The Structure of the Proton at approximate N3LO: MSHTaN3LO PDFs

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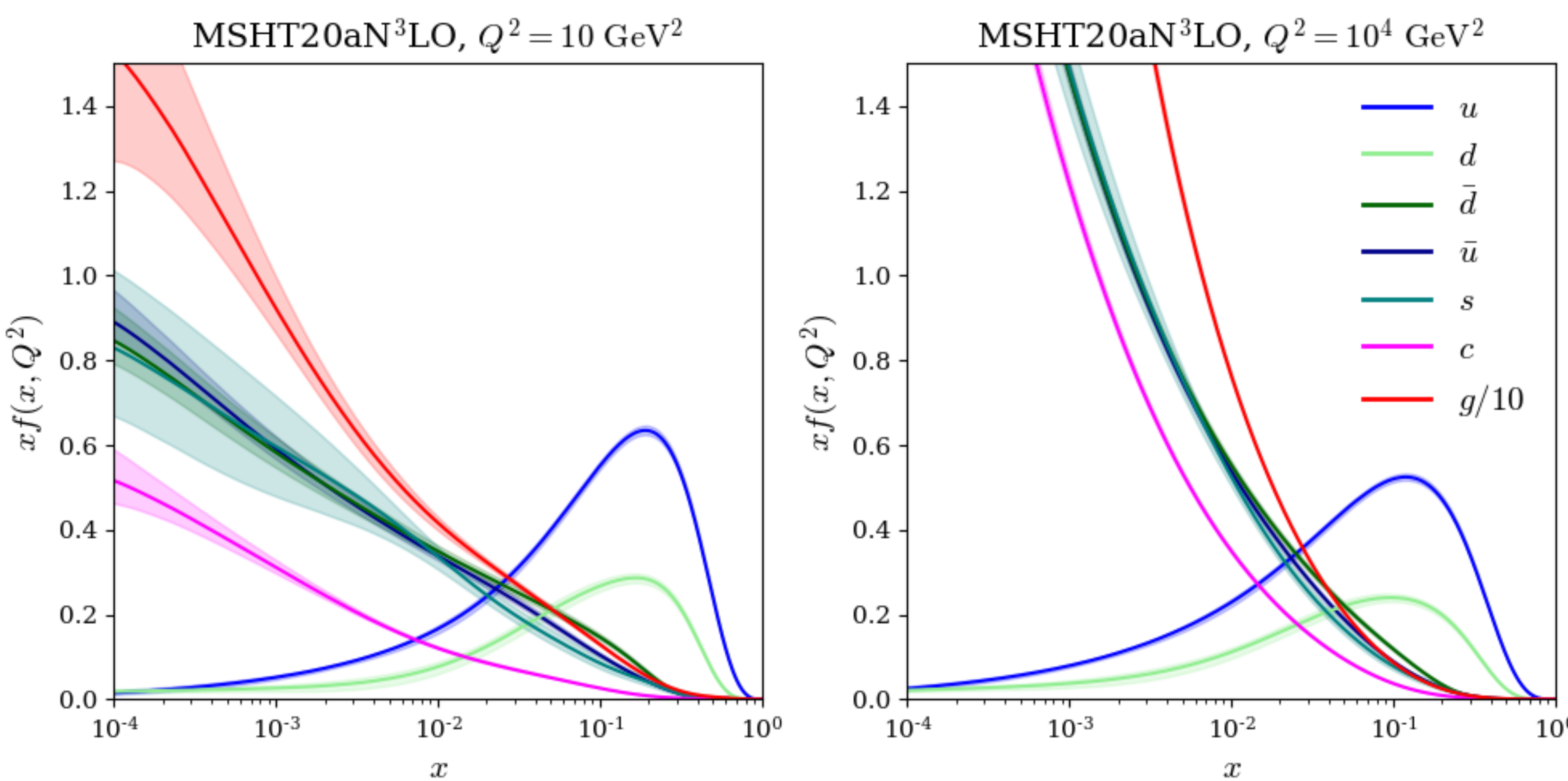
On behalf of Tom Cridge, LHL, Jamie McGowan, Robert Thorne

Based on J. McGowan et al., arXiv:2207.04739

Outline

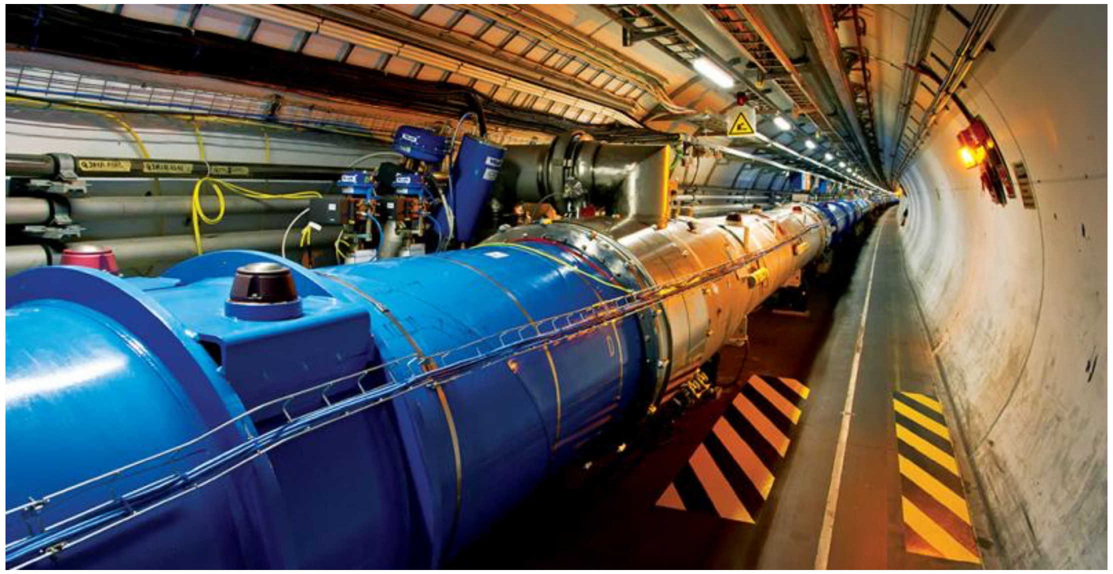
- What are **PDFs** and why are they important?
- How we do fit them?
- A PDF fit at approximate N3LO order: **MSHT20aN3LO**.

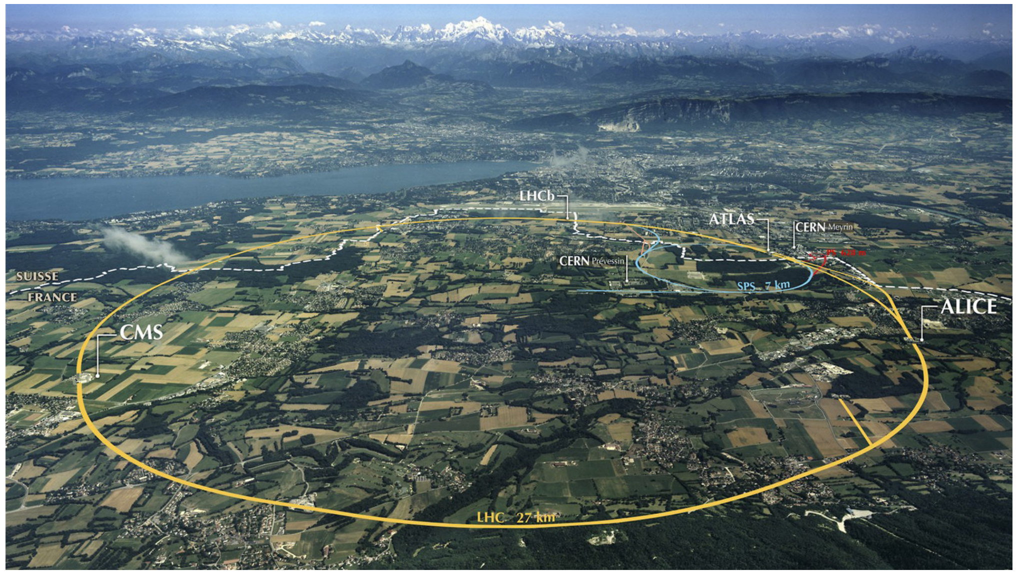


What are PDFs and how do we extract them?

The LHC: a proton-proton collider

- The **LHC** works by colliding proton beams head on at high energy.
- We examine the debris of these interactions in order to probe the Higgs sector, look for physics beyond the Standard Model (SM) and to understand the SM better.
- Before doing any of that that: we need to understand what we are colliding: the **proton.**

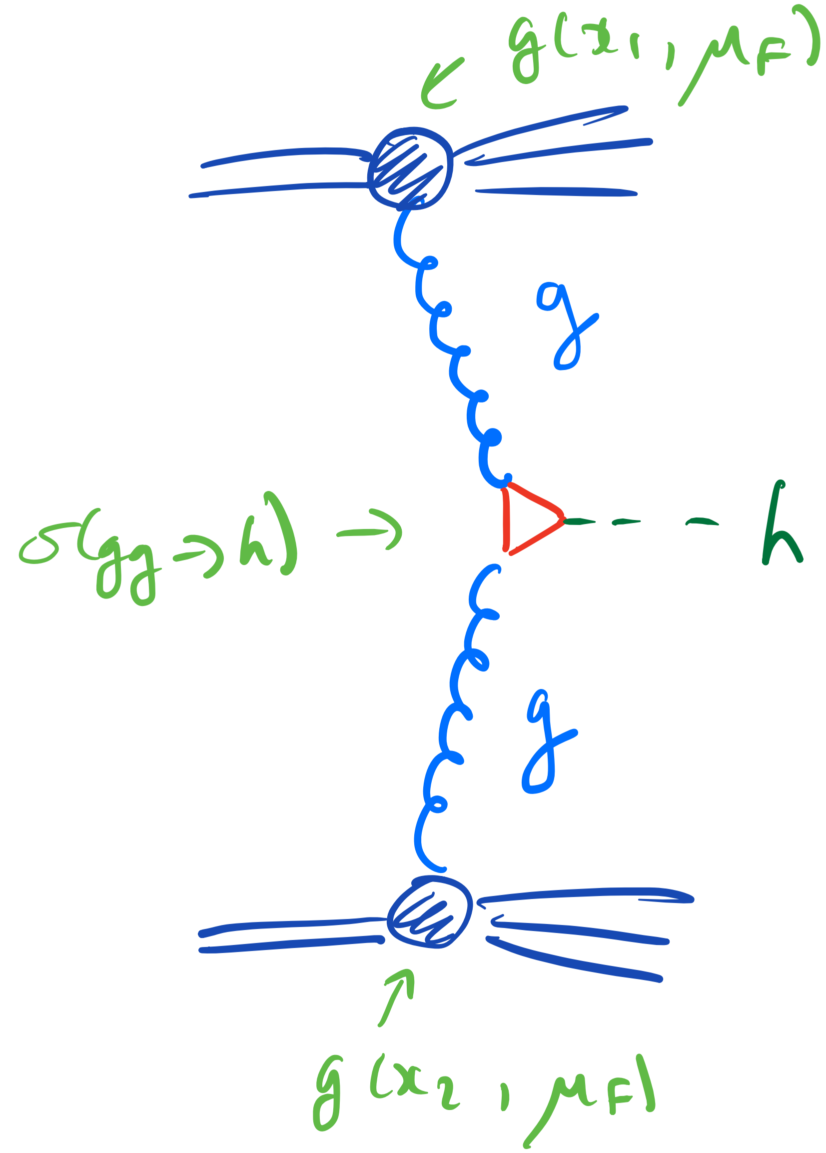




An LHC collision

- How do we model an LHC collision?

Proton is composite - collision involves quarks/gluons:



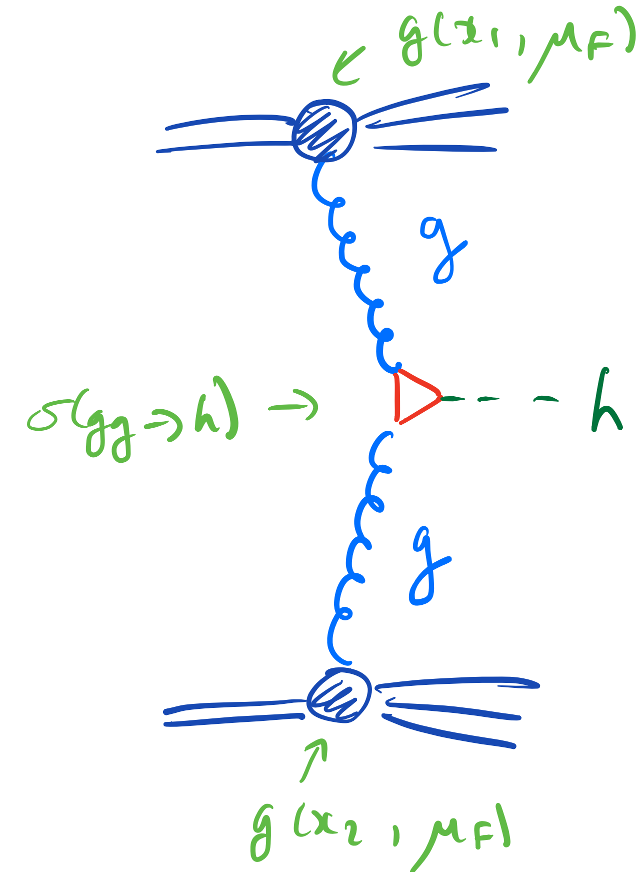
- The \`**parton model**' - proton-proton cross section is convolution of **parton-level cross section** and **Parton Distribution Functions** (PDFs)

$$\sigma(pp \to h + X) \sim \sigma(gg \to h) \otimes g(x_1, Q^2) \otimes g(x_2, Q^2) \ ,$$

$$f(x) \otimes g(x) \sim \int \mathrm{d}y f(x) g(x/y) \ ,$$

Parton Distribution Functions

$$\sigma(pp \to h + X) \sim \sigma(gg \to h) \otimes g(x_1, Q^2) \otimes g(x_2, Q^2) \ ,$$



- Cross section given in terms of:

$\sigma(gg \to h)$: parton-level cross section. $\alpha_S(m_h) \ll 1 \Rightarrow$ perturbative expansion in α_S :

$$\sigma(gg \to h) = \alpha_S(m_h)^2(\sigma_0 + \alpha_S(m_h)\sigma_1 + \cdots)$$

$g(x, Q^2)$: PDF for gluon

x - proton longitudinal **momentum fraction**.

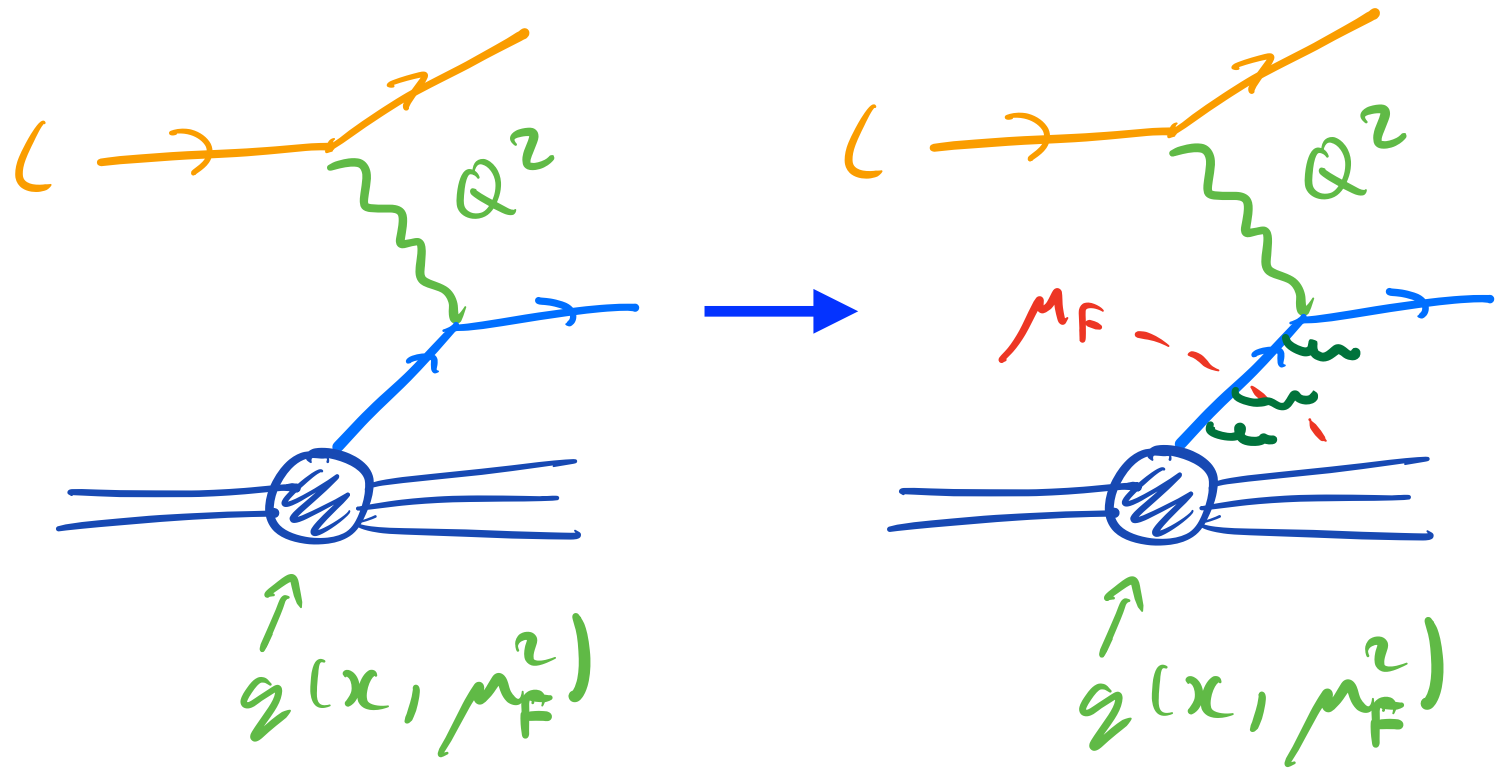
Q - **factorization scale** ~ energy of quark/gluon collision ~ inverse of resolution length.

- At lowest order PDF is probability of finding gluon in the proton carrying momentum fraction x .

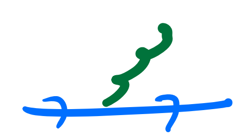
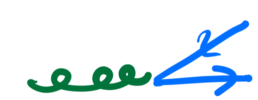
DGLAP

- Quark/gluons like to radiate $\Rightarrow$ PDFs depend on resolution scale. Formally, **factorization** in QCD requires introduction of a scale μ_F

$$\sigma^{lp} \sim \sigma^{lq}(\mu_F) \otimes q(x, \mu_F)$$

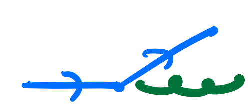


- Requiring that cross section is independent of this to calculated order in α_S gives **DGLAP** evolution equation, e.g.

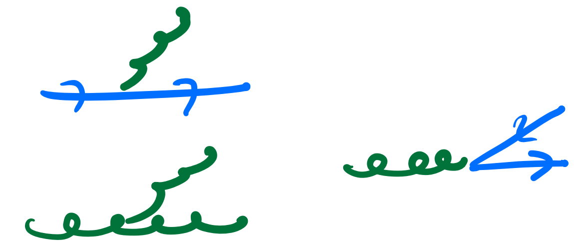



$$\frac{\mathrm{d}\sigma^{lp}}{\mathrm{d}\mu_F} = 0 + \text{higher orders} \rightarrow \frac{\partial q(x,\mu)}{\partial \mu} = P_{qq} \otimes q(x,\mu) + P_{qg} \otimes g(x,\mu)$$

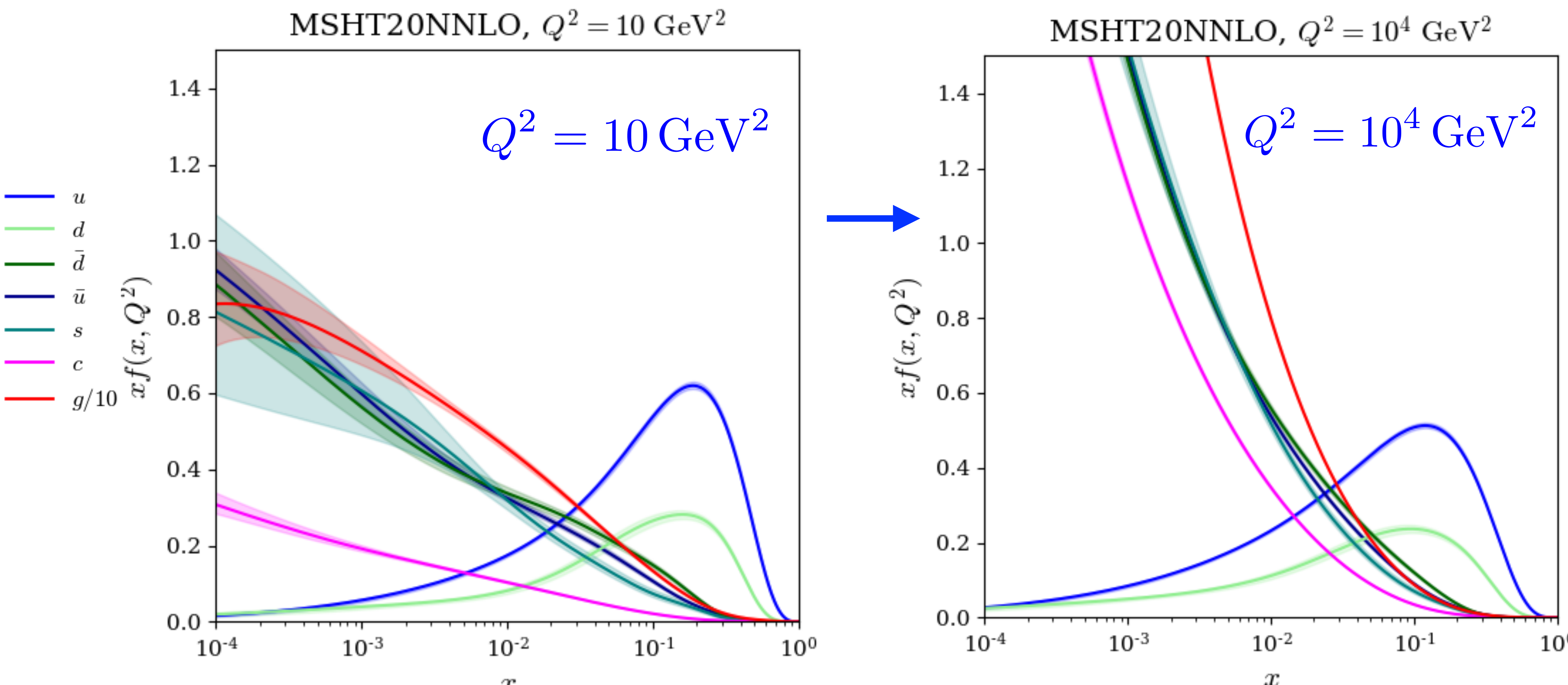
Similarly for gluon: $$\frac{\partial g(x,\mu)}{\partial \mu} = P_{gq} \otimes q(x,\mu) + P_{gg} \otimes g(x,\mu)$$




- Splitting functions P_{ij} encode $j \to i$ QCD splitting probability. Can calculate order by order in pQCD.

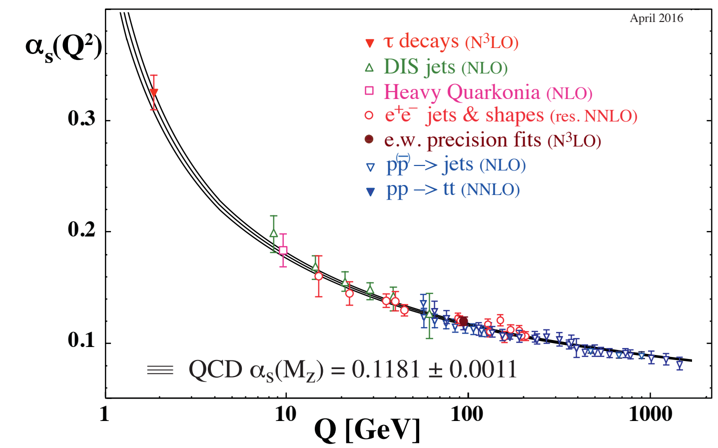


- Basic impact of DGLAP simple: higher $Q^2 \Rightarrow$ more $q, \overline{q}, g$ at low x, less at high x, due to radiation ($q \to qg, g \to q\bar{q}, g \to gg$...).



- **DGLAP** $\Rightarrow$ PDFs at lower scale determine PDFs at higher scales. Thus fits parameterise at low scale Q_0 and fit to a range of energies.

