MSHT PDFs: a First Global Closure Test and aN3LO Determination of the Strong Coupling

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CERN QCD Seminar, June 17 2024, CERN

With Robert Thorne and Tom Cridge

Setting the Scene…

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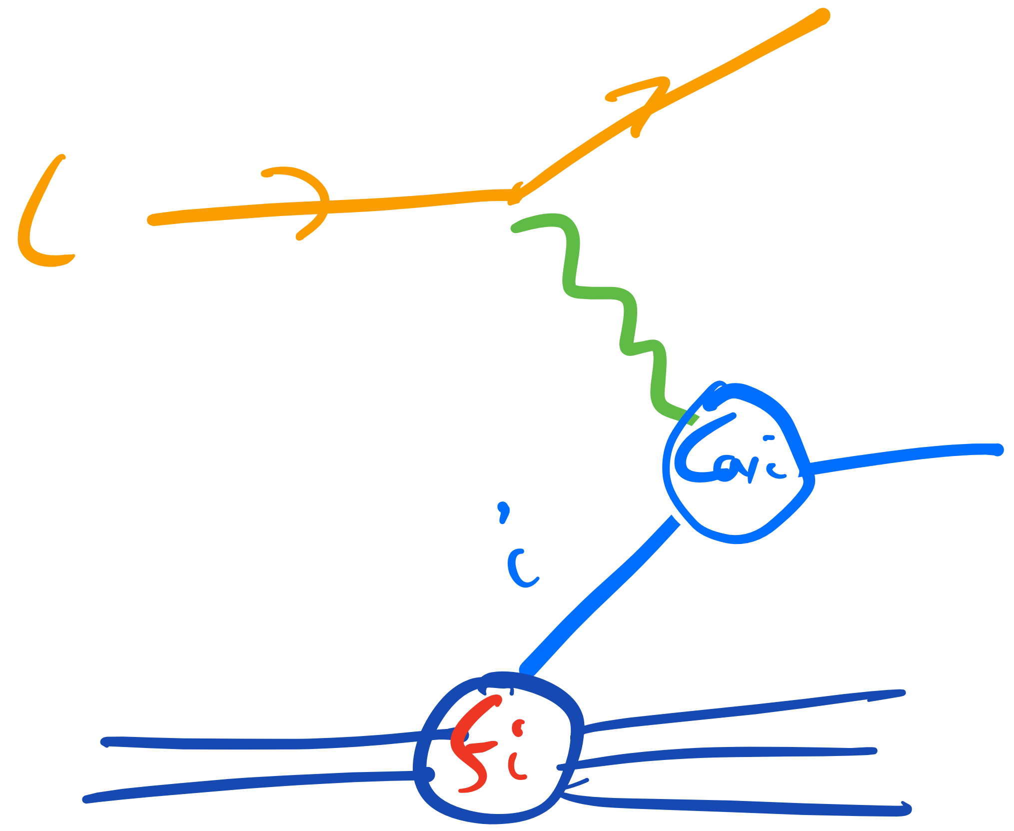
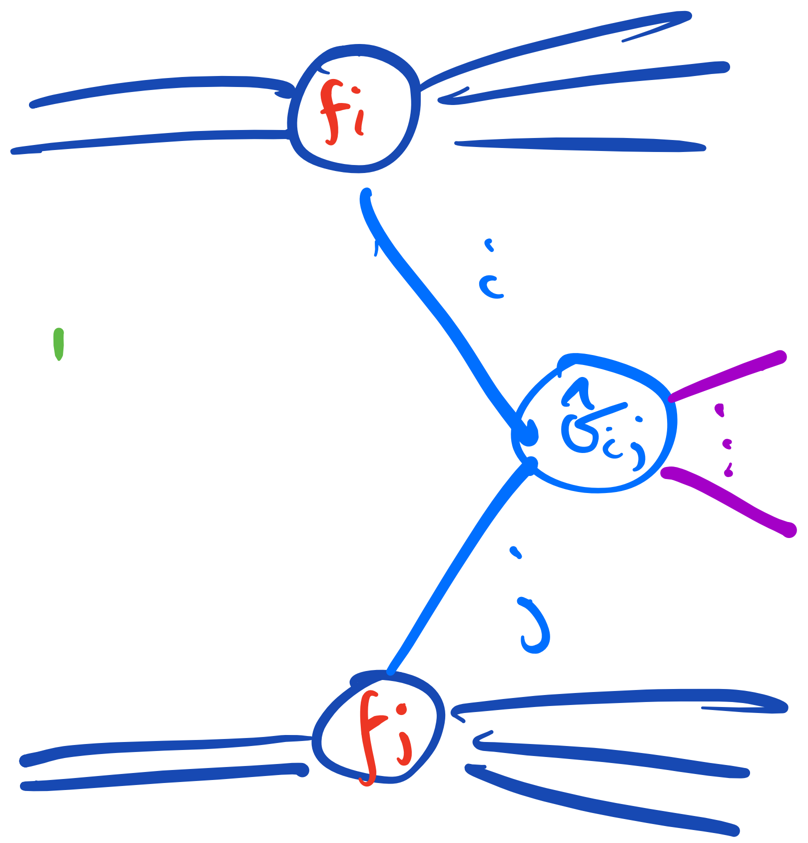
- Parton distribution functions (PDFs): a key ingredient in hadron collider physics!
- QCD factorization: perturbative physics separated from **universal** non-perturbative PDFs





$$F_a(x,Q^2) = \sum_{i=q,\bar{q},g} \int_0^1 \frac{dz}{z} f_i(z,Q^2) C_{a,i}\left(\frac{x}{z}, \alpha_S(Q^2)\right) + \mathcal{O}\left(\frac{\Lambda^2_{QCD}}{Q^2}\right)$$

$$\sigma = \sum_{ij} \int_{x_{min}}^1 dx_1 dx_2\, f_i(x_1,\mu_f^2) f_j(x_2,\mu_f^2) \hat{\sigma}_{ij}(x_1 p_1, x_2 p_2, Q, \mu_F^2)$$

$$\text{Factorization} \Rightarrow f_i^{\text{DIS}}(x,Q^2) \equiv \{f_i^{\text{Collider}}(x,Q^2)\}$$ ← **Drell Yan, Jets, Higgs…**

- PDFs at different scales connected by DGLAP evolution $\frac{\partial f_q^{NS}(x,\mu^2)}{\partial \log \mu^2} = \frac{\alpha_S}{2\pi} \int_x^1 \frac{dz}{z} f_q^{NS}(z,\mu^2) P_{qq}^{NS}(x/z)$ **etc…**
- Foundation of global PDF fits: use data at different scales and processes to extract PDFs.

Global PDF Fits

- Basic idea is simple: $\text{Data} = \text{PDF} \otimes \sigma_H$ but many ingredients enter! Three key areas:

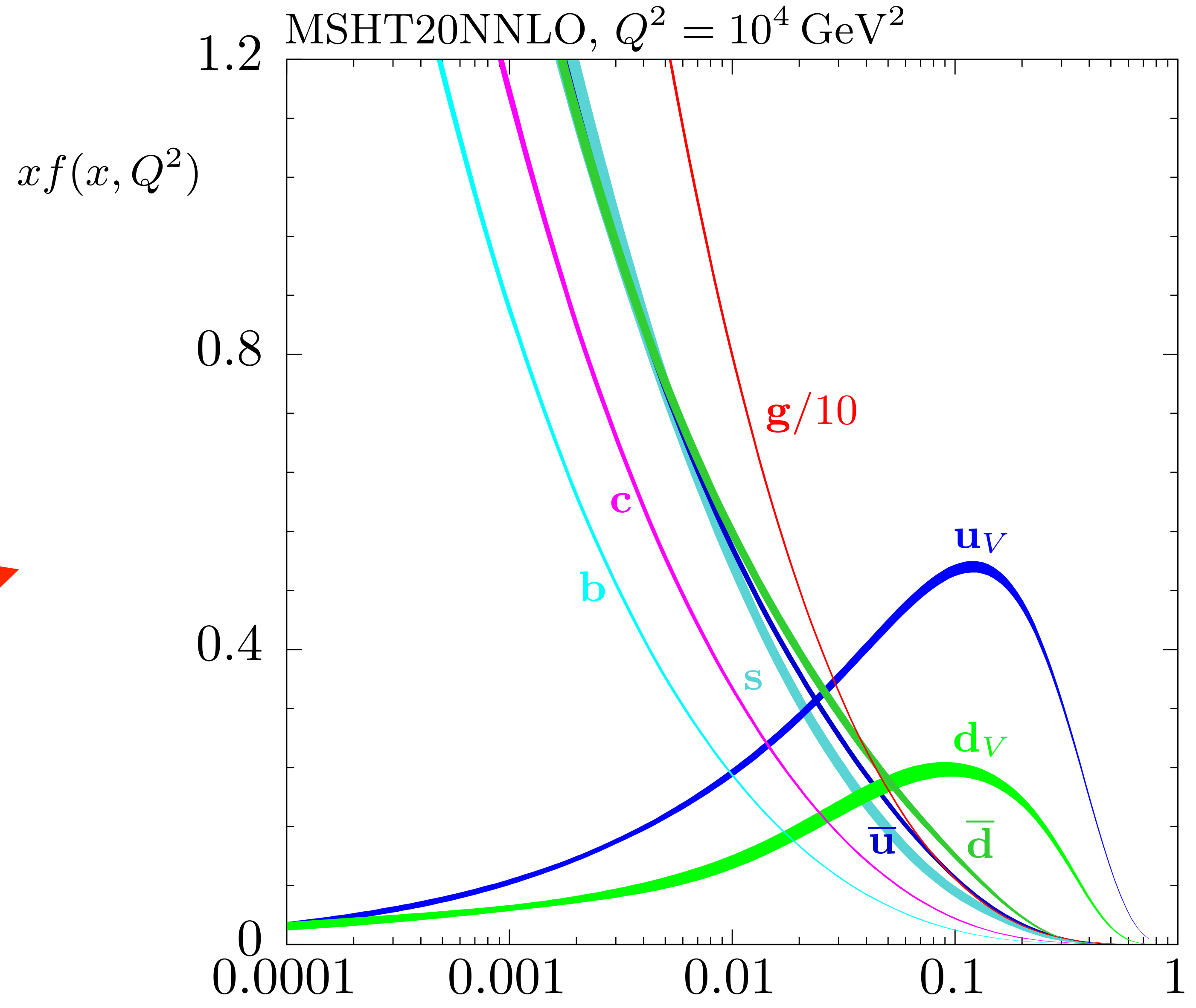
measure (Data) — fit (PDF) — predict (σ_H)

Methodology

- PDF parameterisation, uncertainty prescription…

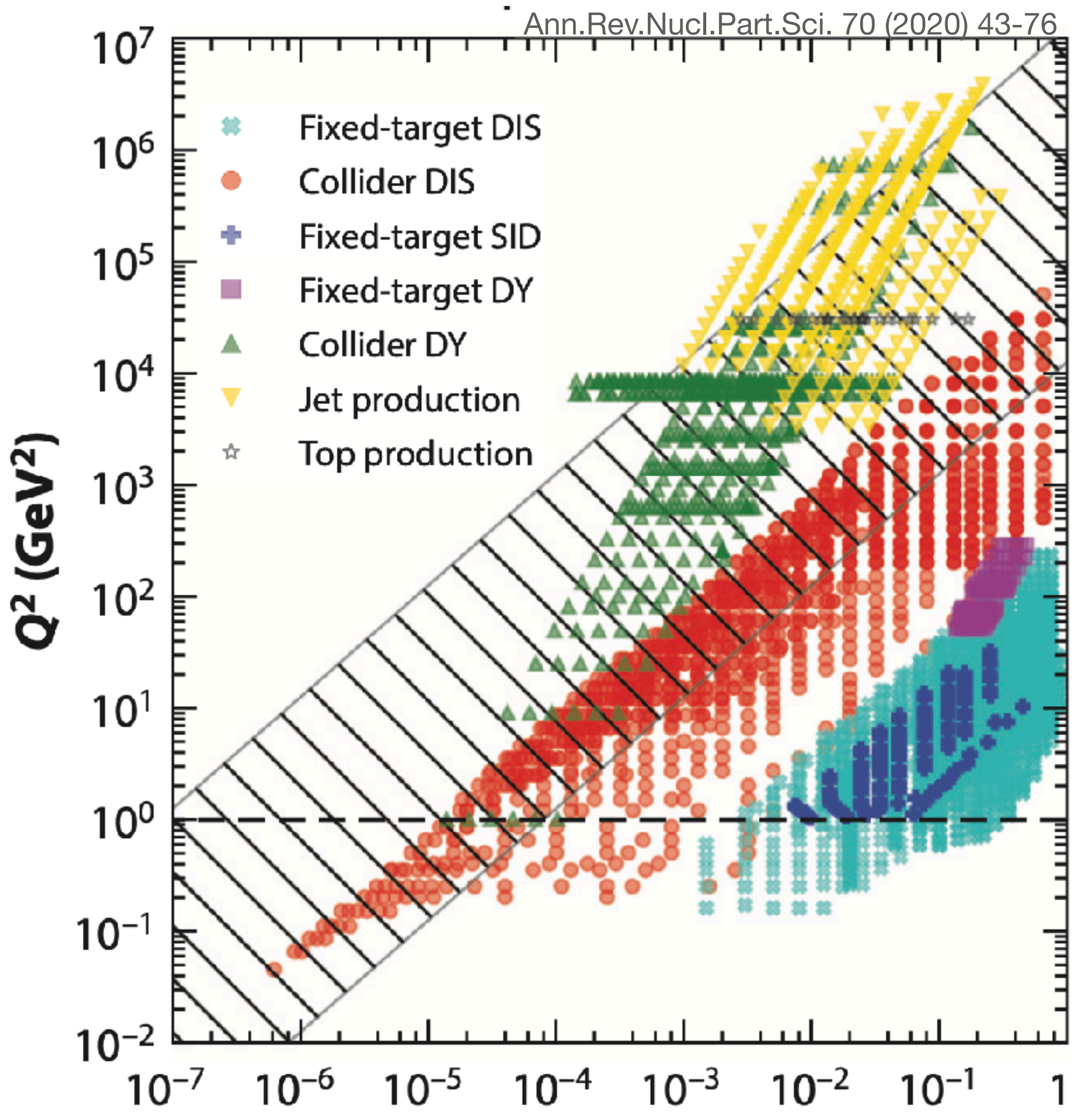
Theory

- High precision: NNLO QCD + NLO EW the standard



Data

- From fixed target, to HERA DIS and collider. LHC data increasingly important.

