Studies of N3LO Fits to DIS Data Using xFitter

EPS-HEP 2025

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N3LO PDF fits

Why and how?

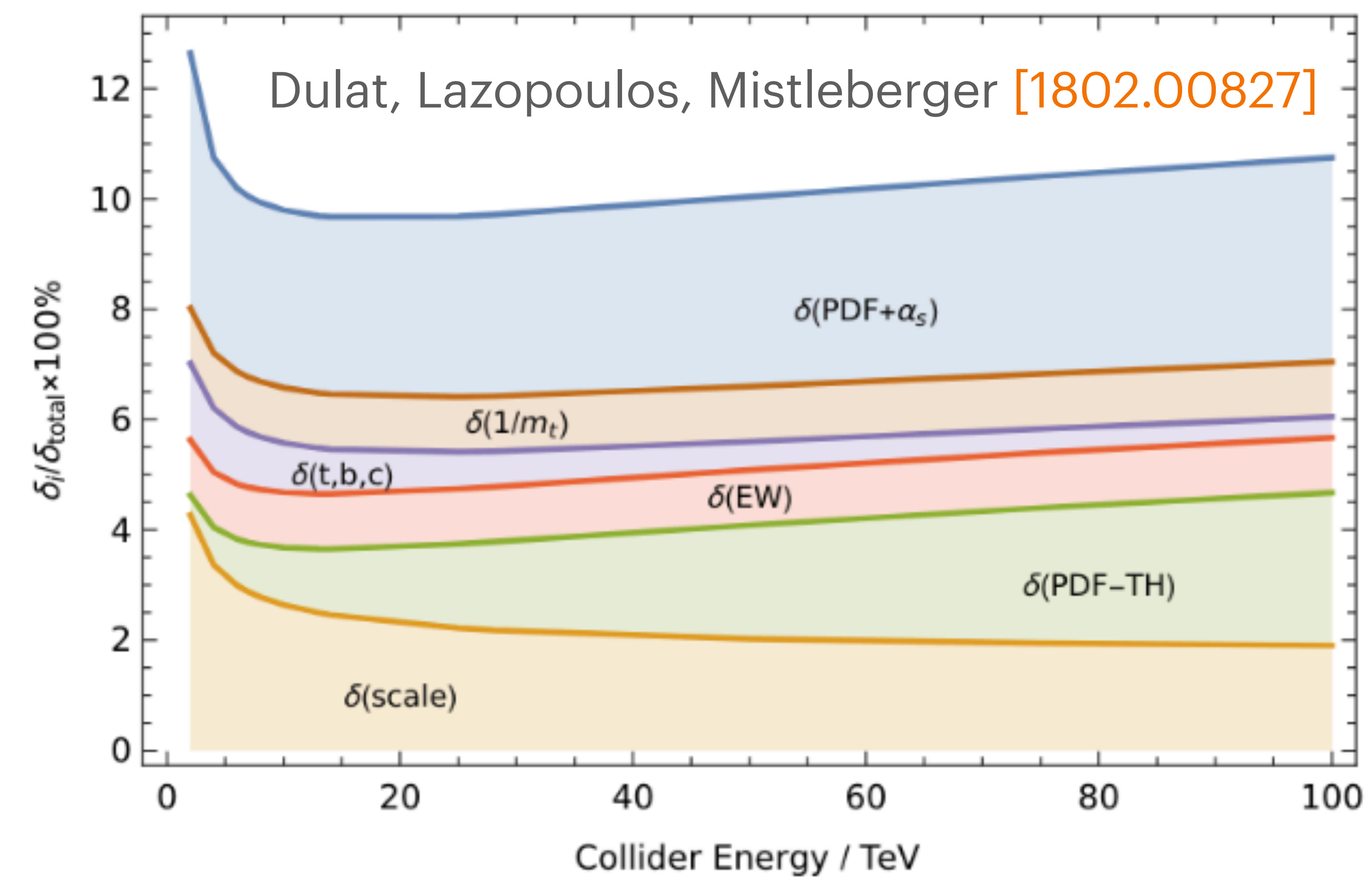
- **Why?** PDF uncertainties are becoming a **bottleneck** for LHC precision measurements

- N3LO cross sections available for Higgs (ggF, VBF, VH) and DY (NC, CC)

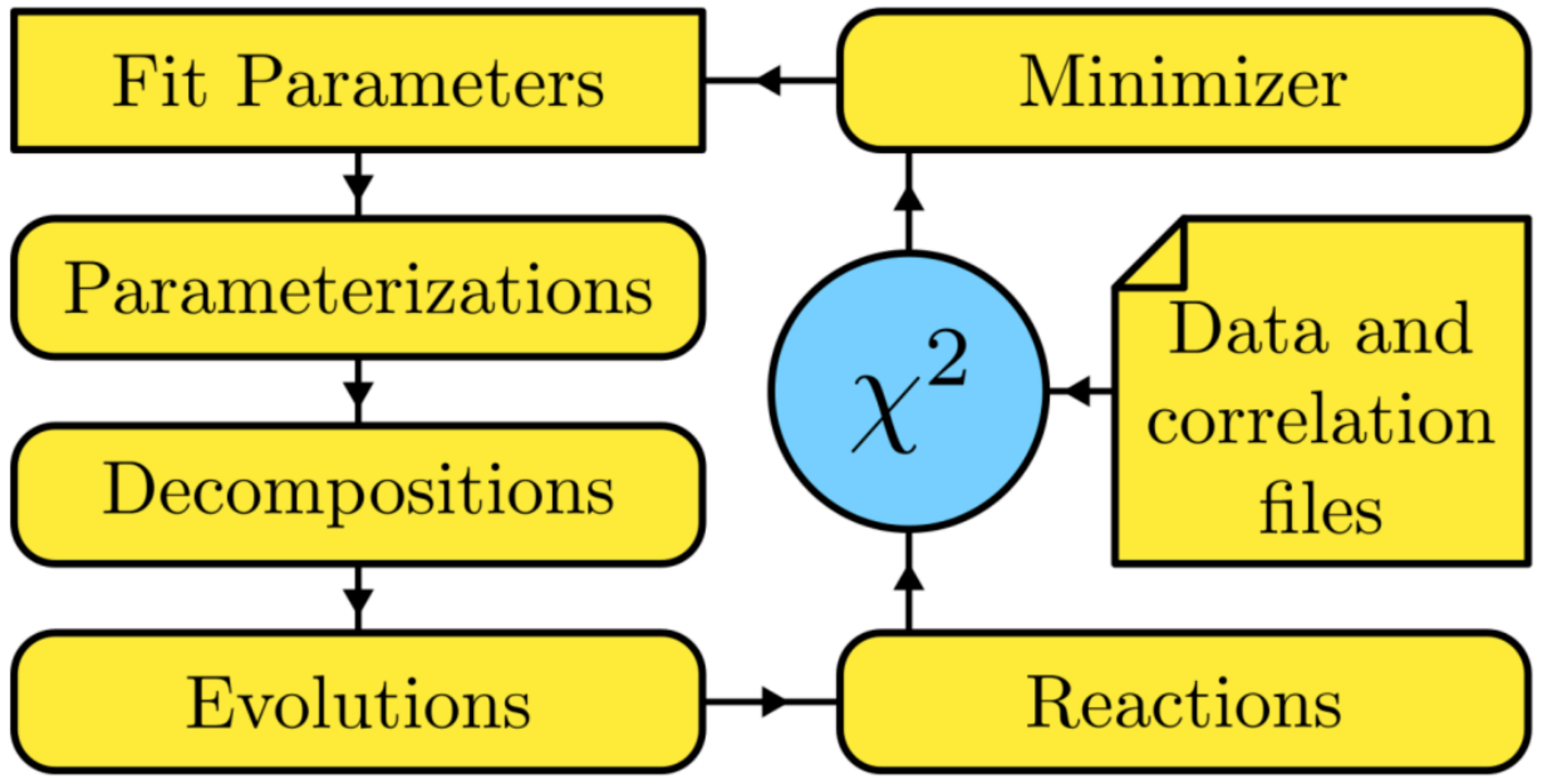
  → call for N3LO PDFs to reduce mismatch and PDF uncertainties

- PDF fits at N3LO: **how?**

Inclusive Higgs production



- **xFitter! Open-source QCD fit framework**



- **Project in active development**
  - Stable release 2.2.0 (“future freeze”)
  - Nightly “master” branch validated vs several public results
  - Interfaces to ploughshare, hoppet, PineAPPL, CIJET, DYTurbo
  - N3LO FONLL for APFEL++
  - Parallel derivatives in CERES, parallel profiling, parallel asymmetric Hessian uncertainties evaluation

N3LO PDF fits

Ingredients for DIS PDF fits at N3LO

- **QCD inputs needed** for N3LO DIS fits can be grouped in 3 categories

- **N3LO (4-loop) DGLAP splitting functions** for PDF evolution

$$Q^2 \frac{\mathrm{d}f_i}{\mathrm{d}Q^2} = P_{ij} \otimes f_j \to P_{ij}(x, \alpha_s) = \alpha_s P_{ij}^{(0)}(x) + \alpha_s^2 P_{ij}^{(1)}(x) + \alpha_s^3 P_{ij}^{(2)}(x) + \alpha_s^4 P_{ij}^{(3)}(x) + \dots$$

- **N3LO matching conditions** to change number of PDF flavours at heavy quark mass (m_h) thresholds

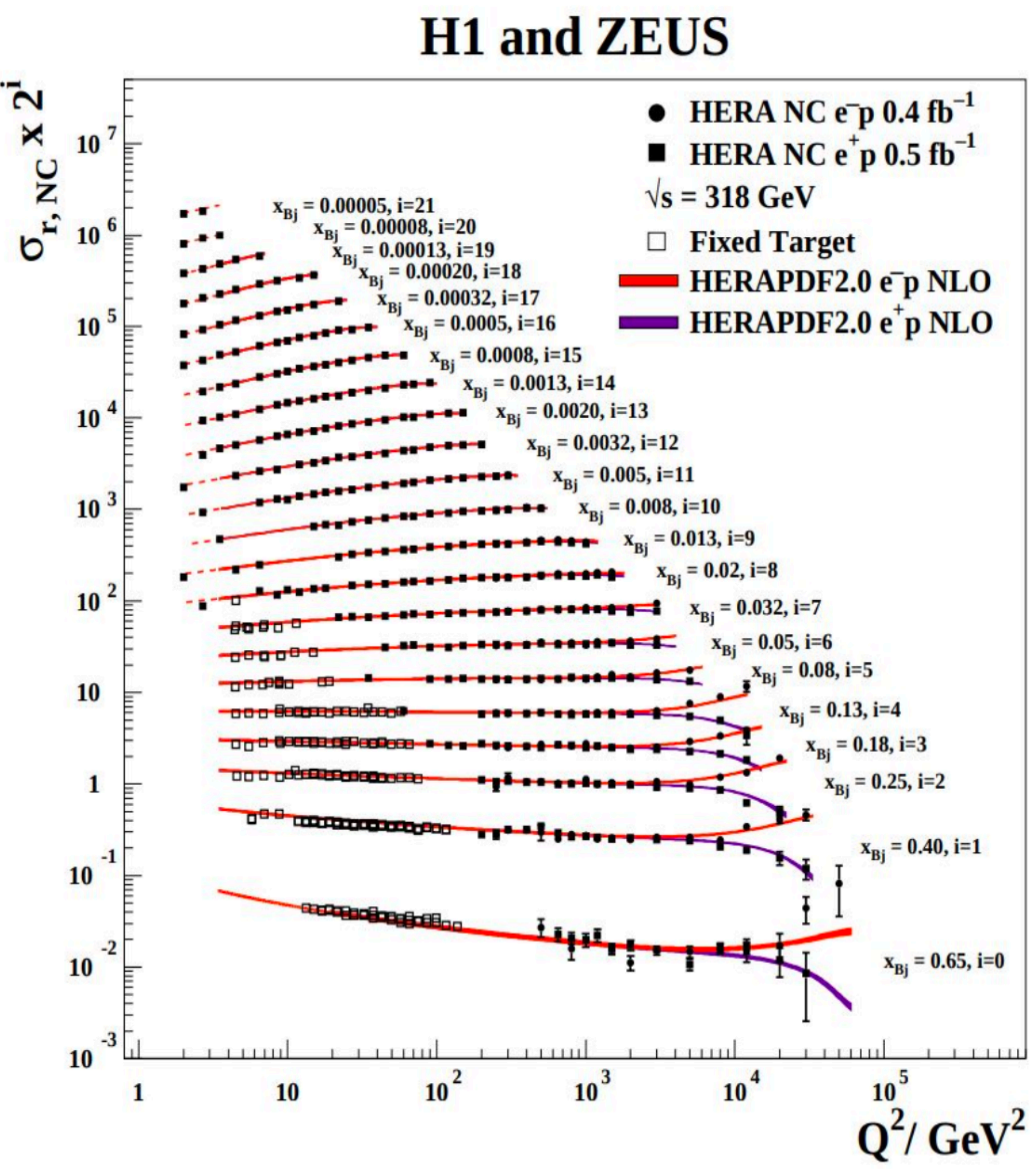
$$f_i^{n_f+1}(x, Q^2) = [A_{ij}(Q^2/m_h^2) \otimes f_i^{n_f}(Q^2)](x)$$