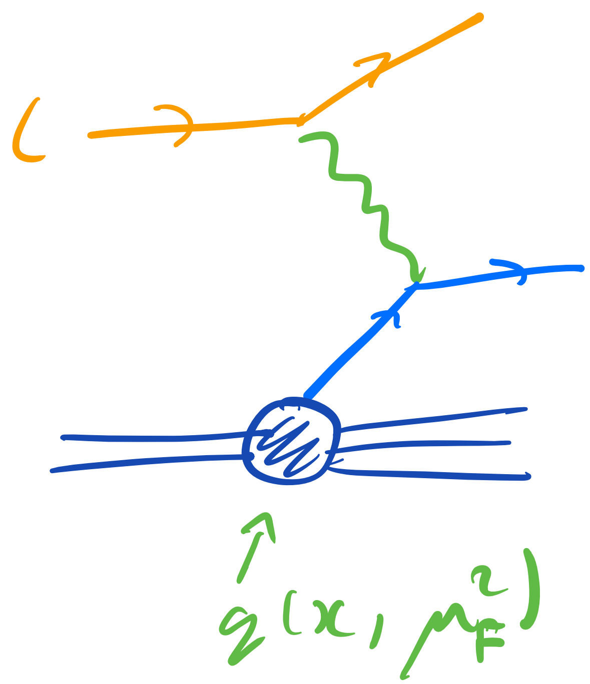
Extracting PDFs



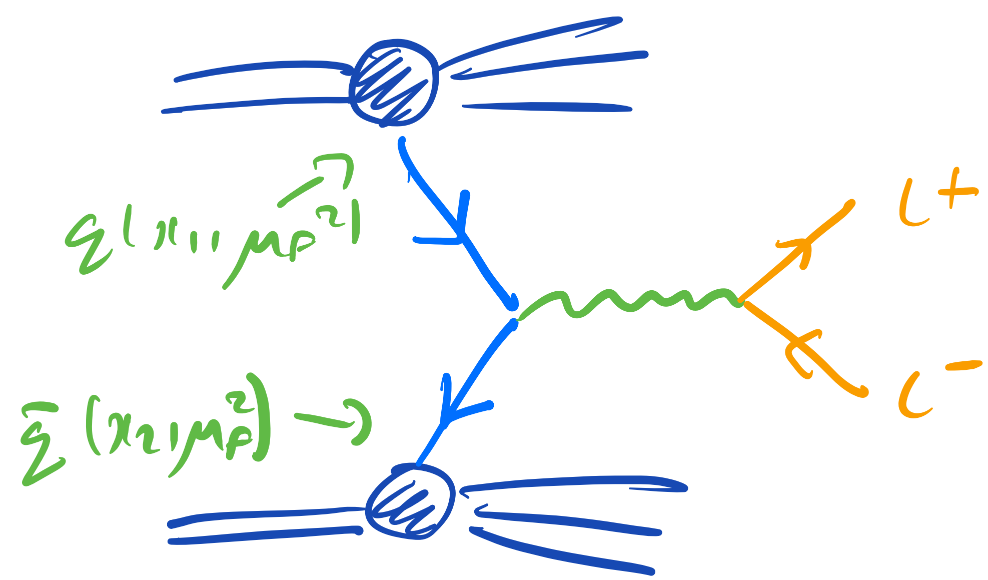
- Binding of quark/gluons in proton due to low-energy QCD ⇒ **cannot** use perturbation theory.

- However **PDFs** are **universal**: same quark (antiquark) PDFs enter DIS and Drell-Yan cross sections.

DIS:



DY:

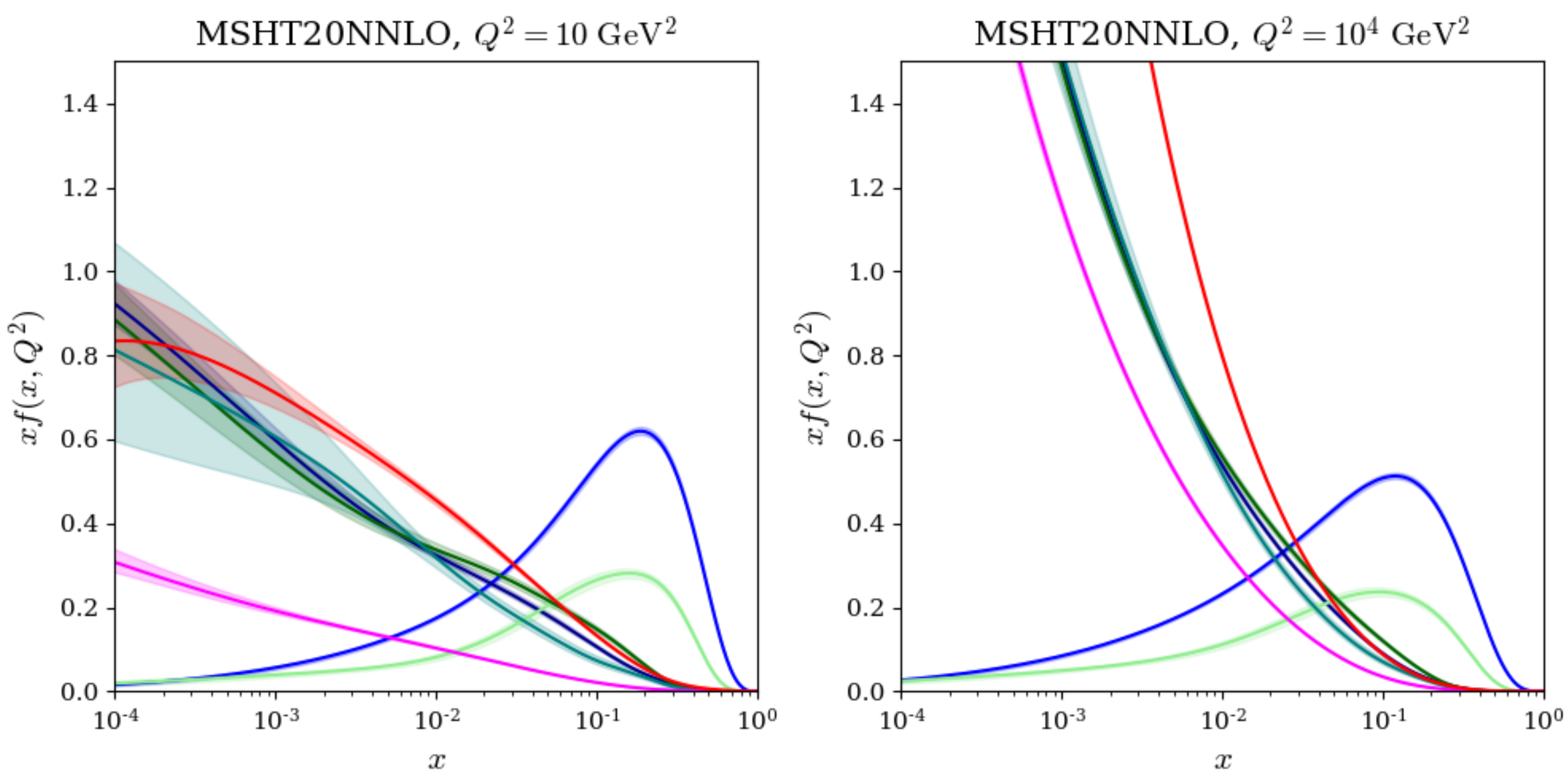


$$\text{Factorization} \Rightarrow q_{DIS}(x, Q^2) \equiv q_{DY}(x, Q^2)$$

⟶ **Fit** PDFs to one dataset (e.g. DIS) and use to make prediction for another (e.g. DY).

PDF Fits

- For LHC (and elsewhere) aim to constrain PDFs to high precision for all flavours (q, $\bar{q}$, g ...) over a wide x region.
- Only so much can be done with DIS $\Rightarrow$ **MSHT** collaboration performs **global PDF fits** to wide range of data.
- One of three major global fitters (**CT, MSHT, NNPDF**).



PDF Fits: Work Flow

$$O \sim f \otimes \sigma$$

Basic idea: **measure (data)** → O; **fit** → f; **predict (pQCD)** → σ

In detail...

Parameterise PDFs at low scale Q_0

↓

Select data & theory

↓

Perform fit

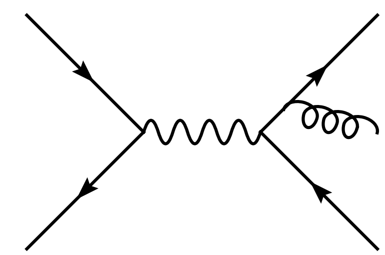
↓

Output PDFs

$$f_i(x, Q_0):\ A_f x^{a_f}(1-x)^{b_f} \times \to \sum_{i=1}^{n} \alpha_{f,i} P_i(y(x))\,,$$ **CT, MSHT...**

$$\to \mathrm{NN}_i(x)$$ **NNPDF**

Perturbative QCD for parton-level theory



$+ \ldots$

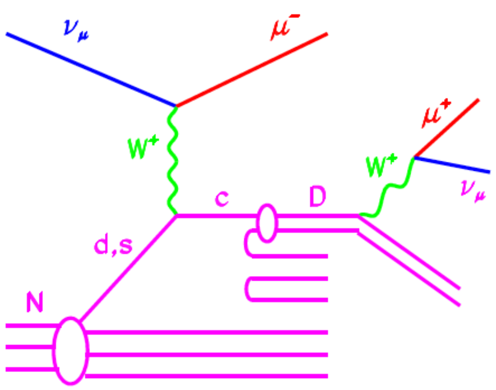
Minimise $\chi^2(\{a\},\{\lambda\}) = \sum_{k=1}^{N_{pt}} \frac{1}{s_k^2}\left(D_k - T_k - \sum_{\alpha=1}^{N_\lambda} \beta_{k,\alpha}\lambda_\alpha\right)^2 + \sum_{\alpha=1}^{N_\lambda} \lambda_\alpha^2\,,$

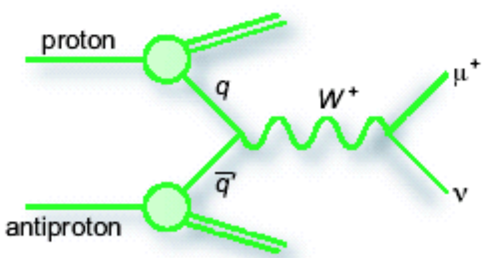
DGLAP: $f(x, Q_0) \to f(x, \mu_{\mathrm{data}})$

$$f(x,\mu) \pm \Delta(x,\mu)$$

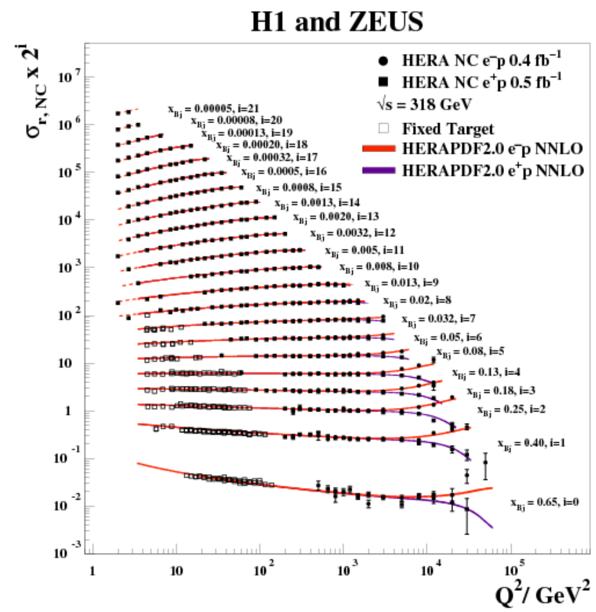
Due to error in data in fit

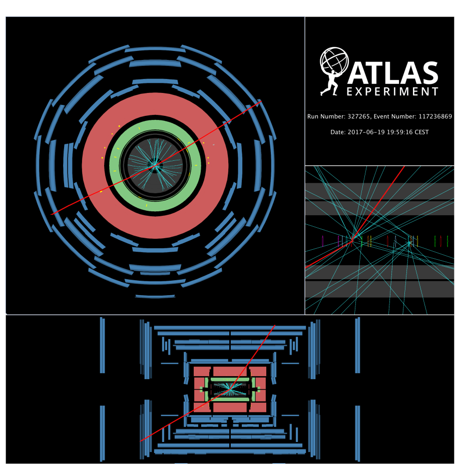
Global Fits: Datasets

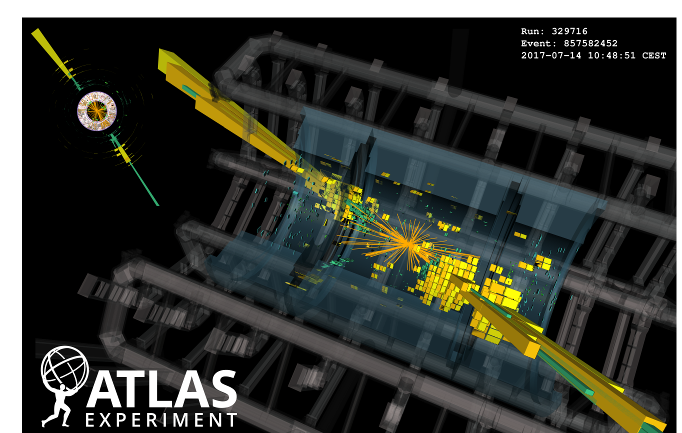




	Process	Subprocess	Partons	x range
Fixed Target	$\ell^\pm\{p,n\} \to \ell^\pm + X$	$\gamma^* q \to q$	$q, \bar{q}, g$	$x \gtrsim 0.01$
	$\ell^\pm\, n/p \to \ell^\pm + X$	$\gamma^*\, d/u \to d/u$	d/u	$x \gtrsim 0.01$
	$pp \to \mu^+\mu^- + X$	$u\bar{u}, d\bar{d} \to \gamma^*$	$\bar{q}$	$0.015 \lesssim x \lesssim 0.35$
	$pn/pp \to \mu^+\mu^- + X$	$(u\bar{d})/(u\bar{u}) \to \gamma^*$	$\bar{d}/\bar{u}$	$0.015 \lesssim x \lesssim 0.35$
	$\nu(\bar{\nu})\, N \to \mu^-(\mu^+) + X$	$W^* q \to q'$	$q, \bar{q}$	$0.01 \lesssim x \lesssim 0.5$
	$\nu\, N \to \mu^-\mu^+ + X$	$W^* s \to c$	s	$0.01 \lesssim x \lesssim 0.2$
	$\bar{\nu}\, N \to \mu^+\mu^- + X$	$W^* \bar{s} \to \bar{c}$	$\bar{s}$	$0.01 \lesssim x \lesssim 0.2$
Collider DIS	$e^\pm\, p \to e^\pm + X$	$\gamma^* q \to q$	$g, q, \bar{q}$	$0.0001 \lesssim x \lesssim 0.1$
	$e^+\, p \to \bar{\nu} + X$	$W^+\{d,s\} \to \{u,c\}$	d, s	$x \gtrsim 0.01$
	$e^\pm p \to e^\pm\, c\bar{c} + X$	$\gamma^* c \to c,\, \gamma^* g \to c\bar{c}$	c, g	$10^{-4} \lesssim x \lesssim 0.01$
	$e^\pm p \to e^\pm\, b\bar{b} + X$	$\gamma^* b \to b,\, \gamma^* g \to b\bar{b}$	b, g	$10^{-4} \lesssim x \lesssim 0.01$
	$e^\pm p \to \text{jet} + X$	$\gamma^* g \to q\bar{q}$	g	$0.01 \lesssim x \lesssim 0.1$
Tevatron	$p\bar{p} \to \text{jet} + X$	$gg, qg, qq \to 2j$	g, q	$0.01 \lesssim x \lesssim 0.5$
	$p\bar{p} \to (W^\pm \to \ell^\pm\nu) + X$	$ud \to W^+, \bar{u}\bar{d} \to W^-$	$u, d, \bar{u}, \bar{d}$	$x \gtrsim 0.05$
	$p\bar{p} \to (Z \to \ell^+\ell^-) + X$	$uu, dd \to Z$	u, d	$x \gtrsim 0.05$
	$p\bar{p} \to t\bar{t} + X$	$qq \to t\bar{t}$	q	$x \gtrsim 0.1$
LHC	$pp \to \text{jet} + X$	$gg, qg, q\bar{q} \to 2j$	g, q	$0.001 \lesssim x \lesssim 0.5$
	$pp \to (W^\pm \to \ell^\pm\nu) + X$	$u\bar{d} \to W^+, d\bar{u} \to W^-$	$u, d, \bar{u}, \bar{d}, g$	$x \gtrsim 10^{-3}$
	$pp \to (Z \to \ell^+\ell^-) + X$	$q\bar{q} \to Z$	$q, \bar{q}, g$	$x \gtrsim 10^{-3}$
	$pp \to (Z \to \ell^+\ell^-) + X,\, p_\perp$	$gq(\bar{q}) \to Zq(\bar{q})$	$g, q, \bar{q}$	$x \gtrsim 0.01$
	$pp \to (\gamma^* \to \ell^+\ell^-) + X$, Low mass	$q\bar{q} \to \gamma^*$	$q, \bar{q}, g$	$x \gtrsim 10^{-4}$
	$pp \to (\gamma^* \to \ell^+\ell^-) + X$, High mass	$q\bar{q} \to \gamma^*$	$\bar{q}$	$x \gtrsim 0.1$
	$pp \to W^+\bar{c}, W^-c$	$sg \to W^+c,\, \bar{s}g \to W^-\bar{c}$	$s, \bar{s}$	$x \sim 0.01$
	$pp \to t\bar{t} + X$	$gg \to t\bar{t}$	g	$x \gtrsim 0.01$
	$pp \to D, B + X$	$gg \to c\bar{c}, b\bar{b}$	g	$x \gtrsim 10^{-6}, 10^{-5}$
	$pp \to J/\psi, \Upsilon + pp$	$\gamma^*(gg) \to c\bar{c}, b\bar{b}$	g	$x \gtrsim 10^{-6}, 10^{-5}$
	$pp \to \gamma + X$	$gq(\bar{q}) \to \gamma q(\bar{q})$	g	$x \gtrsim 0.005$

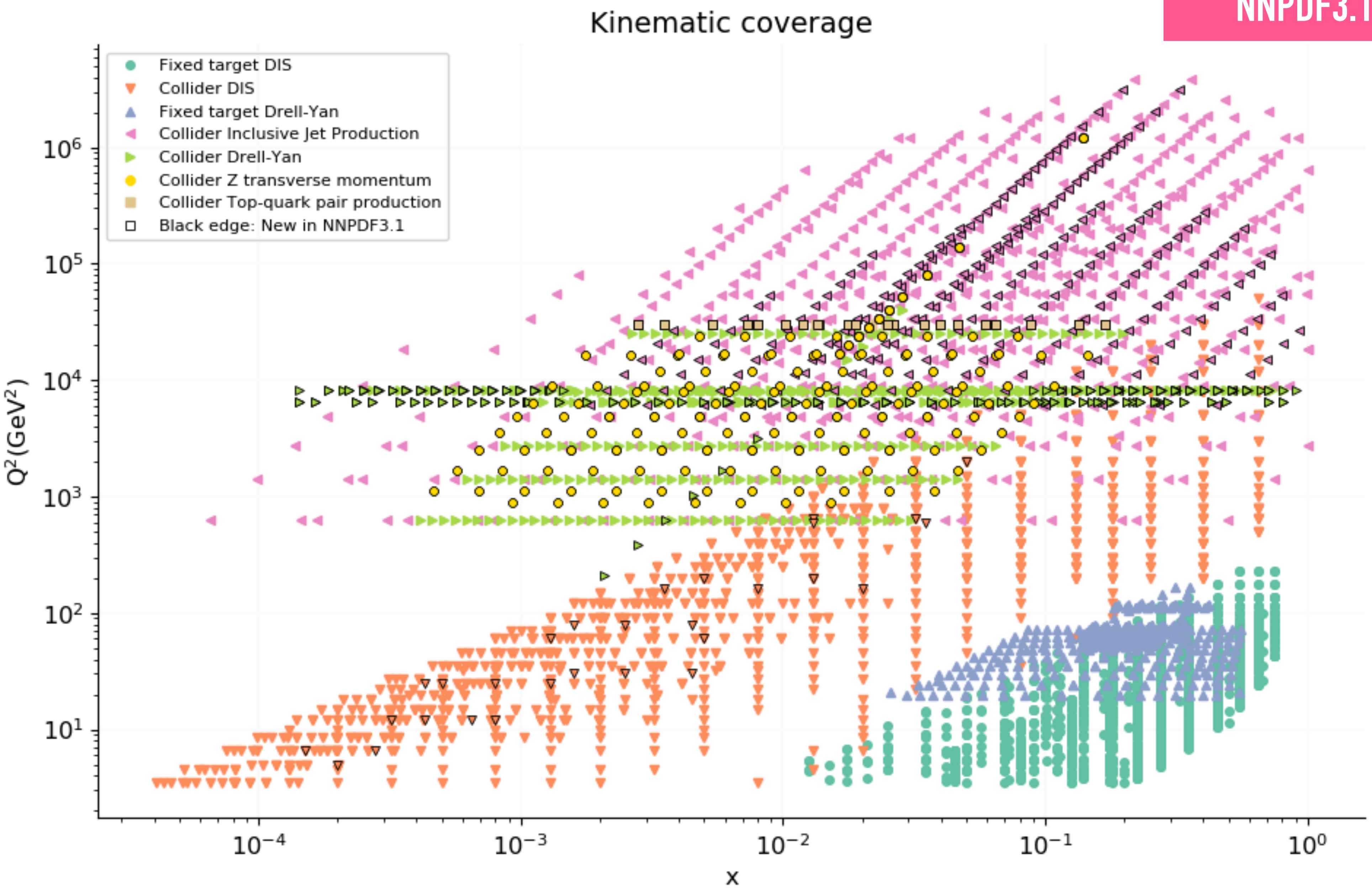






Global Fits: Kinematic Coverage

NNPDF3.1



- Global fits achieve **broad coverage** from low to high x , and over many orders of magnitude in Q^2.

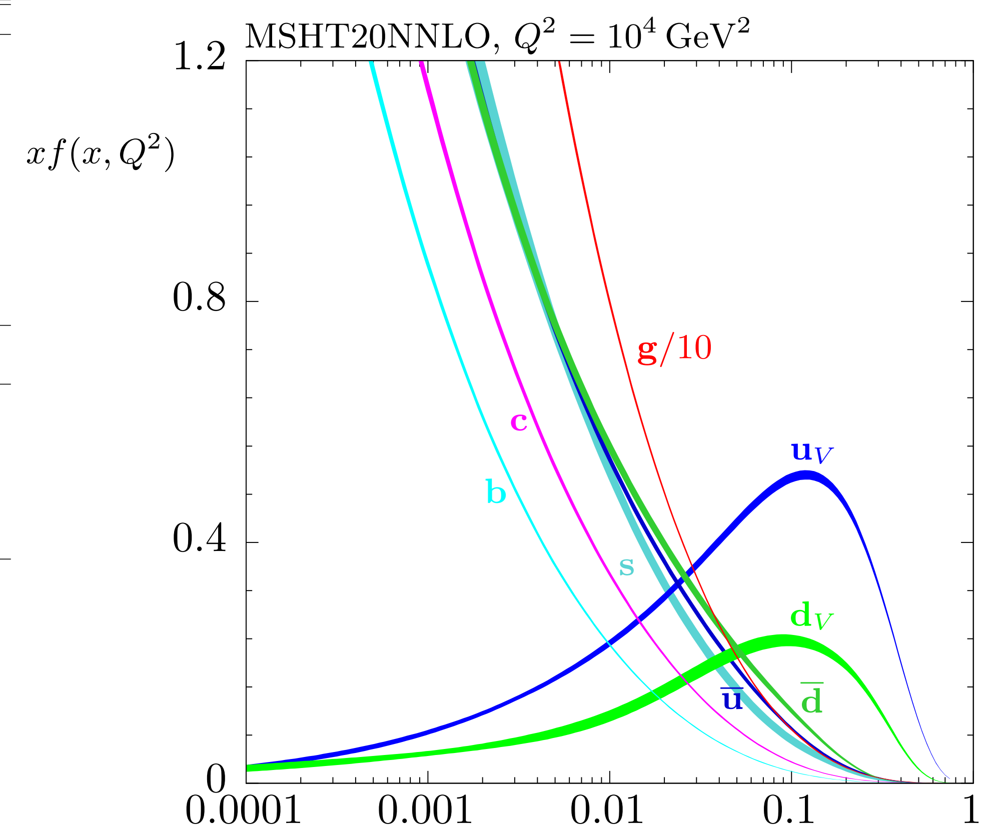
Fit Quality

- Fits to wide range of data from different colliders/experiments. Is a good/ reliable fit possible from this? **Yes**!