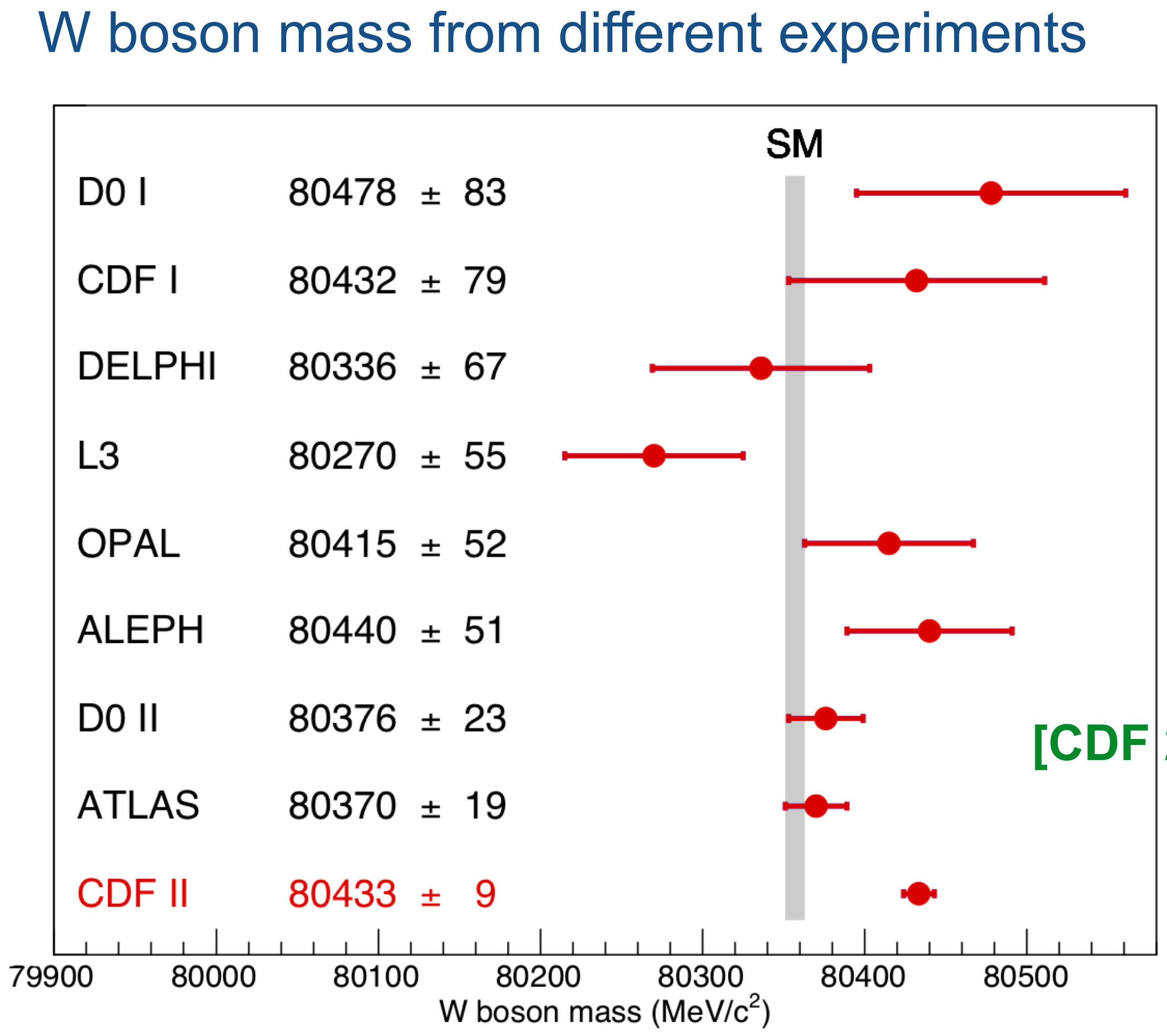


- Aim: high precison theory + wide range of data $\longrightarrow$ **precise** + **accurate** PDFs
- Alternative/complementary route: input from lattice.

Why do we care about PDFs?

- The LHC is a Standard Model precision machine, and PDFs are a key ingredient in this. Increasingly a limiting factor:

W mass



[CDF 2022]

Fig. 5

SM expectation: $M_W = 80{,}357 \pm 4_{\text{inputs}} \pm 4_{\text{theory}}$ (PDG 2020)

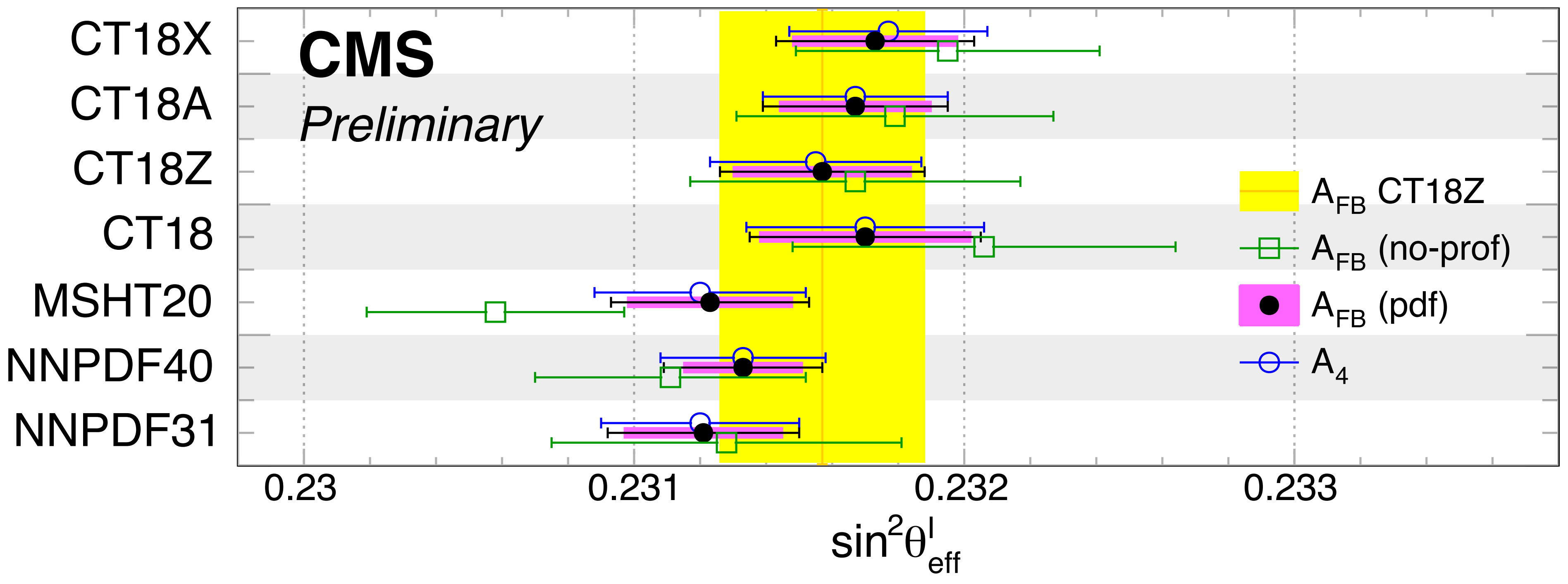
LHCb measurement : $M_W = 80{,}354 \pm 23_{\text{stat}} \pm 10_{\text{exp}} \pm 17_{\text{theory}} \pm 9_{\text{PDF}}$ *[JHEP* **2022,** 36 (2022)]

PDF unc. of CDF / ATLAS / LHCb: 3.9 / 8 / 9 MeV

$$\sigma_{\text{PDF}} \sim \sigma_{\text{tot}}/2$$

(up to)

$\sin^2 \theta^l_{\text{eff}}$

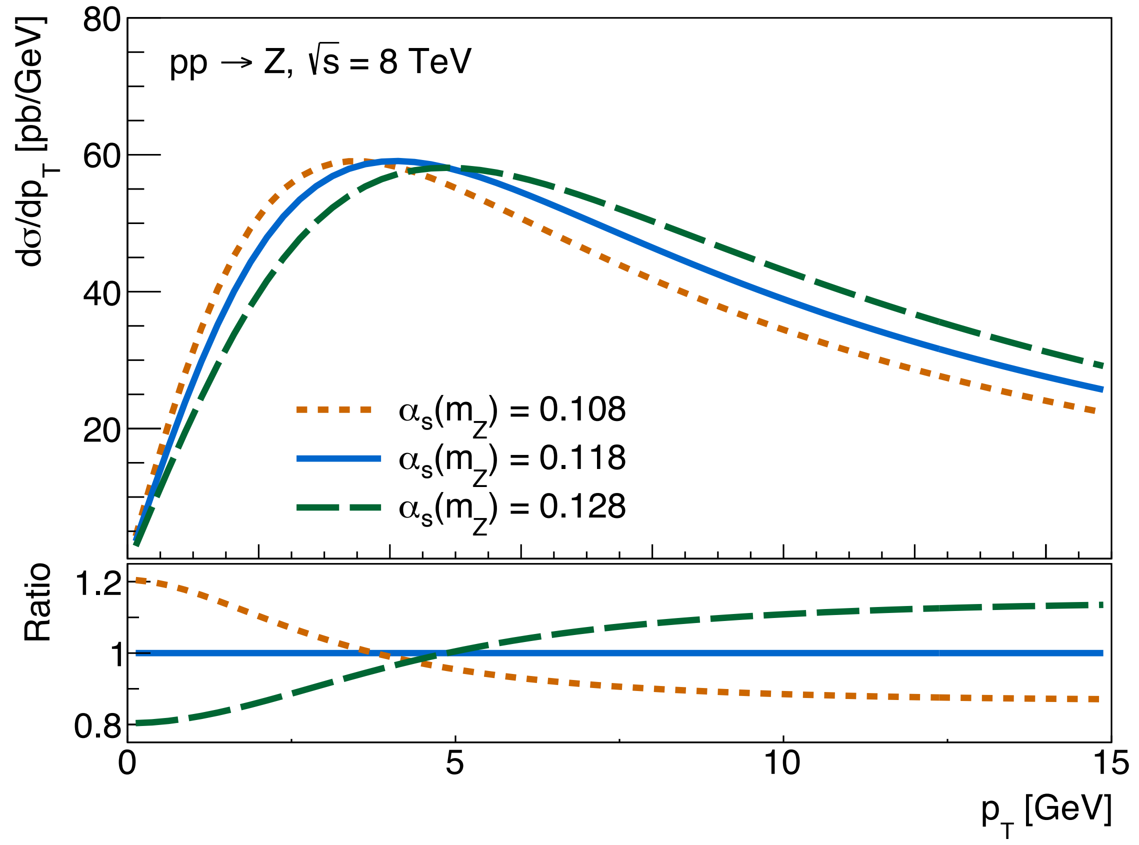


CMS PAS SMP-22-010

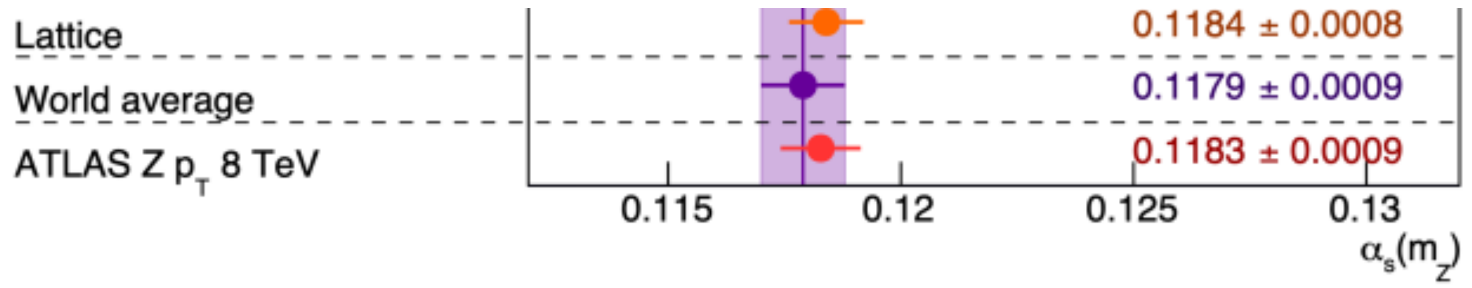
$$\sin^2 \theta^\ell_{\text{eff}} = 0.23157 \pm 0.00010(\text{stat}) \pm 0.00015(\text{syst}) \pm 0.00009(\text{theo}) \pm 0.00027(\text{PDF}),$$