- **N3LO coefficient functions** to determine DIS structure functions

$$F_i^V(x, Q^2) = \sum_a [C_{i,a}^V \otimes f_a](x, Q^2)$$

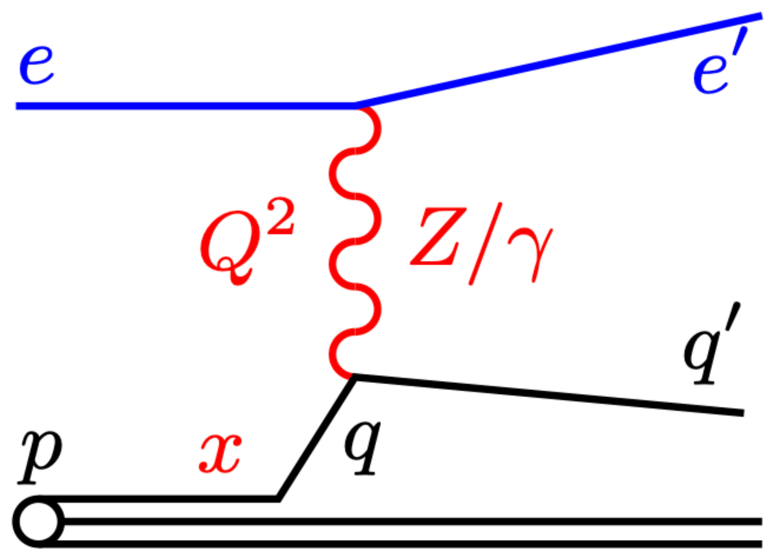
Analysis of HERA DIS data at N3LO

HERA DIS data



[Eur.Phys.J.C 75 (2015) 12, 580]

- **xFitter analysis** based on **HERAI+II** inclusive [1506.06042] and charm+bottom data [1804.01019]
  - HERA *ep* collider: H1&ZEUS collected ~1/fb of data ($E_p = 460/575/820/920\,\text{GeV}$, $E_e = 27.5\,\text{GeV}$)



$$\frac{d\sigma^{\pm}_{\text{NC}}}{dx\, dQ^2} = \frac{2\pi\alpha^2}{xQ^4} y_+ \left[F_2^{\gamma/Z} \mp \frac{y_-}{y_+} xF_3^{\gamma/Z} - \frac{y^2}{y_+} F_L^{\gamma/Z} \right], \quad y_\pm = 1 \pm (1-y)^2$$

$$\sigma^{\pm}_{\text{NC,red}} = \left[\frac{2\pi\alpha^2}{xQ^4} y_+ \right]^{-1} \frac{d\sigma^{\pm}_{\text{NC}}}{dx\, dQ^2} = F_2^{\gamma/Z} \mp \frac{y_-}{y_+} xF_3^{\gamma/Z} - \frac{y^2}{y_+} F_L^{\gamma/Z}$$

$$F_2 \approx x \sum e_q^2 (q(x) + \bar{q}(x)), \quad xF_3 \approx x \sum 2 e_q a_q (q(x) - \bar{q}(x))$$

- At HERA dominant contribution photon exchange: ***u(x)*** best determined PDF
- Sizeable charm ***c(x)*** at low *x*: up to 30% of F_2
- **Gluon** measured from Q^2 dependence of F_2 or from charm production
- Lower accuracy at high *x*, ***d***

Analysis of HERA DIS data at N3LO

Framework and model

- HERAPDF2.0 parametrization [1506.06042]

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

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

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

$$x\bar{d}(x,\mu_0^2) = A_{\bar{d}} x^{B_{\bar{d}}} (1-x)^{C_{\bar{d}}}, \quad xs(x,\mu_0^2) = x\bar{s}(x,\mu_0^2) = r_s x\bar{d}(x,\mu_0^2) \text{ with } r_s = \frac{f_s}{1-f_s} \quad (f_s = 0.4)$$

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

- **N3LO evolution** as implemented in APFEL++ [1708.00911]

- **Exact** [DESY 24-037] **and approximate N3LO flavor matching conditions** implemented in APFEL++ [2404.15711]

- FONLL VFNS implemented in xFitter, validated with fortran APFEL for N2LO

- **Model variations**
  - $Q_0^2 = 1.9 \pm 0.2\,\mathrm{GeV}^2$
  - $Q_{\mathrm{min}}^2 = 3.5 \pm 1.0\,\mathrm{GeV}^2$
  - $m_c = 1.47 \pm 0.06\,\mathrm{GeV}$
  - $m_b = 4.50 \pm 0.25\,\mathrm{GeV}$
  - $f_s = 0.40 \pm 0.08$

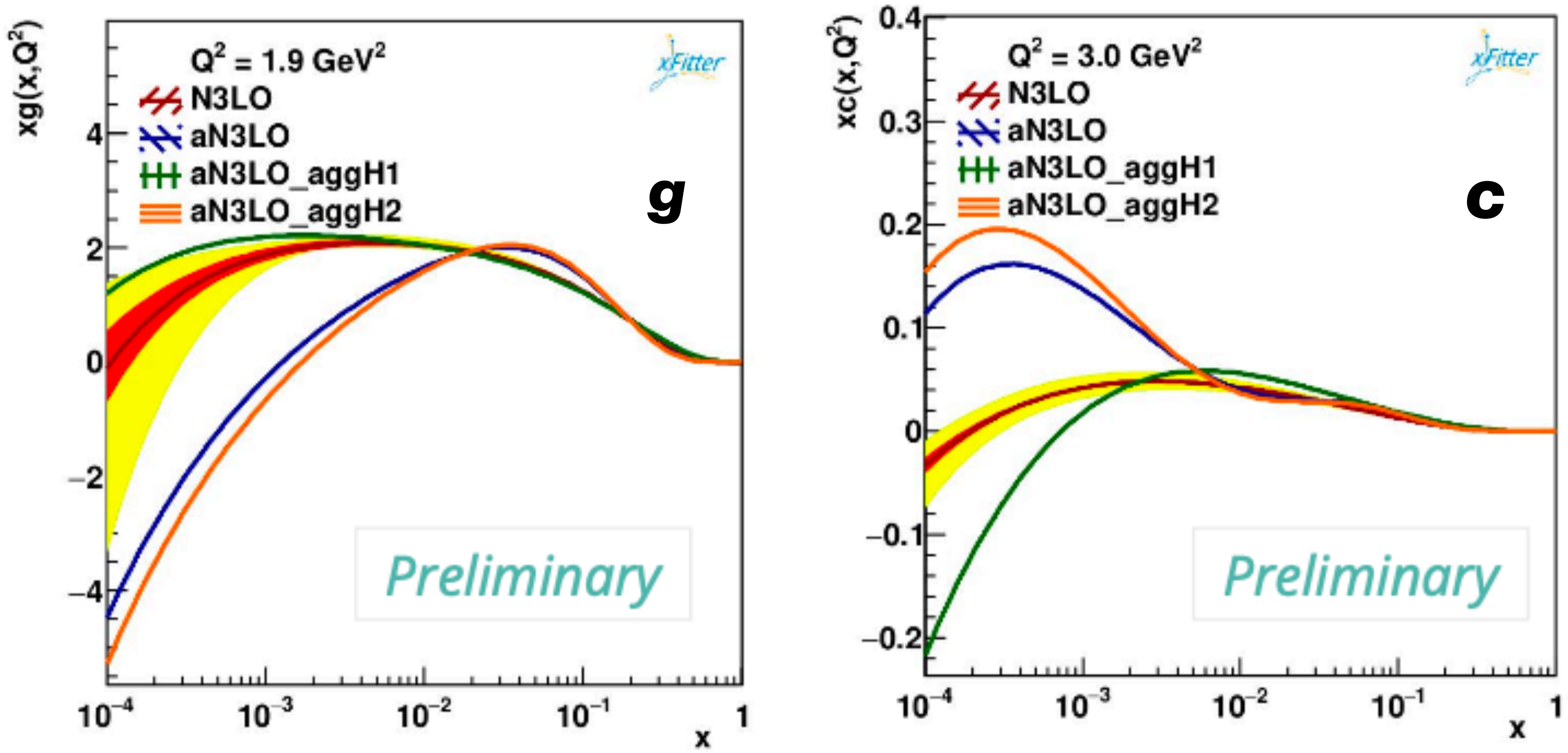
N3LO fits with xFitter

Validation at N3LO

- Fit HERA DIS data using **exact N3LO matching conditions** and validate against approximate N3LO matching (aN3LO) based on MSHT20 prescription [2207.04739]