$\chi^2/\mathrm{dof} \sim 1$

$\Rightarrow$ **Non-trivial check of QCD.**

Data set	NLO	NNLO
BCDMS μp F_2 [49]	169.4/163	180.2/163
BCDMS μd F_2 [49]	135.0/151	146.0/151
NMC μp F_2 [50]	142.9/123	124.1/123
NMC μd F_2 [50]	128.2/123	112.4/123
NMC $\mu n/\mu p$ [51]	127.8/148	130.8/148
E665 μp F_2 [52]	59.5/53	64.7/53
E665 μd F_2 [52]	50.3/53	59.7/53
SLAC ep F_2 [53, 54]	29.4/37	32.0/37
SLAC ed F_2 [53, 54]	37.4/38	23.0/38
NMC/BCDMS/SLAC/HERA F_L [49, 50, 54, 146–148]	79.4/57	68.4/57
E866/NuSea pp DY [149]	216.2/184	225.1/184
E866/NuSea pd/pp DY [150]	10.6/15	10.4/15
NuTeV νN F_2 [55]	43.7/53	38.3/53
CHORUS νN F_2 [56]	27.8/42	30.2/42
NuTeV νN xF_3 [55]	37.8/42	30.7/42
CHORUS νN xF_3 [56]	22.0/28	18.4/28
CCFR $\nu N \to \mu\mu X$ [57]	73.2/86	67.7/86
NuTeV $\nu N \to \mu\mu X$ [57]	41.0/84	58.4/84
HERA e^+p CC [84]	54.3/39	52.0/39
HERA e^-p CC [84]	80.4/42	70.2/42
HERA e^+p NC 820 GeV [84]	91.6/75	89.8/75
HERA e^+p NC 920 GeV [84]	553.9/402	512.7/402
HERA e^-p NC 460 GeV [84]	253.3/209	248.3/209
HERA e^-p NC 575 GeV [84]	268.1/259	263.0/259
HERA e^-p NC 920 GeV [84]	252.3/159	244.4/159
HERA ep F_2^{charm} [26]	125.6/79	132.3/79
DØ II $p\bar{p}$ incl. jets [125]	117.2/110	120.2/110
CDF II $p\bar{p}$ incl. jets [124]	70.4/76	60.4/76
CDF II W asym. [90]	19.1/13	19.0/13
DØ II $W \to \nu e$ asym. [151]	44.4/12	33.9/12
DØ II $W \to \nu \mu$ asym. [152]	13.9/10	17.3/10
DØ II Z rap. [153]	15.9/28	16.4/28
CDF II Z rap. [154]	36.9/28	37.1/28
DØ W asym. [21]	13.1/14	12.0/14

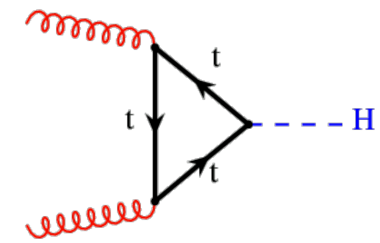


	NLO	**NNLO**
Total, LHC data in MSHT20	1.79	1.33
Total, non-LHC data in MSHT20	1.13	1.10
Total, all data	1.33	1.17

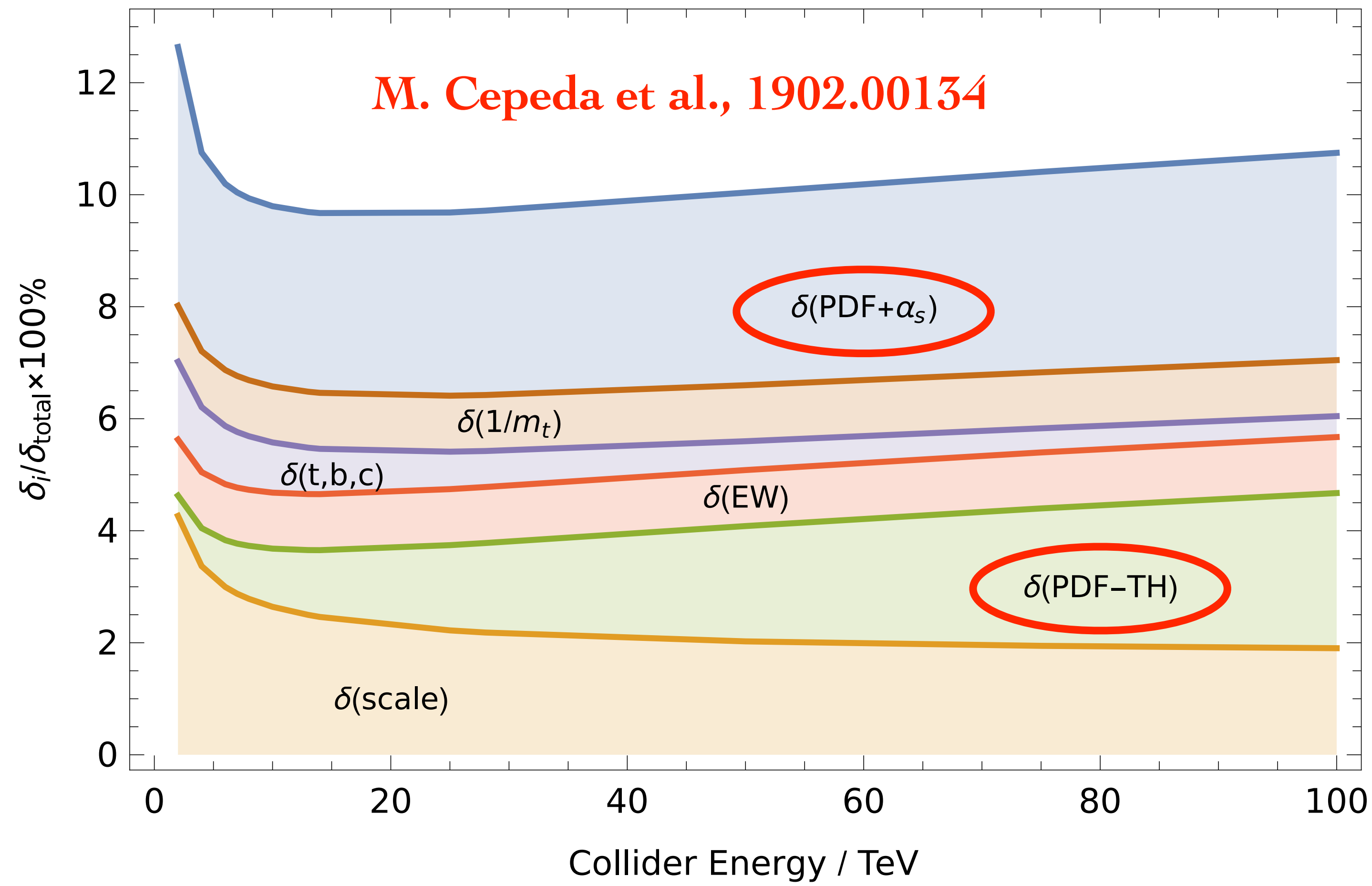
Why do we care about them at the LHC?

Higgs

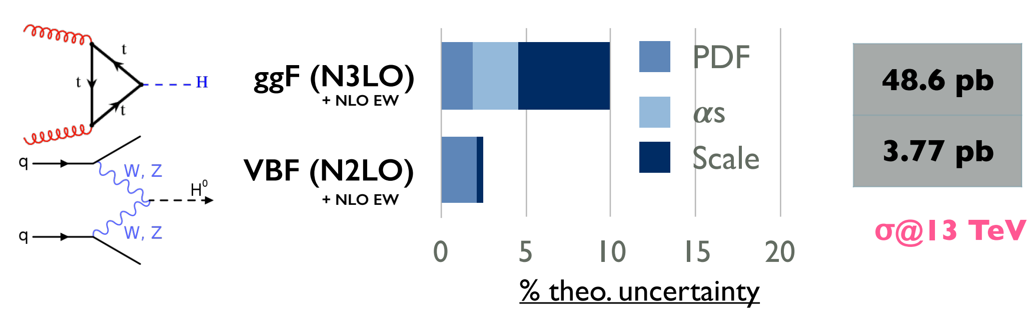
- Major (ongoing) aim of LHC: pin down the **Higgs sector** as precisely as we can.



★ PDF uncertainty important limiting factor in this.



★ Not just gg fusion: significant for VBF, associated production…

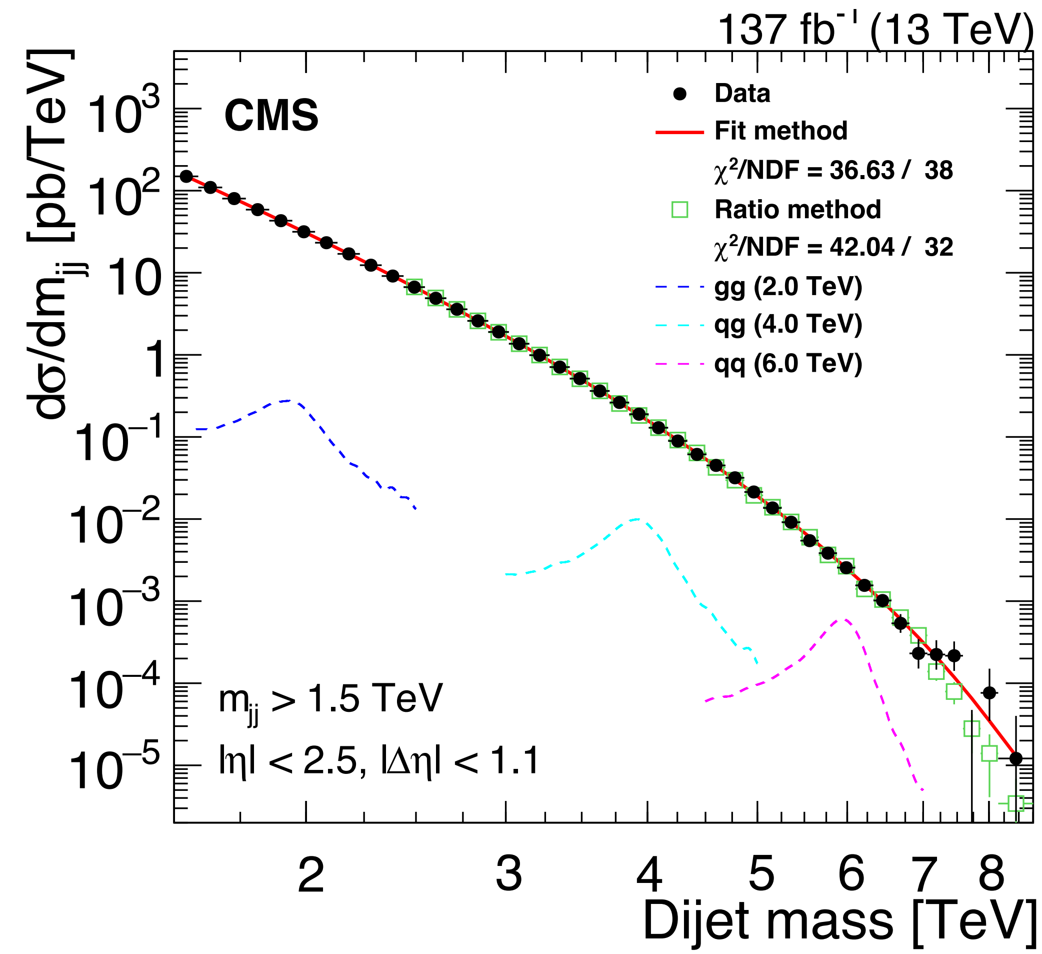


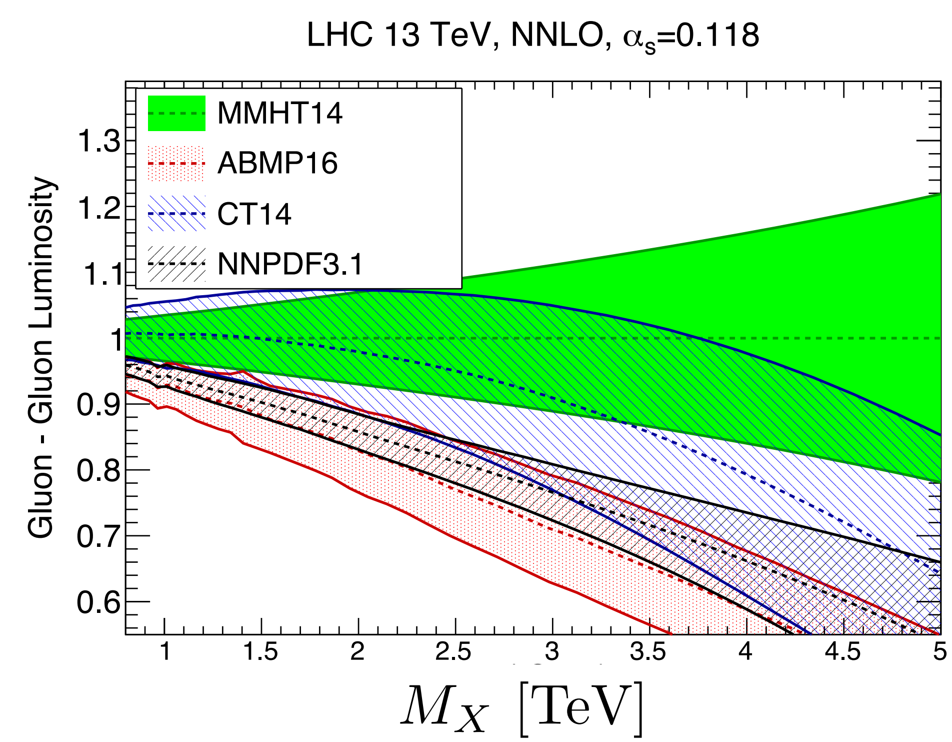
BSM

- **High mass searches** for new resonances/contact interactions - PDFs in high x region.

- PDF uncertainties larger here (less constraints). Though see later for more on that.

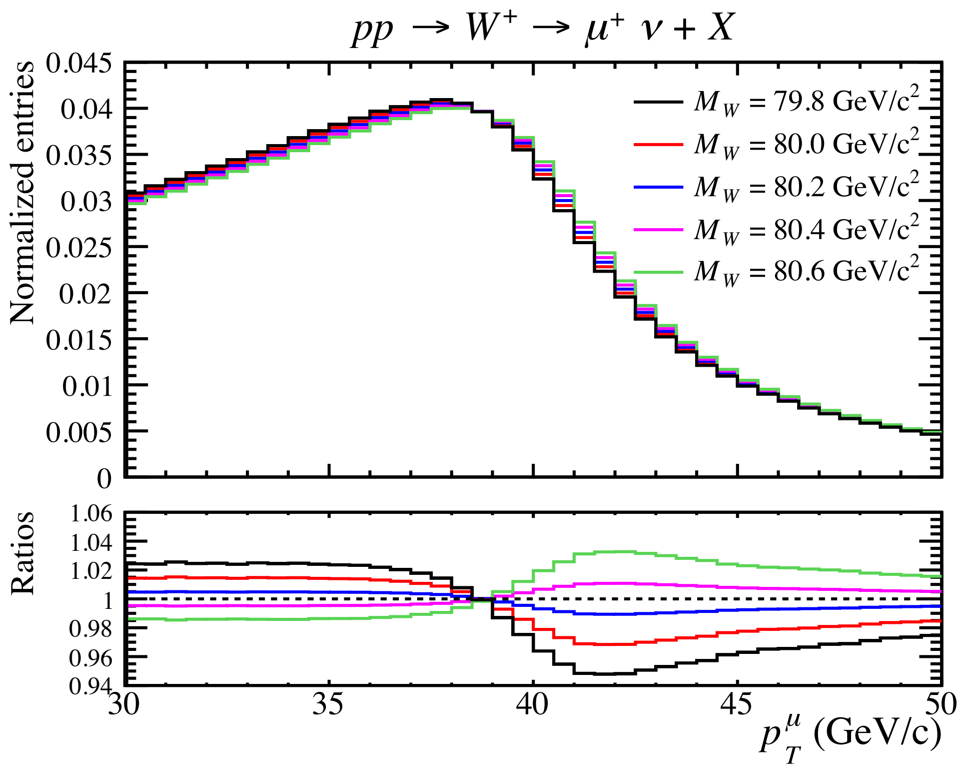
[1911.03947 (JHEP05 (2020) 033)](1911.03947)



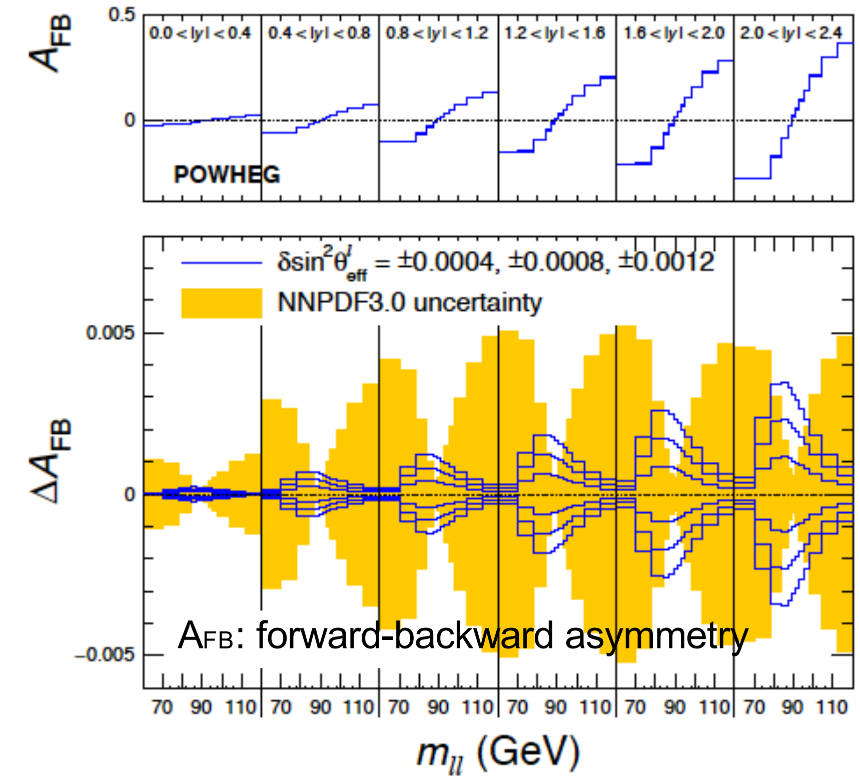


SM Precision

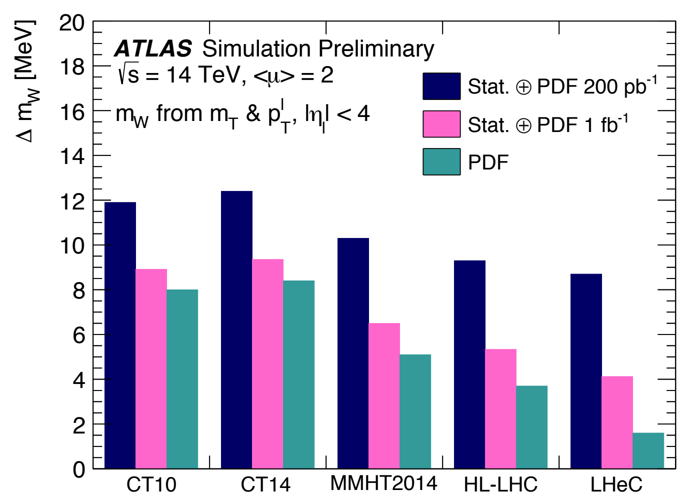
S. Farry et al., EPJC79 (2019) no.6, 497



CMS collab., EPJC78 (2018) no.9, 701

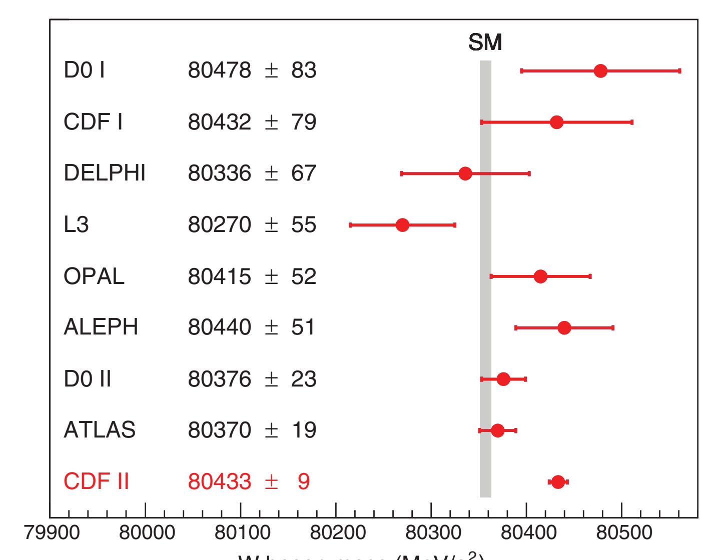


- W mass: fit to lepton ($W \to l\nu$) kinematics.



- Weak mixing angle θ_W : lepton decay distribution ($Z \to l^+ l^-$) w.r.t. initial quark.

- Both approaching level of indirect EW determination, but strongly sensitive to **PDF uncertainties.**
- Not to forget recent CDF W mass measurement!



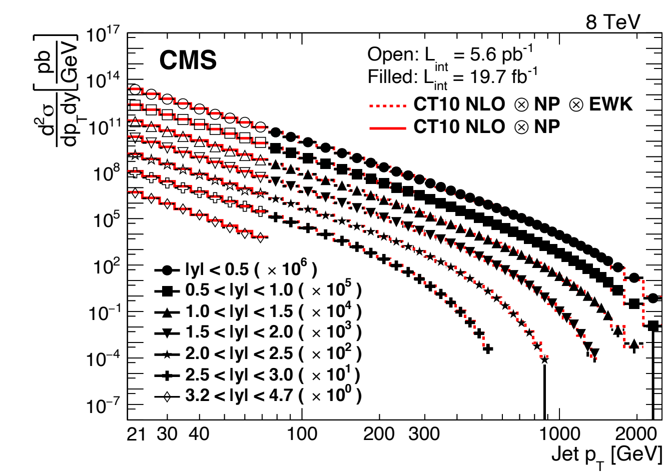
The MSHT20aN3LO fit

T. Cridge et al., *Eur.Phys.J.C* 81 (2021) 4, 341

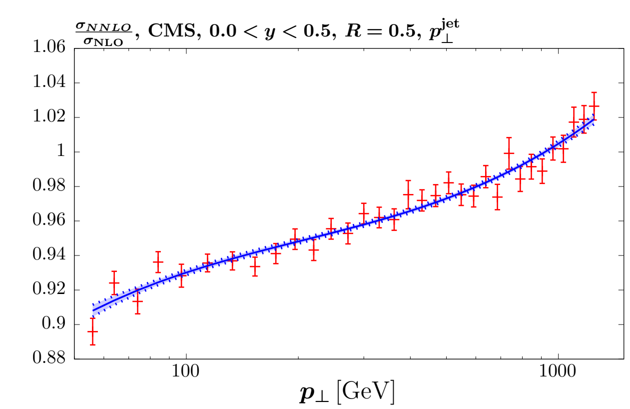
MSHT20 (in a slide)

- The 'Post-Run I' set from the MSTW, MMHT… group: **MSHT20**
- Focus on including significant amount of **new data**, higher **precision theory** and on **methodological improvements**.

★ **New data**: Updated data from HERA and LHC, including much high precision and multi-differential data. LHC data (DY, jets, top quark, V + jets…) playing increasing role.



★ **Precision theory**: NNLO theory input standard, and essential describing high precision data. EW/QED corrections also included where relevant.



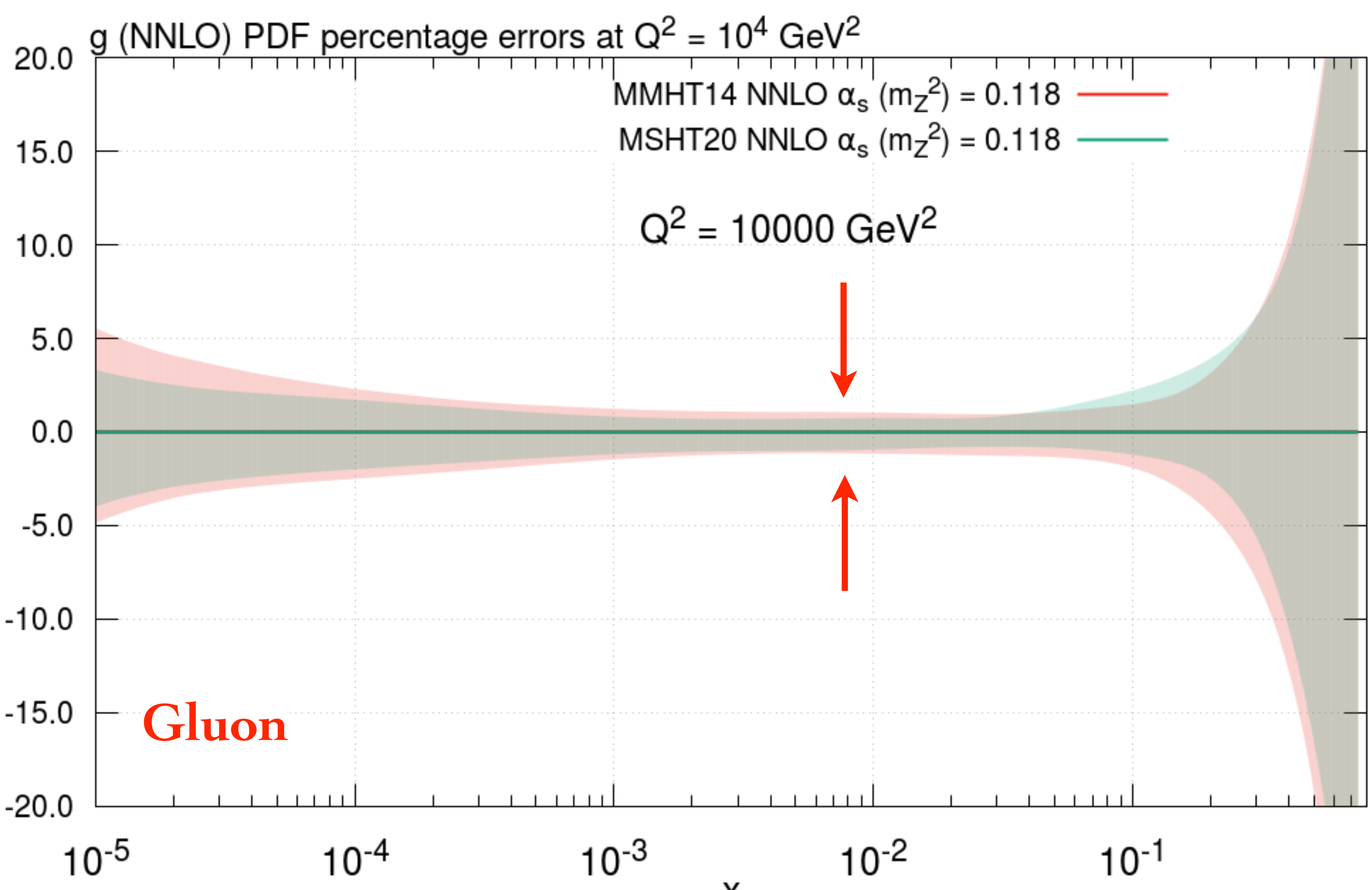
★ **Methodological improvements**: Flexible parameterisation in terms of Chebyshev polynomials (sub 1% level precision).

$$xf(x, Q_0^2) \;=\; A(1-x)^\eta x^\delta \left(1 + \sum_{i=1}^{n} a_i T_i^{\rm Ch}(y(x))\right)$$

How well do know PDFs?

- All previous major PDF releases: uncertainty given by propagating experimental uncertainty on data through to PDFs. $f(x,\mu) \pm \Delta(x,\mu)$

- Result depends on x, Q^2 and PDF type but can be as low as 1-2%.