$$\sigma_{\text{PDF}} \sim \sigma_{\text{tot}}$$

α_S



ATLAS, 2309.12986

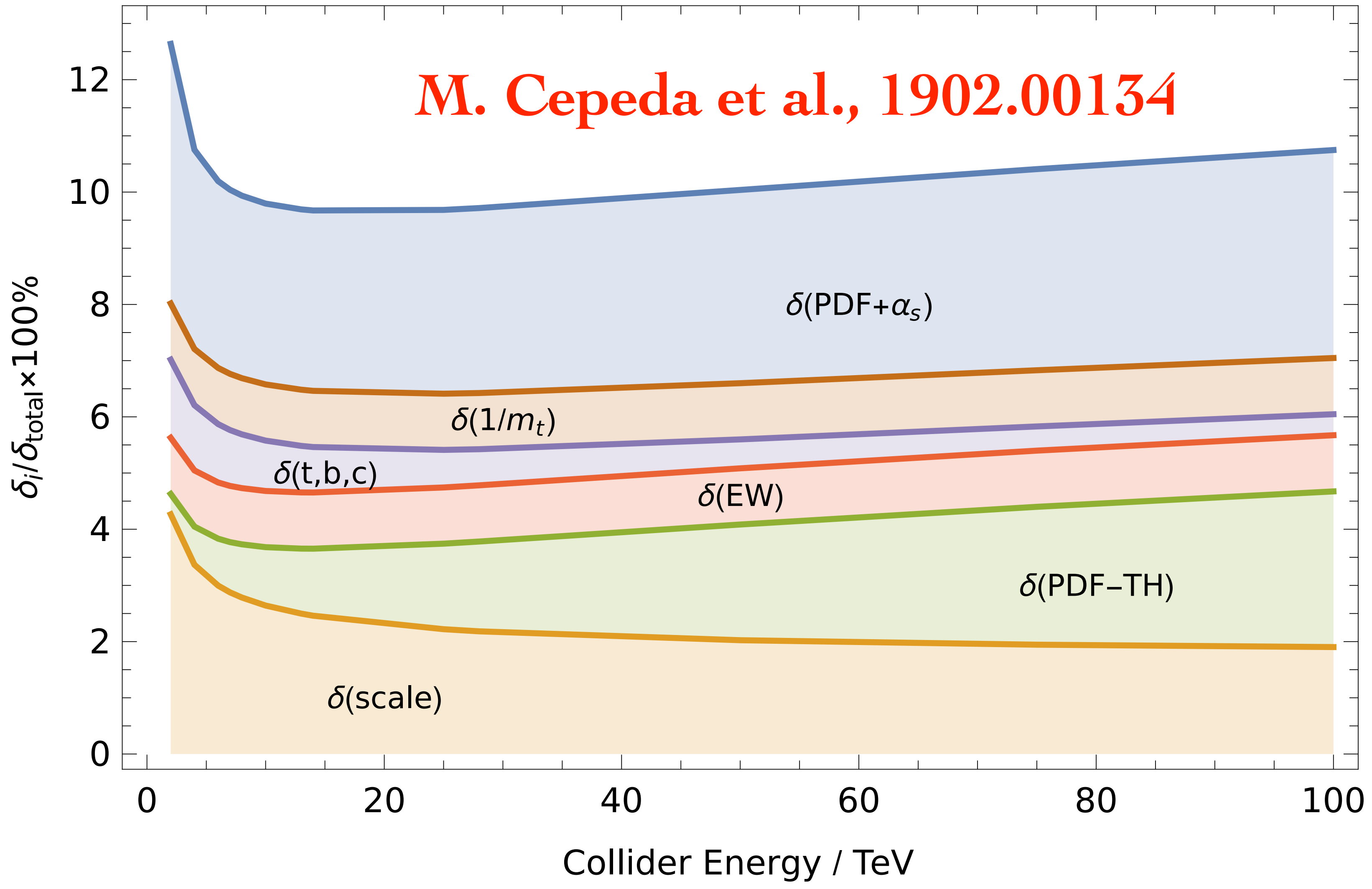


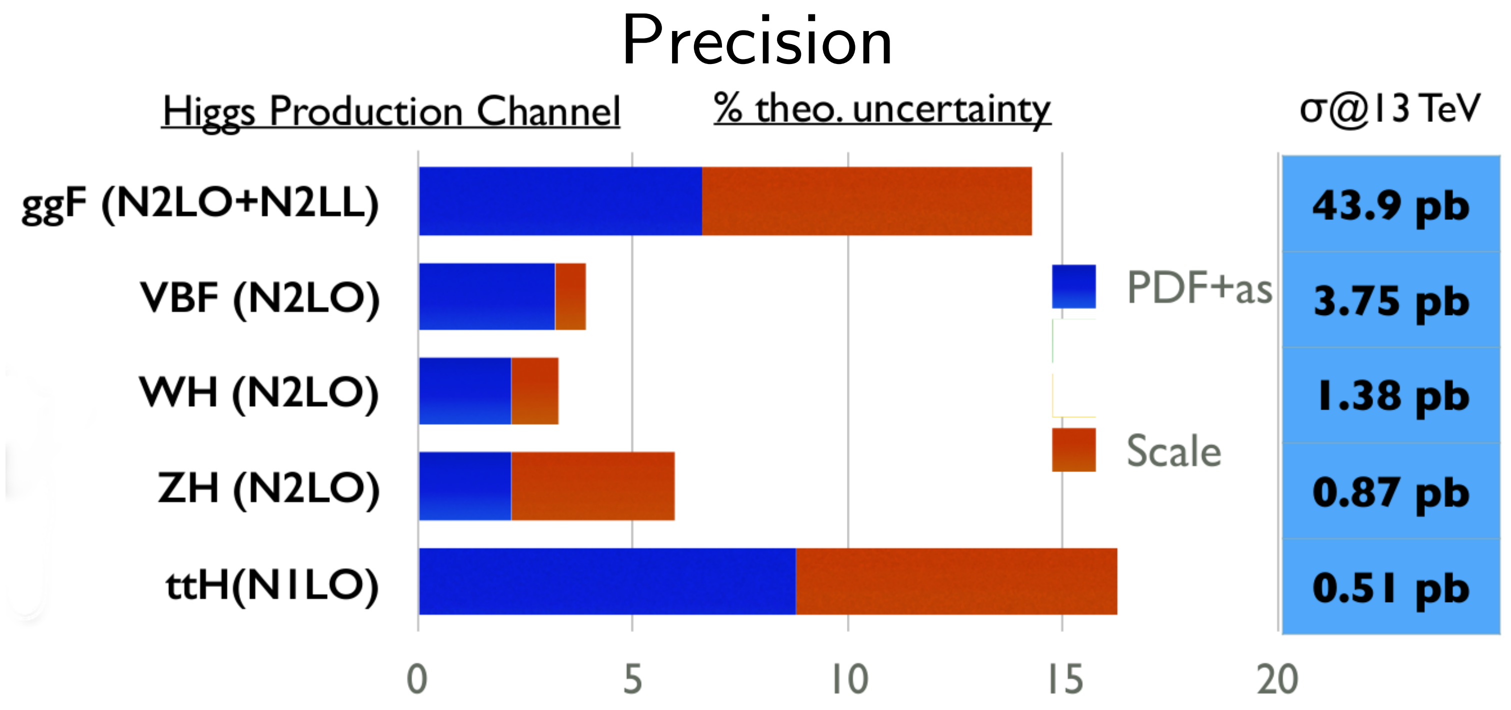
$$\sigma_{\text{PDF}} \sim \sigma_{\text{tot}}/2$$

Disclaimer: will generally refer to papers by their arxiv number, even if published.

- The LHC is a **Higgs** factory: PDFs play a key role here.

Image Credit: Emanuele Nocera





- The LHC is a **BSM** search machine. Often need PDFs here.
- High mass = high x , where PDFs are less well known. Key when looking for small/smooth deviations.

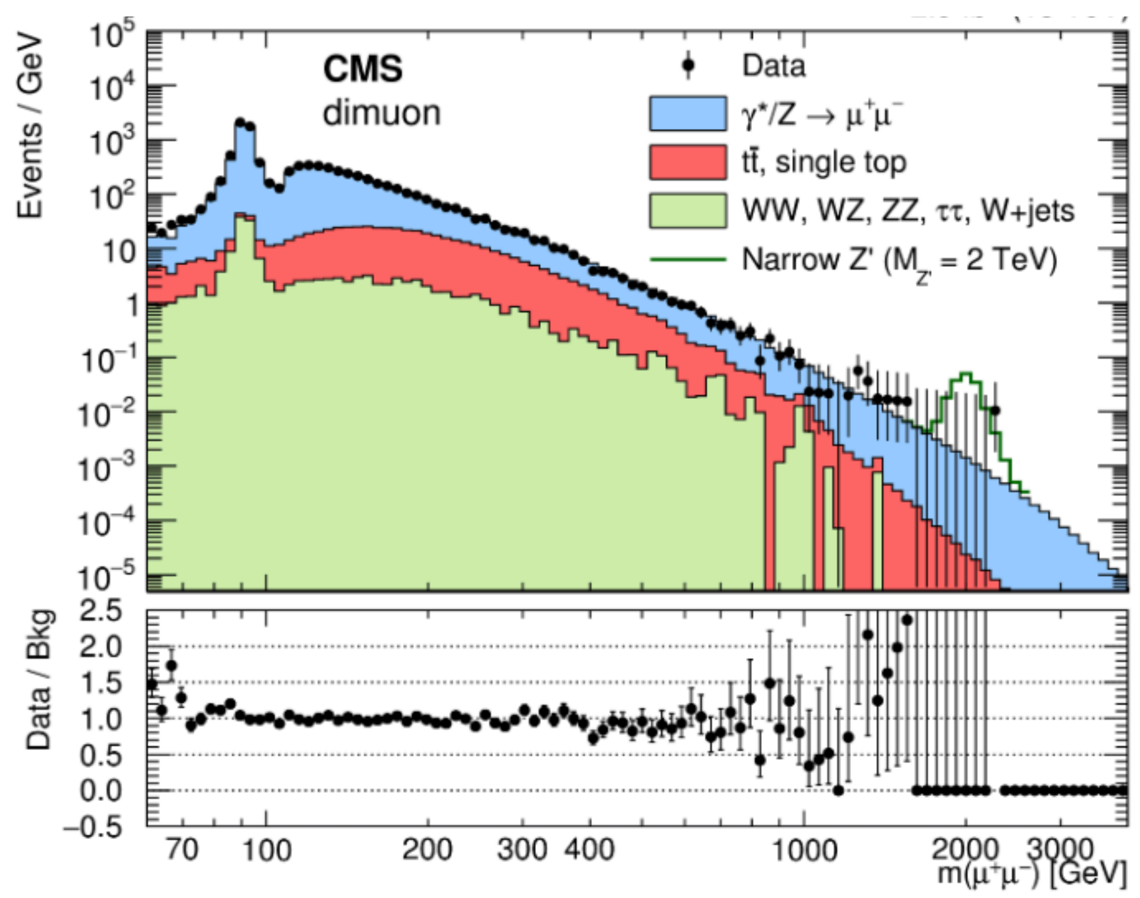
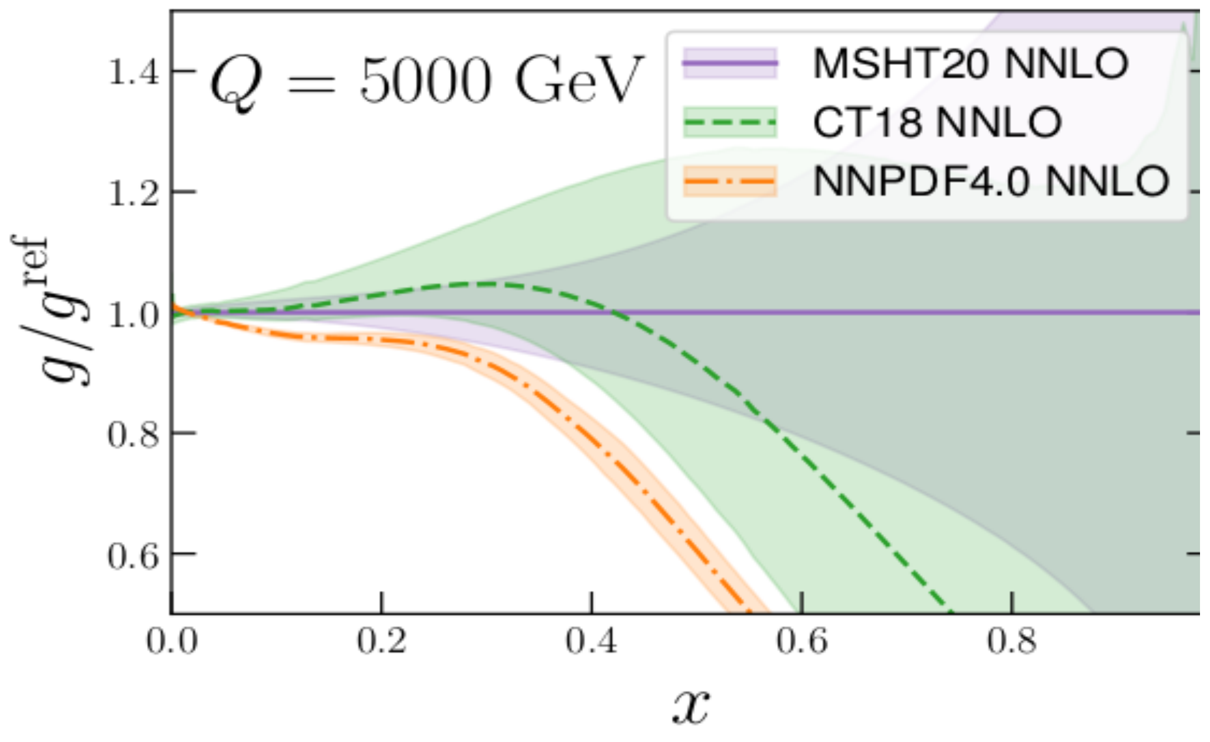


Image Credit: Tom Cridge



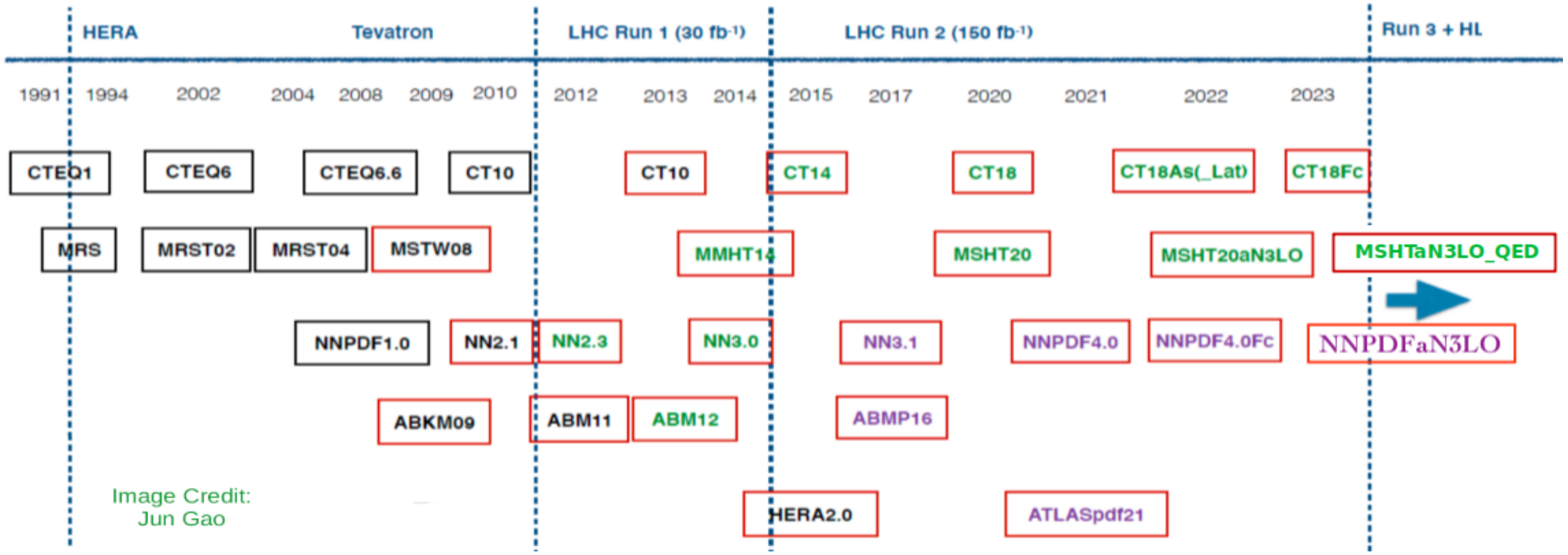
Major PDF Analyses

- Multiple PDF analyses, with different methodogies and datasets. Cannot cover these all here!
- Major releases from 3 global fitters (CT, MSHT, NNPDF) ~ 2 or more years ago. But they have been busy:

★ Major push to approximate N3LO + theoretical uncertainties

★ QED/EW corrections standard

★ Many dedicated studies



- These advances all build towards next generation of releases.