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



- No sizeable difference in the fit quality

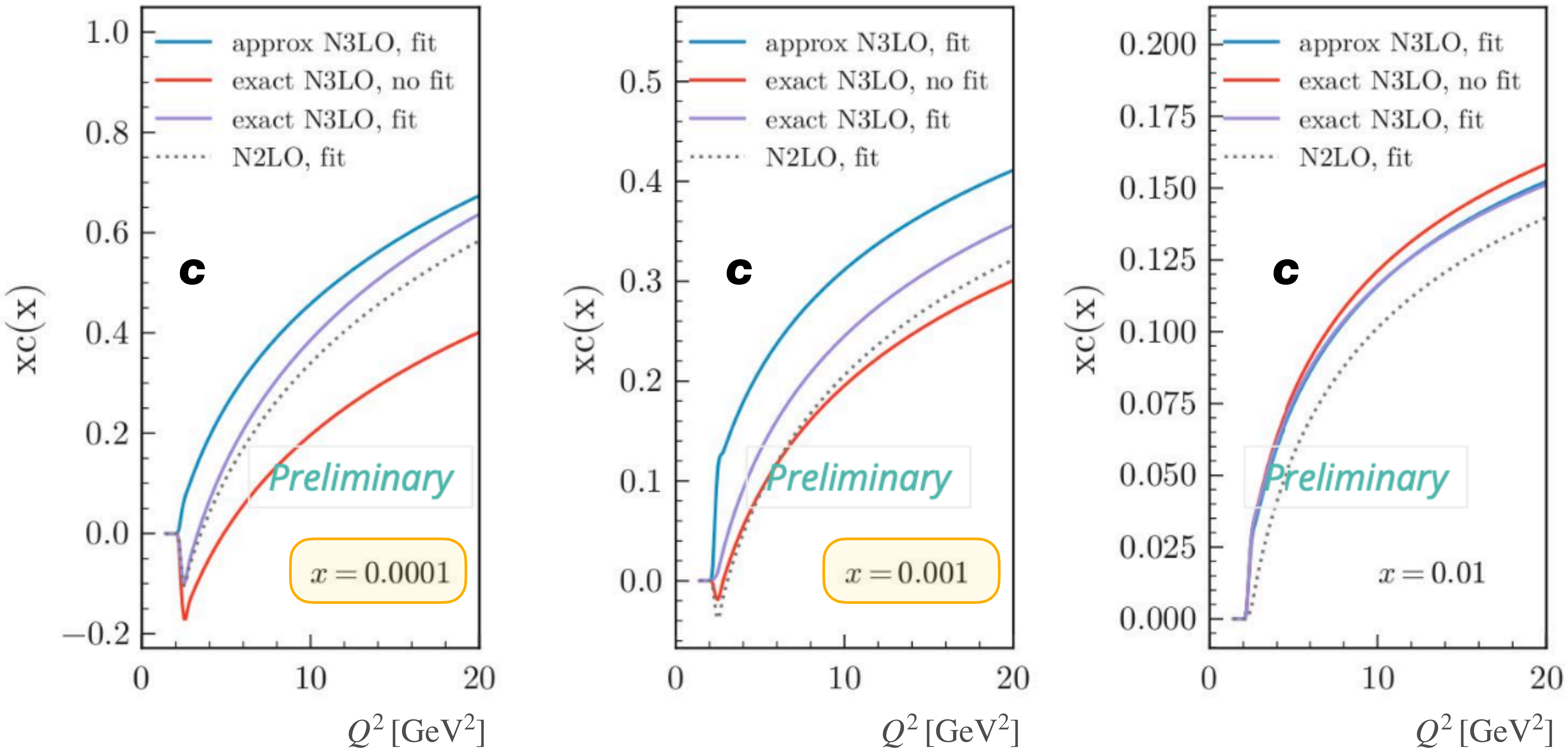
- Exact N3LO fit shown with experimental + model uncertainty bands
- Large difference for exact N3LO gluon and charm at low x compared to aN3LO, but within aN3LO uncertainty (aggH1, aggH2)

N3LO fits with xFitter

Validation at N3LO: **effect of exact matching conditions on charm**

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

- Compare results from fits using **exact N3LO** and **approximate N3LO** matching schemes (and N2LO fits)

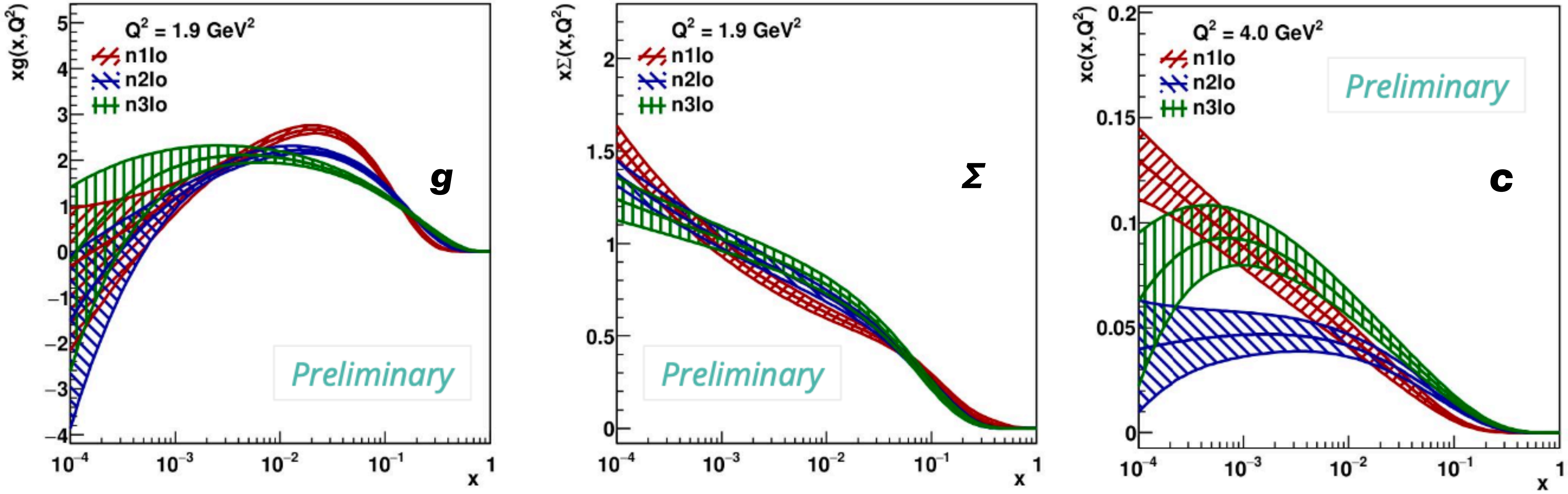


- Significant differences observed at low *x*

xFitter PDFs at N3LO

PDFs at N3LO vs NNLO and NLO

- ***xg***, ***xΣ*** and ***xc*** PDFs compared for **N3LO**, **N2LO** and **NLO** perturbative accuracy of the PDF fit



- Fits with alternative gluon parametrisation consistent with HERAPDF style
- N3LO gluon (***g***) is hardest, also largest at small x
- General good agreement at $x \geq 0.01$