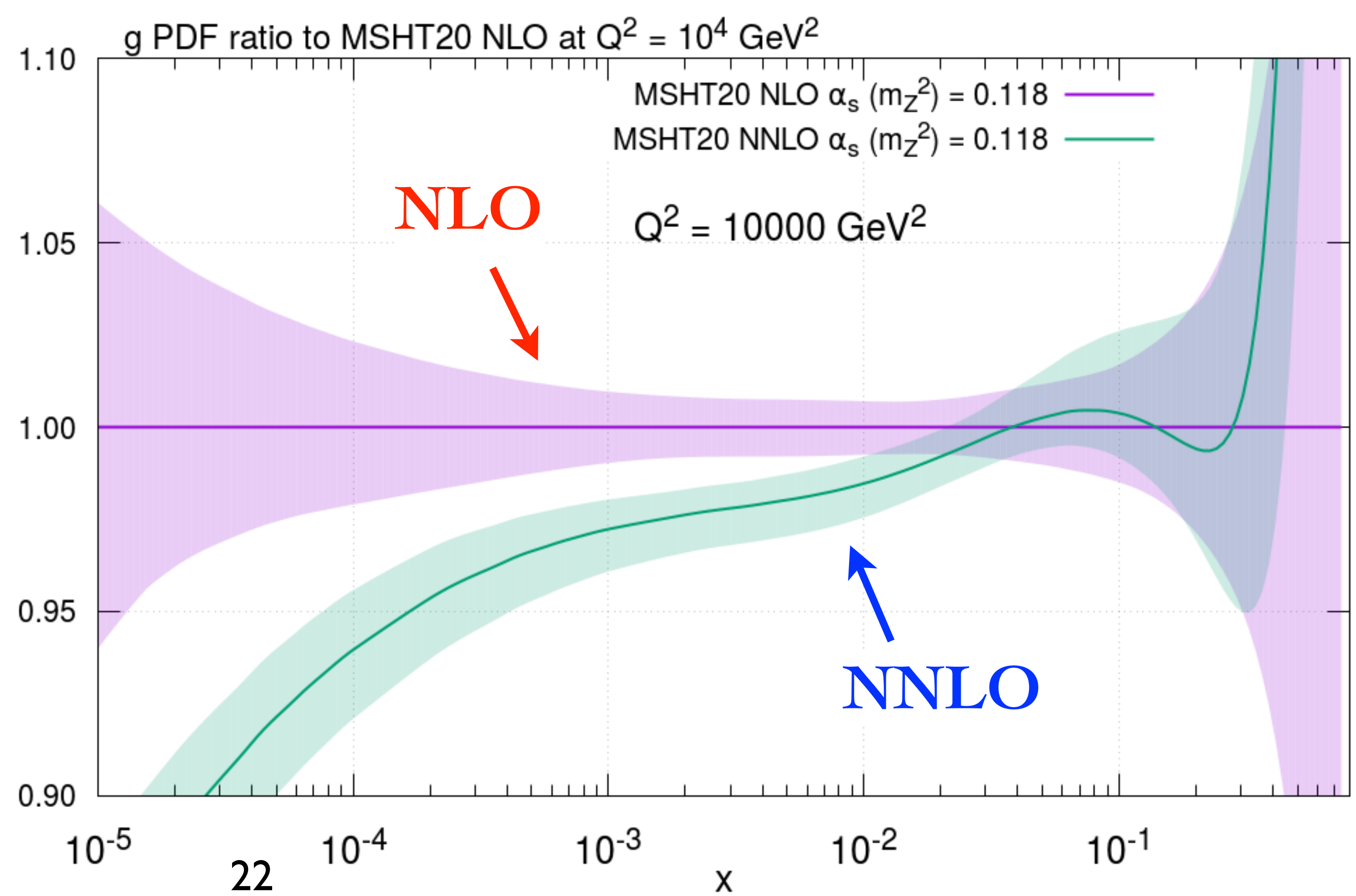
- However this is not the only source of uncertainty!
- Dependence on α_S , heavy quark masses, parameterisation can be accounted for. But recall:

$$O \sim f \otimes \sigma$$

Basic idea: **measure (data)** **fit** **predict (pQCD)**

- σ in fit not known exactly: calculated in pQCD to given order.

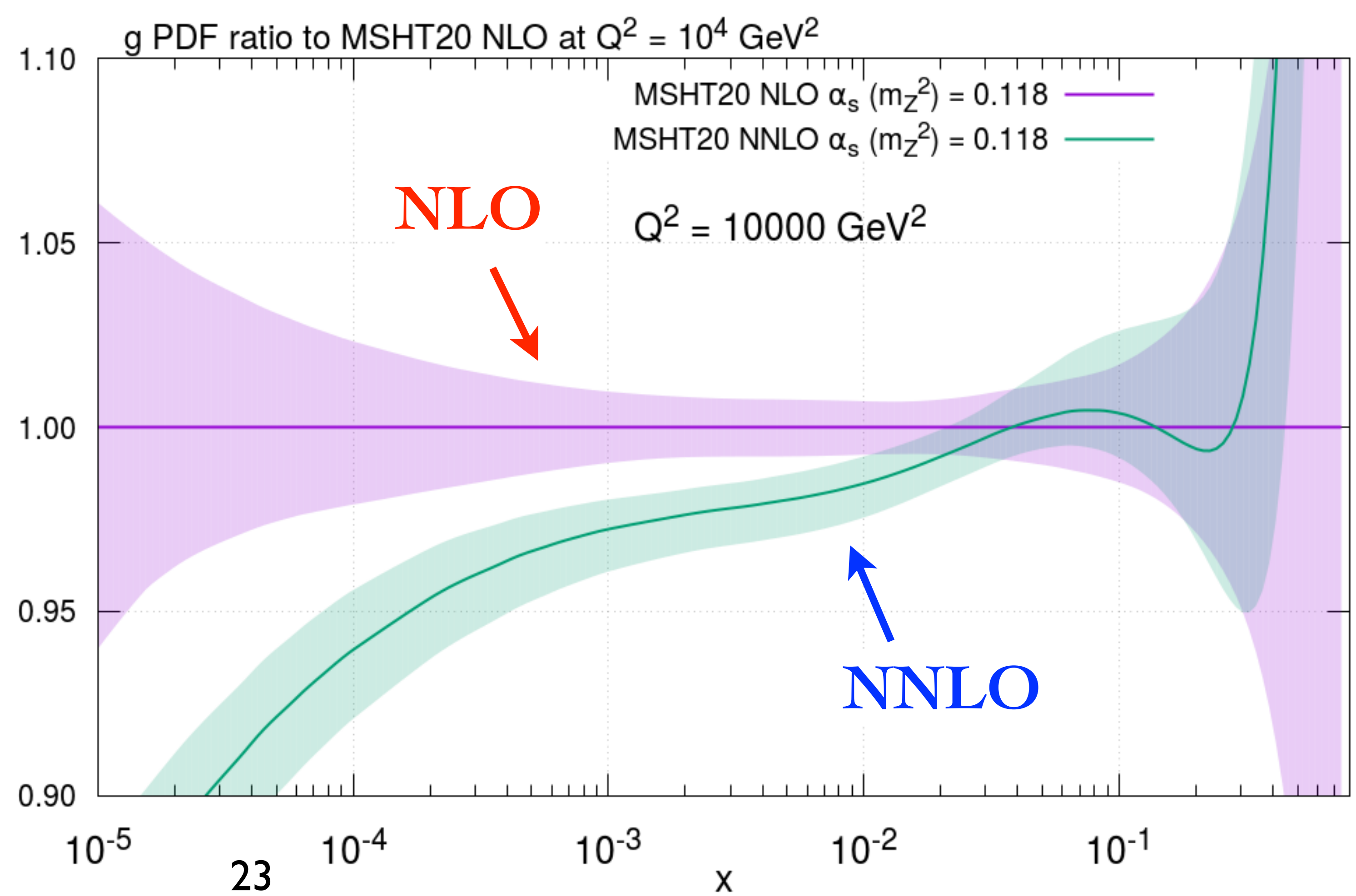
- Compare e.g. gluon between NLO and NNLO fits. Can differ by more than PDF errors.



- Now NLO and NNLO fits not to be treated on equal footing. Precision increases with order in α_S.
- Indeed this is reflected in fit quality, e.g. NLO fails dramatically for higher precision LHC data.

	NLO	NNLO
Total, LHC data in MSHT20	1.79	1.33
Total, non-LHC data in MSHT20	1.13	1.10
Total, all data	1.33	1.17

- But question remains: what might happen if we go beyond NNLO?



Missing Higher Orders

- How to estimate uncertainty due to missing higher orders (MHOs)? Standard approach is use scale variations:

$$\sigma = \sigma_0 \left(1 + c_1 \alpha_S + \cdots c_n \alpha_S^n\right) \quad \frac{\mathrm{d}\sigma}{\mathrm{d}\mu} = O(\alpha_S^{n+1}) \quad \delta\sigma = \sigma(2\mu_0) - \sigma(\mu_0/2)$$

- Can then propagate through to fit:

$$\underbrace{O}_{\substack{\textbf{measure}\\\textbf{(data)}}} \sim \underbrace{f}_{\textbf{fit}} \otimes \underbrace{\sigma}_{\substack{\textbf{predict}\\\textbf{(pQCD)}}}$$

NNPDF, *Eur.Phys.J.* C (2019) 79:838

- However this is just a rule of thumb:

★ Why 2? ★ What value for μ_0 ? ★ Does this really follow pert. series?

$n = 2$

- Moreover for NNLO PDF fit: we actually know quite a bit already about the next (N3LO) order up. Should use this!

$n = 3$

Basic Idea

- In general terms: parameterise higher order (~N3LO) corrections via nuisance parameters given by prior probability distribution.
- That is, starting with original fit probability:

$$P(T|D) \propto \exp\left(-\frac{1}{2}\underbrace{(T-D)^T H_0 (T-D)}_{\chi^2}\right)$$

T: Theory (NNLO)

D: Data

$H_0 \sim \frac{1}{\sigma^2_{\mathrm{exp}}}$

- Then we model N3LO theory via: $\underset{\text{N3LO theory}}{T'} = \underset{\text{N3LO (central)}}{T'_0} + \underset{\text{Allowed variation}}{\theta' u}$

- With shift given by prior probability:

$$P(\theta') = \frac{1}{\sqrt{2\pi}\sigma_{\theta'}} \exp(-\theta'^{\,2}/2\sigma^2_{\theta'})$$

- To give final result: $P(T|D) \propto \exp\left(-\frac{1}{2}M^{-1}(\theta' - \underset{\text{Best fit (error < }\sigma_{\theta'}\text{)}}{\overline{\theta}'})^2 - \frac{1}{2}(T'-D)^T H (T'-D)\right)$

- Question: How do we determine prior?

Splitting Functions

- Start with QCD splitting functions:

$$\frac{\partial f}{\partial \mu} \sim P \otimes f$$

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

- While these are not known exactly at N3LO, we do know quite a lot already:

  ★ Form at low x:

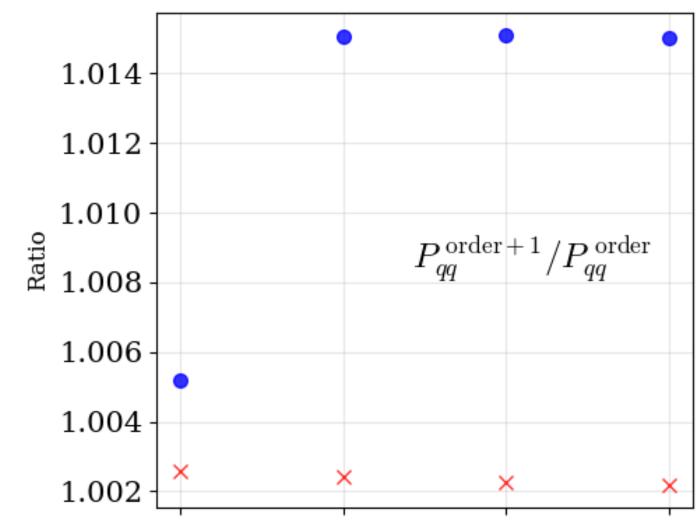
$$\boldsymbol{P}_{qg}^{(3)}(x) \to \frac{C_A^3}{3\pi^4}\left(\frac{82}{81} + 2\zeta_3\right)\frac{1}{2}\frac{\ln^2 1/x}{x} + \rho_{qg}\frac{\ln 1/x}{x},$$

  ★ Even Mellin moments up to $N = 8$

$$\int_0^1 \mathrm{d}x\, x^{N-1} P(x)$$

  $\Rightarrow$ intermediate to high x constraints.

  ★ Intuition from lower orders about what to expect.



- Idea is to parameterise $P(x)$ using set of basis functions:

$$P(x) = \sum_{i=1}^{N_m} A_i f_i(x) + f_e(x,\rho)$$

with N_m known moments used to solve for A_i .

- $f_e(x,\rho)$ is given known leading low x term + next-to-leading with nuisance parameter ρ , e.g. for $\boldsymbol{P}_{qg}^{(3)}(x)$:

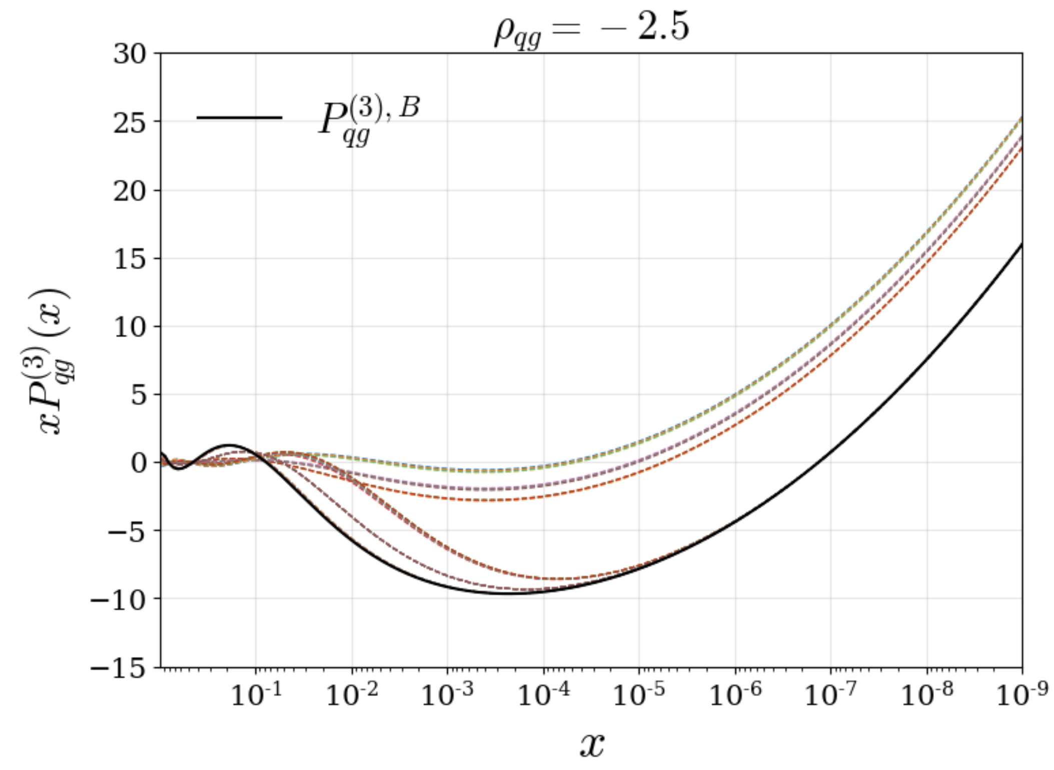
$$f_e(x,\rho_{qg}) \quad = \quad \frac{C_A^3}{3\pi^4}\left(\frac{82}{81} + \quad 2\zeta_3\right)\frac{1}{2}\frac{\ln^2 1/x}{x} + \;\rho_{qg}\,\frac{\ln 1/x}{x}.$$

Coefficient known

Form known
Coefficient unknown

- For $f_i(x)$ range of choices are made, guided by what appears at lower orders

$$\begin{aligned}
f_1(x) &= \frac{1}{x} \quad \text{or} \quad \ln^4 x \quad \text{or} \quad \ln^3 x \quad \text{or} \quad \ln^2 x,\\
f_2(x) &= \ln x,\\
f_2(x) &= 1 \quad \text{or} \quad x \quad \text{or} \quad x^2,\\
f_3(x) &= \ln^4(1-x) \quad \text{or} \quad \ln^3(1-x) \quad \text{or} \quad \ln^2(1-x) \quad \text{or} \quad \ln(1-x),
\end{aligned}$$



- For a given value of ρ and set of $f_i(x)$ splitting function predicted entirely. Varying these gives prior uncertainty band.

- More precisely, range of ρ set by requiring that 'reasonable' result:

  ★ Low $x < 10^{-5}$: full function cannot be in large tension with leading term.

$$\frac{C_A^3}{3\pi^4}\left(\frac{82}{81} + 2\zeta_3\right)\frac{1}{2}\frac{\ln^2 1/x}{x}$$

  ★ High x: N3LO correction small, following general trend of NNLO.

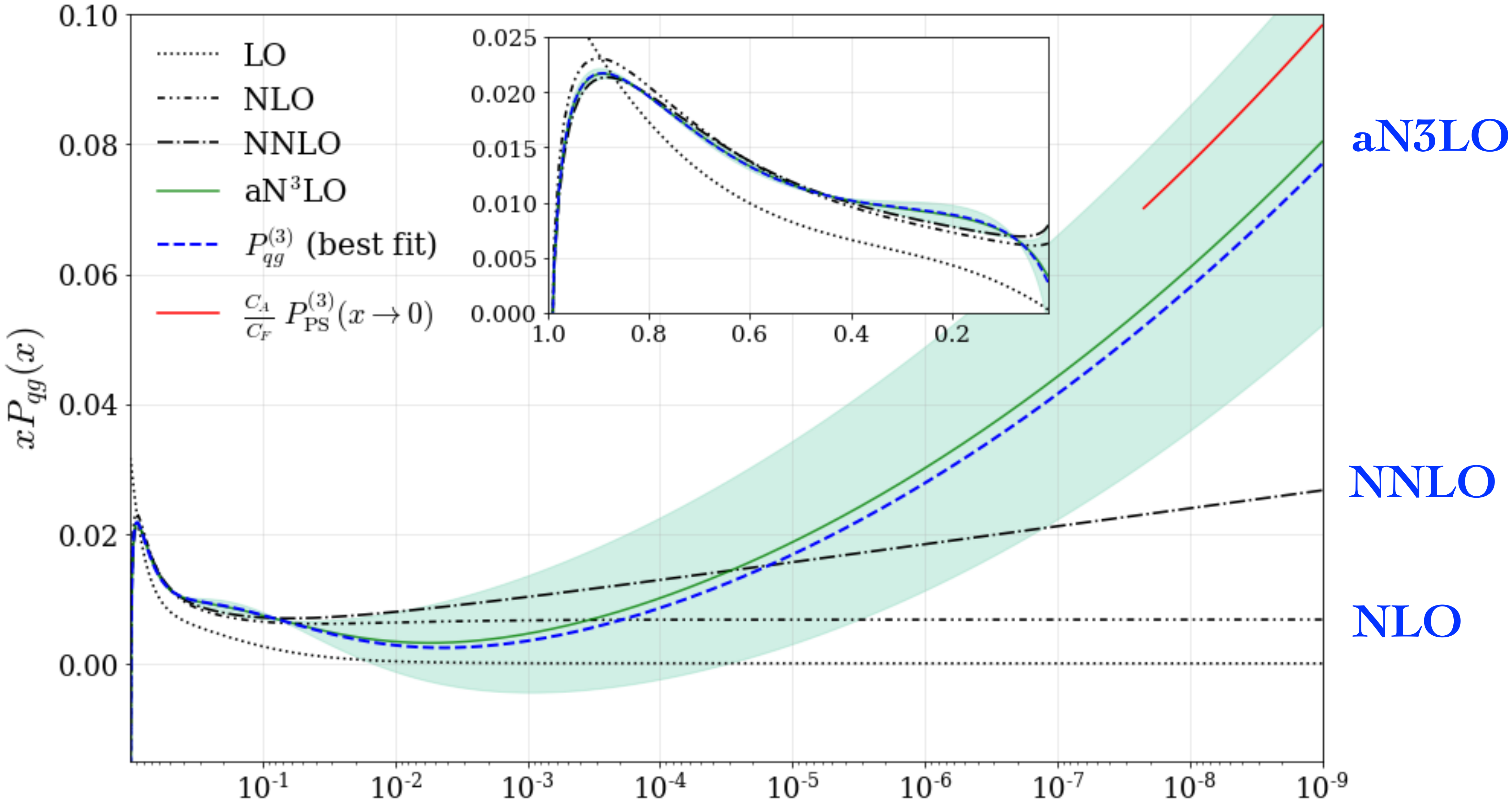
- In the end choose one set of $f_i(x)$ and range of ρ to satisfy this.

- Some subjectivity here, but result does not depend sensitively on precise prior.

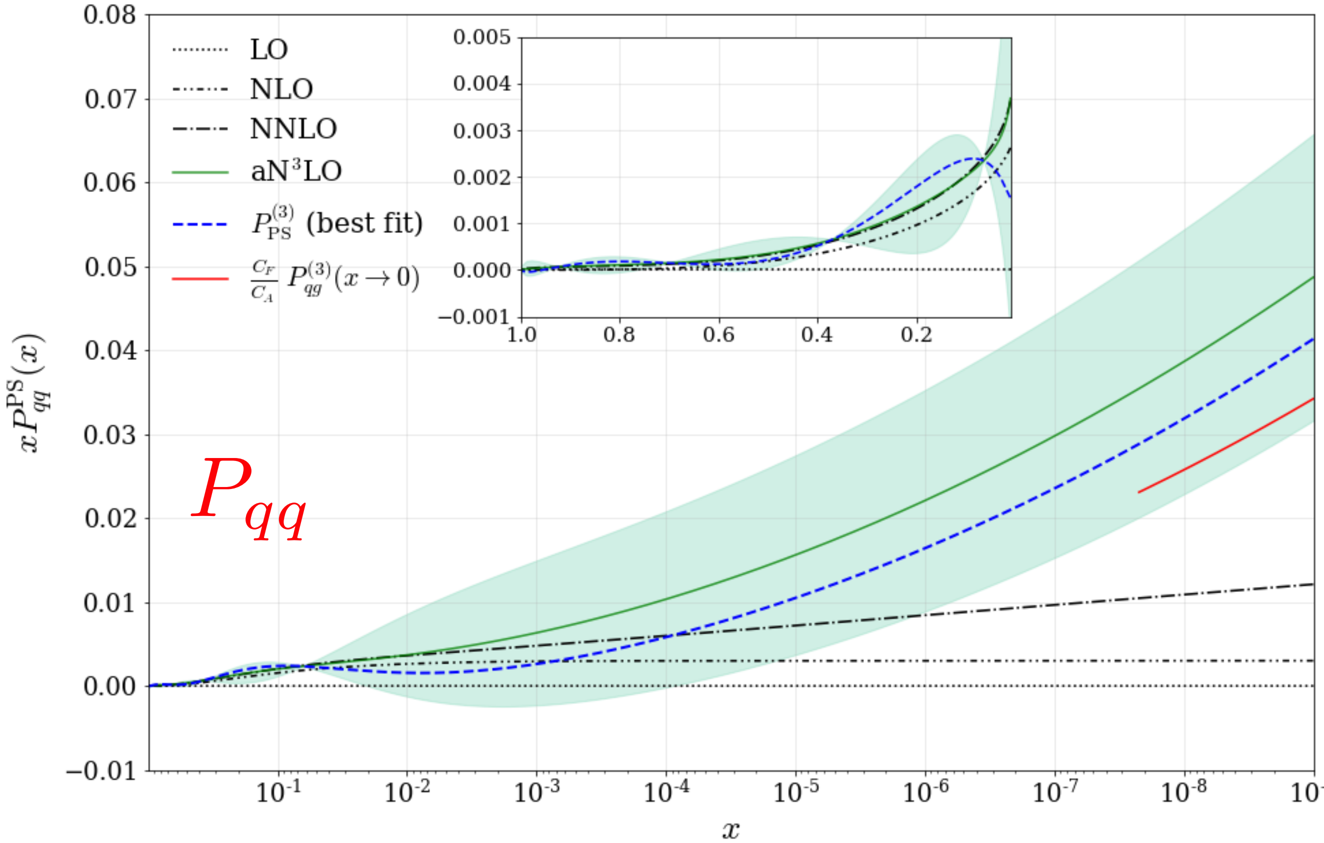
- A similar approach was used before the full NNLO was known, and found to match the exact NNLO result well!