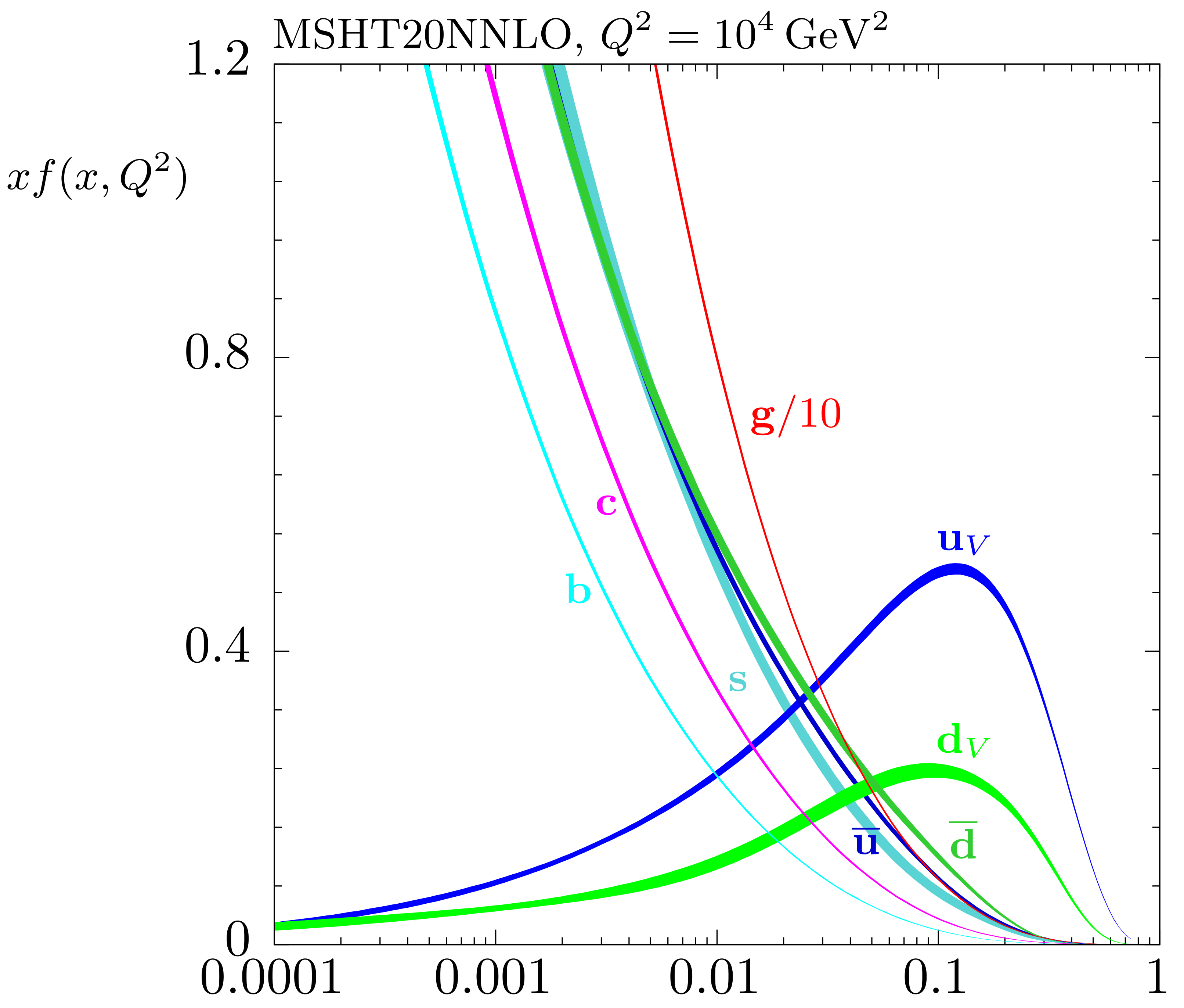
- Will focus here on MSHT.

Image Credit:
Jun Gao

Stress Testing the MSHT Approach

MSHT PDFs

- 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**.
- Although no official NNLO release since MSHT20, we have been busy! Recent highlights:



★ First global aN3LO PDF analysis. **J. McGowan et al., arXiv: 2207.04739**

★ First global QED and aN3LO PDF analysis. **T. Cridge, LHL, R. Thorne, arXiv: 2312.07665**

★ First global determination of strong coupling at aN3LO. **T. Cridge, LHL, R. Thorne, arXiv: 2404.02964**

- Will focus on third study here, but before getting there, need to lay some ground work…

Understanding the Fitting Methodology

- Two distinct methodologies on the market to parameterising PDFs: **Neural Nets** (NNPDF) or **Explicit Parameterisation** (CT, MSHT).

✦ **MSHT**: **52** free parameters in terms of Chebyshev polynomials.

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

$$\searrow \; \mathrm{NN}_i(x) \quad \textbf{NNPDF}$$

$$u_V(x,Q_0^2) = A_u(1-x)^{\eta_u} x^{\delta_u}\left(1+\sum_{i=1}^{6} a_{u,i} T_i(y(x))\right)$$

$$d_V(x,Q_0^2) = A_d(1-x)^{\eta_d} x^{\delta_d}\left(1+\sum_{i=1}^{6} a_{d,i} T_i(y(x))\right)$$

$$S(x,Q_0^2) = A_S(1-x)^{\eta_S} x^{\delta_S}\left(1+\sum_{i=1}^{6} a_{S,i} T_i(y(x))\right)$$

$$s_+(x,Q_0^2) = A_{s_+}(1-x)^{\eta_{s+}} x^{\delta_S}\left(1+\sum_{i=1}^{6} a_{s_+,i} T_i(y(x))\right)$$

$$g(x,Q_0^2) = A_g(1-x)^{\eta_g} x^{\delta_g}\left(1+\sum_{i=1}^{4} a_{g,i} T_i(y(x))\right) + A_{g-}(1-x)^{\eta_{g-}} x^{\delta_{g-}}$$

$$s_-(x,Q_0^2) = A_{s_-}(1-x)^{\eta_{s-}}(1-x/x_0)x^{\delta_{s-}}$$

$$(\bar{d}/\bar{u})(x,Q_0^2) = A_\rho(1-x)^{\eta_\rho}\left(1+\sum_{i=1}^{6} a_{\rho,i} T_i(y(x))\right)$$

A.D. Martin et al., arXiv: 1211.1215

✦ **NNPDF**: neural net with (in principle) many more free parameters.

- Two important questions to address here:

★ Is such a fixed **parameterisation flexible** enough for LHC precision physics requirements?

★ Are the **PDF uncertainties** appropriate?

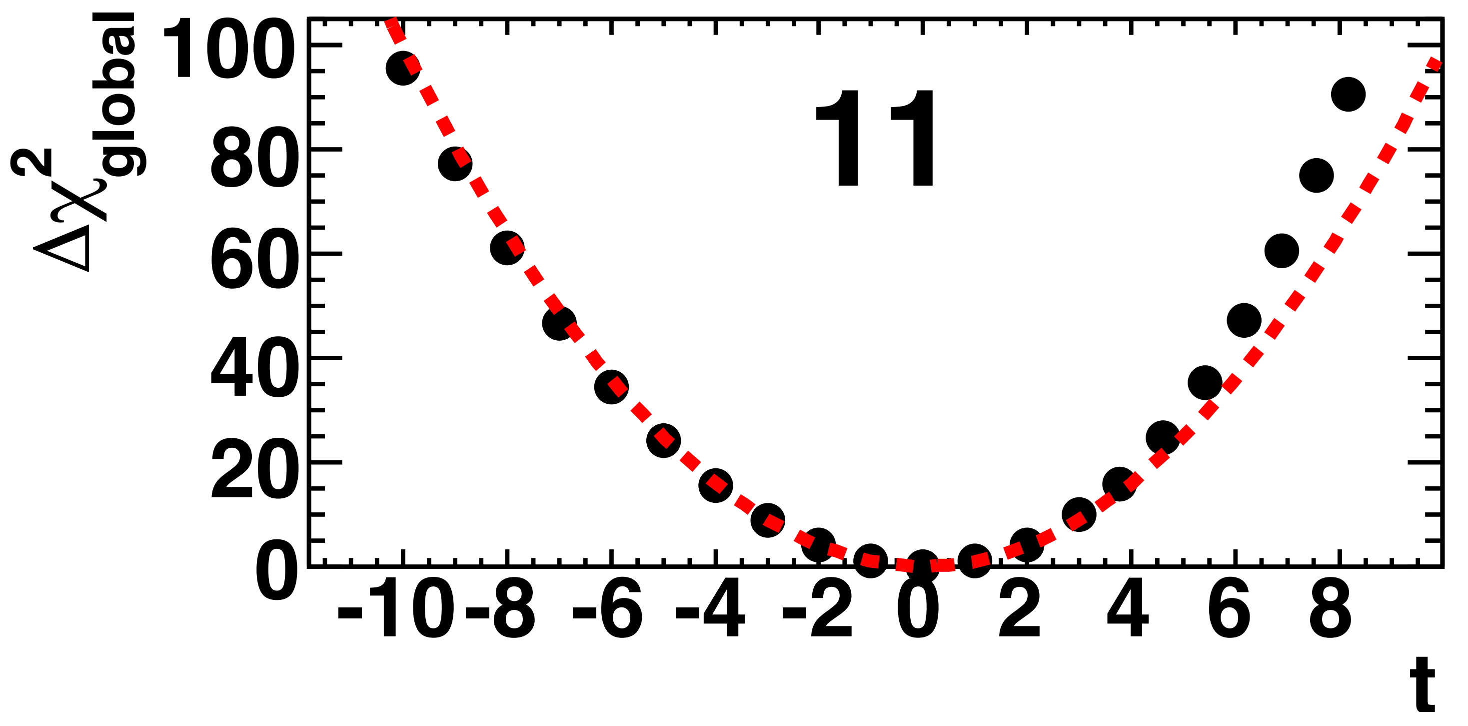
MSHT PDF Uncertainty

$$\chi^2_{\rm global} \sim \frac{(D_{\rm ata} - T_{\rm heory})^2}{\sigma^2}$$

- Find global minimum of χ^2 and evaluate eigenvectors of Hessian matrix at this point.
- Parameter shifts corresponding to given $\Delta\chi^2$ criteria given in terms of these

$$H_{ij} = \frac{1}{2} \frac{\partial^2 \chi^2_{\rm global}}{\partial a_i \partial a_j}\bigg|_{\rm min}$$

$$a_i(S_k^\pm) = a_i^0 \pm t\, e_{ik}, \qquad \text{with } t \text{ adjusted to give desired } T = \Delta\chi^2_{\rm global}$$



- $T = 1$: `textbook' criterion for 68% C.L., would apply if:
  - ★ Complete statistical compatibility between multiple datasets entering fit.
  - ★ Completely faithful evaluation of experimental uncertainties within each dataset.
  - ★ Theoretical calculations that match these exactly.

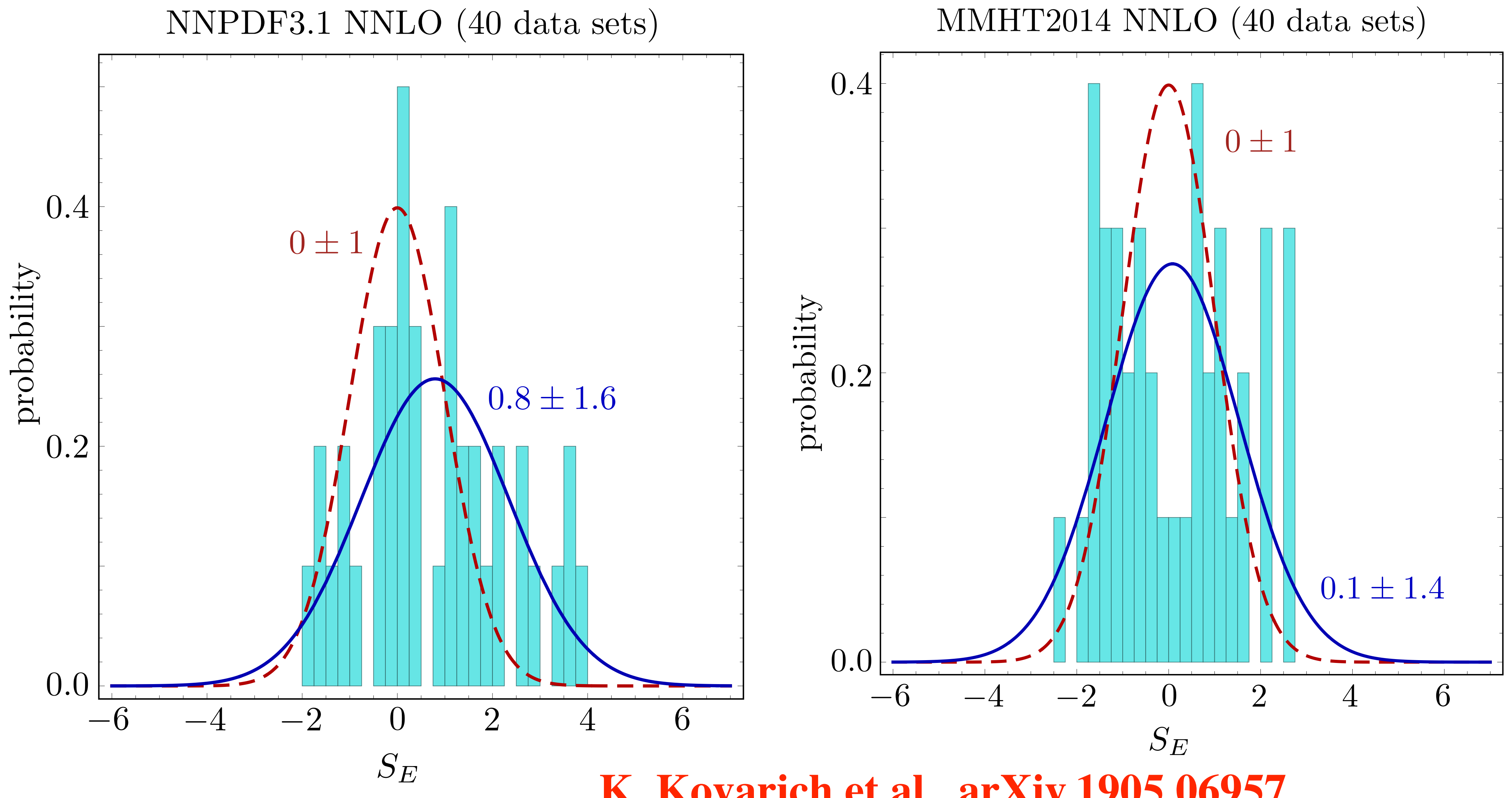
- $T = 1$: `textbook' criterion for 68% C.L., would apply if:

Fixed target, DIS, Tevatron, LHC

  - ★ Complete statistical compatibility between multiple datasets entering fit. $N_{\rm dataset} \sim 50 - 60$
  - ★ Completely faithful evaluation of experimental uncertainties within each dataset.
  - ★ Theoretical calculations that match these exactly.

- Good evidence that first two points do not always hold, while last point known not be true (though progress towards missing higher order uncertainties made).