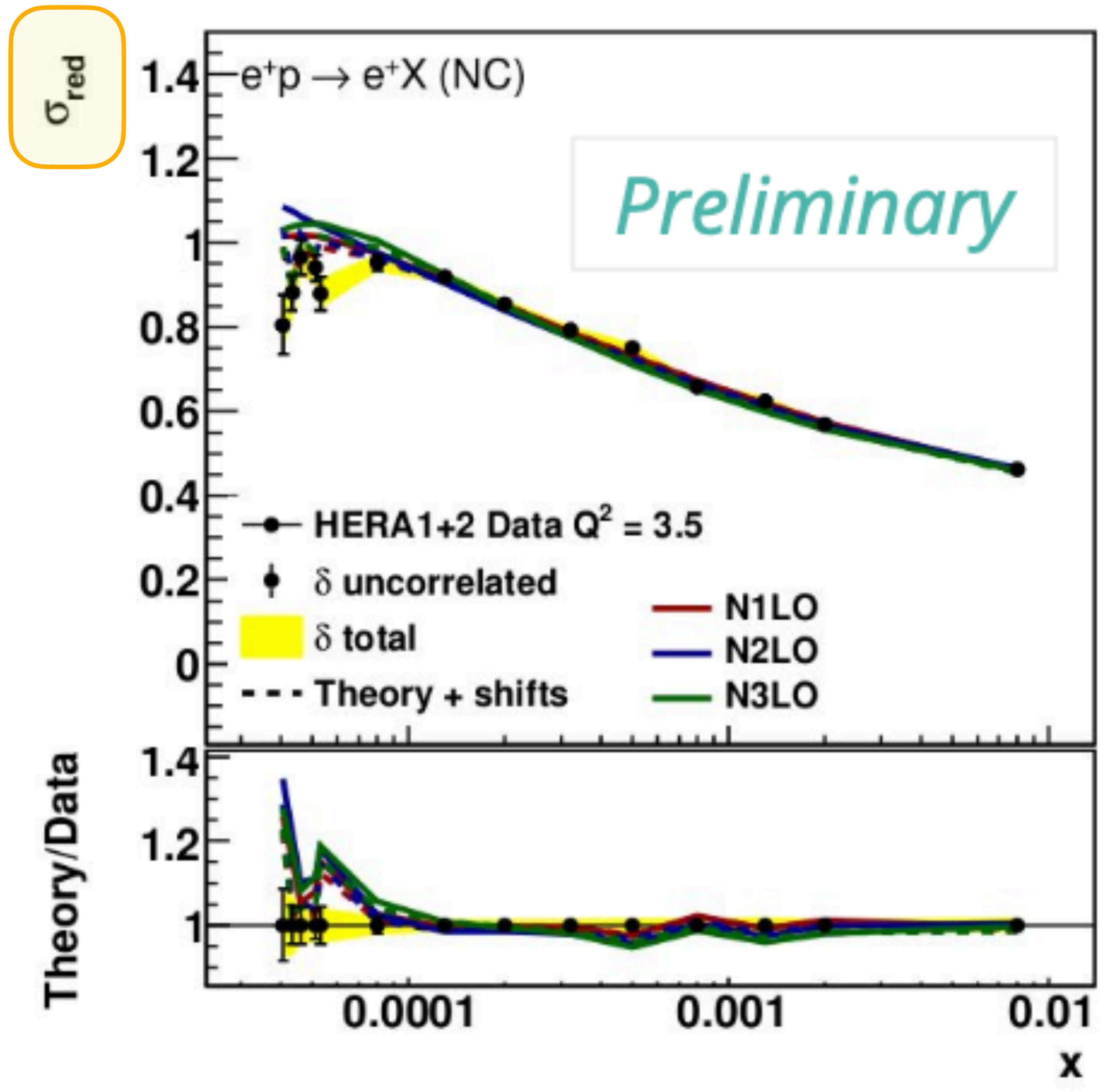
Fit results at N3LO

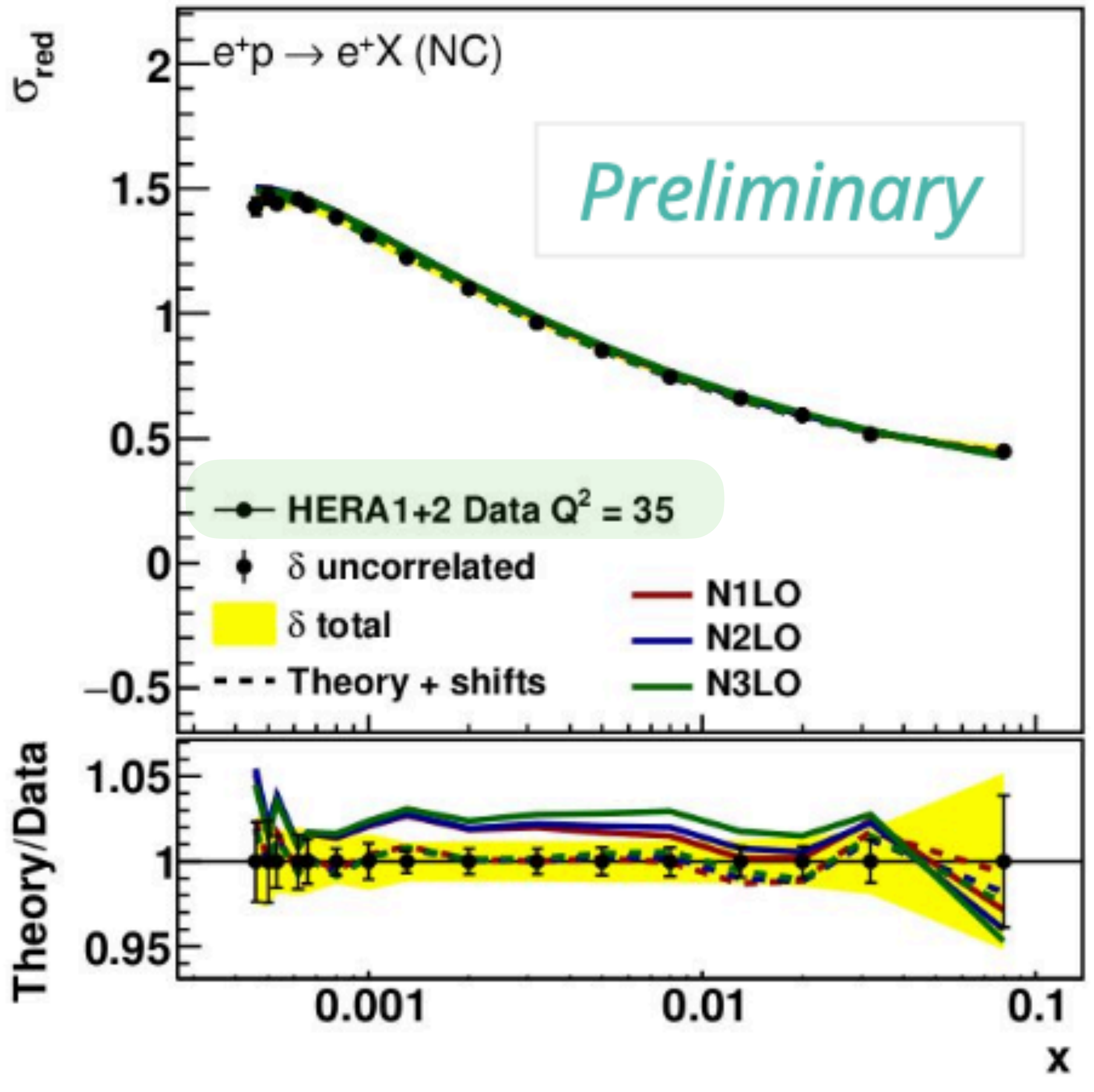
√s=920 GeV data

- Most precise HERA data: all fixed-order fits do not describe well data at lowest x / highest inelasticity y
- Slight low-x improvement at N3LO compared to N2LO

  → **need** ln(1/x)-resummation corrections — **small-x resummation** [1802.00064]
- Enhanced pre-fit normalisation: excess over data for N3LO at intermediate $Q^2 = 35\,\mathrm{GeV}^2$ (absorbed post-fit)

$$\sigma^{+}_{\mathrm{NC,red}} = F_2^{\gamma/Z} - \frac{y_-}{y_+} x F_3^{\gamma/Z} - \frac{y^2}{y_+} F_L^{\gamma/Z} \rightarrow \sigma_{\mathrm{red}}$$