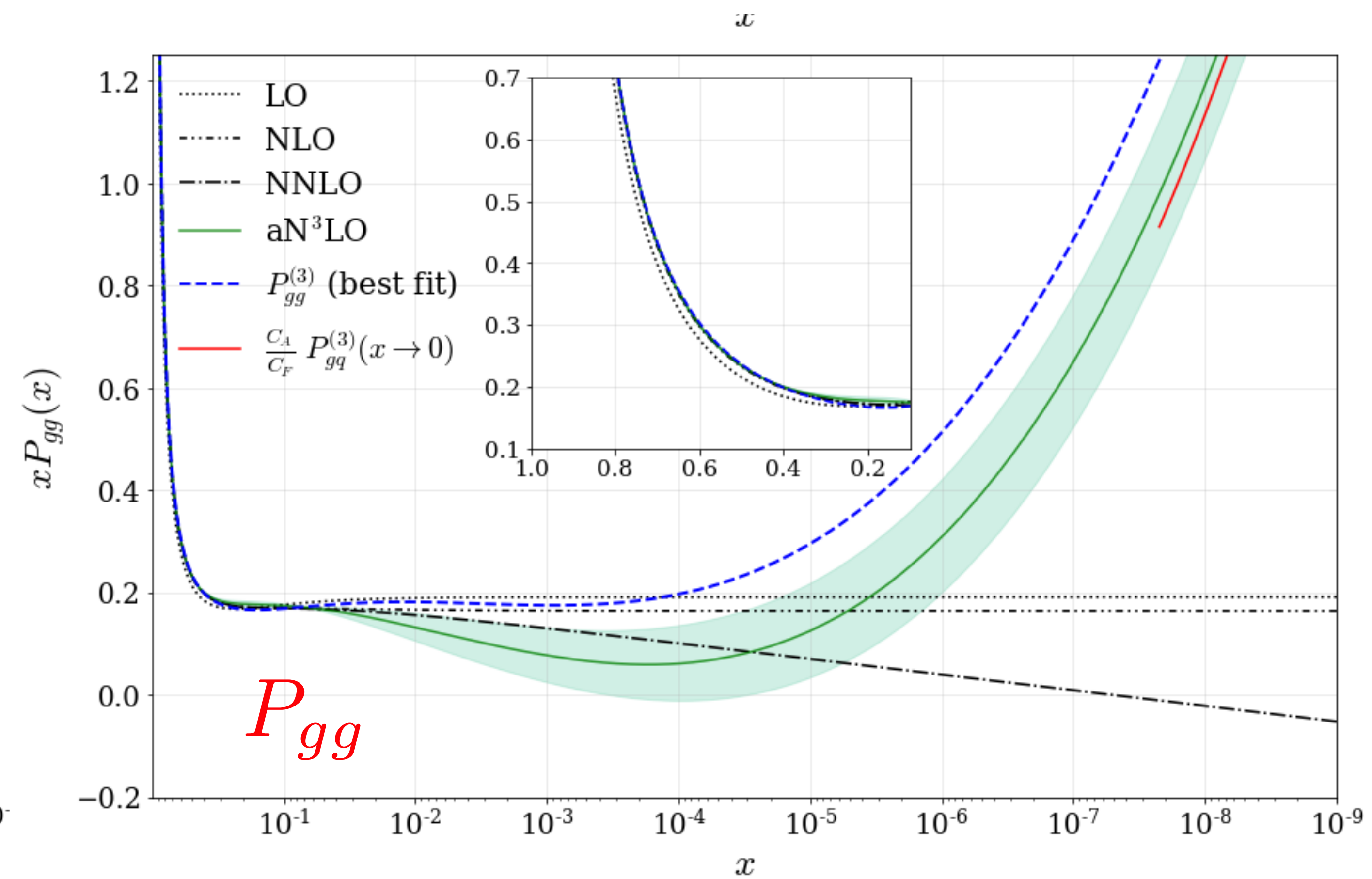
W. L. van Neervan and A. Vogt,
***Nucl.Phys.B* 588 (2000) 345-373,**
***Nucl.Phys.B* 568 (2000) 263-286**

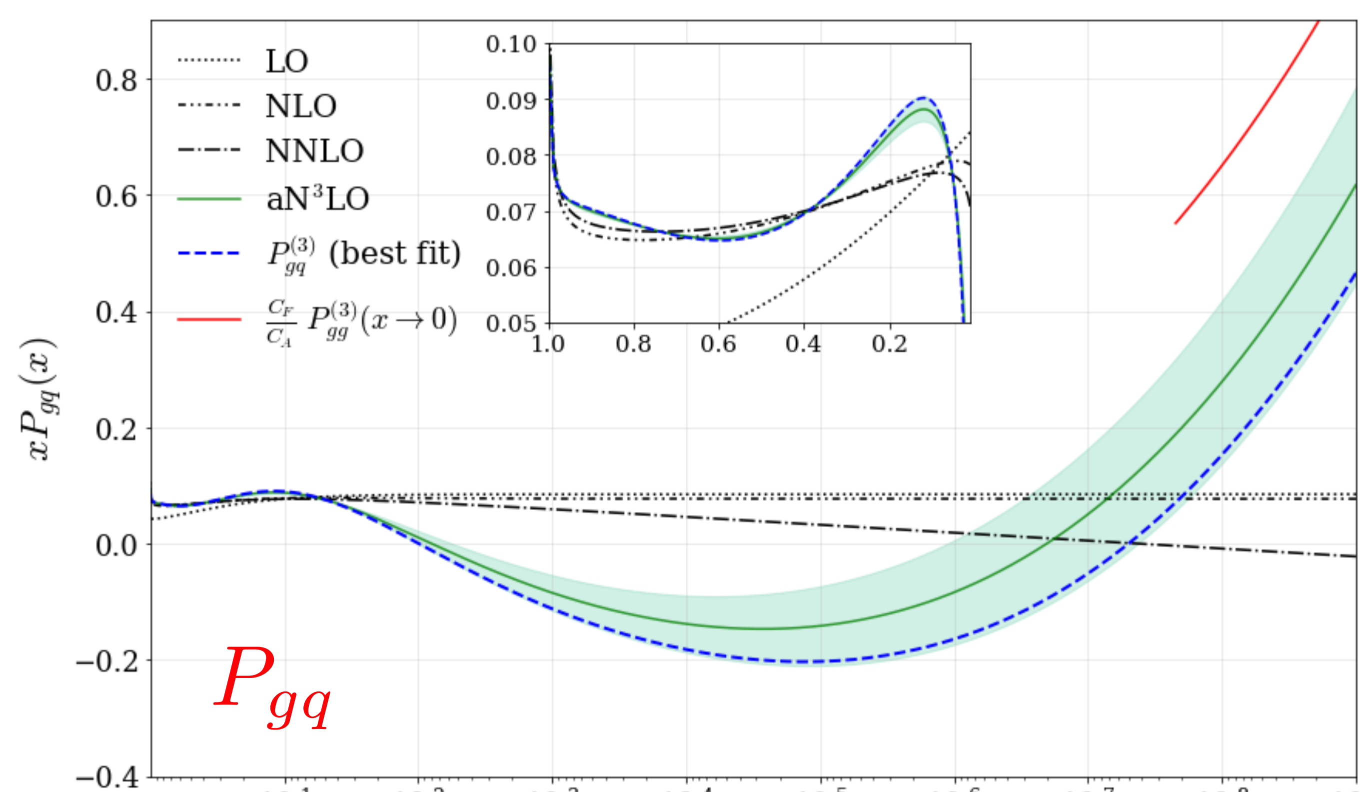
- Result for P_{qg} :
  - ★ Largest deviations at low x - corrections here larger.
  - ★ But also differences at high x , driven by known moments.
  - ★ Green curve: central result of prior. Not centred on NNLO $\longrightarrow$ known information from N3LO.
  - ★ Dashed curve: result after fitting, i.e. agrees well with prior.



- Similar trends for other splitting functions







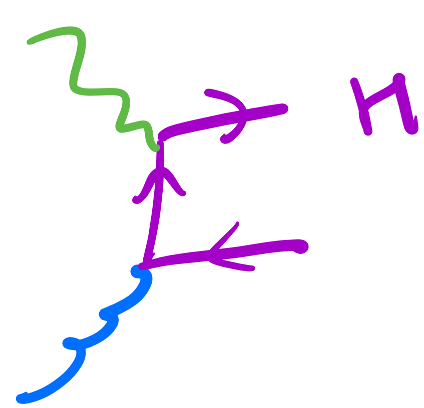
DIS Coefficient Functions

- Deep inelastic scattering (DIS) : backbone of PDF fits.
- DIS cross section given in terms of coefficient functions C_i :

$$\sigma_{\mathrm{DIS}} \sim C_i \otimes f_i$$

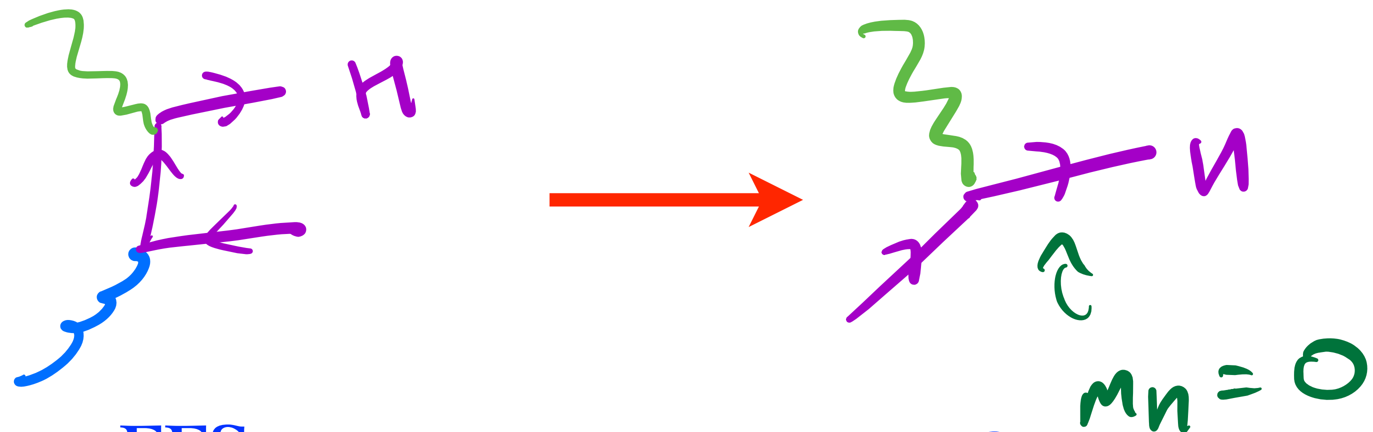
are known at N3LO for the light quarks ($m_q = 0$)!

- Is this enough? Not quite - heavy quark contributions ($m_{c,b} \neq 0$) play important role. Here some information is known but not everything.
- In more detail: one could in principle just include heavy quarks in final state ('fixed flavour scheme'):



as non-zero quark mass regulates collinear ($g \to H$) divergence.

- However if we do this then for larger photon Q^2 cross section develops large logs in Q^2/m_H^2 and perturbation theory breaks down.
- At large $Q^2 \gg m_H^2$ essential to instead include heavy quark PDFs, with DGLAP evolution resumming these ('zero mass flavour scheme').



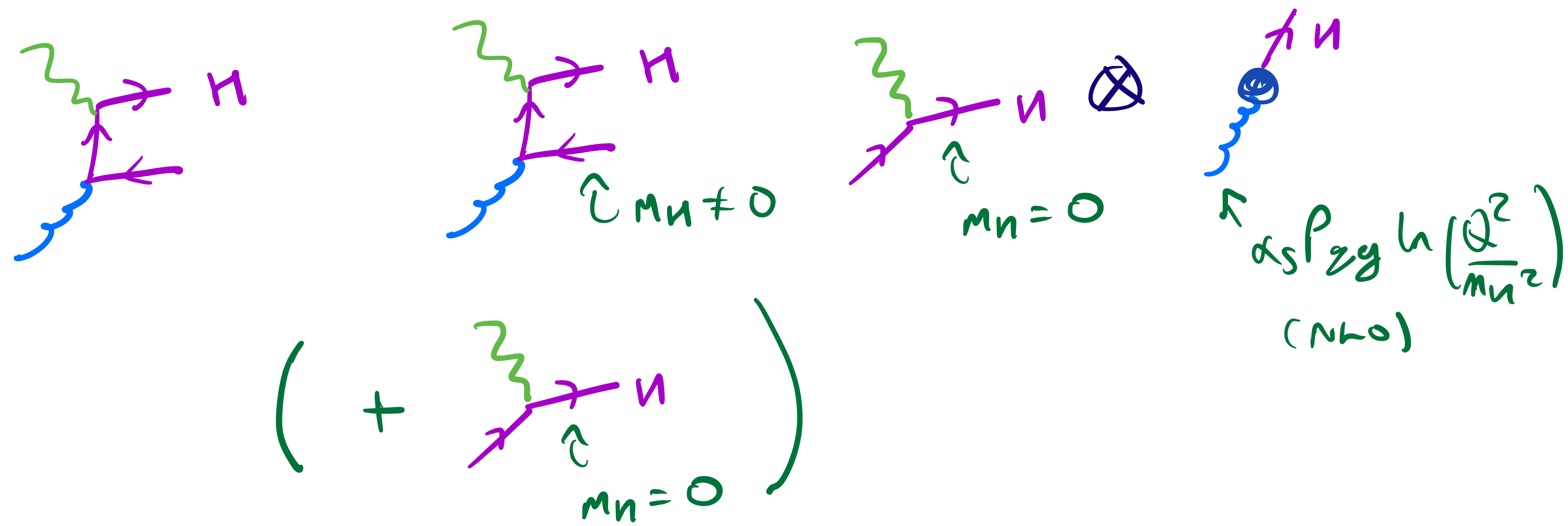
FFS **ZMFS**

- The heavy quark PDFs are completely predicted in pQCD via so-called `transition matrix elements':

$$f_H^{n_f+1}(x, Q^2) = \left[A_{Hq}(Q^2/m_h^2) \otimes f_q^{n_f}(Q^2) + A_{Hg}(Q^2/m_h^2) \otimes f_g^{n_f}(Q^2)\right](x)$$

- Better still is to interpolate between $Q^2 \sim m_H^2$ and $Q^2 \gg m_H^2$ regions. Keep exact m_H dependence in former and $\ln Q^2/m_H^2$ resummation in latter - 'general mass variable flavour number scheme' (GM-VFNS).
- For e.g. gluon-initiated heavy flavour production at NLO:

$$C^{VF}_{H,g} = C^{FF,(1)}_{H,g} - C^{VF,(0)}_{H,H} \otimes A^{(1)}_{Hg}$$



- Beyond this order, can build up contributions systematically.
- So we need at N3LO:
  - ★ Transition matrix elements.
  - ★ DIS coefficient functions with $m_H \neq 0$.

Transition Matrix Elements

- Situation in some cases similar to splitting functions, e.g. for $A_{Hg}^{(3)}$ we know:

  ★ Form at low x: $\left(224\,\zeta_3 - \frac{41984}{27} - 160\,\frac{\pi^2}{6}\right)\frac{\ln 1/x}{x} + a_{Hg}\,\frac{1}{x}$

  ★ Even Mellin moments up to $N = 10$ $\quad \int_0^1 \mathrm{d}x\, x^{N-1} A_{Hg}^{(3)}$

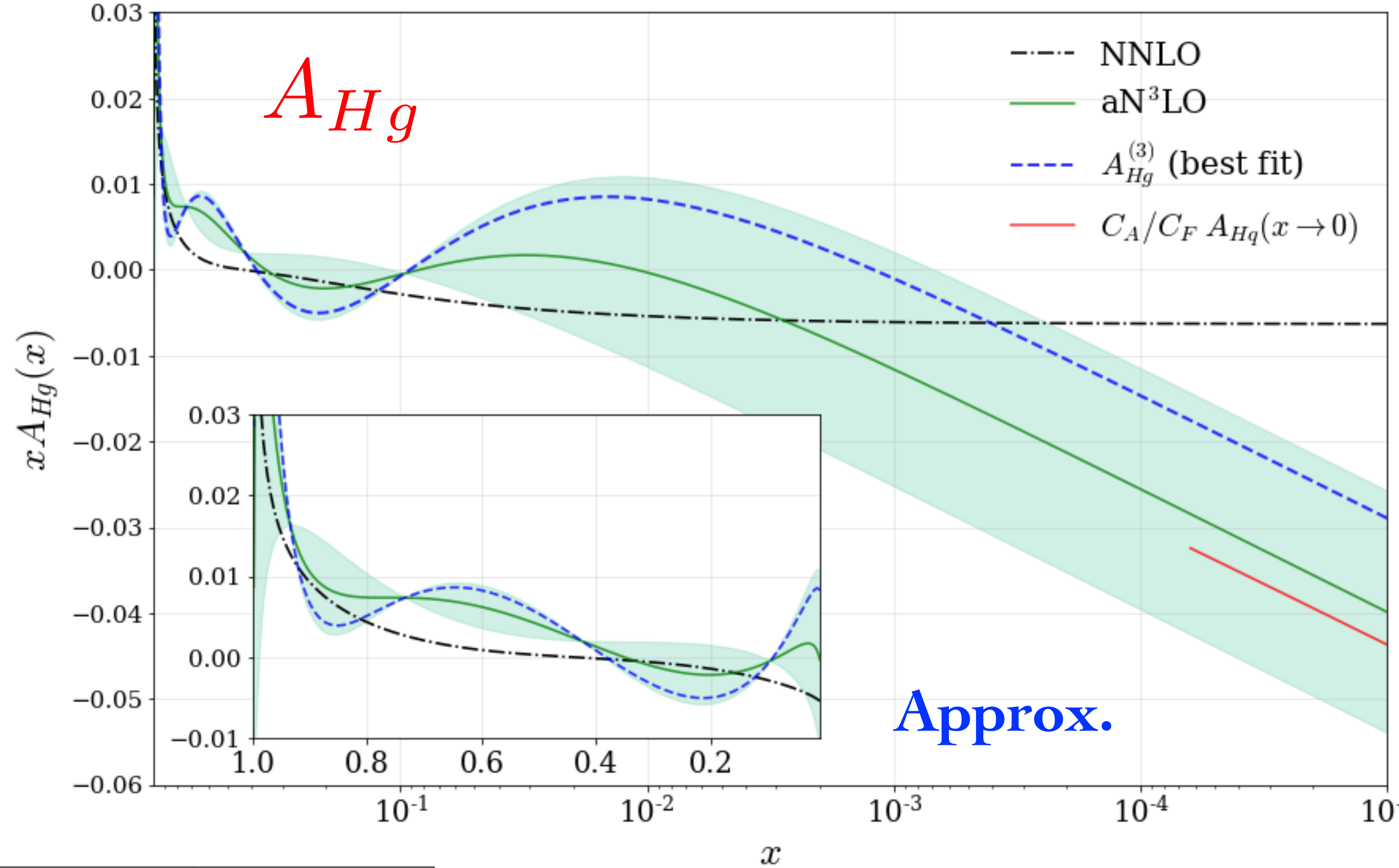
  $\Rightarrow$ high x constraints.

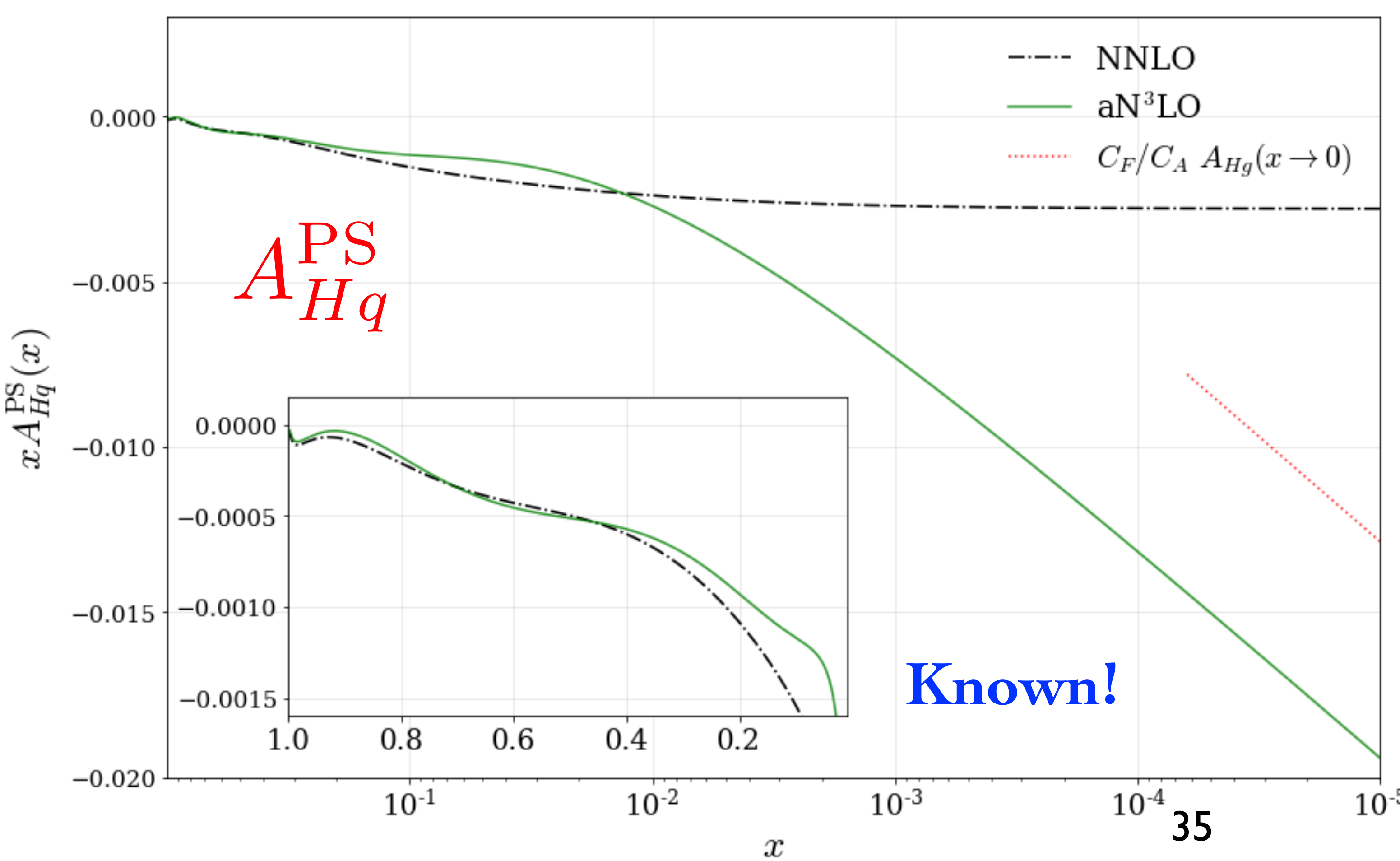
- We therefore follow a similar procedure as before for this…

$$
\begin{aligned}
f_{1,2}(x) &= \ln^5(1-x) \quad \text{or} \quad \ln^4(1-x) \quad \text{or} \quad \ln^3(1-x) \quad \text{or} \quad \ln^2(1-x) \\
&\quad \text{or} \quad \ln(1-x), \\
f_{3,4}(x) &= 2-x \quad \text{or} \quad 1 \quad \text{or} \quad x \quad \text{or} \quad x^2, \\
f_5(x) &= \ln x \quad \text{or} \quad \ln^2 x, \\
f_e(x, a_{Hg}) &= \left(224\,\zeta_3 - \frac{41984}{27} - 160\,\frac{\pi^2}{6}\right)\frac{\ln 1/x}{x} + a_{Hg}\,\frac{1}{x}
\end{aligned}
\tag{5.3}
$$

- For other cases ($A_{gq,H}^{(3)}, A_{Hq}^{\mathrm{PS},(3)}$) exact results are known - simply use these.

- A similar picture to before builds up.

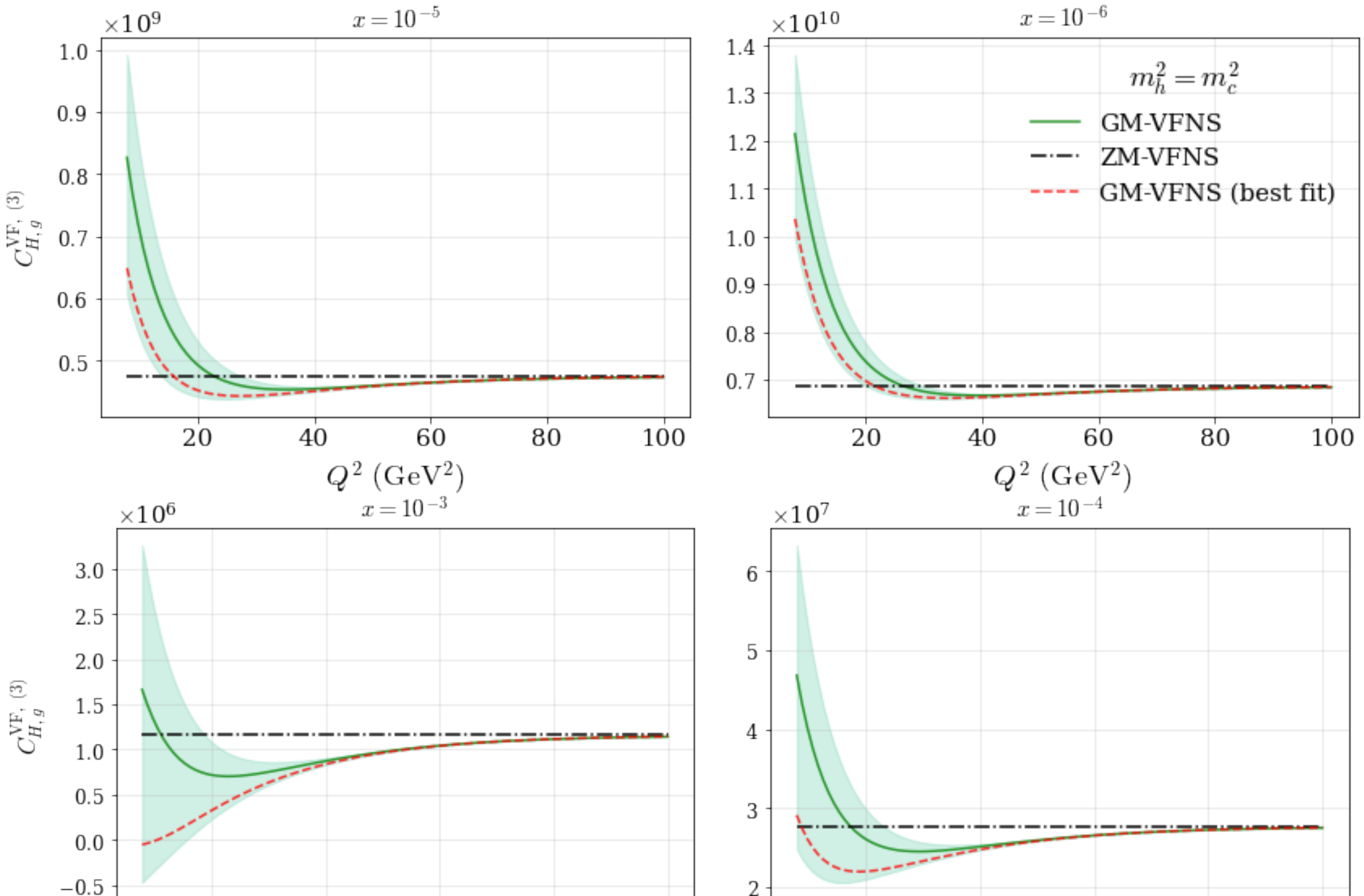




Coefficient Functions

- Massless ($Q^2 \to \infty$) case known as well as approximations for massive close to threshold ($Q^2 \leq m_H^2$). Use this to build up approximate GMVFNS prediction.

$C_{H,g}$



Hadronic Collisions

- So far have only consider DIS. What about hadron-hadron collisions as in e.g. the LHC?
- Here much less is known about cross sections at N3LO:

  ★ Higgs - does not go in PDF fit!

  ★ Drell-Yan - not yet for relevant fiducial cross sections.