G. Watt and R. Thorne, arXiv:1205.4024 M. Yan et al., arXiv.2406.01664
J. Pumplin, arXiv:0909.0268



K. Kovarich et al., arXiv.1905.06957

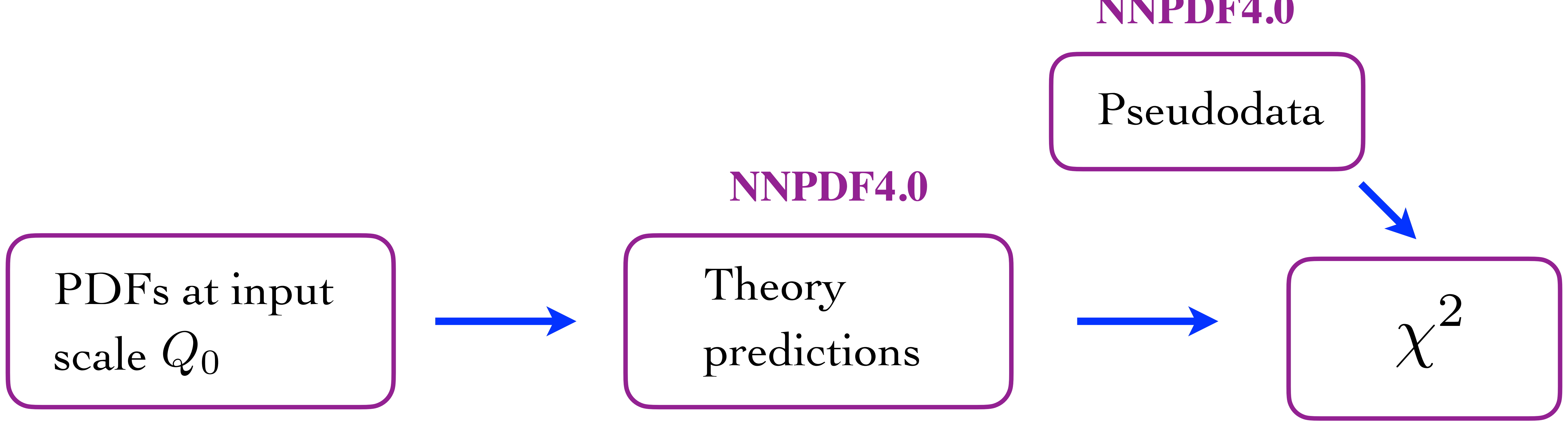
$N_{\rm pts} \sim 4000 - 5000$

- Given complete statistical compatibility, global PDF fit very constraining. Danger is claimed (high) precision will increasingly not match accuracy with $T = 1$. Motivates enlarged tolerance $T > 1$ (more later).
- Equally possible that parameterisation inflexibility may require this. Does it? To see we will present results of 'closure tests'…

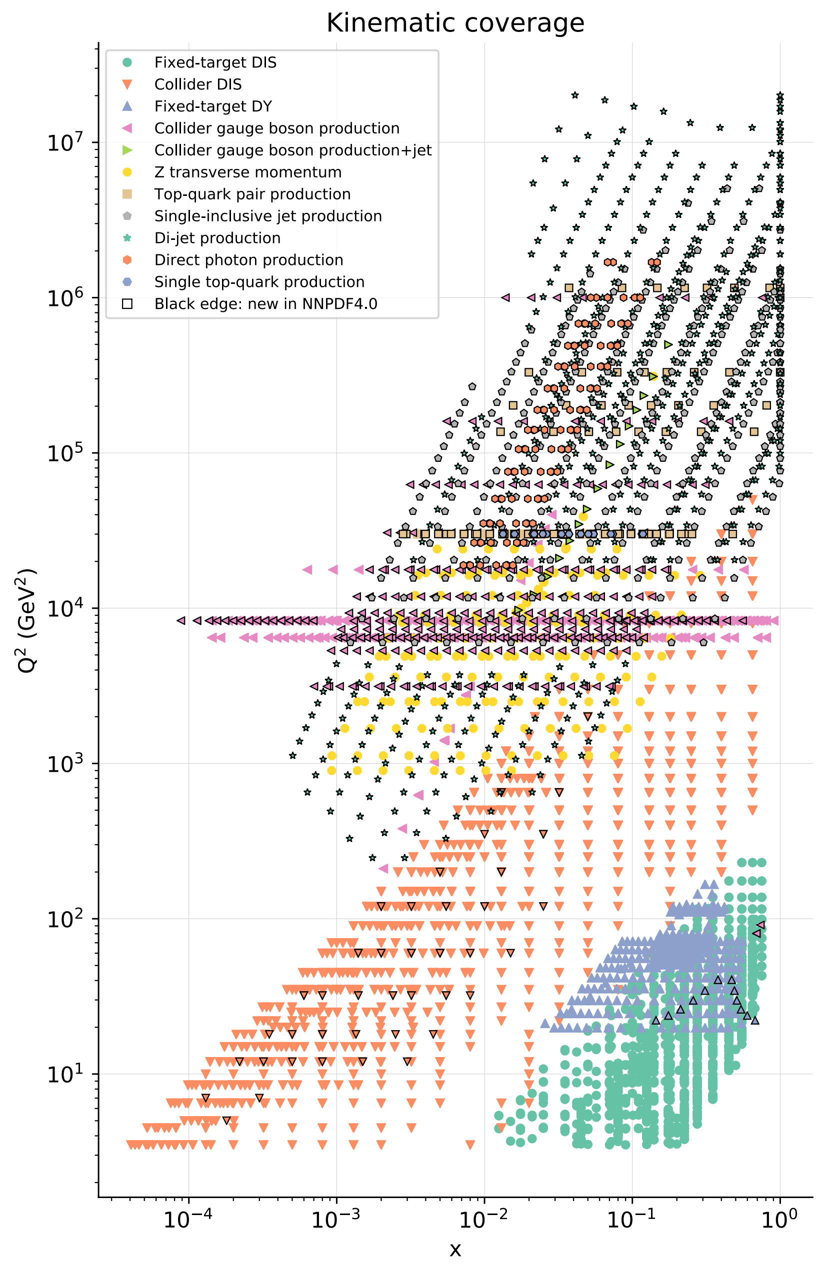
Global Closure Test

- Global Closure Test: generate pseudodata corresponding to global dataset with a particular input PDF set and perform usual MSHT fit to this. Then determine how faithfully underlying input is reproduced.
- To do this we will make use of publicly available NNPDF fitting code.

https://docs.nnpdf.science/



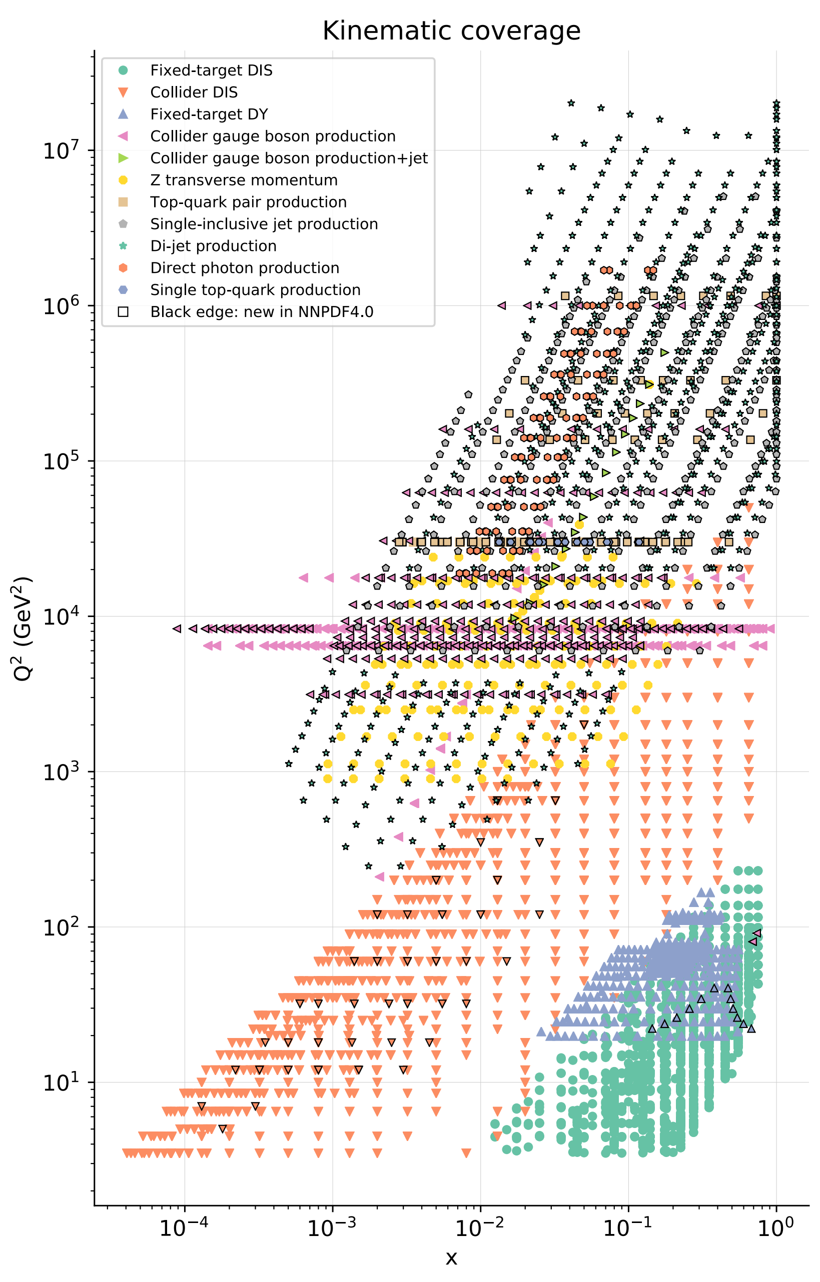
NNPDF, arXiv:2109.02653



- This allows us to evaluate corresponding fit quality with a (MSHT) fixed parameterisation, but to NNPDF data/theory - **only difference** is **input parameterisation.**
- Will use for closure tests (though not essential) - but setting things up in this way will allow direct comparison at level of full fit (not focus of current talk, but stay tuned!).

Always NNLO

- For direct comparison will consider perturbative charm - NNPDF4.0pch set as input.
- Then generate unshifted pseudodata for 4.0 global dataset ($N_{\rm pts} = 4627$). In principle exact agreement possible, with $\chi^2 = 0$.
- Then perform fit with default MSHT parameterisation. What do we find?



NNPDF, arXiv:2109.02653

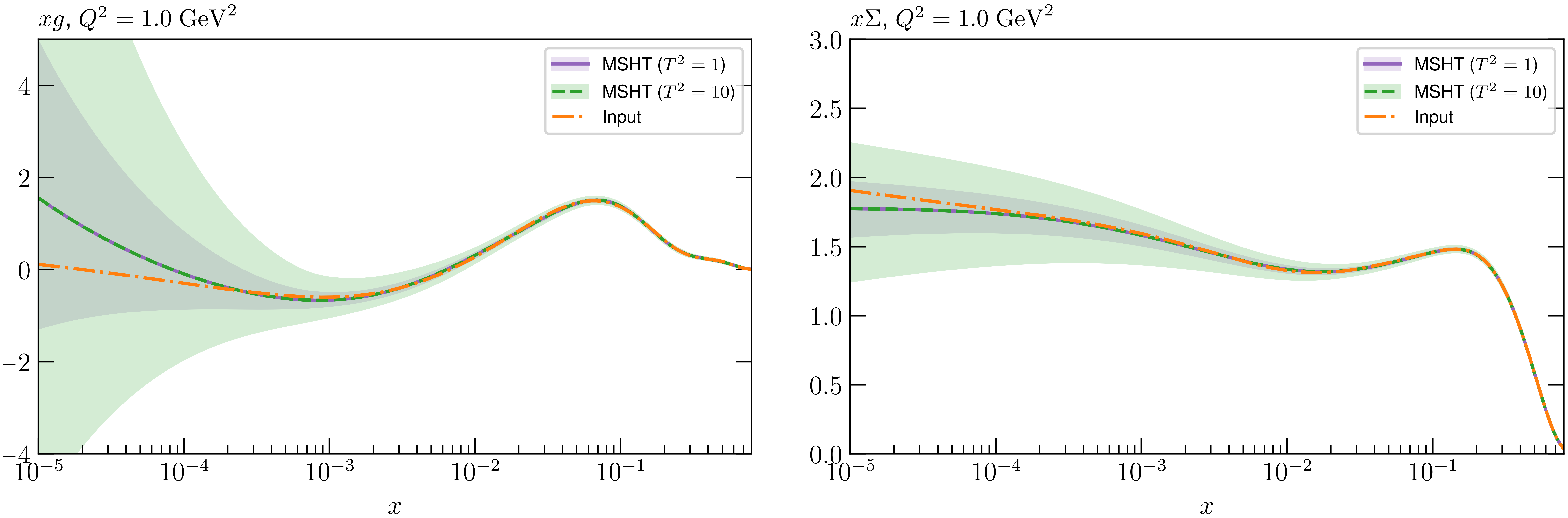
	χ^2	$\chi^2/N_{\rm pts}$
Fit quality:	2.4	0.0005

- **Remarkably good!** In fact lower than reported result of NNPDF L0 closure test.

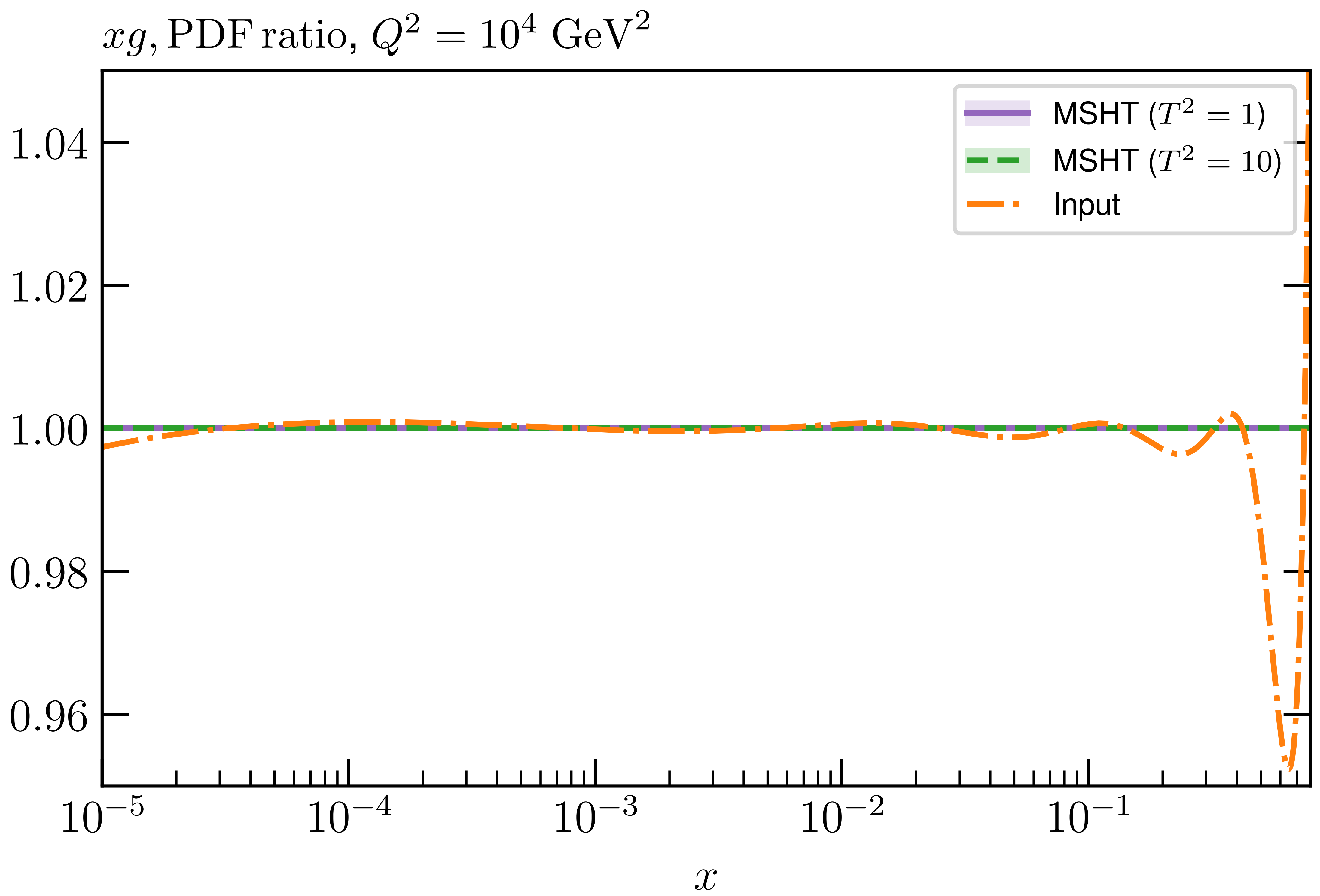
L. Del Debbio, T. Giani and M. Wilson, arXiv:2111.05787