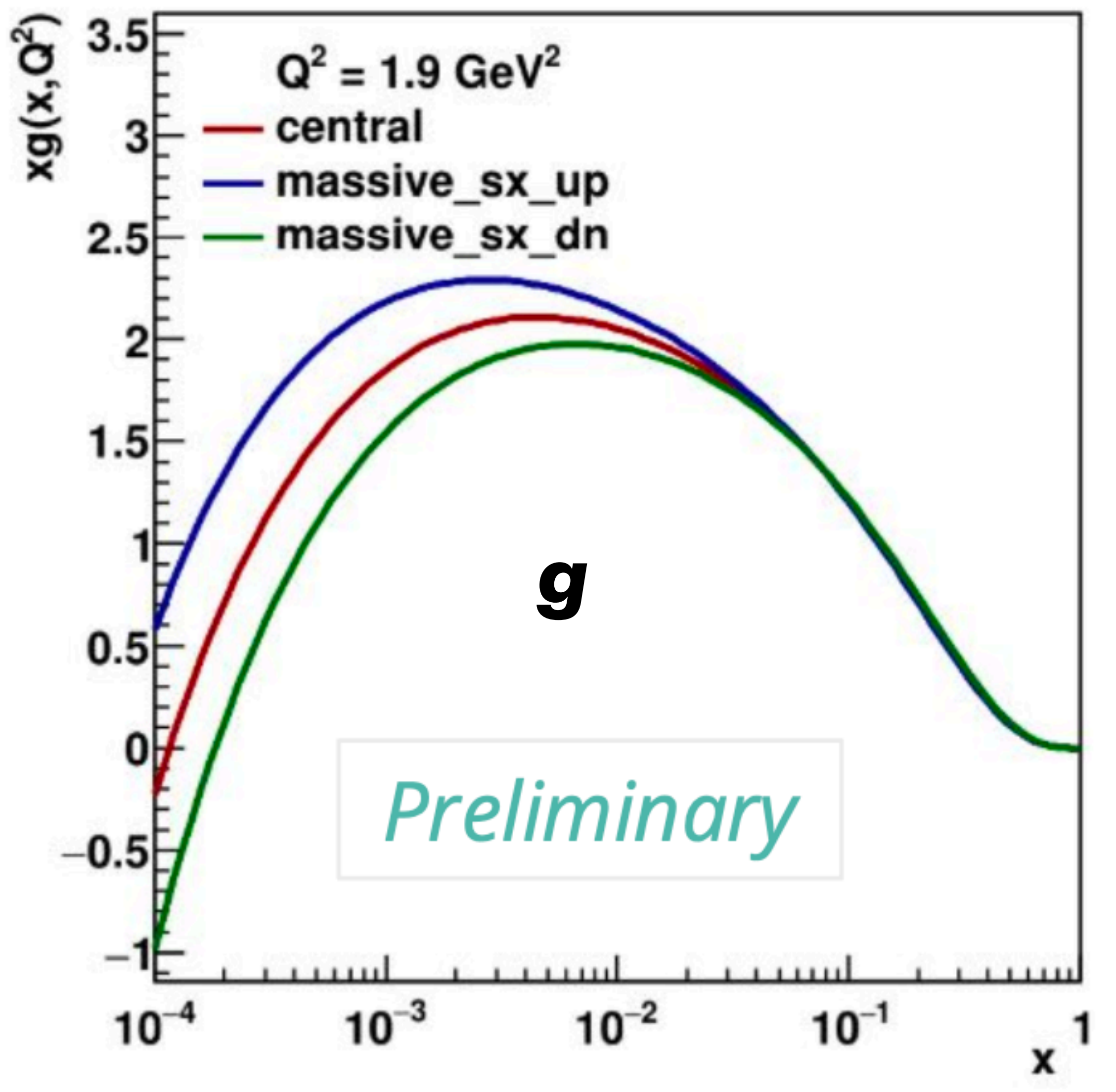


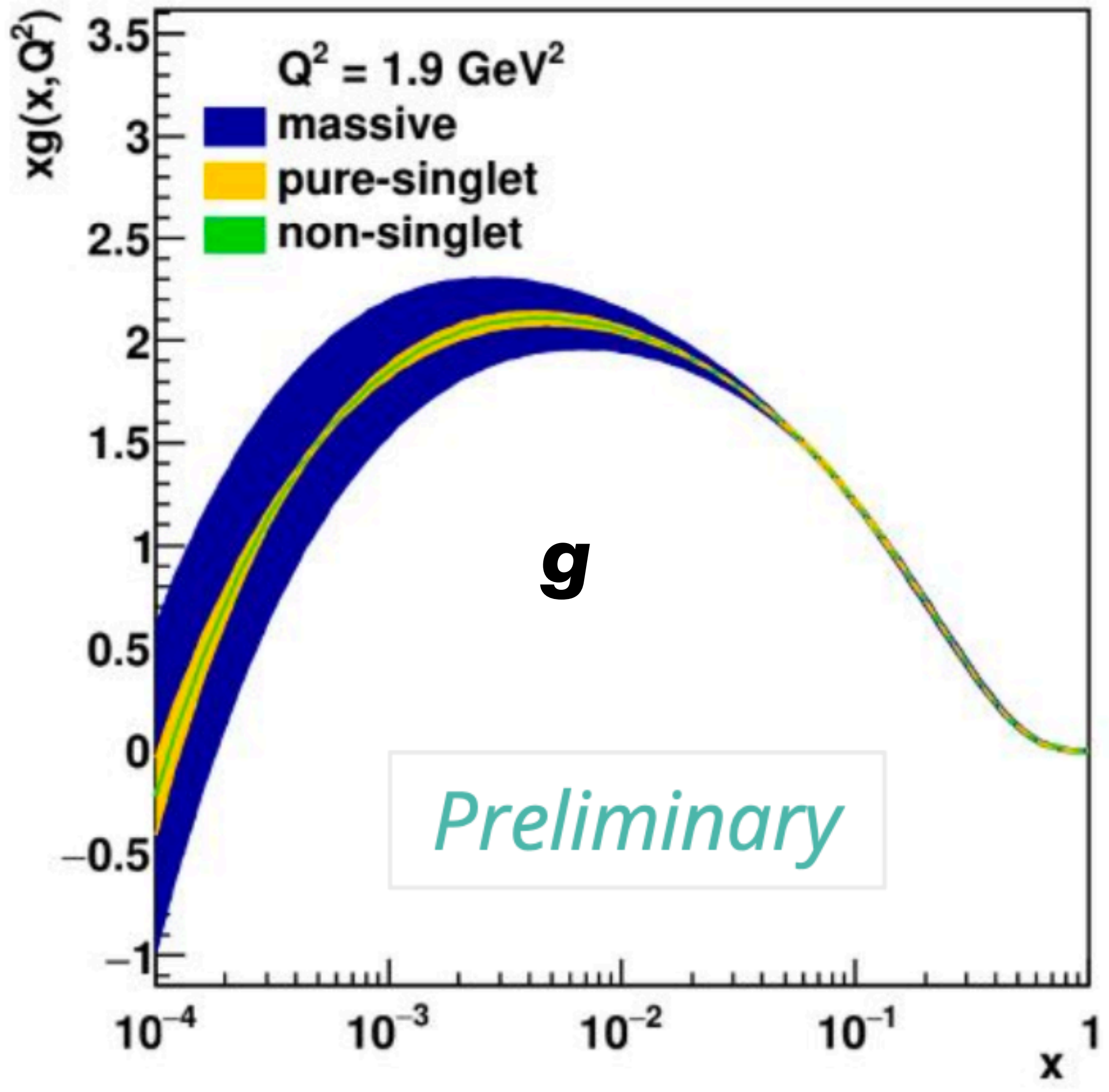


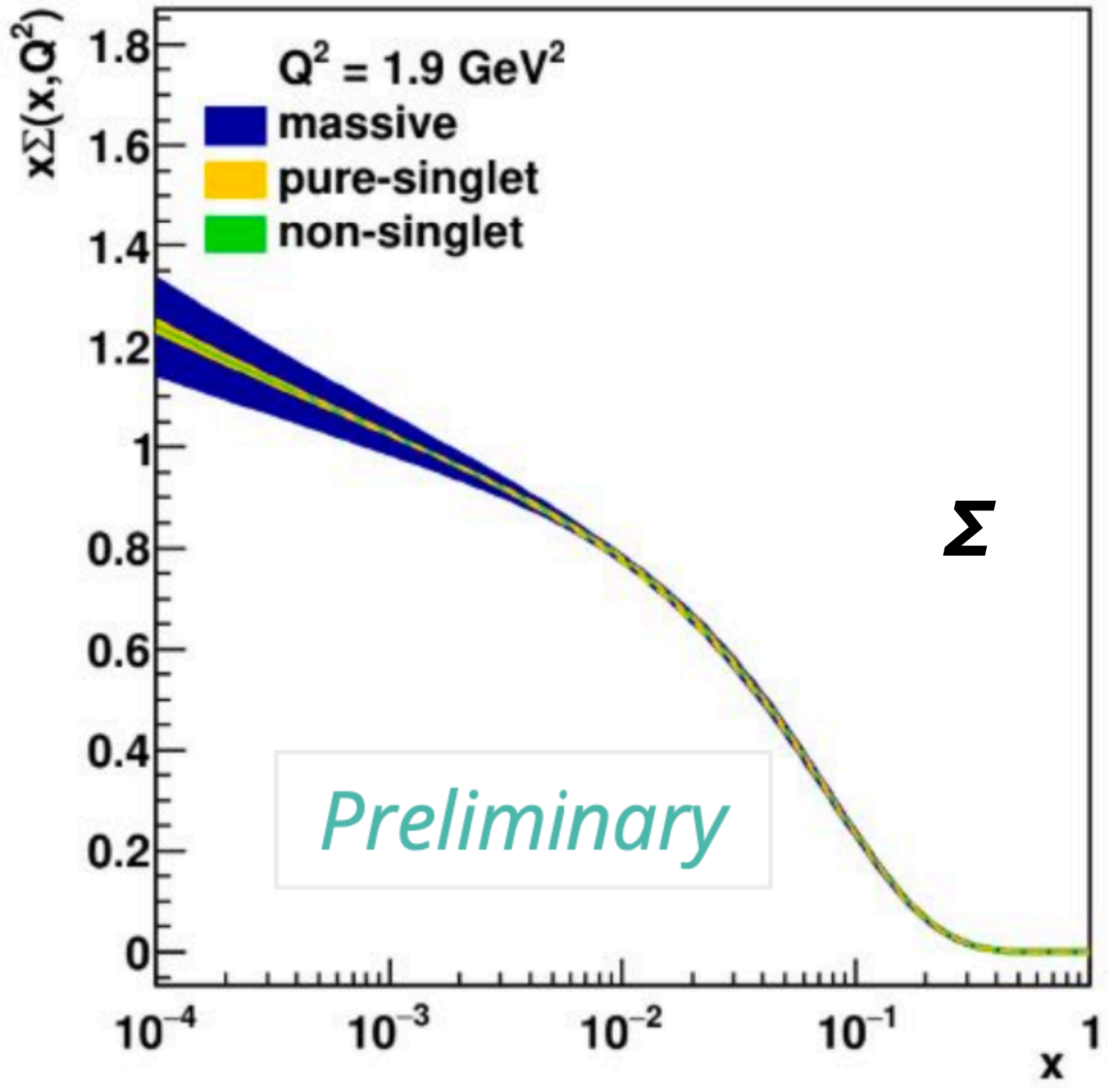
DIS coefficient functions at N3LO

Massive coefficient functions and related 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
- **Larger uncertainty** compared to variations due to approximated **singlet** and **non-singlet splitting functions**





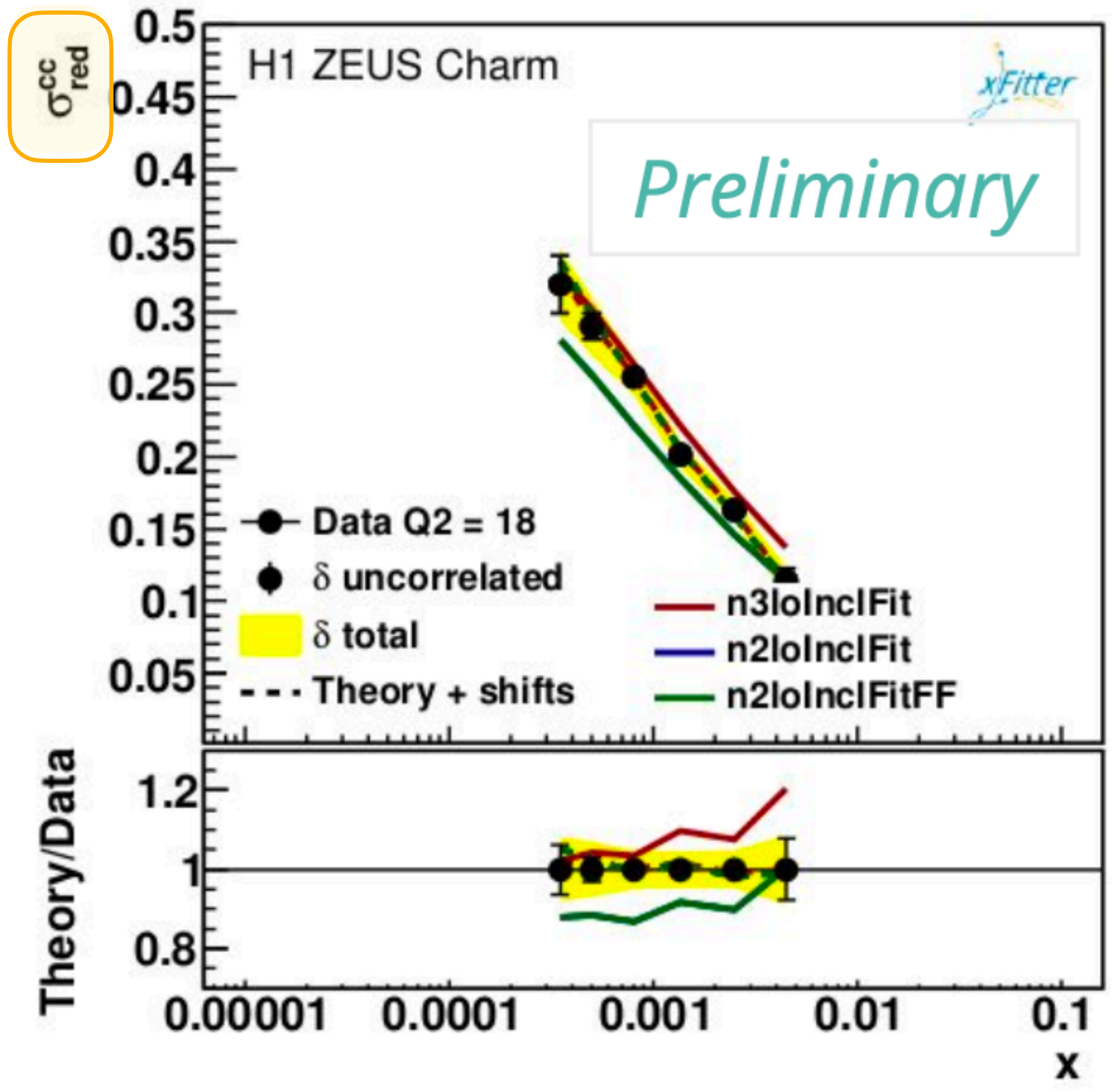


N3LO for charm data

Charm predictions from N2LO and N3LO fits

- Compare $\sigma_{\text{red}}^{c\bar{c}}$ predictions from **N2LO** and **N3LO** fits to inclusive HERA data with charm data from H1 and ZEUS combined analysis [1804.01019]

$$\sigma_{\text{red}}^{c\bar{c}} = F_2^{c\bar{c}} - \frac{y^2}{1+(1-y)^2} F_L^{c\bar{c}} \rightarrow \sigma_{\text{red}}^{cc}$$