- So for now we assume nothing is known about this, and instead include a MHO uncertainty (= approx. N3LO K-factor) on cross sections.
- Do not use scale variations, rather base on known NLO and NNLO:

$$\sigma_{N3LO} = K(y) \cdot \sigma_{LO}$$

y: rapidity, $p_\perp$...

$$K(y) = 1 + \frac{\alpha_s}{\pi} D(y) + \left(\frac{\alpha_s}{\pi}\right)^2 E(y) + \left(\frac{\alpha_s}{\pi}\right)^3 F(y) + \mathcal{O}(\alpha_s^4).$$

NLO (known) **NNLO (known)** **N3LO (unknown)**

$$K(y) = 1 + \frac{\alpha_s}{\pi} D(y) + \left(\frac{\alpha_s}{\pi}\right)^2 E(y) + \left(\frac{\alpha_s}{\pi}\right)^3 F(y) + \mathcal{O}(\alpha_s^4).$$

NLO (known) **NNLO (known)** **N3LO (unknown)**

- Take: $$K^{\mathrm{N^3LO/LO}} = K^{\mathrm{NNLO/LO}} \left(1 + \alpha_s^3 \hat{a}_1 \frac{\mathcal{N}^2}{\pi} D + \alpha_s^3 \hat{a}_2 \frac{\mathcal{N}}{\pi^2} E\right).$$

with $a_{1,2}$ free nuisance parameters.

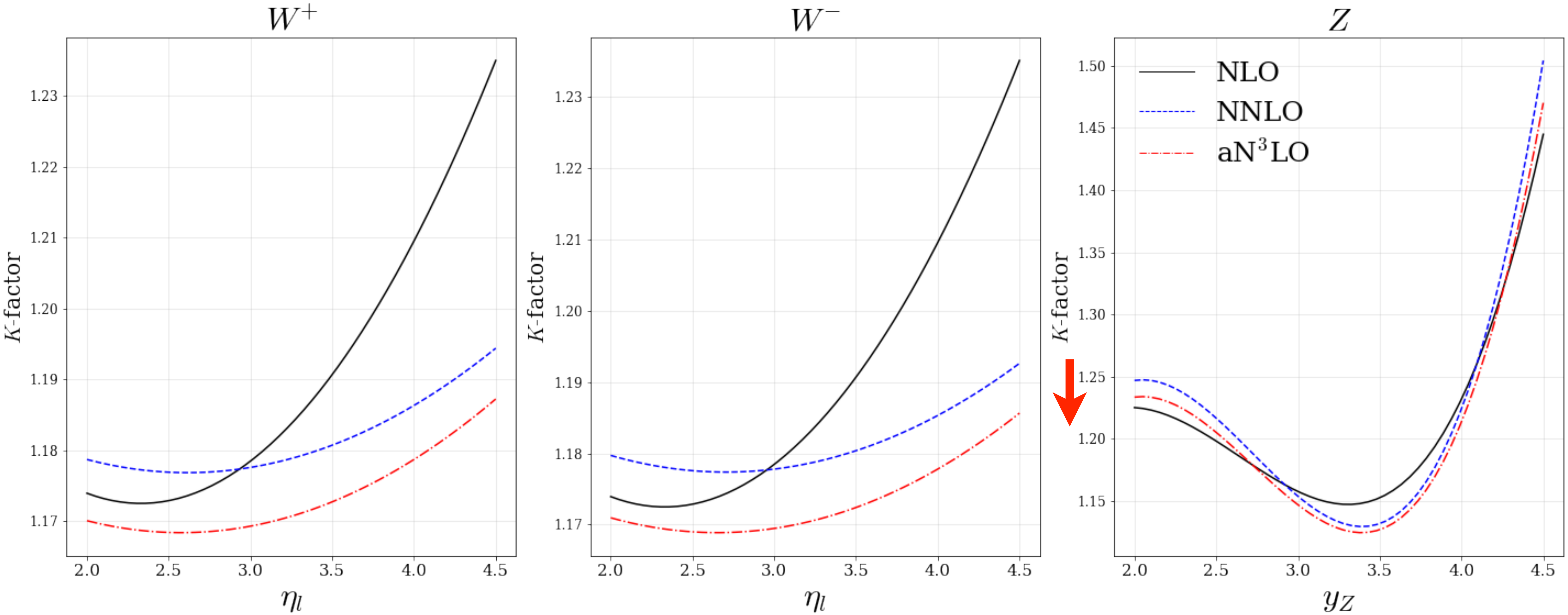
- Can show that if $\mathcal{N} = 3$ is taken then have $a_{1,2} \sim O(1)$ in order to match expected trend with increasing orders.

$\Rightarrow$ Prior distribution is $a_{1,2}^{\mathrm{cent}} = 0$ with $\sigma_{1,2} = 1$.

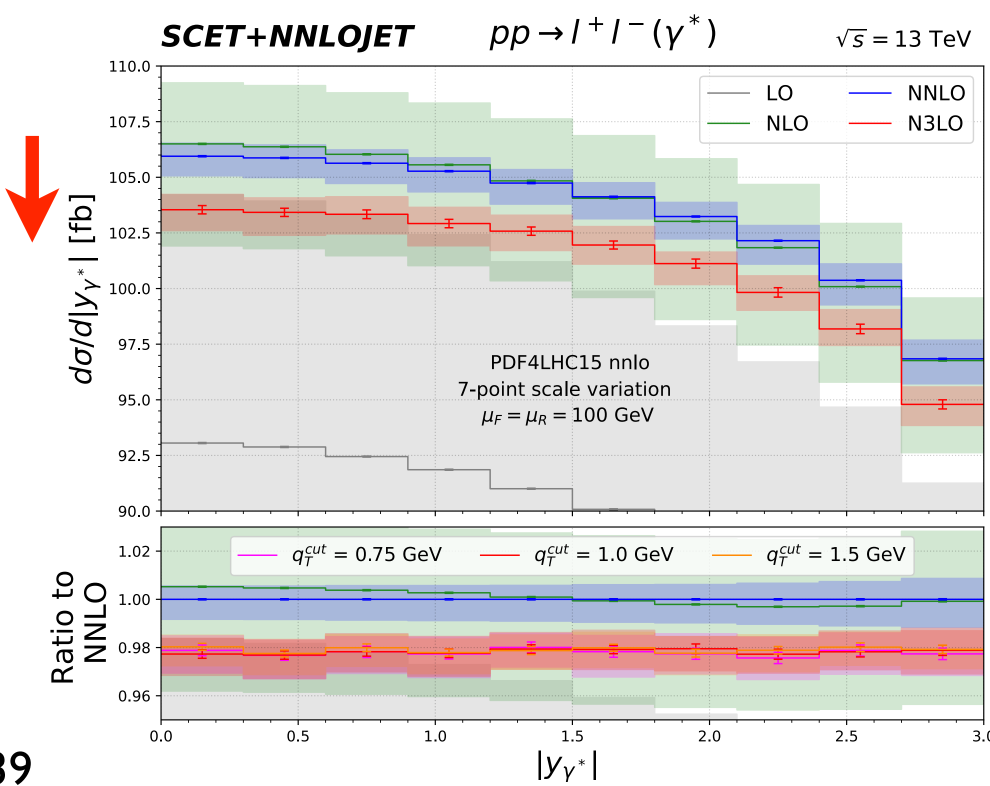
- As expect K-factors to behave ~ similarly between similar processes, correlate these between 5 classes of process:

★ Jets ★ $t\bar{t}$ ★ Drell Yan ★ $Zp_\perp$ and V + jets ★ Neutrino-induced 'dimuon' DIS

★ Resulting K-factors: **Drell Yan**.

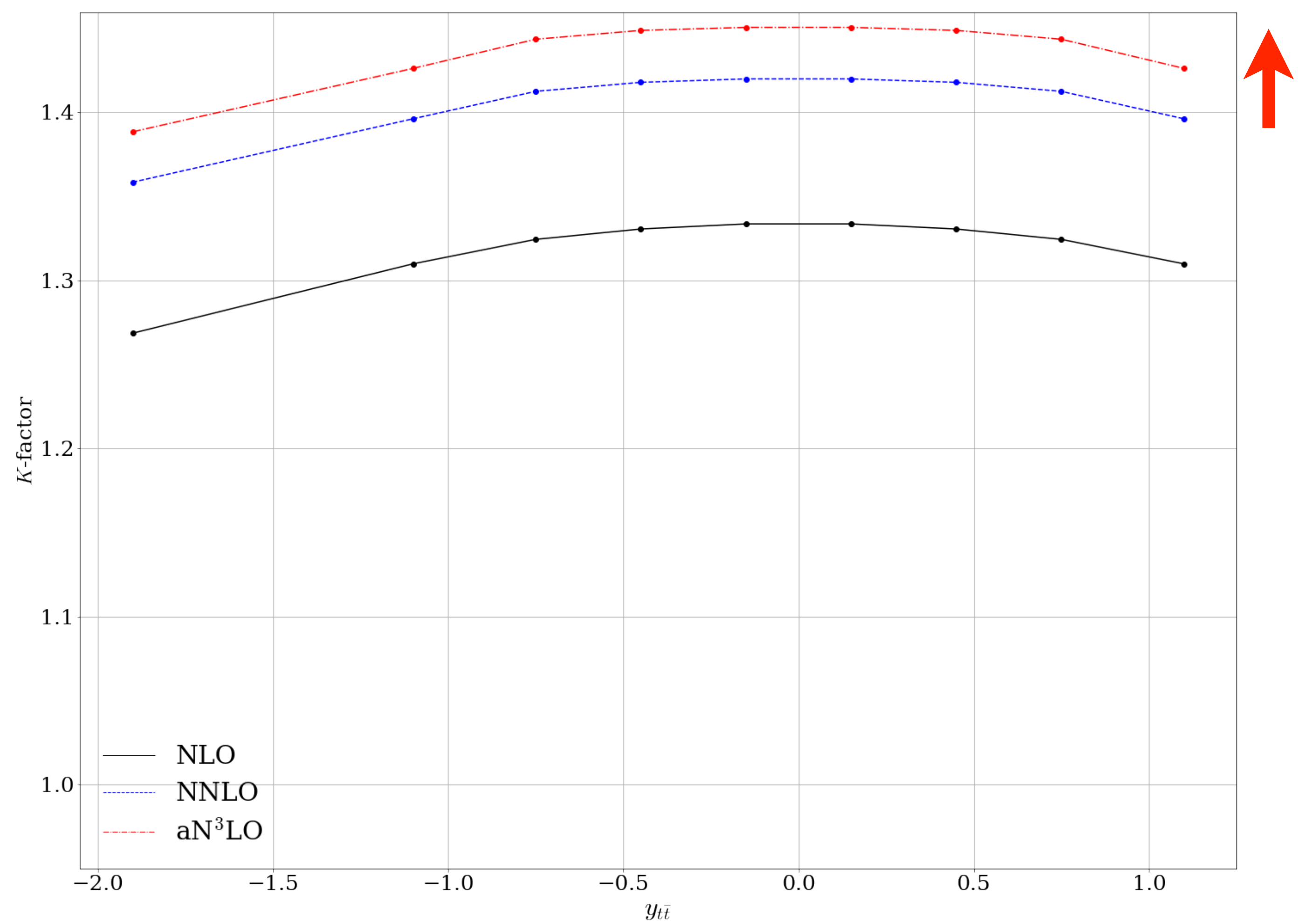


- Fit prefers a ~ 1% decrease from NNLO to aN3LO.
- This is in nice agreement with expectations from exact N3LO calculations!
- Implies improved perturbative convergence with aN3LO PDFs.

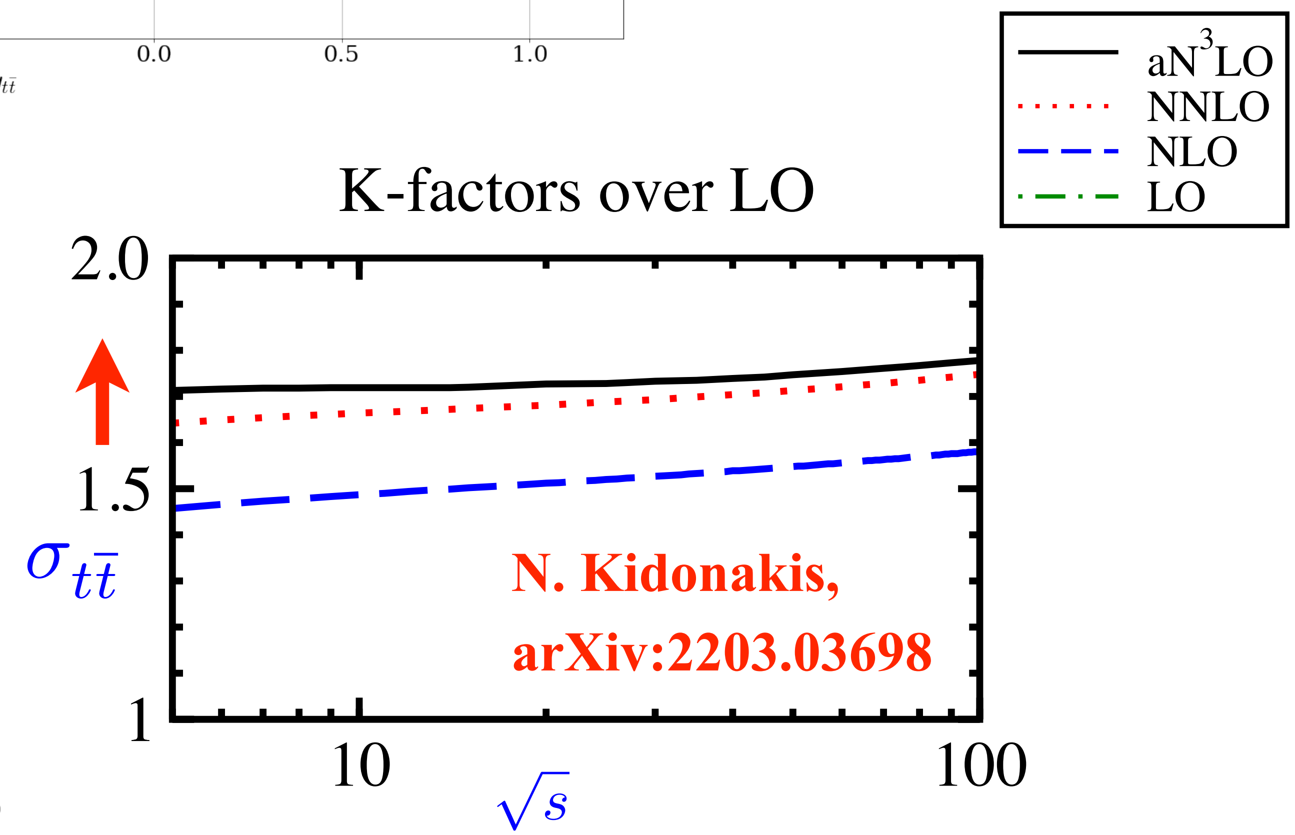


X. Chen et al., Phys.Rev.Lett. 128 (2022) 5, 052001

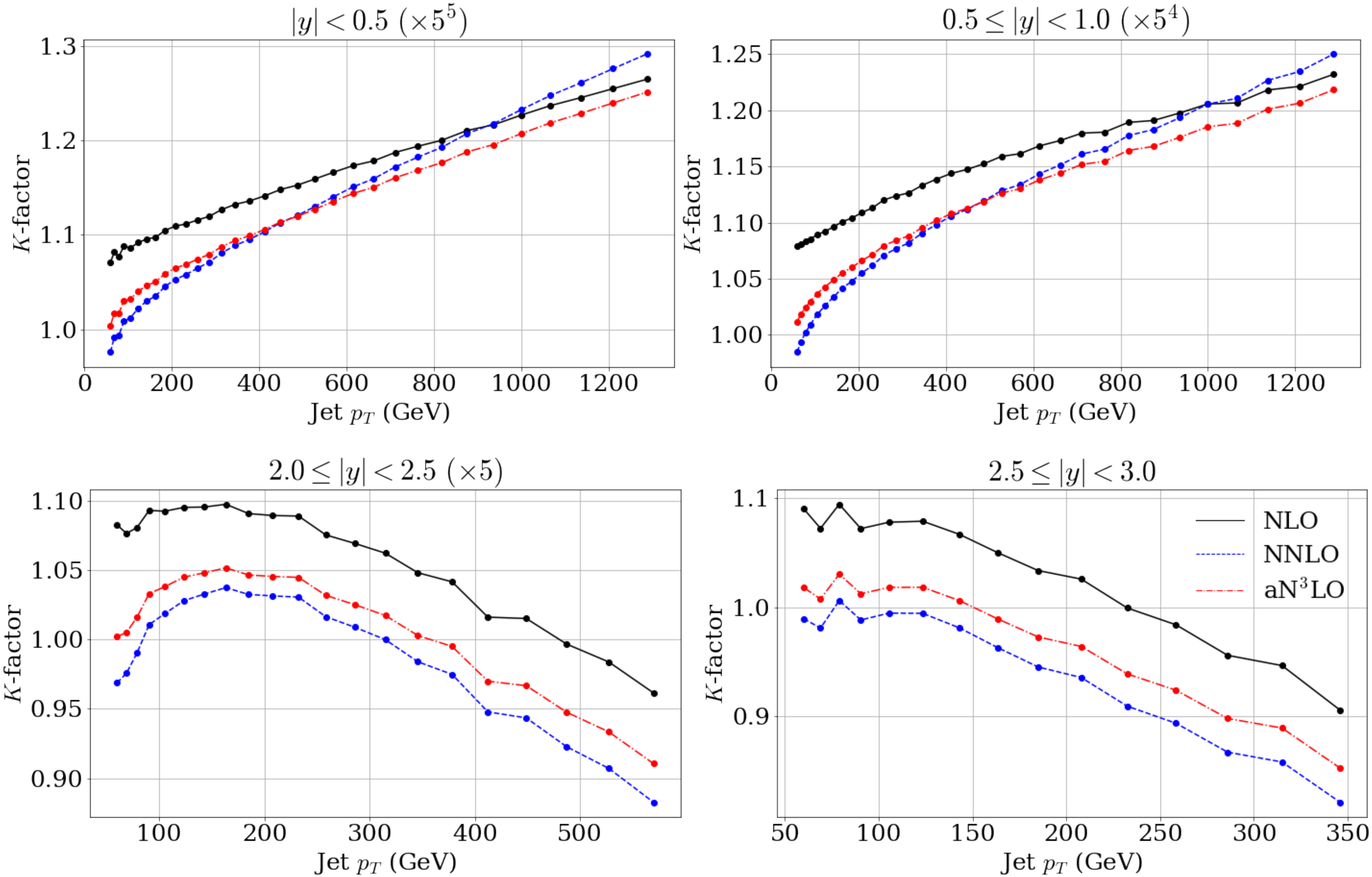
★ Resulting K-factors: $t\bar{t}$.



- Fit prefers overall increase in magnitude from NNLO to N3LO.
- Consistent with approximation N3LO calculation.

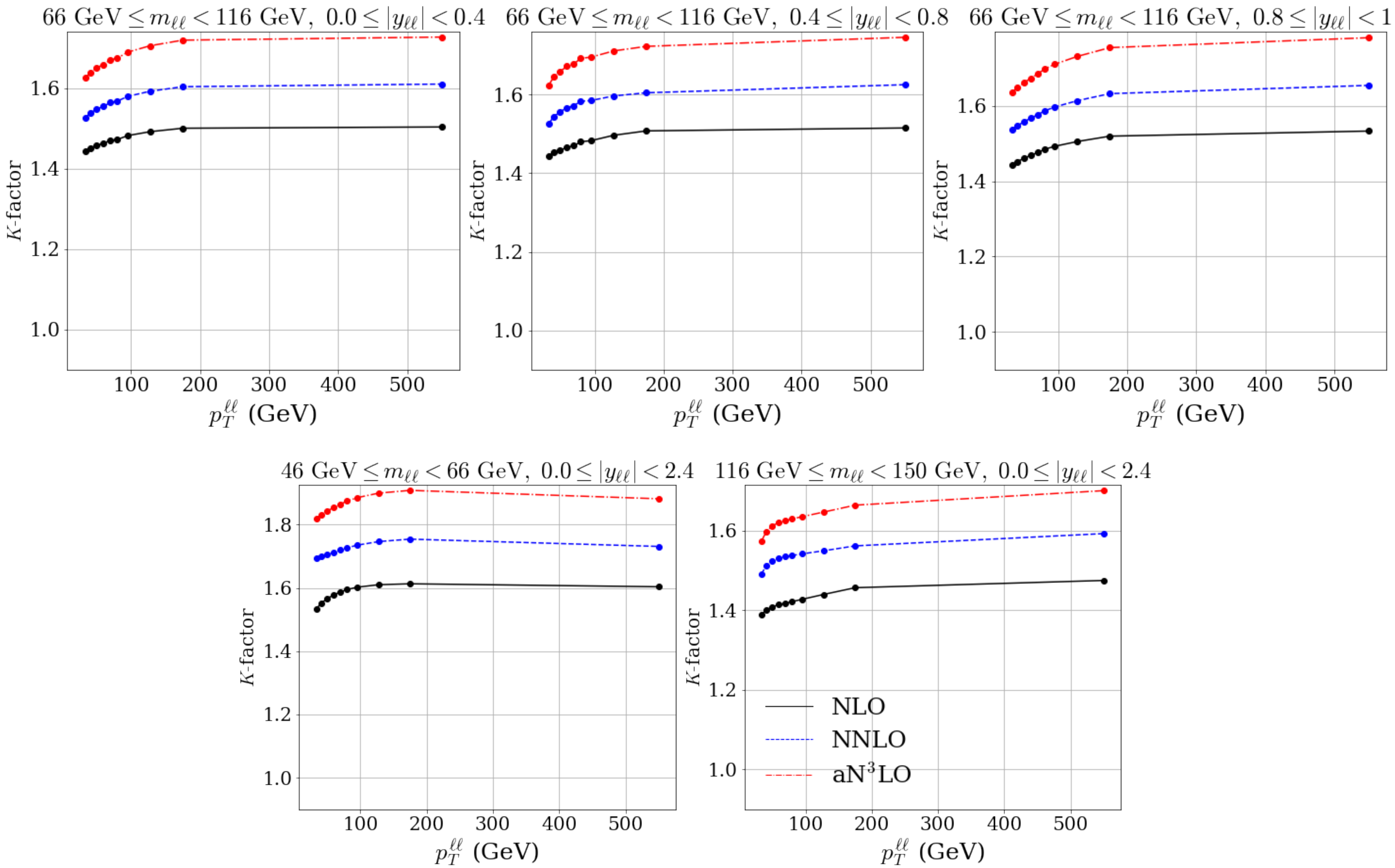


★ Resulting K-factors: **jets**.



- Fairly mild shift from NNLO to N3LO, as one might expect/hope for.

★ Resulting K-factors: $Z\, p_\perp$



- Somewhat larger shift here. Arguably consistent with rather larger lower order corrections.
- **Note**: here (and elsewhere) K-factor is one preferred by fit $\Rightarrow$ may be tendency for this to lie towards 'all orders' result. Important when interpreting wrt perturbative stability.

Results

Fit Quality

- Using the results above, perform aN3LO fit to exactly same dataset as MSHT20 NNLO global fit.
- Start with total χ^2 per point. General trend for improvement at aN3LO, as we would expect from pQCD. Corresponds to $\sim 1-2\sigma$ from NNLO.

	LO	NLO	NNLO	N^{3}LO
$\chi^2_{N_{pts}}$	2.57	1.33	1.17	1.14

- Some of this improvement comes from additional freedom in LHC K-factors. However:
  - ★ Over half remains if we turn these off.
  - ★ We have seen for DY + $t\bar{t}$ that these follow what we could expect from pQCD calculations.
- **Key point**: much of theory changes are not centred on NNLO. Can depart quite strongly from this due to known information about N3LO. The fit is preferring this!

- Breaking things down more:

Dataset	N_{pts}	χ^2	$\Delta\chi^2$ from
DY data Total	864	1069.4	-18.5
Top data Total	71	75.1	-4.2
Jets data Total	739	963.6	$+21.5$
p_T Jets data Total	144	138.0	-77.2
Dimuon data Total	170	125.0	-1.2
DIS data Total	2375	2580.9	-90.8
Total	4363	4961.2	-160.1

- Significant improvement in DIS - driven by N3LO input.
- Also large improvement in '$p_\perp$ Jets' - driven by ATLAS 8 TeV $Z\,p_\perp$ data: from 1.81 to 1.04 per point (104 points).
- $Z\,p_\perp$ constrains high x gluon, and similar level of improvement found if we exclude HERA DIS from NNLO fit, i.e. aN3LO is alleviating tension between low and high x regions.
- Milder improvement in $t\bar{t}$ and DY. Interestingly inclusive jet data actually gets worse - issues with fitting inclusive jet data?