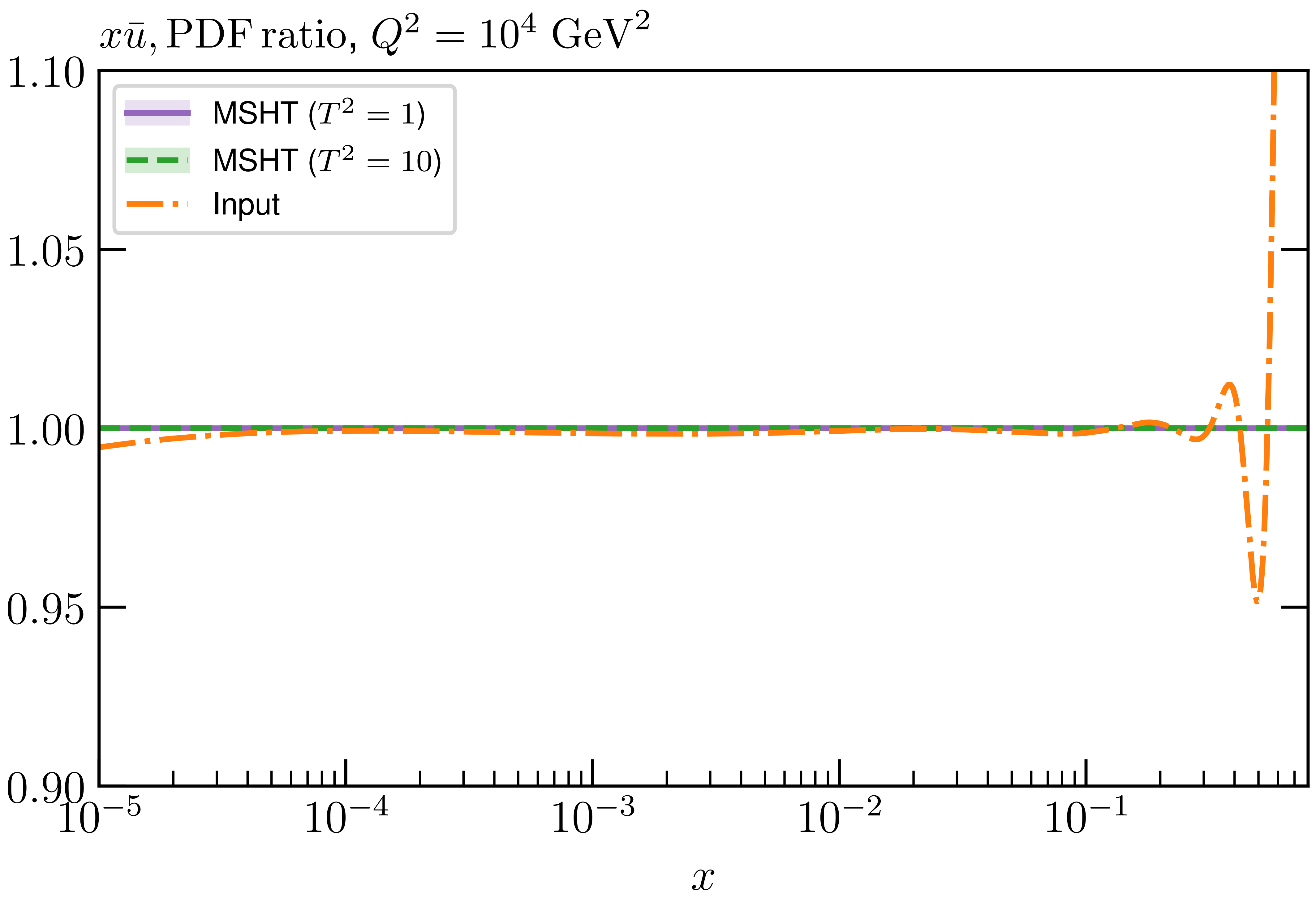
	3.1 meth.	**4.0 meth.**
$\chi^2/N_{\rm pts}$	0.012	0.002

- **Caveat**: only one input set, may well be different (not quite as good) for others. Trend should be similar.
- But apparently no issue with parameterisation inflexibility in this case. But what about PDFs?



- First look: encouraging results! In more detail…





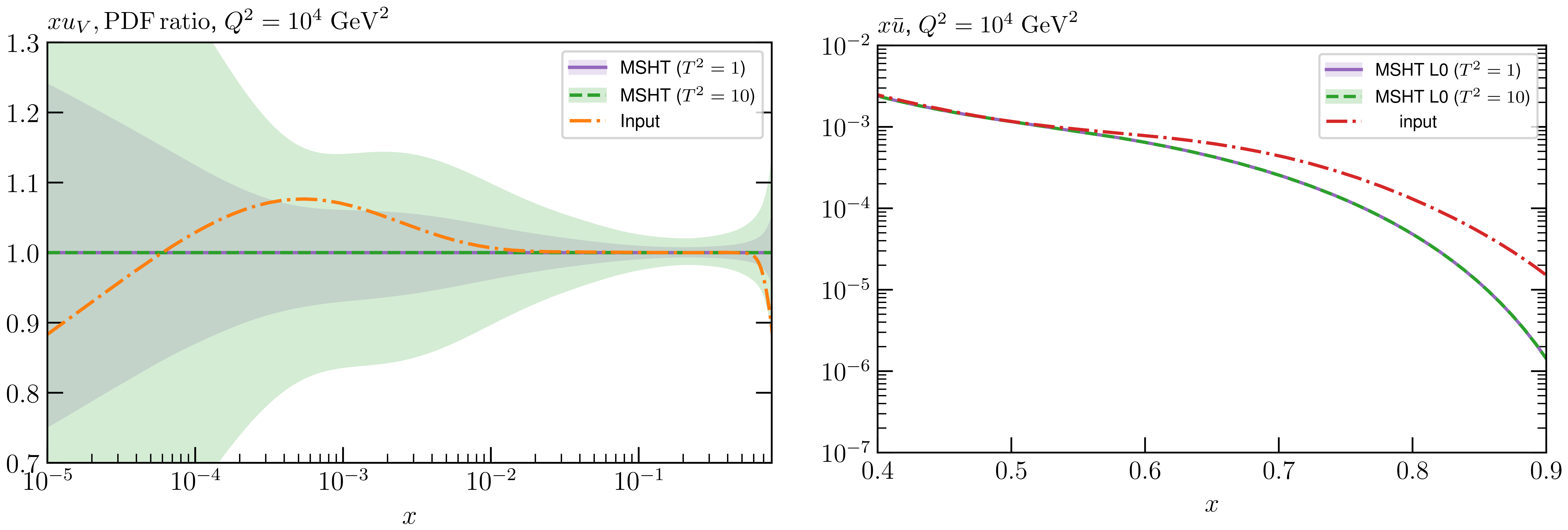
- Ratio of (NNPDF4.0pch) input to fit result, including PDF uncertainties with $T^2 = 1$ and 10 that come from the closure test fit. Latter is ~ result of dynamic tolerance used in MSHT20 (checked here).

Similar results for other quarks - see backup

★ **Deviation** in general (in data region) **per mille** level and well within the $T^2 = 1$ uncertainties.

★ More precisely, deviation is ~ 10% or less of $T^2 = 1$ uncertainty, and a factor of $\sim 2 - 5$ lower as a fraction of the $T^2 = 10$ uncertainty.

$\longrightarrow$ In **data region** input PDF matched very well, and much better than $T^2 = 1$ uncertainties. **No evidence** that the increased tolerance is driven by **parameterisation inflexibility** for MSHT.

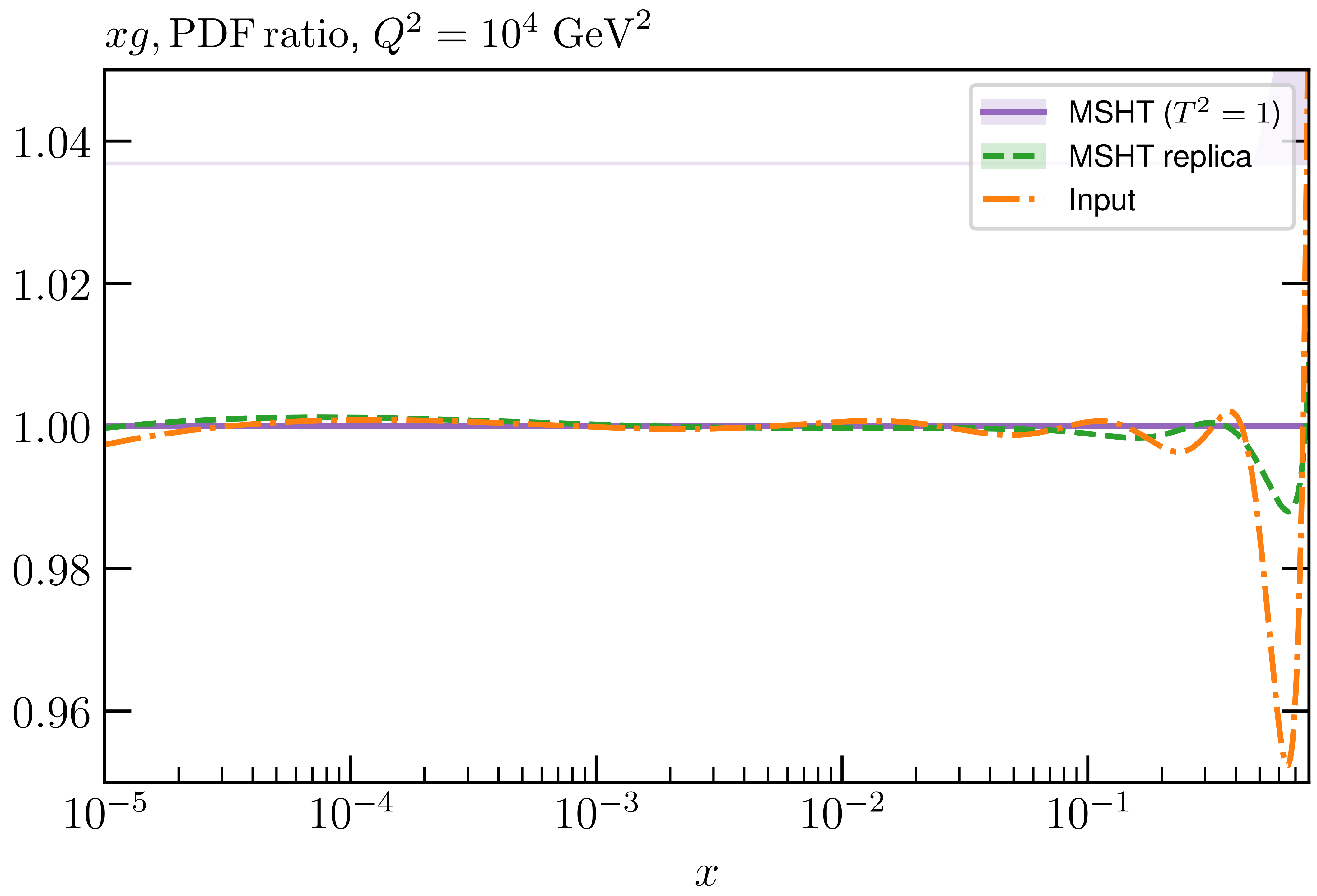


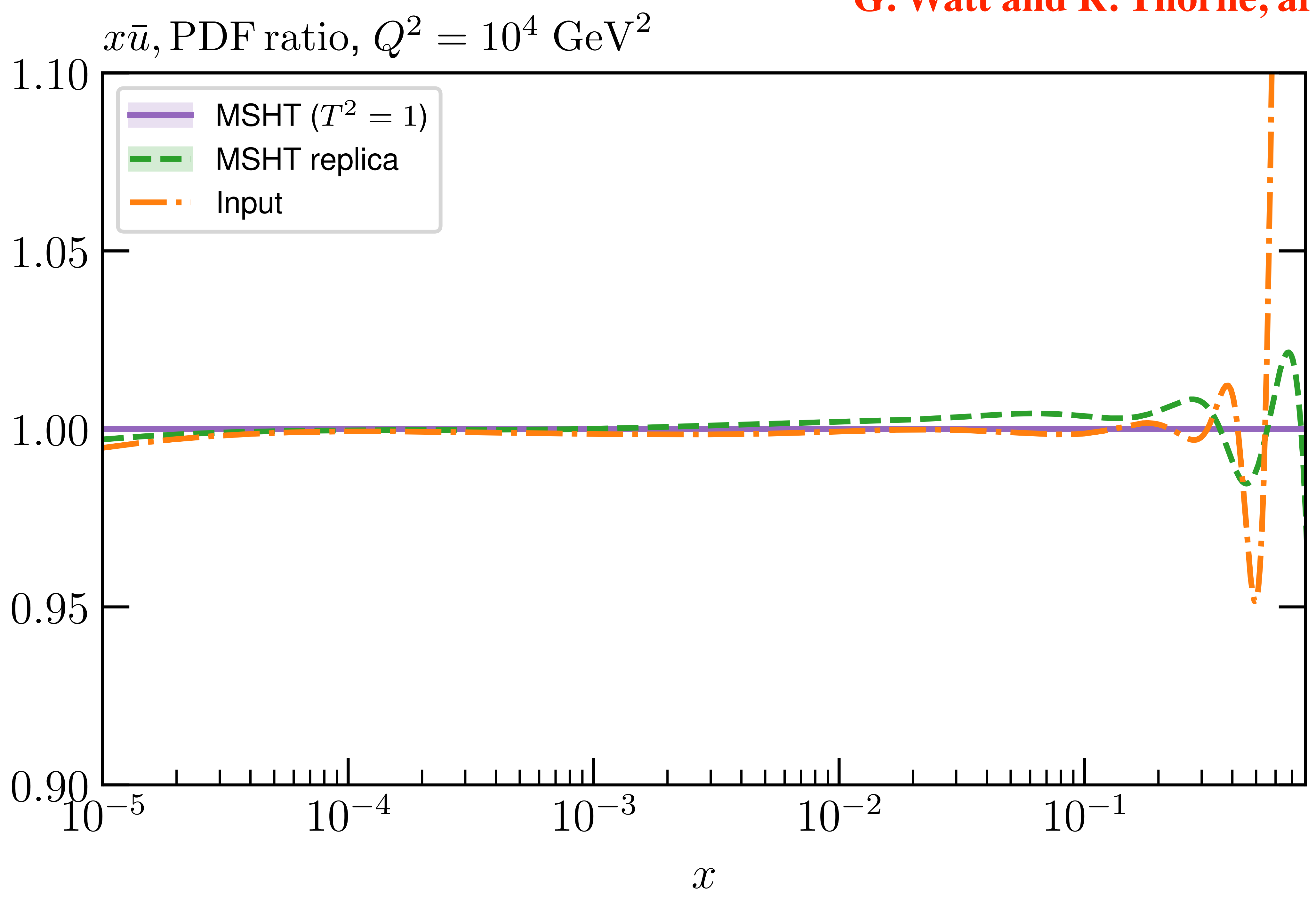
- In less well constrained regions deviation larger, e.g for u_V, d_V at low and high x and the $\overline{u}, \overline{d}$ at high x .
- Hence in extrapolation region input not always consistent within uncertainties
- As ~ outside data region not inconsistent (errors driven by data), but indicates more conservative error definition in these regions may be desirable (as tends to happen in NN approach).
- Though arguably no 'right' answer in true extrapolation region (too conservative vs. over-conservative).