Preliminary

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

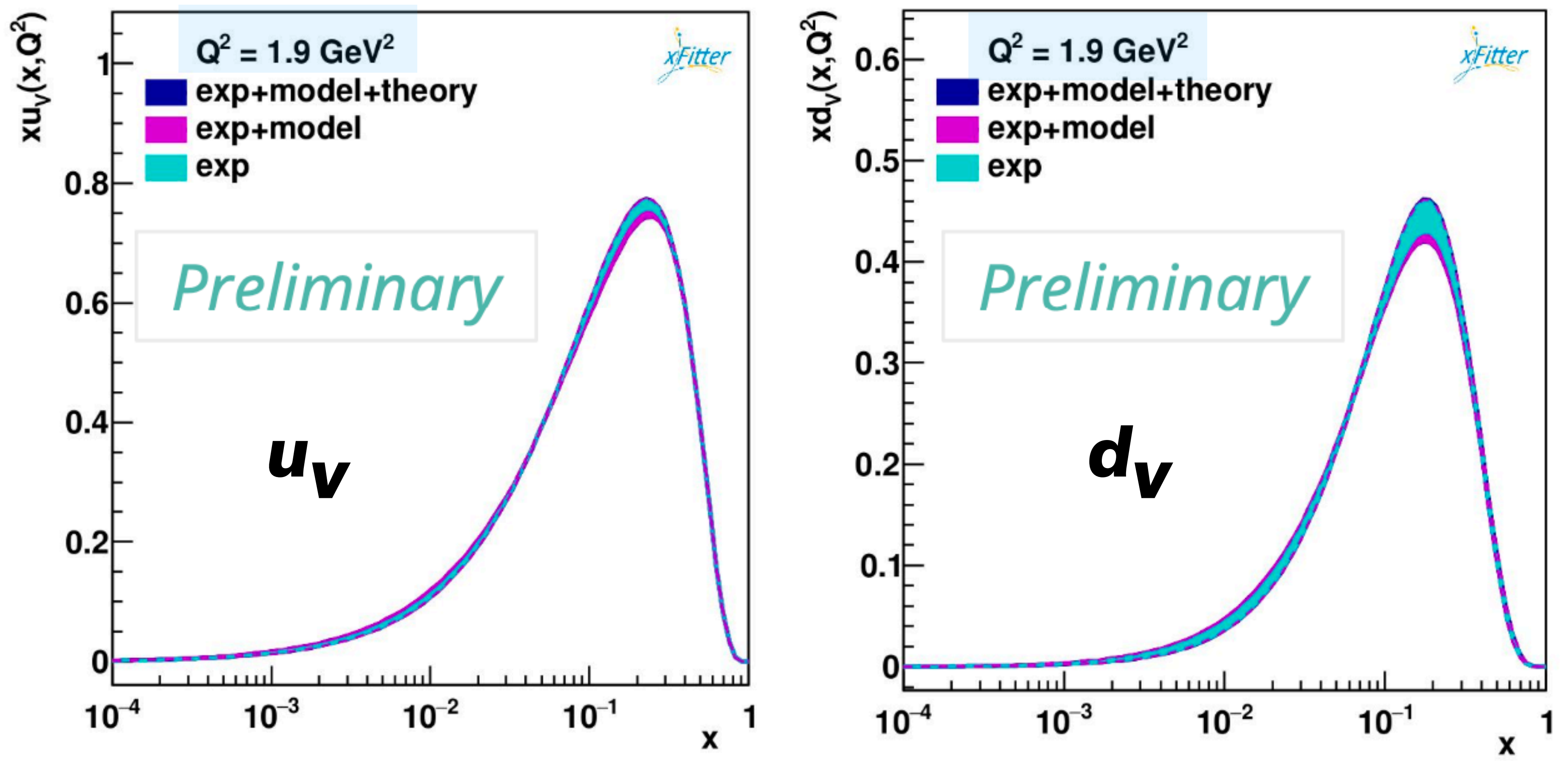
- Improved χ^2 / dof for the N3LO fit

Overview of N3LO xFitter PDFs

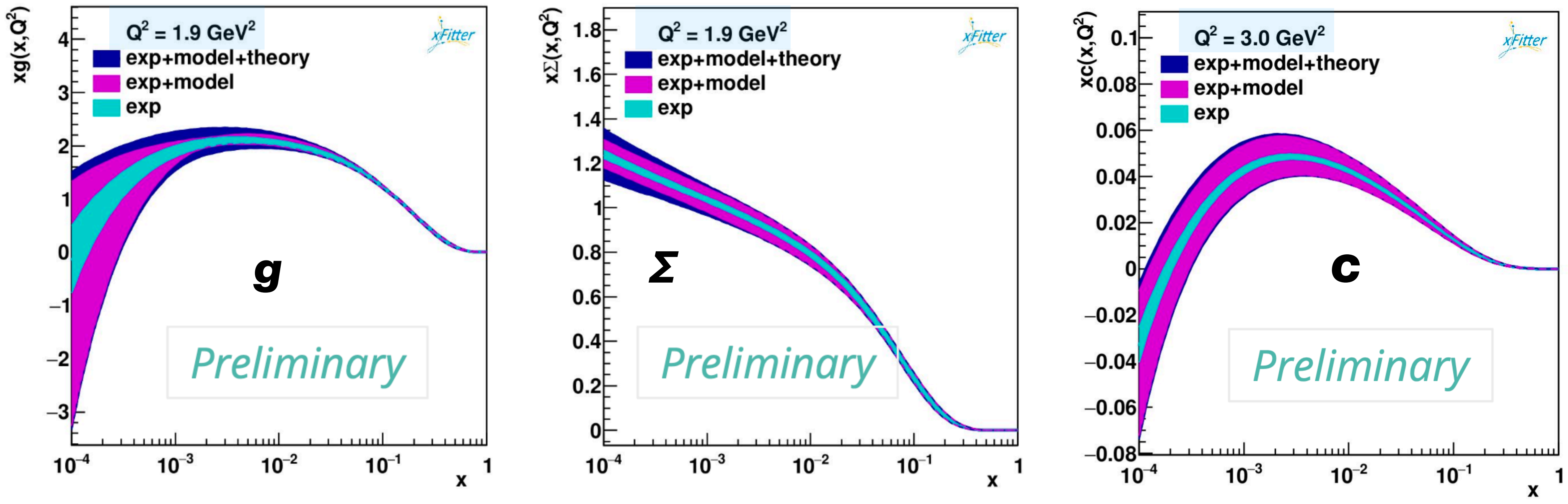
Complete PDF uncertainty *budget*

- PDFs from N3LO fit to HERA inclusive + charm and bottom data

- **Model** and **theory uncertainties** included
  - Approximation of singlet and non-singlet 4-loop splitting functions based on known Mellin moments
  - NLL small-x approximation of exact DIS massive coefficients
  - Leading model uncertainties from m_b, m_c variations



PDFs at the starting scale →



Overview of N3LO xFitter PDFs

Complete PDF uncertainty *budget*

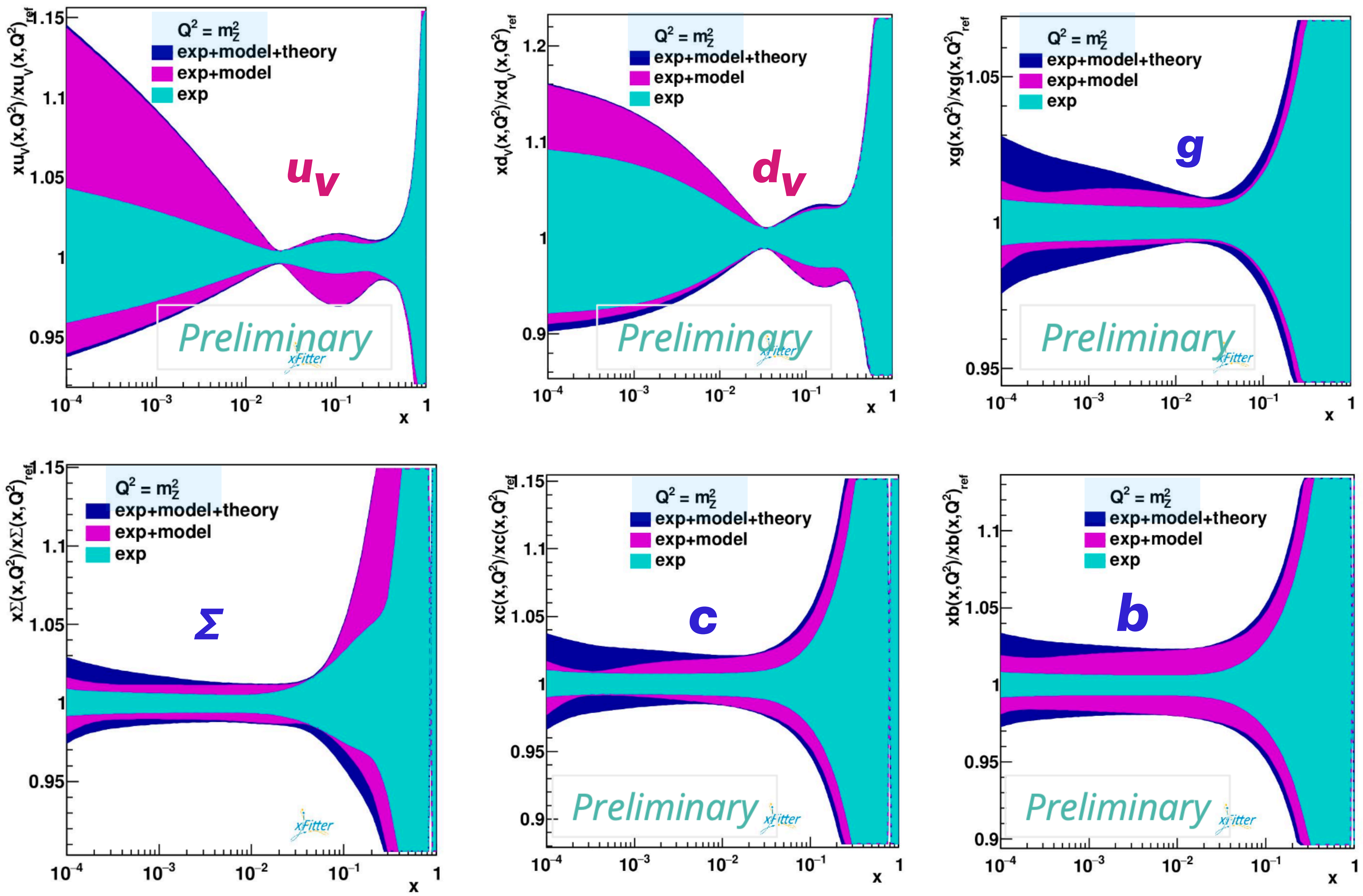
- PDFs from N3LO fit to HERA inclusive + charm and bottom data

  - **Model** and **theory uncertainties** included

- PDF relative uncertainties at $Q^2 = M_Z^2$

- Large uncertainties for ***$xd_v(x)$*** and ***$xu_v(x)$*** at low x
- Significant theory uncertainty for ***xg(x)*** at $x < 0.01$
- ***xc(x)*** and ***xb(x)*** uncertainties driven by m_c and m_B variations

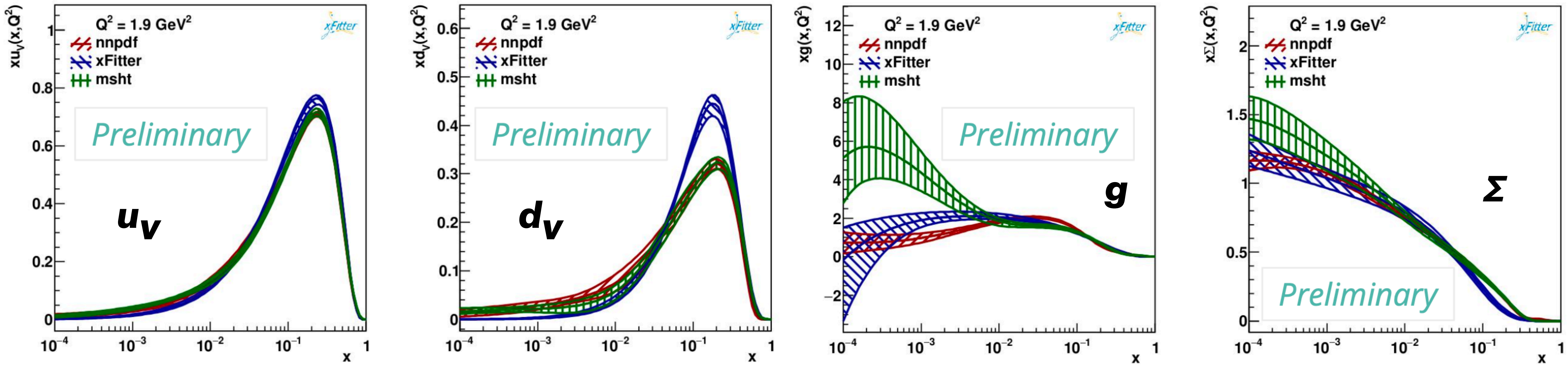
$$Q^2 = M_Z^2$$

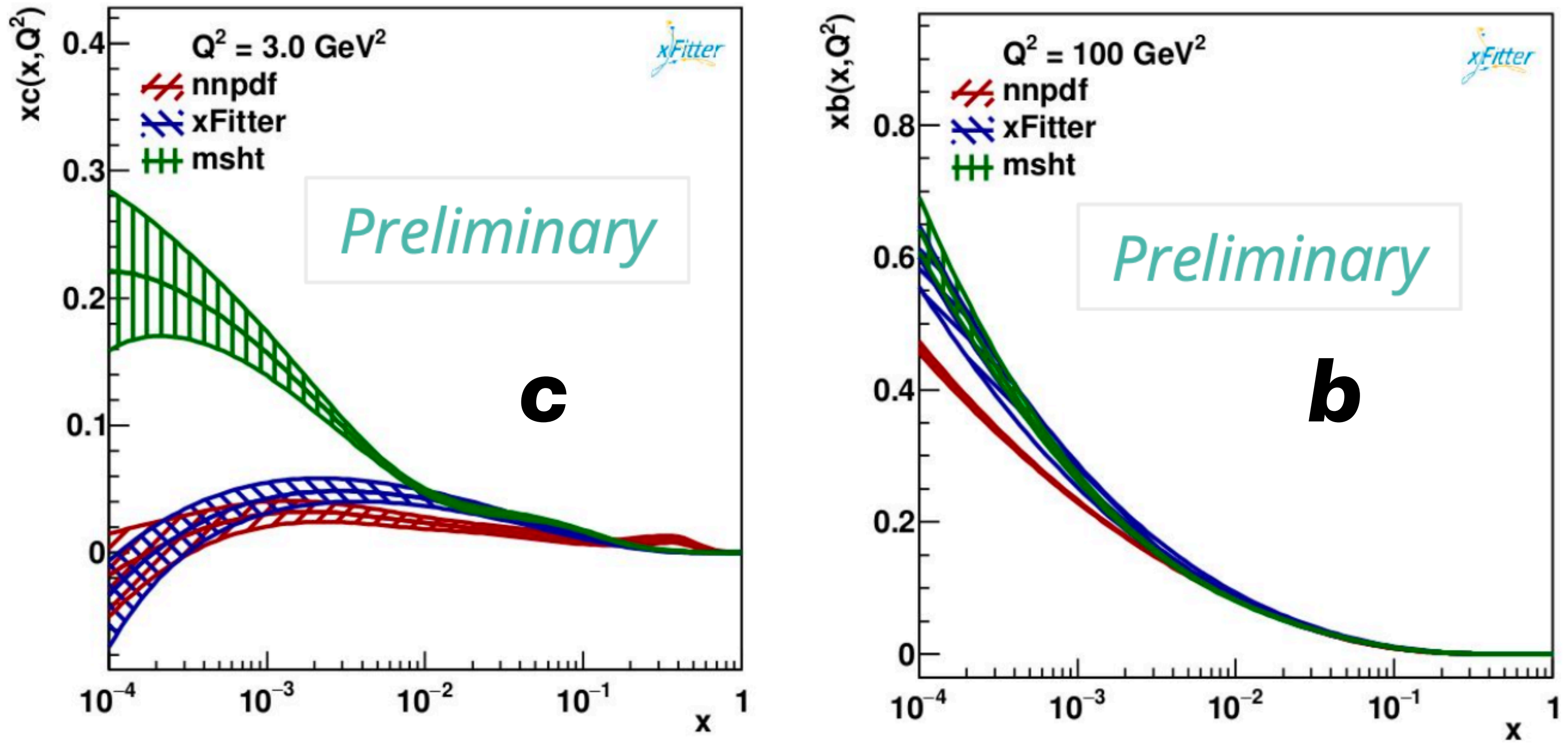


Overview of N3LO xFitter PDFs

Comparisons to existing aN3LO sets from global PDF fits

- PDFs from N3LO **xFitter fit** to HERA inclusive + charm and bottom data in comparison with **NNPDF40_an3lo** and **MSHT20an3lo**