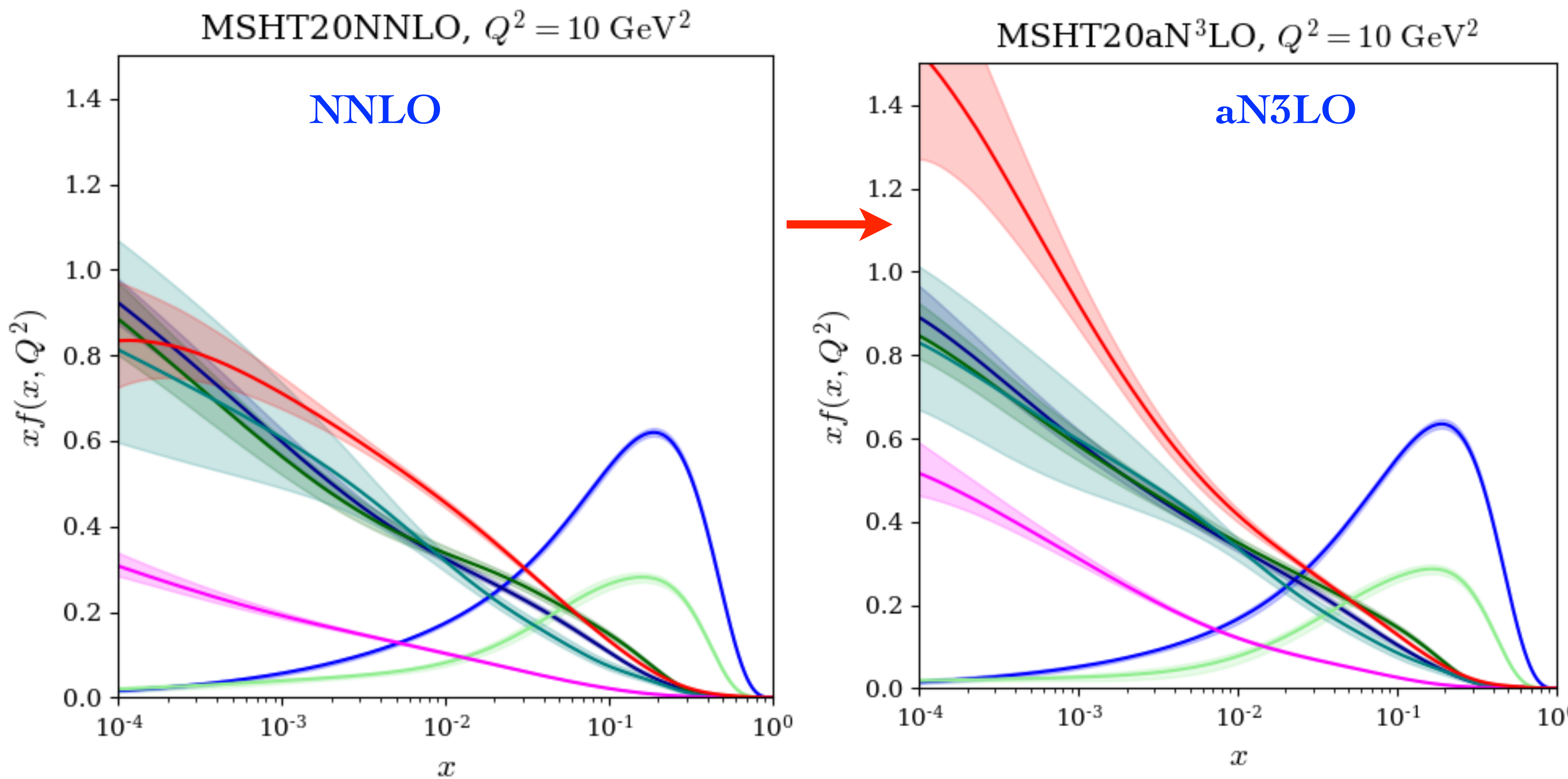
Nuisance parameters

Low-Q^2 Coefficient			
$c_q^{\rm NLL} = -3.868$	0.004	$c_g^{\rm NLL} = -5.837$	0.844
Transition Matrix Elements			
$a_{Hg} = 12214.000$ $a_{gg,H} = -1951.600$	0.601 0.857	$a_{qq,H}^{\rm NS} = -64.411$	0.001
Splitting Functions			
$\rho_{qq}^{NS} = 0.007$ $\rho_{qq}^{PS} = -0.501$ $\rho_{qg} = -1.754$	0.000 0.186 0.015	$\rho_{gq} = -1.784$ $\rho_{gg} = 19.245$	0.802 3.419
K-factors			
$\mathrm{DY}_{\rm NLO} = -0.307$ $\mathrm{Top}_{\rm NLO} = 0.041$ $\mathrm{Jet}_{\rm NLO} = -0.300$ $p_T\mathrm{Jets}_{\rm NLO} = 0.583$ $\mathrm{Dimuon}_{\rm NLO} = -0.444$	0.094 0.002 0.090 0.339 0.197	$\mathrm{DY}_{\rm NNLO} = -0.230$ $\mathrm{Top}_{\rm NNLO} = 0.651$ $\mathrm{Jet}_{\rm NNLO} = -0.691$ $p_T\mathrm{Jets}_{\rm NNLO} = -0.080$ $\mathrm{Dimuon}_{\rm NNLO} = 0.922$	0.053 0.424 0.478 0.006 0.850
N^{3}LO Penalty Total	9.262 / 20	Average Penalty	0.463
		Total $\Delta\chi^2$ from NNLO	4961.2 / 4363 -160.1

- Average penalty for 20 aN3LO parameters is 0.46, i.e. on average fit prefers values well within prior.

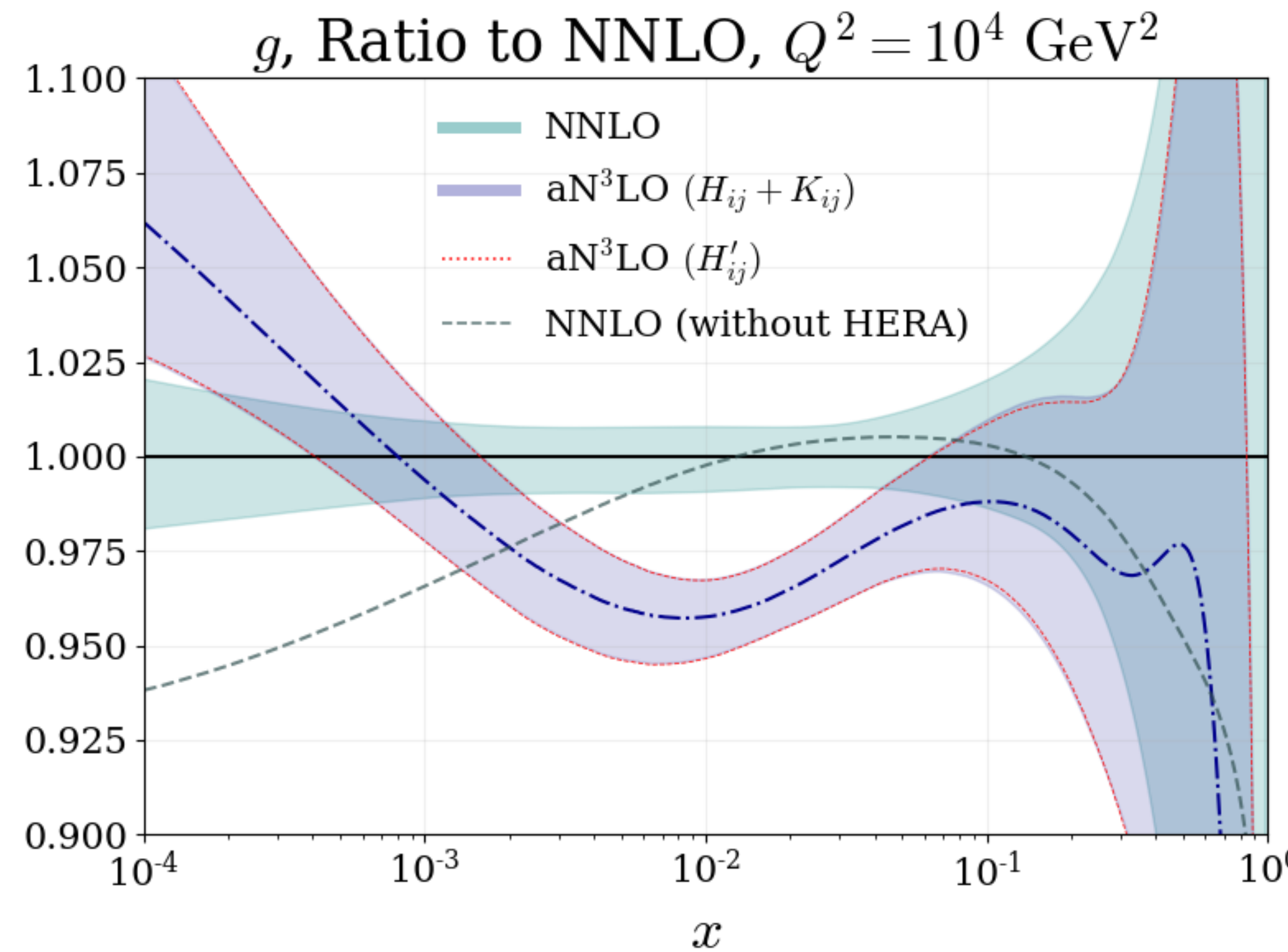
PDFs

- Broad picture:

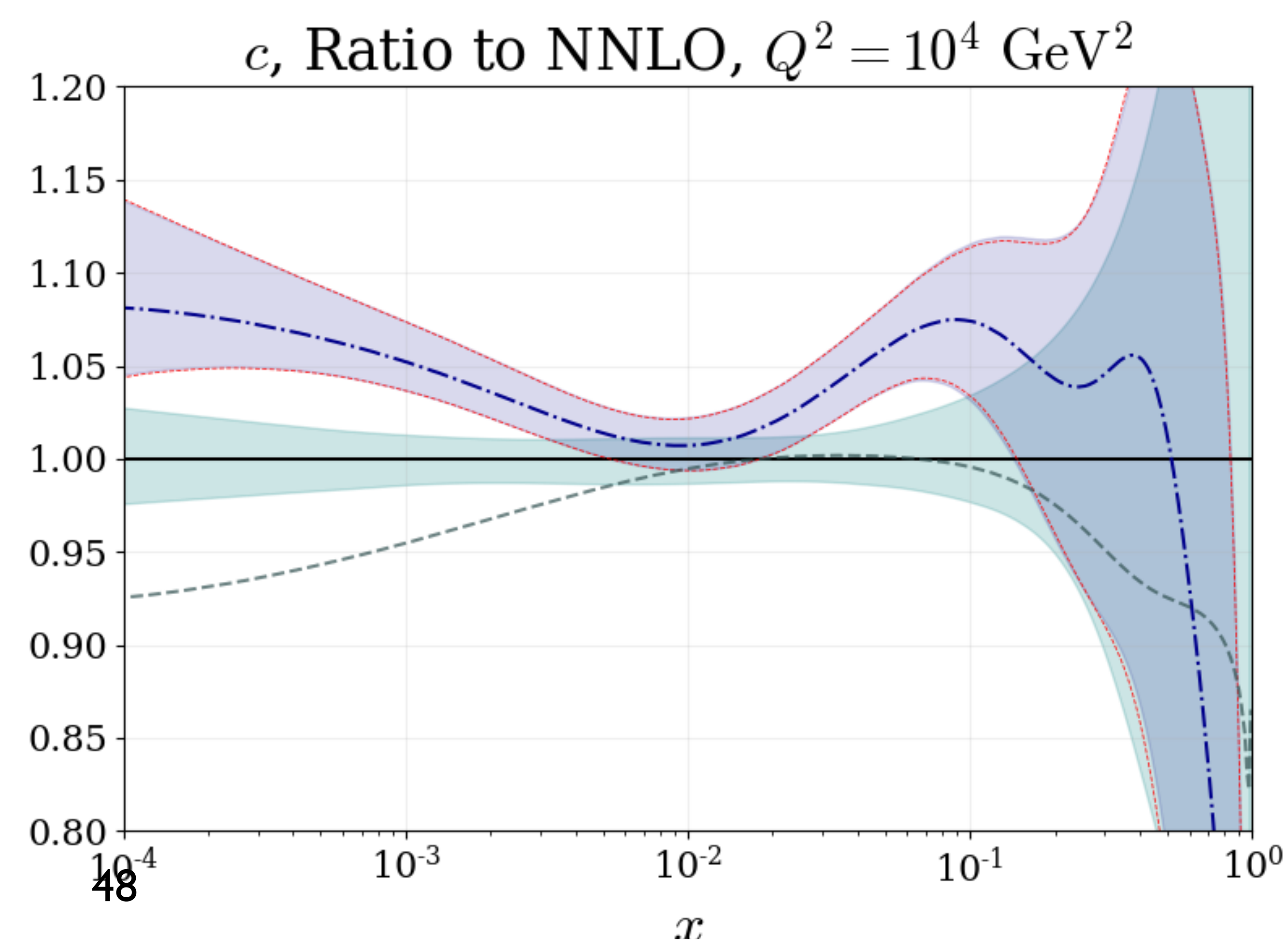


- Most noticeable difference: gluons and quarks larger at low x .
- In more detail…

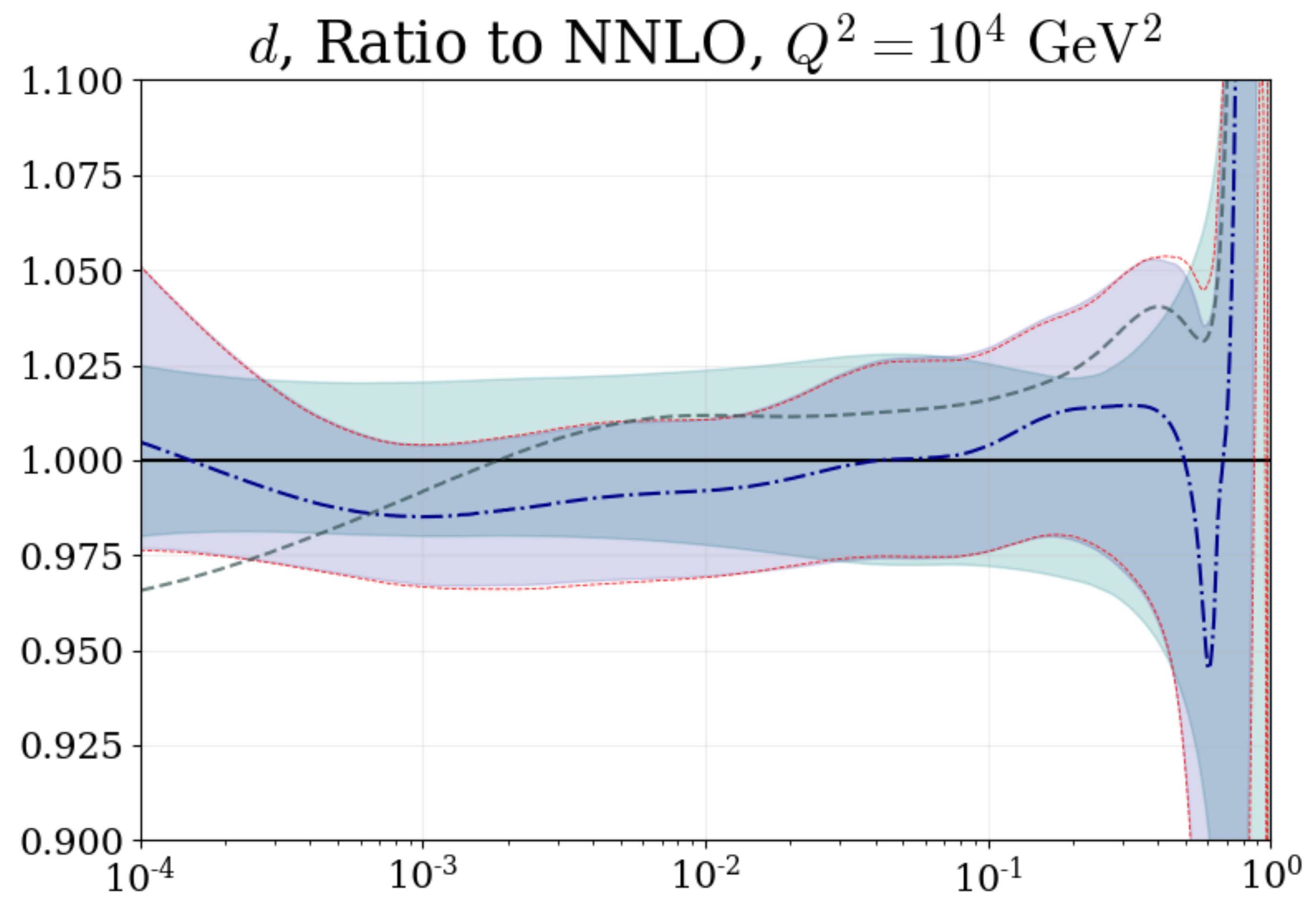
- Gluon enhanced at low x due to large logs in splitting functions.
- But also reduced at $x \sim 10^{-2}$ due to reduction in P_{qg} and compensation for increased gluon at low x .



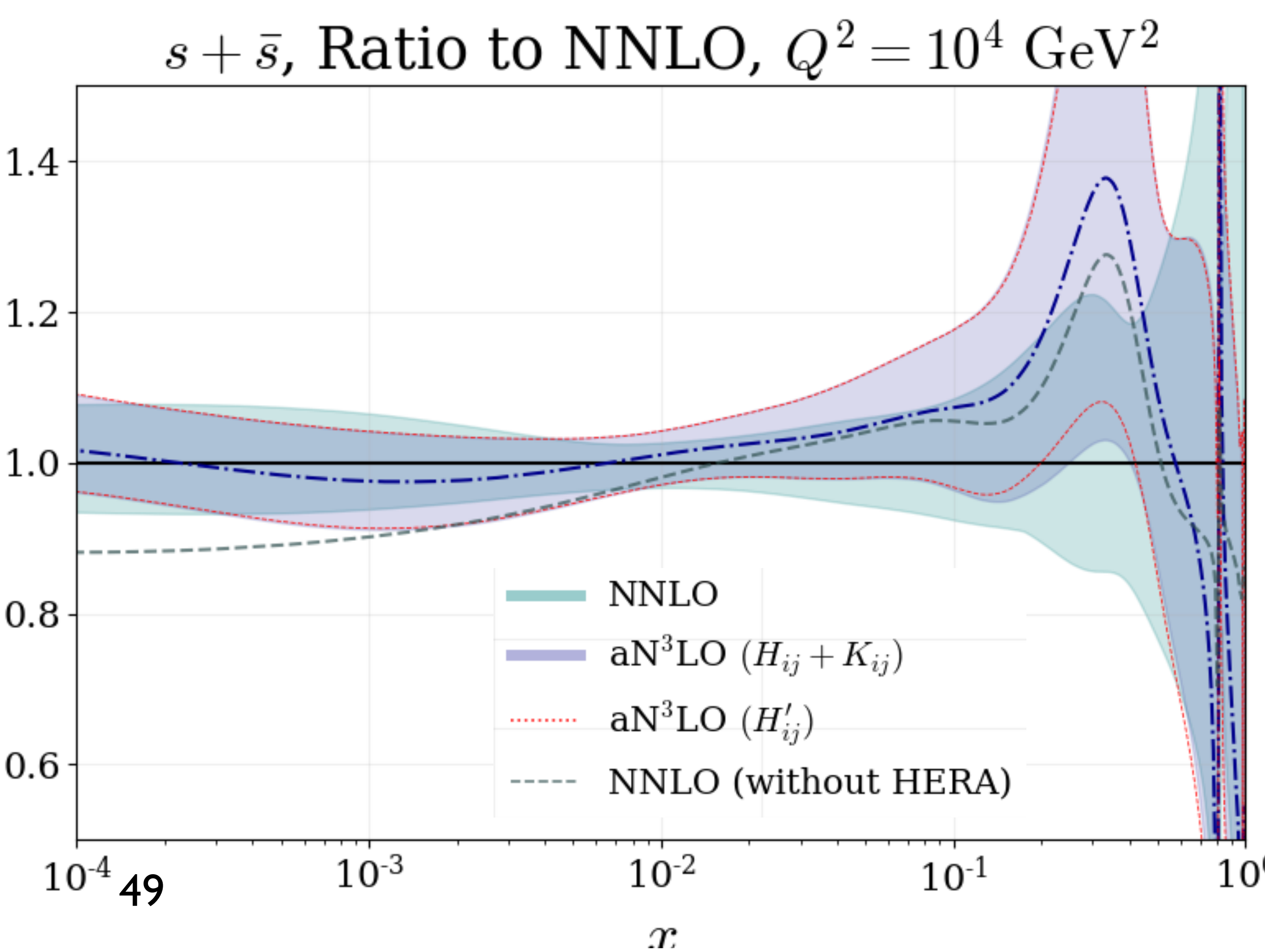
- Charm (generated perturbatively) increased due to increase in gluon at low x and change in A_{Hg} .



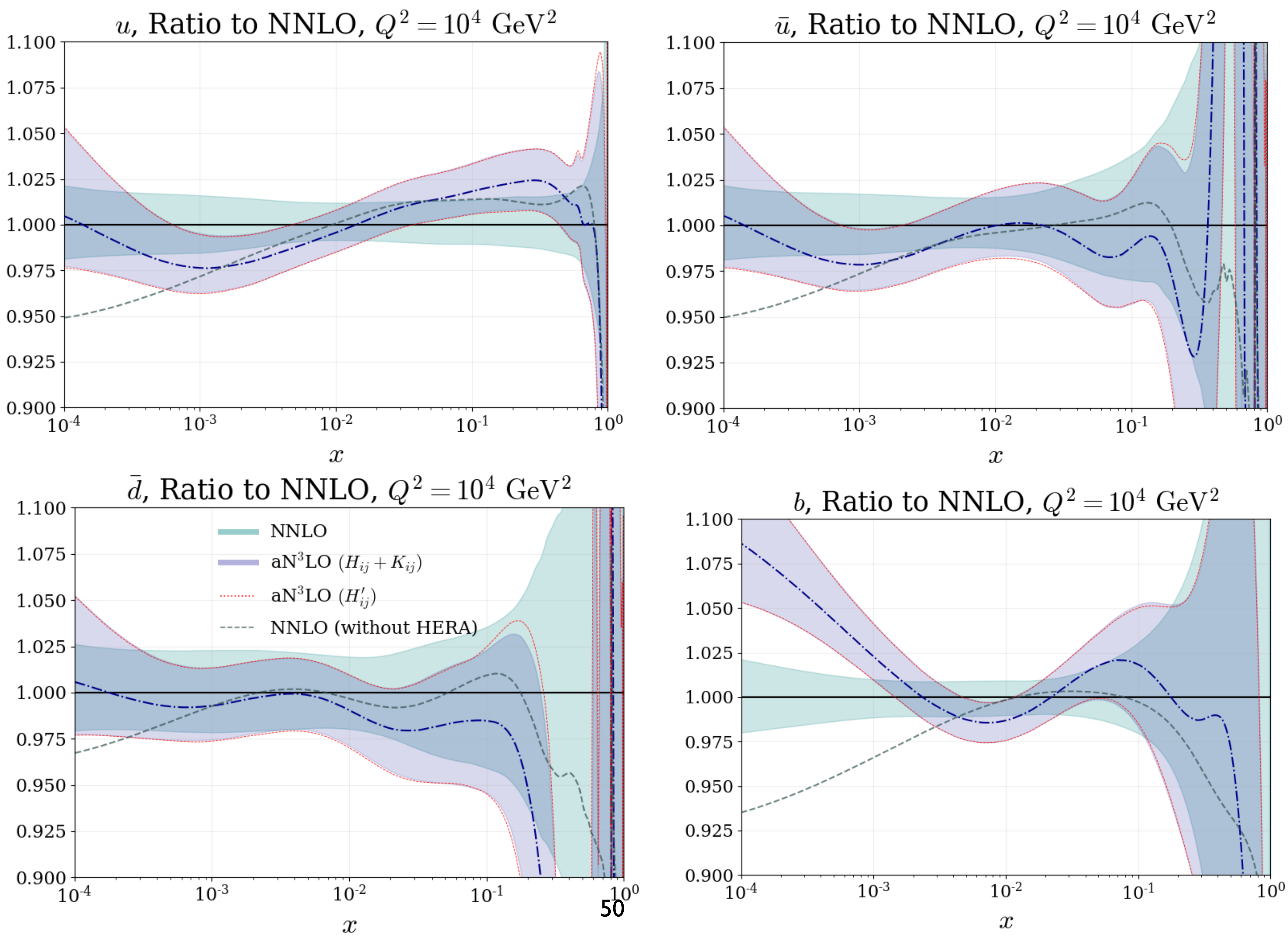
- Some enhancement in light quarks at high x .



- Strange quark enhanced at high x .
- Follows the NNLO (no HERA) rather closely - reduced tensions.