Global Fluctuated Closure Test

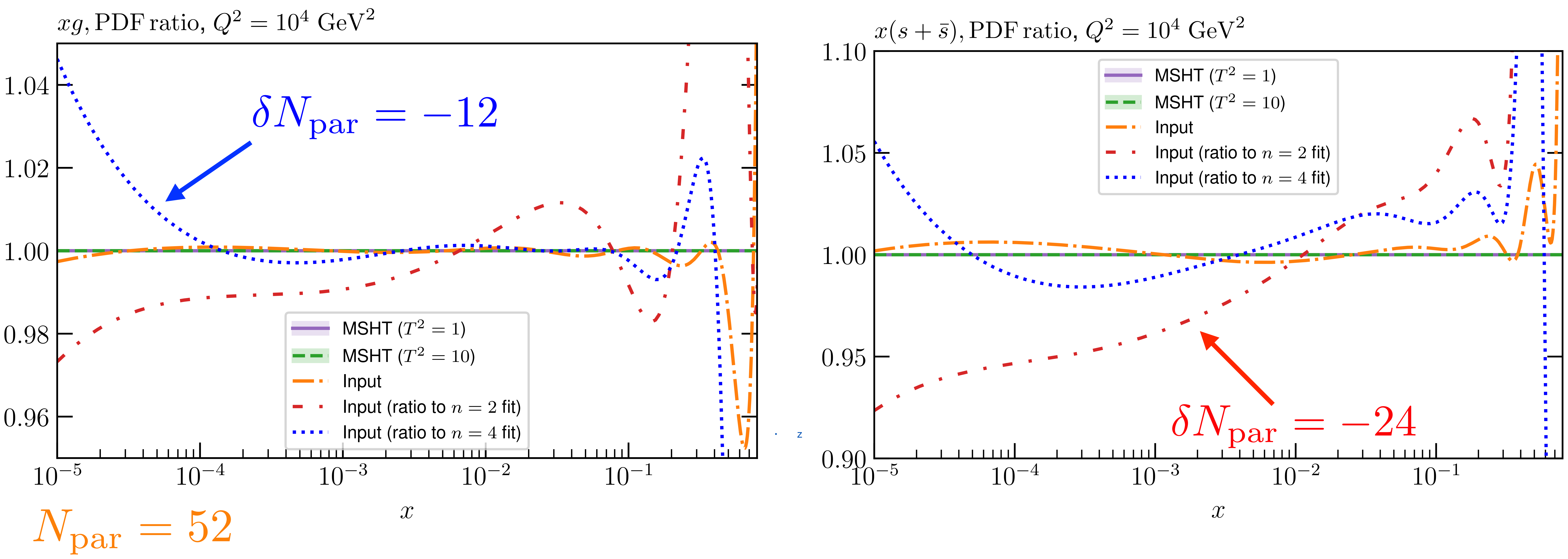
- Exactly the same closure test settings, but fluctuate pseudodata according to experimental uncertainties. Fit quality $\chi^2 \sim N_{\rm dat} \pm \sqrt{2N_{\rm dat}}$ expected (and found).
- Test faithfulness of MSHT parameterisation by producing MC replica set - perform 100 replica fits.
- Error propagation used by NNPDF. Shown to be equivalent to Hessian $T^2 = 1$ w. fixed parameterisation.

G. Watt and R. Thorne, arXiv:1205.4024





- Encouraging agreement between MC replica and Hessian uncertainties. Would not expect if issues with parameterisation inflexibility. PDF uncertainties more representative at high x .



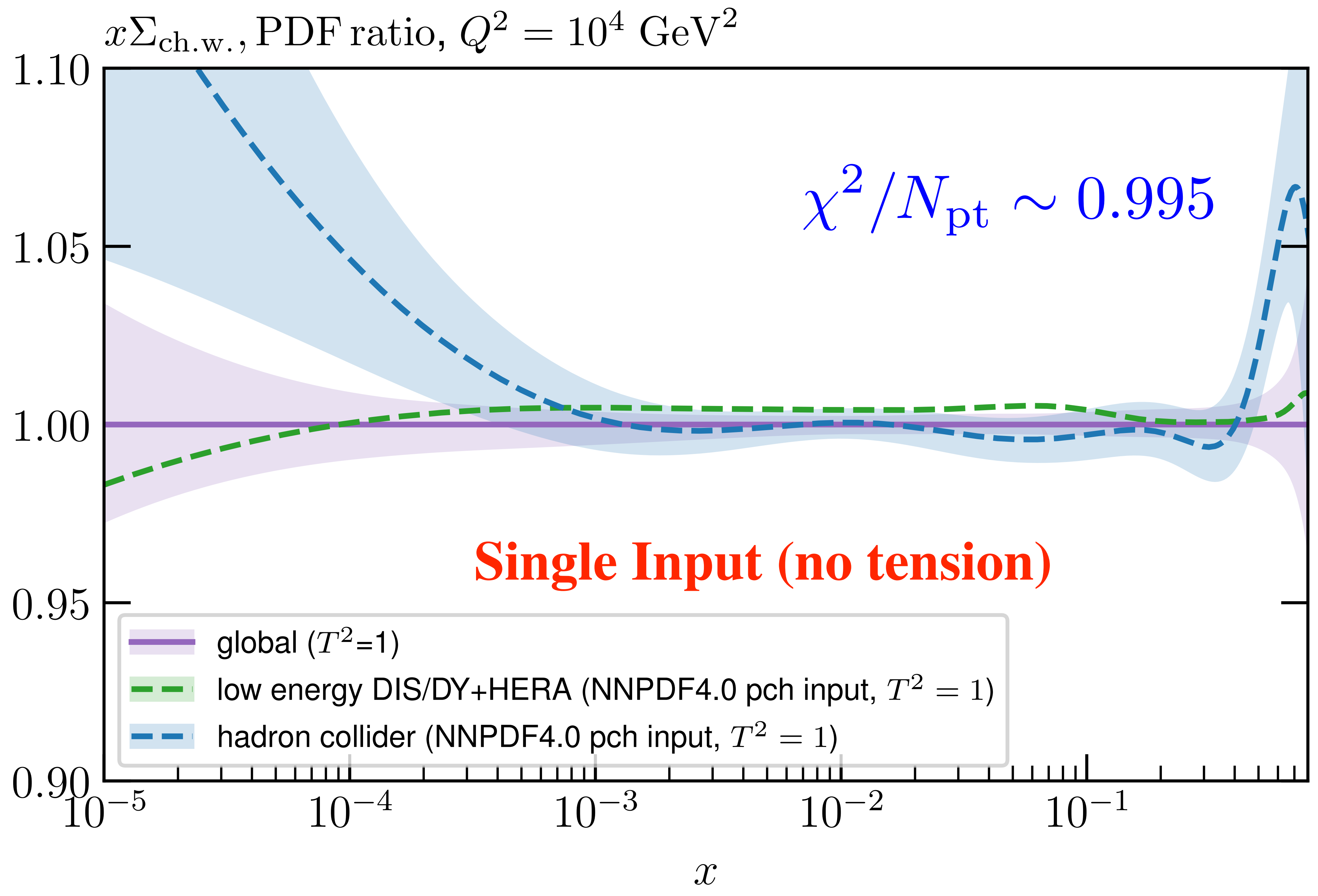
- Note this level of agreement is not automatic! Need flexible enough parameterisation: restricting number of free parameters gives much poorer agreement.
- Is also not coincidental: parameterisation chosen in order to provide 1% precision.

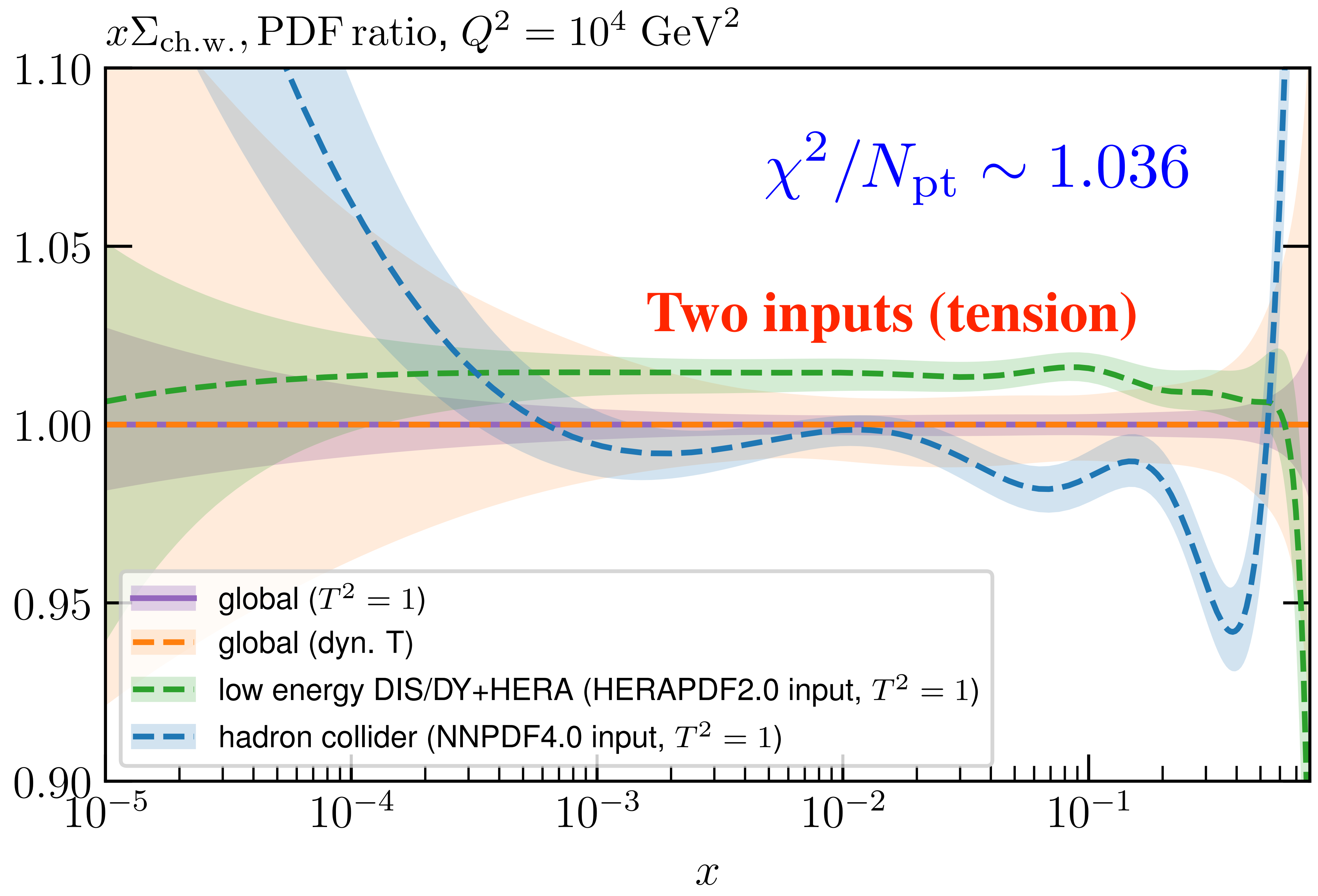
A.D. Martin et al., arXiv: 1211.1215

Tolerance (Again)

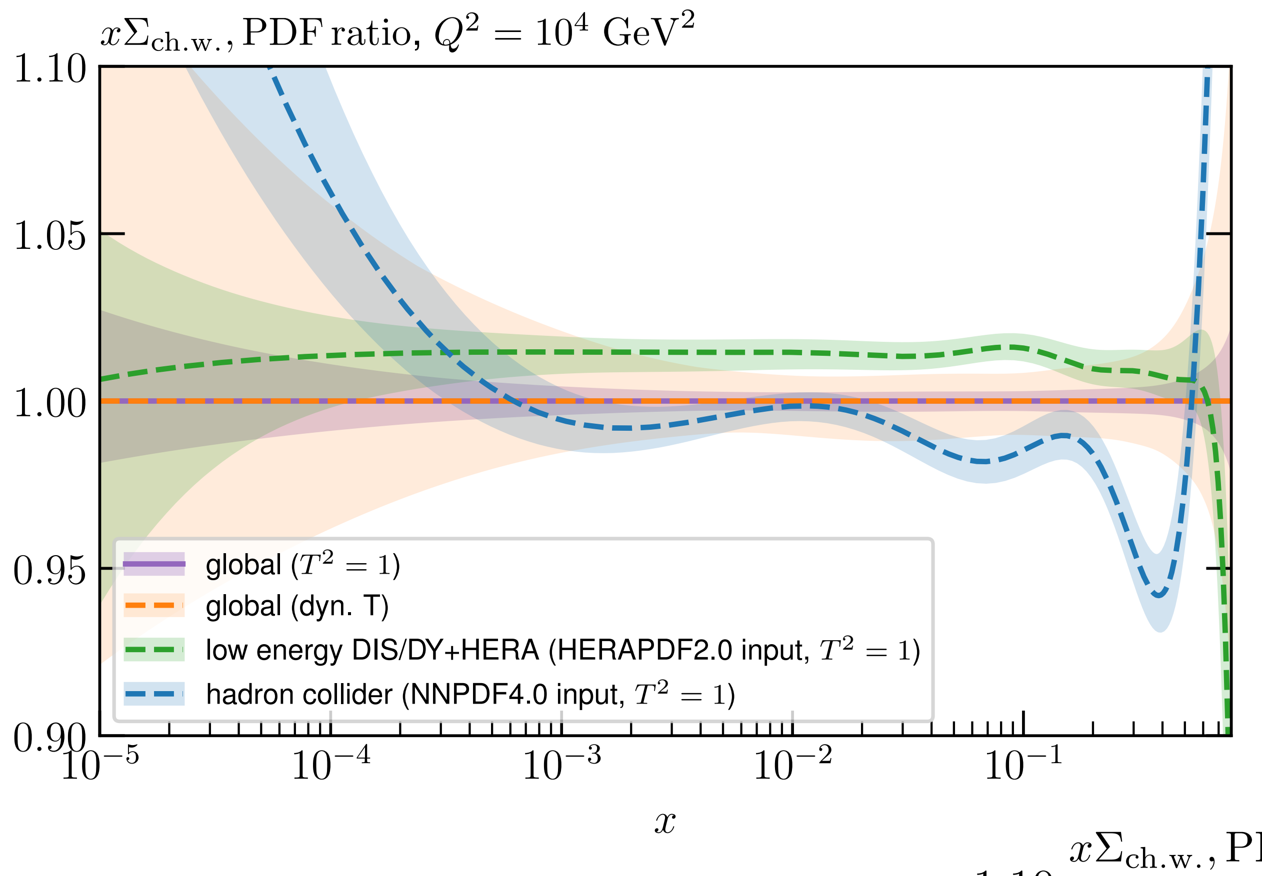
See also G. Watt and R. Thorne, arXiv:1205.4024

