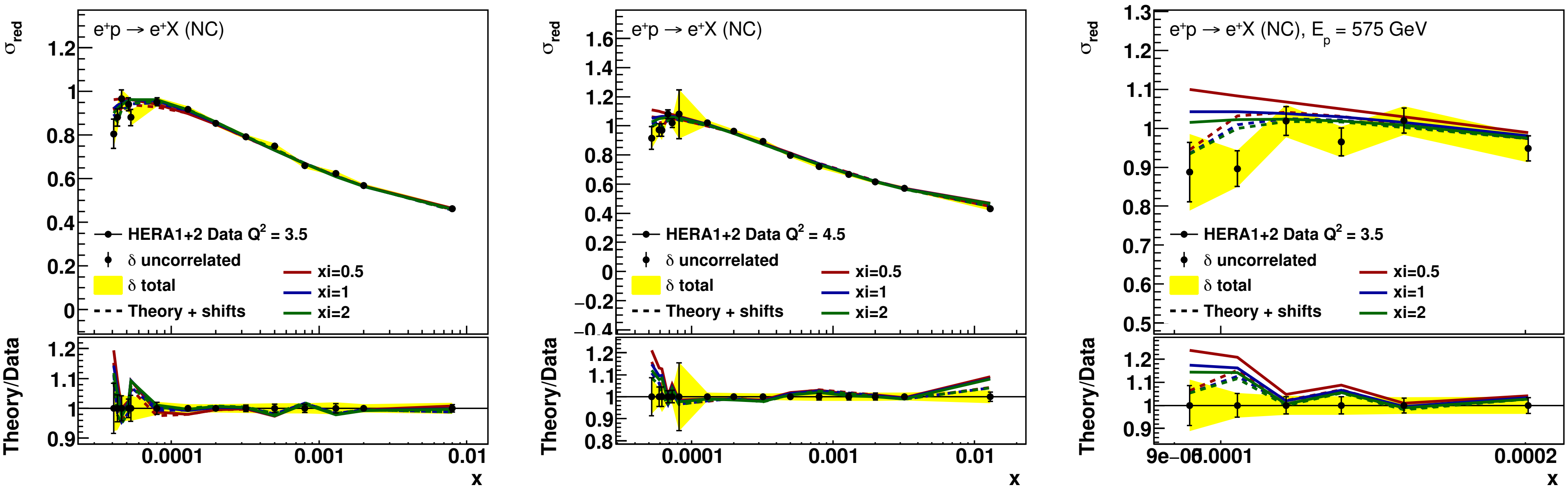
PDF fit with resummation scale

- Study the impact of resummation scale variations in a PDF fit using inclusive HERA data



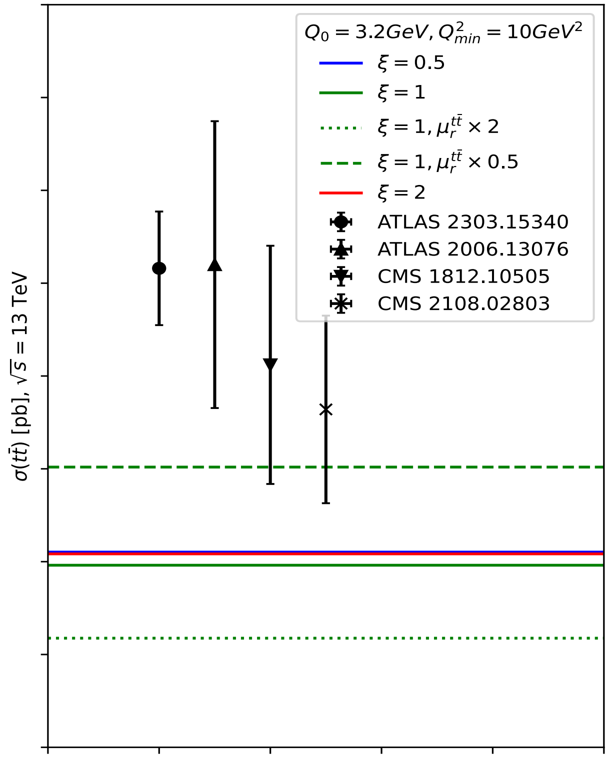
- PDF parametrization and fit setting follow the Bonvini-Giuli paper
- Q_0 = 1.6 GeV, Q^2_{min} = 3.5 GeV² (top)
- Q_0 = 3.2 GeV, Q^2_{min} = 10 GeV² (bottom)
- Significant dependence on the resummation scale
- Ignored in global fits so far
- Impact of μ_{res} reduced if Q_0 is higher i.e. ~2-3 GeV

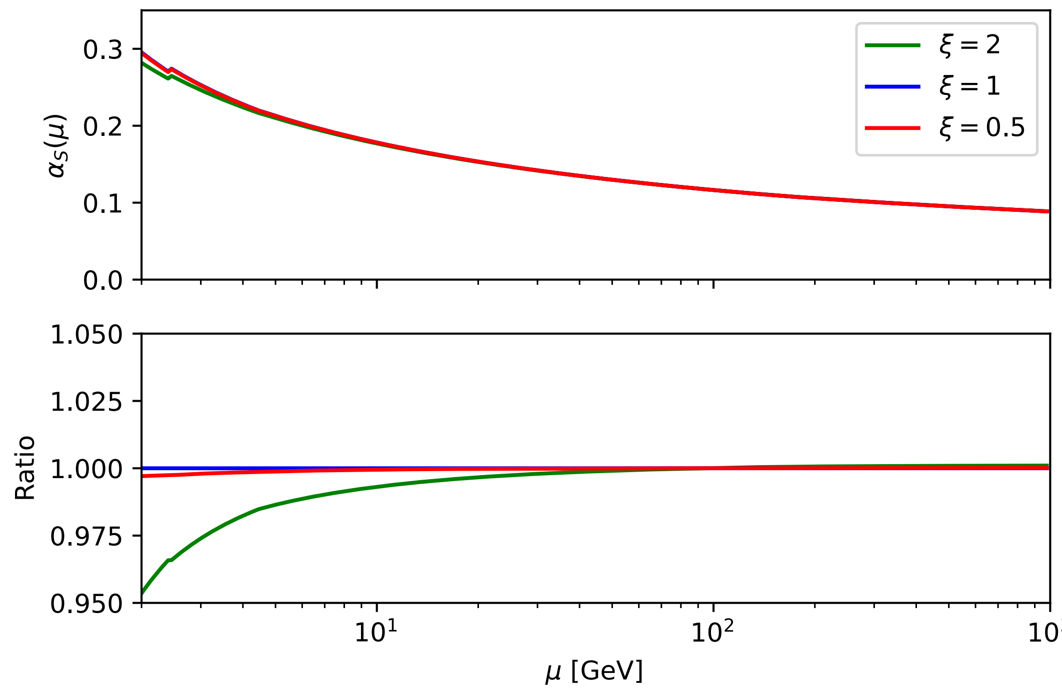
PDF fit with resummation scale



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

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 GeV, Q^2_{min} = 10 GeV^2 is used
- Study on the α_s running - **huge impact at low scales**, but **~negligible at Q^2 = m_Z^2 GeV^2**