- Other PDFs…


u, Ratio to NNLO, $Q^2 = 10^4$ GeV^2
$\bar{u}$, Ratio to NNLO, $Q^2 = 10^4$ GeV^2
$\bar{d}$, Ratio to NNLO, $Q^2 = 10^4$ GeV^2
b, Ratio to NNLO, $Q^2 = 10^4$ GeV^2
1.100
1.075
1.050
1.025
1.000
0.975
0.950
0.925
0.900
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^{0}
x
NNLO
aN^{3}LO ($H_{ij} + K_{ij}$)
aN^{3}LO (H'_{ij})
NNLO (without HERA)

PDFs - theoretical uncertainty

- Recall we have added in additional freedom via aN3LO nuisance parameters:

$$T' = T'_0 + \theta' u$$

N3LO theory

N3LO (central)

Allowed variation

$$P(\theta') = \frac{1}{\sqrt{2\pi}\sigma_{\theta'}} \exp(-\theta'^{\,2}/2\sigma^2_{\theta'})$$

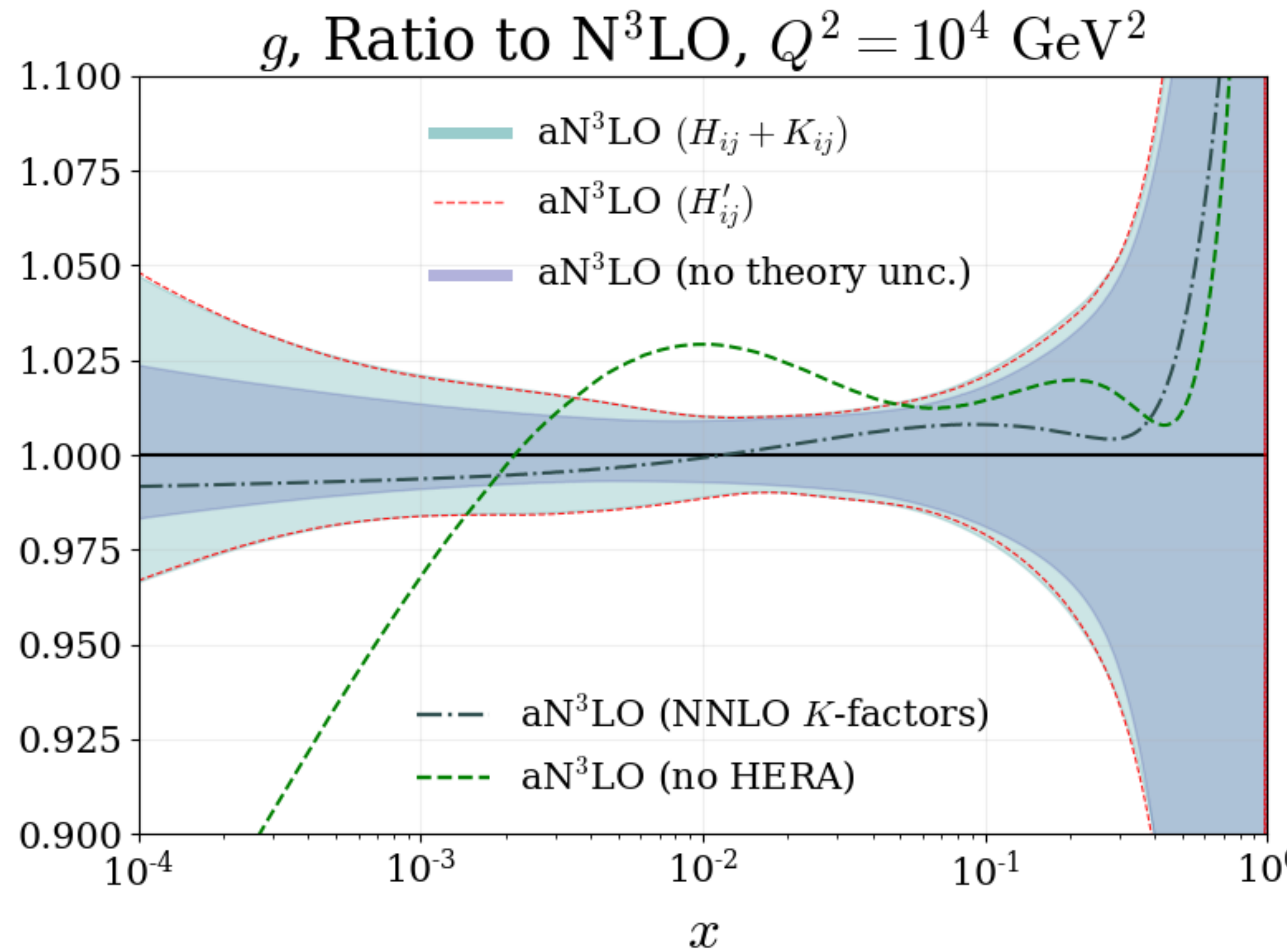
- This will also impact on PDF uncertainties - an additional uncertainty due to unknown higher order corrections:

$$P(T'|D) \propto \int d\theta' \exp\left(-\frac{1}{2}M^{-1}(\theta' - \overline{\theta}')^2 - \frac{1}{2}(T' - D)^T (H_0^{-1} + uu^T)^{-1}(T' - D)\right).$$

Additional uncertainty

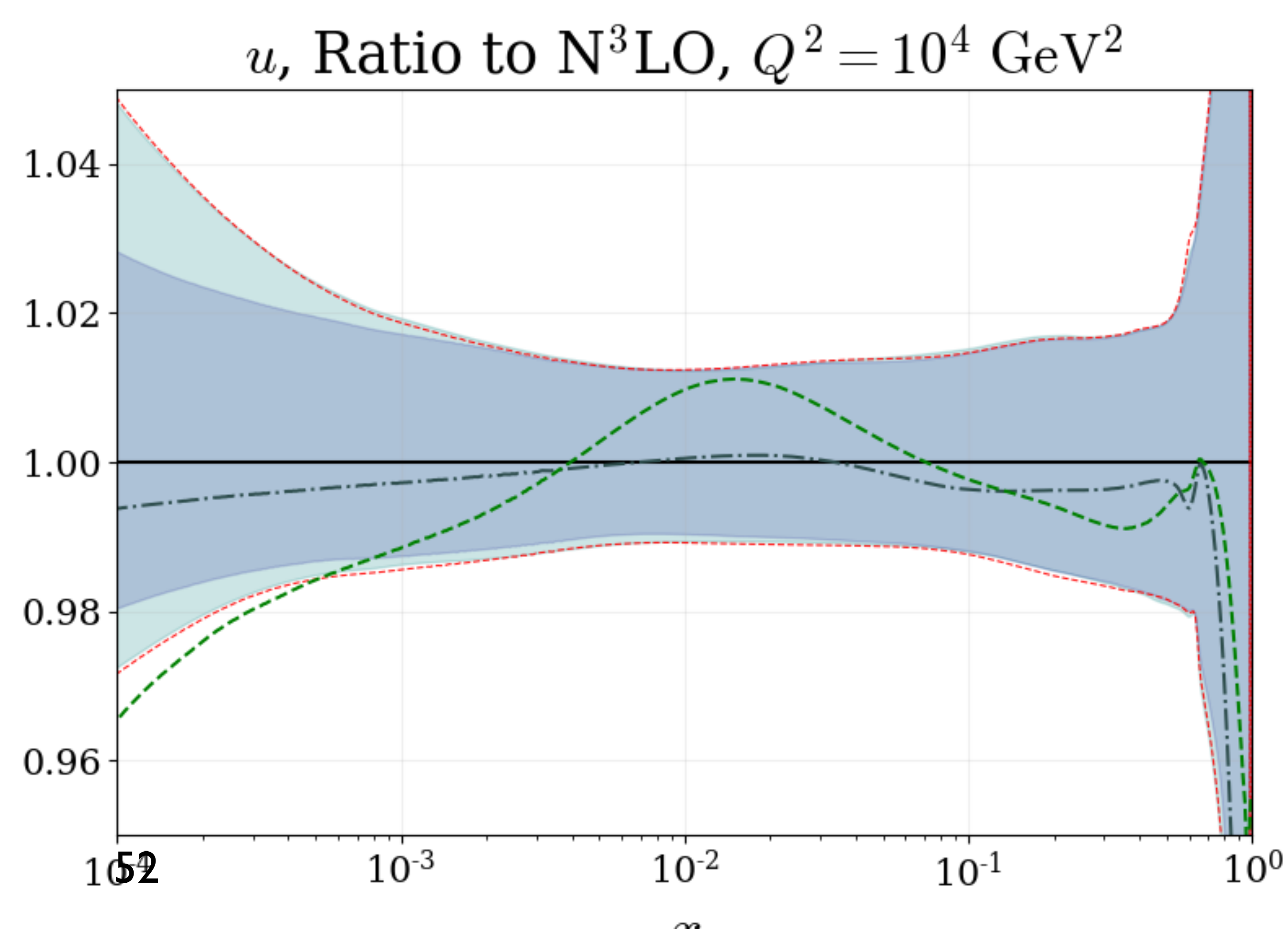
  - In principle uncertainty from these is correlated with other (experimental) PDF uncertainties.
  - However for K-factors find these largely separate out: can provide separately with little loss in accuracy.

- Gluon uncertainty most affected - increased at low x due to larger uncertainty in splitting functions.



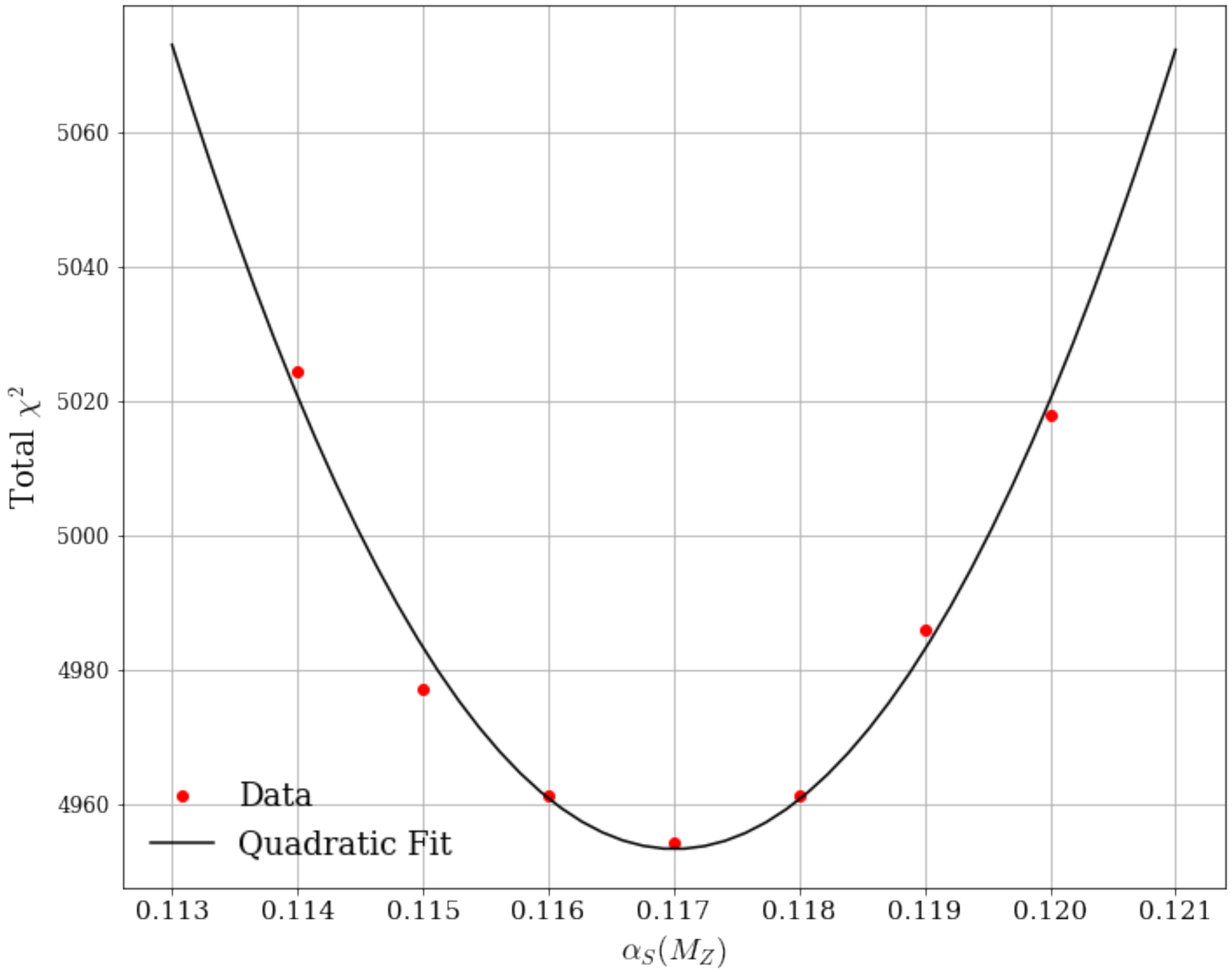
- Some increase in light quarks at low x .
- But at high x impact tiny - much more known here and uncertainty lower.

- Correlated and decorrelated errors very similar.



Strong Coupling

- Can also allow α_S to be free in fit. Find for best fit: $\alpha_S(M_Z^2)^{\rm bf} = 0.117$
- Consistent with world average.

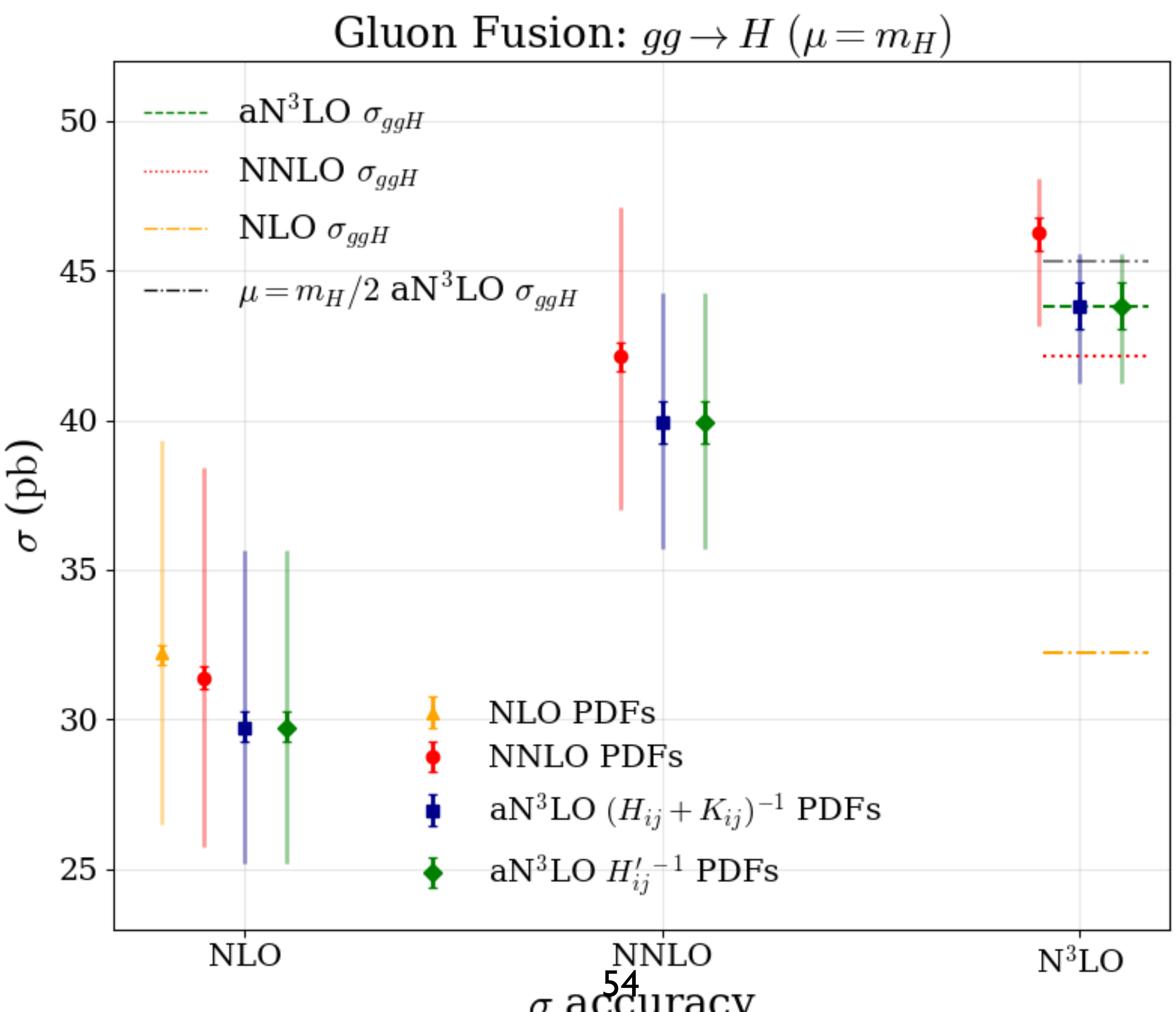


MSHT20 NNLO: $\alpha_S(M_Z^2) = 0.1174 \pm 0.0013$.

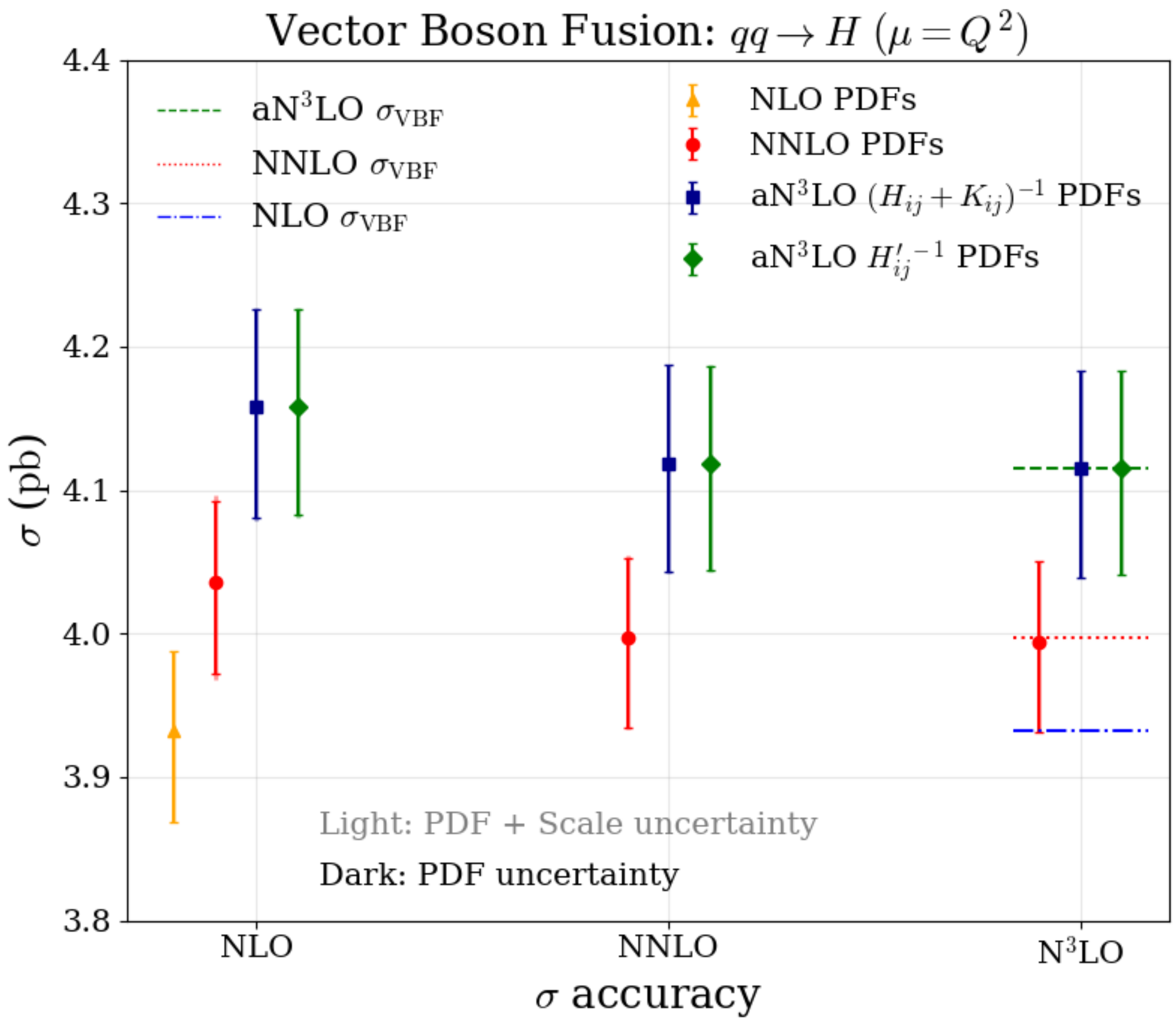
MSHT20 NLO: $\alpha_S(M_Z^2) = 0.120 \pm 0.0015$.

Implications for the Higgs

- **Higgs via gg fusion**: reasonable shift down induced due to change in gluon.
- Perturbative convergence improved once aN3LO PDFs used. This cancellation not guaranteed (not driven by e.g. change in P_{gg}).



- **Higgs via VBF**: less cancellation although here variation between orders is smaller.



Dijet Data

Preliminary

- Try fitting (2D and 3D) dijet data rather than inclusive jets.
- Recall fit quality to inclusive jets worse from NNLO at aN3LO.
- For dijets this is no longer the case! Improvement in going to aN3LO and also in overall fit to other data.

	N_{pts}	χ^2/N_{pts}	
		NNLO	aN^{3}LO
ATLAS 7 TeV jets	140	1.58	1.54
CMS 7 TeV jets	158	1.11	1.18
CMS 8 TeV jets	174	1.50	1.56
Total	472	1.39	1.43

	N_{pts}	χ^2/N_{pts}	
		NNLO	aN^{3}LO
ATLAS 7 TeV dijets	90	1.05	1.12
CMS 7 TeV dijets	54	1.43	1.39
CMS 8 TeV dijets	122	1.04	0.83
Total	266	1.12	1.04

- Impact on PDFs similar (not identical). Closer at aN3LO.

Low x and resummation

- Interesting to observe that impact on gluon and improvement in fit quality to HERA DIS data rather similar to earlier fits including low x resummation.

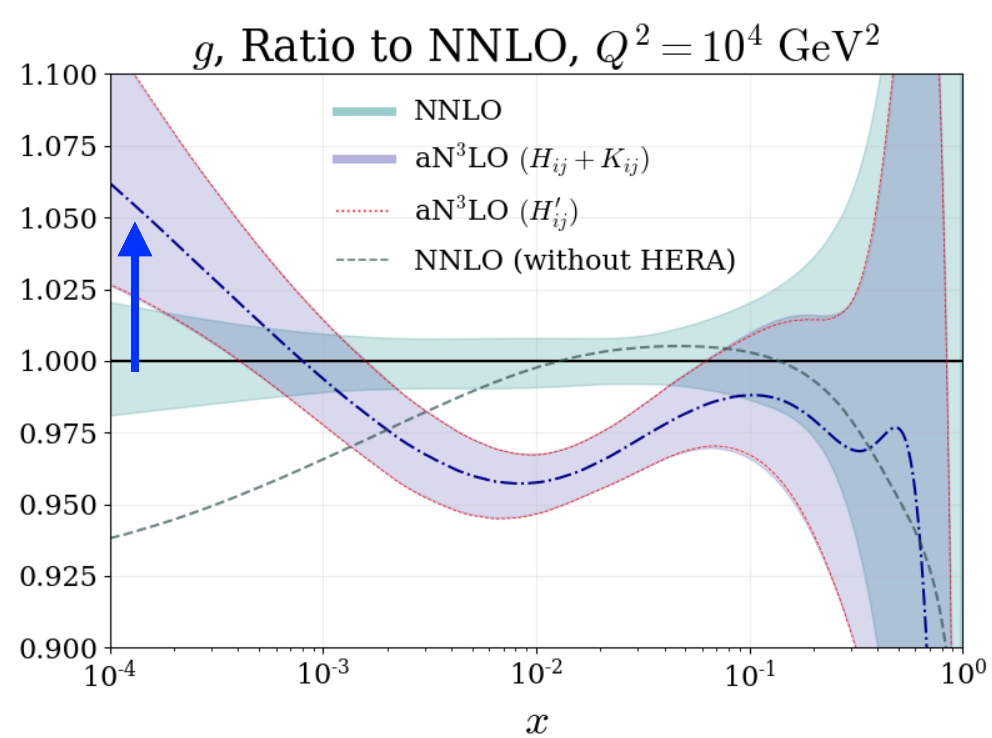
aN3LO

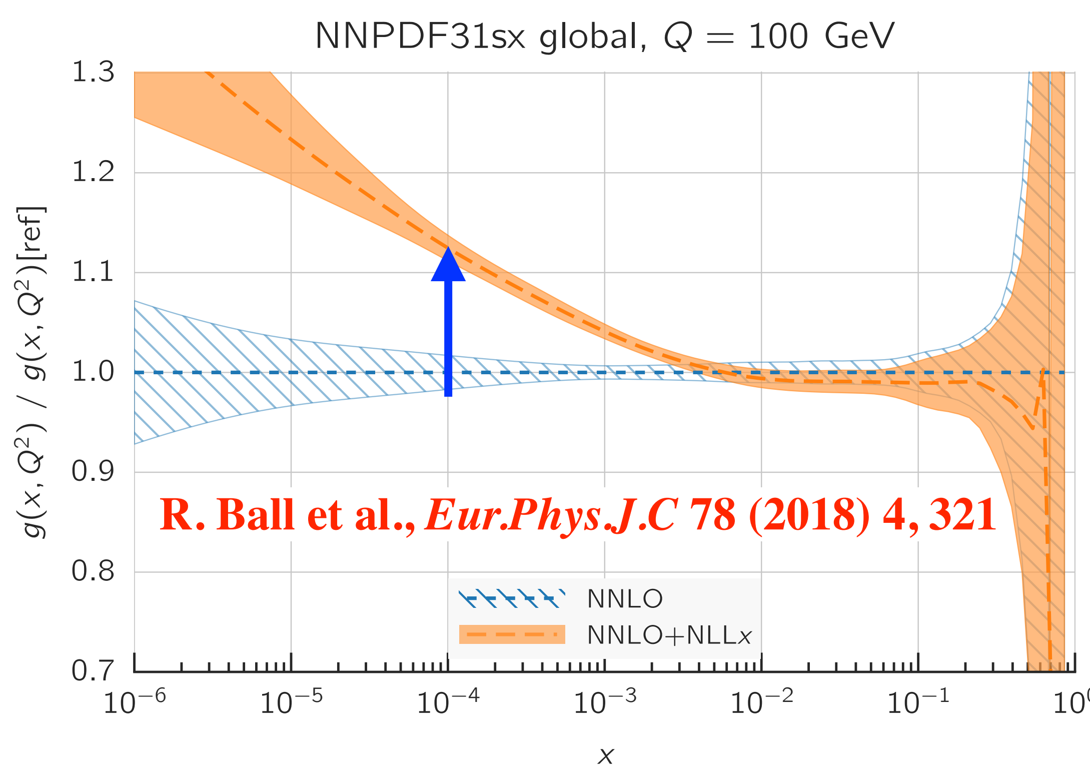
DIS Dataset	χ^2	$\Delta\chi^2$ from NNLO
HERA e^+p NC 820 GeV [144]	84.3 / 75	−5.6
HERA e^-p NC 460 GeV [144]	247.7 / 209	−0.6
HERA e^+p NC 920 GeV [144]	474.0 / 402	−38.7
HERA e^-p NC 575 GeV [144]	248.5 / 259	−14.5
HERA e^-p NC 920 GeV [144]	243.0 / 159	−1.4
Total	2580.9 / 2375	−90.8

Resummation

$\chi^2/N_{\rm dat}$ NNLO	NNLO+NLLx	$\Delta\chi^2$
1.17	1.11	−62
1.25	1.24	−1

xFitter, *Eur.Phys.J.C* 78 (2018) 8, 621





Interpretation/Usage

- We assume for now that dominant MHO uncertainty is from missing N3LO. However fit can pick up corrections beyond this.
- Can update in future to account for more N3LO information as it comes in. At some point as this becomes more constrained can update procedure to include uncertainty from N4LO (in principle!).
- Recommendation for usage:
    - ⋆ If N3LO cross sections are known, use aN3LO PDF + their theoretical uncertainties.
    - ⋆ For DIS processes advised to use aN3LO PDF with aN3LO coefficient functions.
    - ⋆ For any processes included in fit we provide full details of fitted K-factors.
    - ⋆ For processes not included in fit, the change between using NNLO and N3LO can be taken as a corresponding uncertainty.

Summary and Outlook

- ⋆ As precision of data continues to improve and we continue to stress test the SM as precisely as possible essential to account for all sources of uncertainty in PDFs.
- ⋆ Have presented first aN3LO PDF set release: MSHT20aN3LO. Can be used where N3LO is known or where it is not to evaluate uncertainty due to missing higher orders in fit.
- ⋆ Provides intuitive and controllable way to include theoretical uncertainties in PDF fit but also use all available information about higher order.
- ⋆ PDFs as LHAPDF grids are available here:

  `www.hep.ucl.ac.uk/msht/`

- ⋆ Stay tuned for further studies!