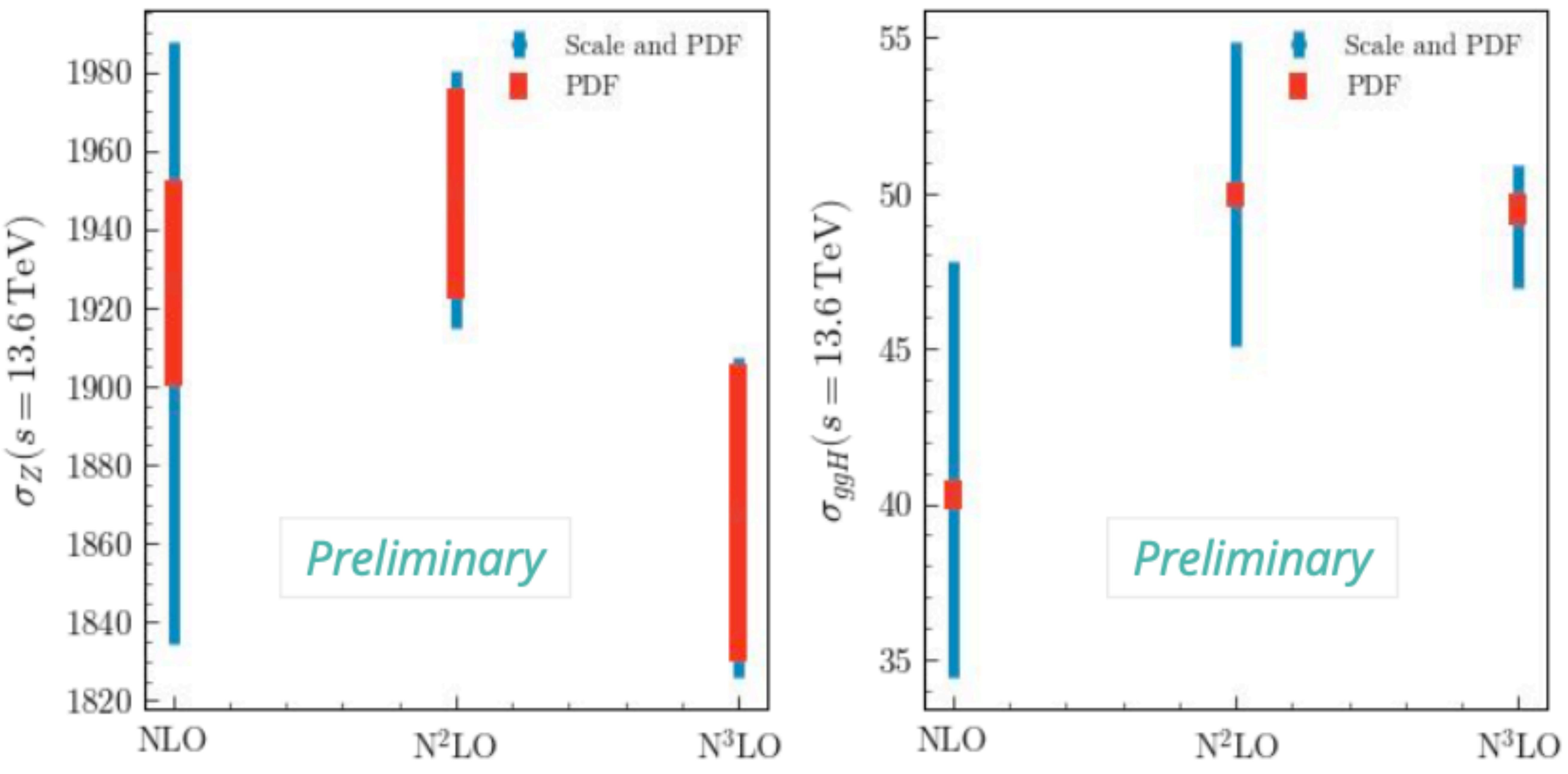


- Good overall agreement for u_v
- **xFitter** d_v in disagreement with **NNPDF40** and **MSHT20**
- **MSHT20** outlier for g and **c**
- **NNPDF40** outlier for b

xFitter N3LO PDF fit in action

Impact on LHC predictions

- **Put xFitter N3LO PDF fit in action:** compute inclusive cross sections for gluon-fusion Higgs (*ggH*) and neutral-current DY (*Z*) production with the n3loxs program [2209.06138] using xFitter PDFs



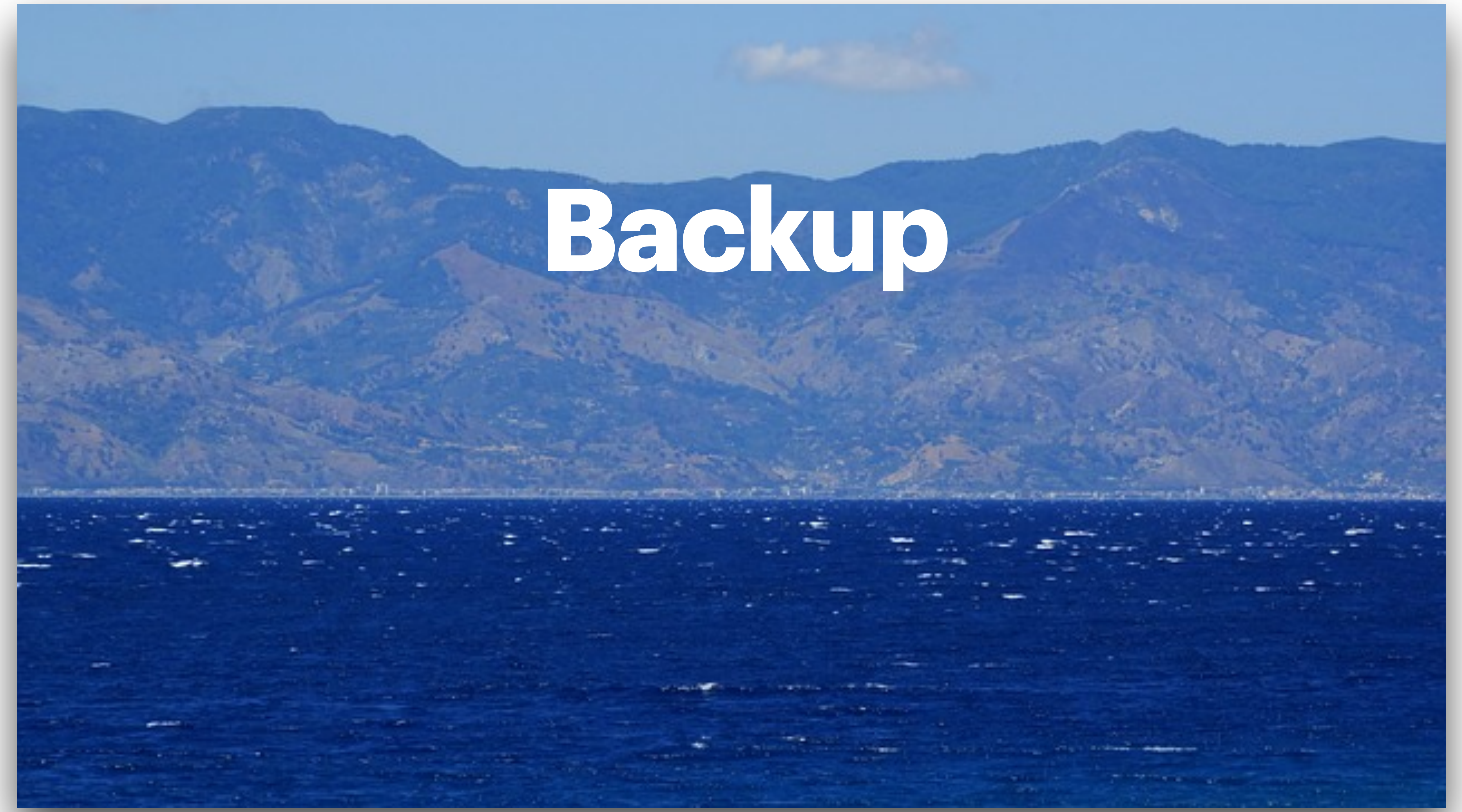
- Compare predictions at NLO, N2LO and N3LO using input PDFs from xFitter fits performed at the same perturbative accuracy
- PDF uncertainties for N3LO predictions include theory uncertainties
- Better perturbative convergence for *ggH*
- PDF uncertainty remains large for *Z* at N3LO

Conclusion

Summary and outlook

- xFitter DIS-only analysis with consistent **N3LO** modelling of **evolution** and **coefficient functions**
- **First analysis** including **exact matching** conditions
- Residual uncertainties originating from heavy flavour coefficient functions
- Visible impact on PDF (i.e. largest gluon at small-x) and predictions for the LHC
- Further **studies including small-*x* resummation** ongoing

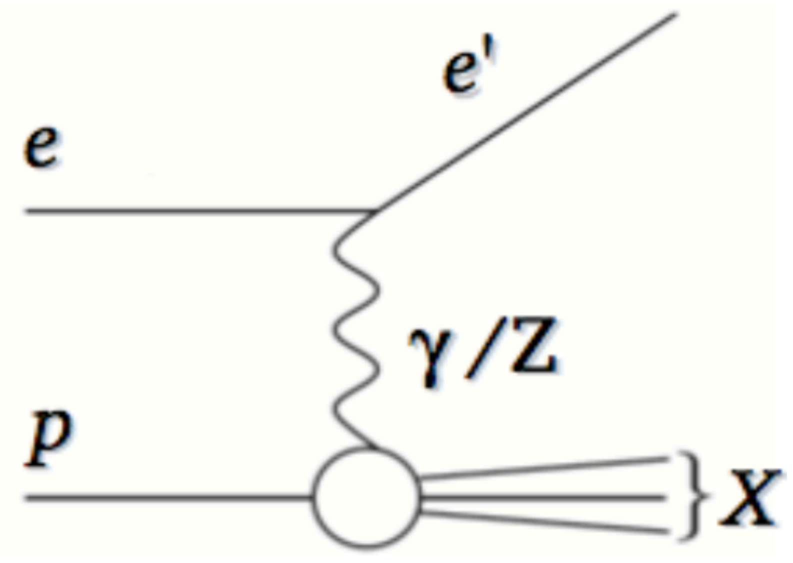
xFitter


Backup

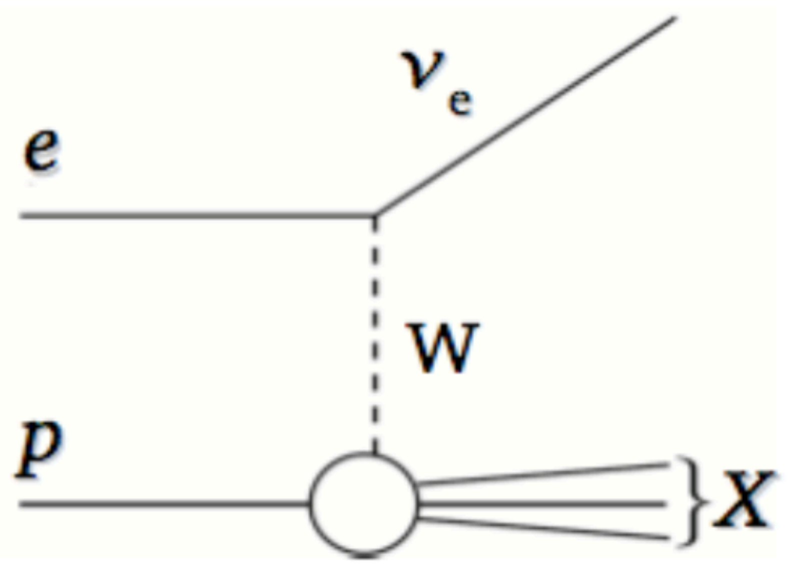
Analysis of HERA DIS data at N3LO

HERA DIS data

NC : $e\,p \rightarrow e'\,X$



CC : $e\,p \rightarrow \nu_e\,X$

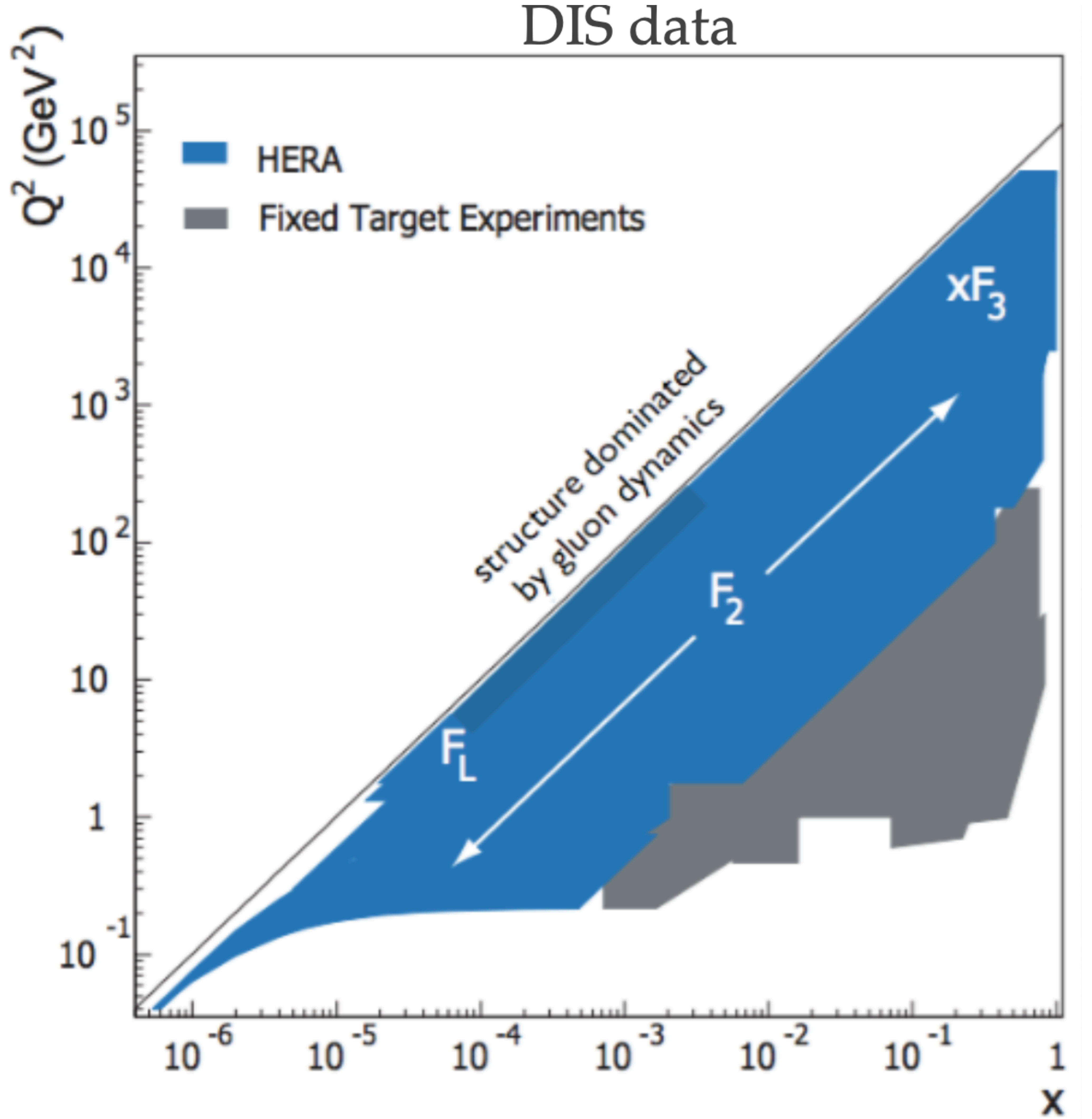


$$\frac{d\sigma^{\pm}_{NC}}{dxdQ^2} = \frac{2\pi\alpha^2}{x}\left[\frac{1}{Q^2}\right]^2\left[Y_+\tilde{F}_2 \mp Y_- x\tilde{F}_3 - y^2\tilde{F}_L\right]$$

$$\frac{d\sigma^{\pm}_{CC}}{dxdQ^2} = \frac{G_F^2}{4\,\pi\,x}\left[\frac{M_W^2}{M_W^2+Q^2}\right]^2\left[Y_+\tilde{W}_2^{\pm} \mp Y_- x\tilde{W}_3^{\pm} - y^2\tilde{W}_L^{\pm}\right]$$

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

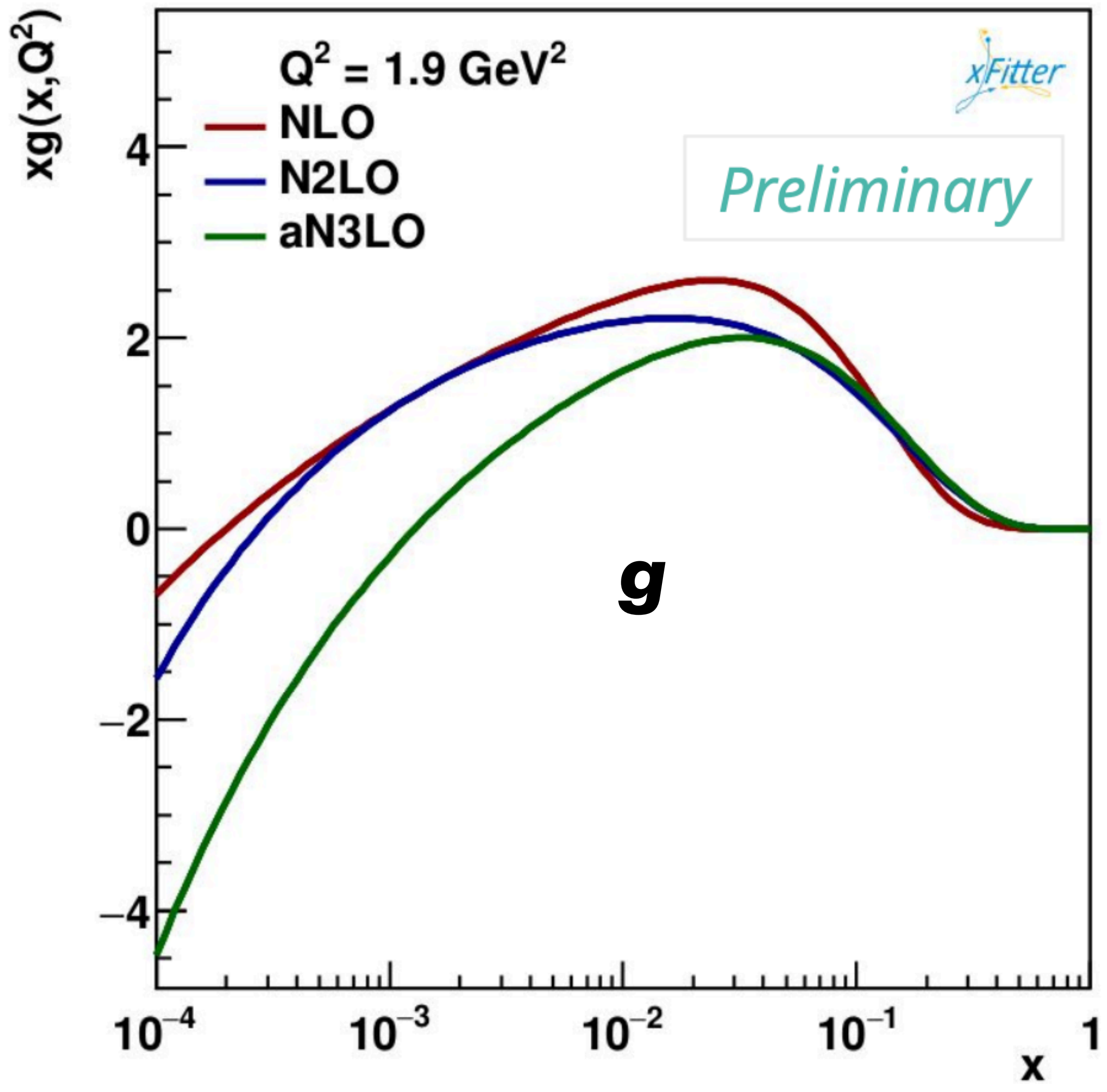
$$\tilde{F}_2 \propto \sum(xq_i + x\bar{q}_i) \quad x\tilde{F}_3 \propto \sum(xq_i - x\bar{q}_i) \quad \tilde{F}_L \propto \alpha_s \cdot xg(x,Q^2)$$



Approximate N3LO

N3LO with approximate matching vs N2LO and NLO

- Compare fits to HERA DIS data at NLO and N2LO with **approximate N3LO (aN3LO)**



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 N3LO flavour matching conditions based on MSHT20 approximation [2207.04739]

- aN3LO gluon is more negative at low x at the starting scale → **Worst $\chi2$ / dof**

Approximate N3LO

N3LO with approximate matching vs N2LO and NLO

- Prescription based on MSHT20 allows variations of approximated transition matrix elements accounting for missing corrections

- $A^{(3)}_{gg,H} = A_1 \ \ln^2(1-x) + A_2 \ \ln(1-x) + A_3 \ x^2 + A_4 \ \ln x + A_5 \ x + \boxed{a_{gg,H} \ \frac{\ln x}{x}}$ $\leftarrow -2000 < a_{gg,H} < -700$

- $-2000 < a_{gg,H} < -700$ induces large effect on gluon/charm at low x (aggh1, aggh2)