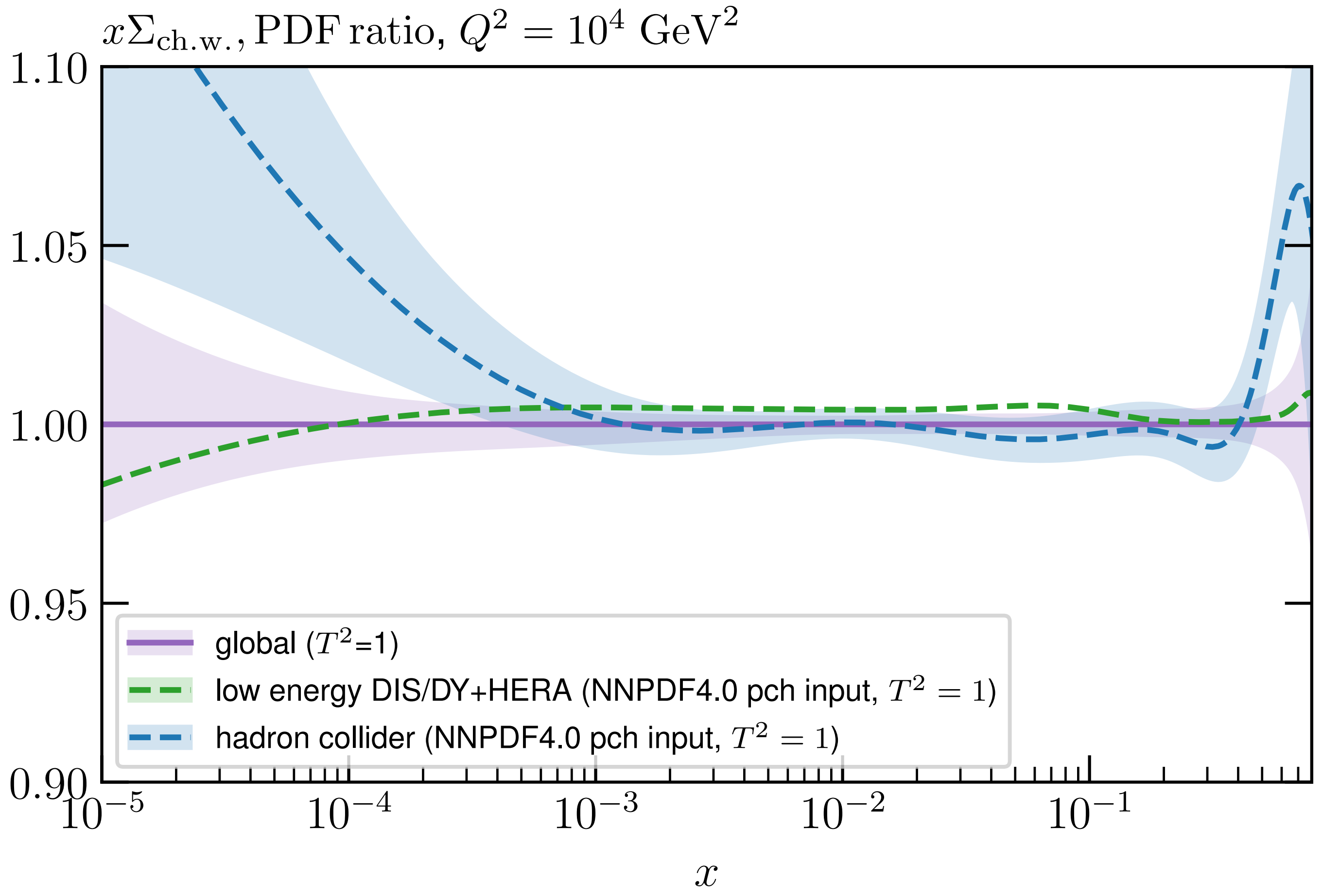
- Can also use closure test to motivate need for tolerance. Generate:
  - ★ **Fixed-Target DY + DIS** data with **HERAPDF2.0** input.
  - ★ **Hadron Collider** data with **NNPDF4.0** (pch) input.
- Inputs are indeed in tension for various PDFs - simply model of incompatibility in fit. What do we find?

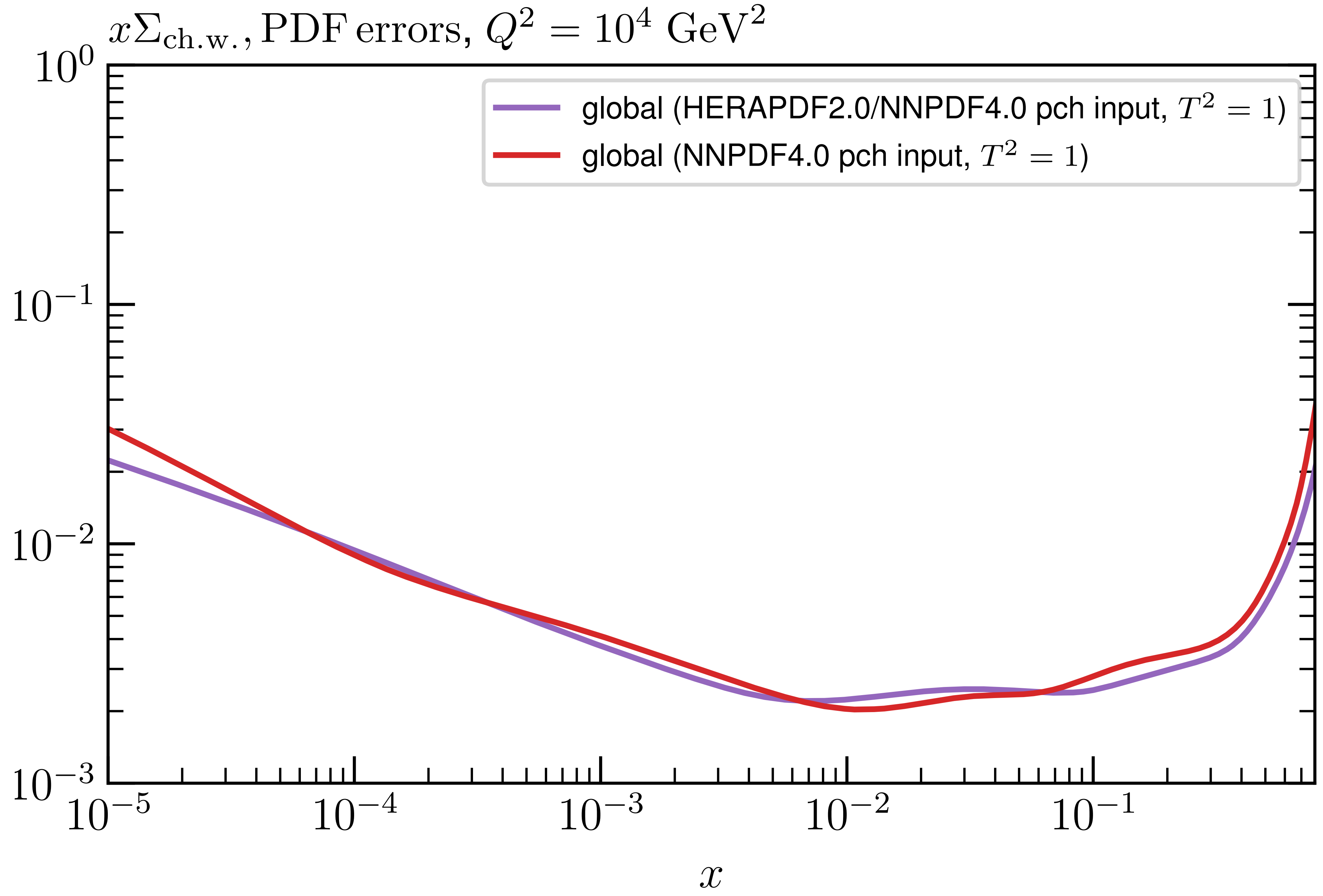




- Fit including tension lies ~ in the middle where tension appears. The $T = 1$ error clearly too small - enlarged MSHT tolerance does rather better. Crucially the $T = 1$ error v. similar between left + right…







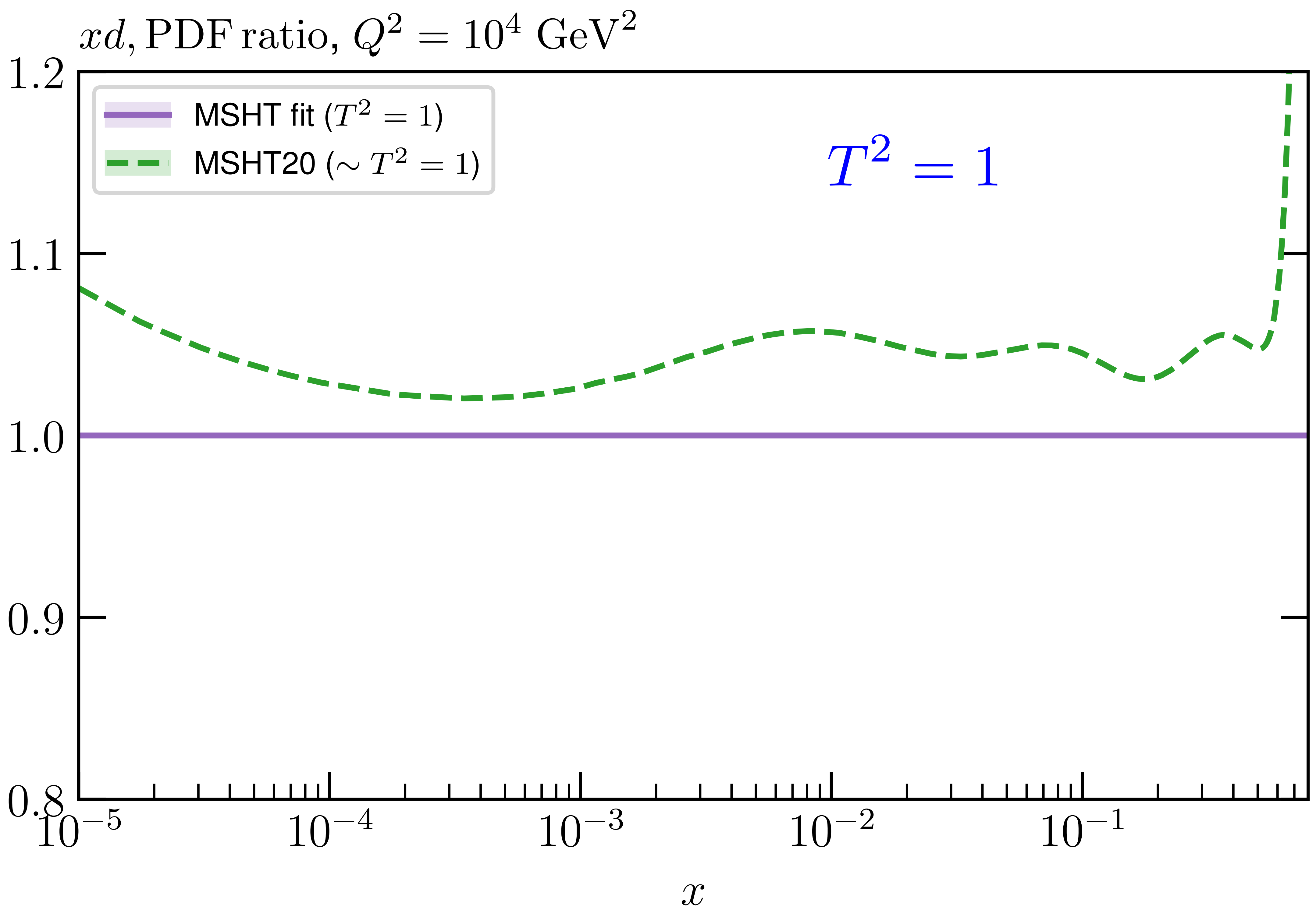
Backup

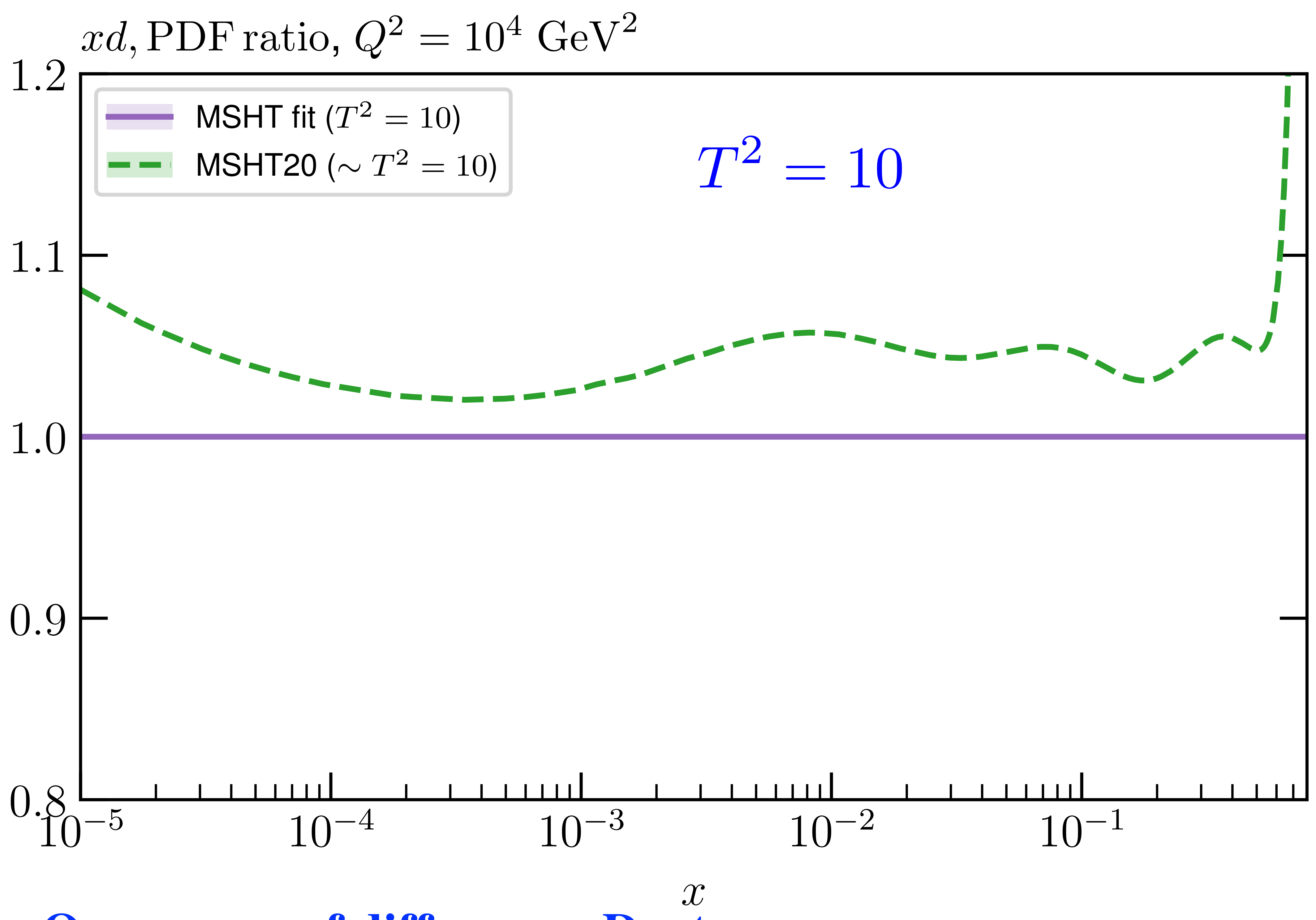
- This effect is completely expected. Can show in simple toy model: PDF uncertainties driven by the quoted experimental (theoretical) uncertainties whether underlying fit is self—consistent or not.
- Naive application of $T = 1$ criterion in such a scenario will lead to overly **aggressive errors**.

Tolerance (and Again)

Stay tuned for more!

- Final indication here. Perform fit to real NNPDF4.0 data + theory but with MSHT20 parameterisation.
- Compare to public MSHT20 fit: only difference due to differing data + theory.



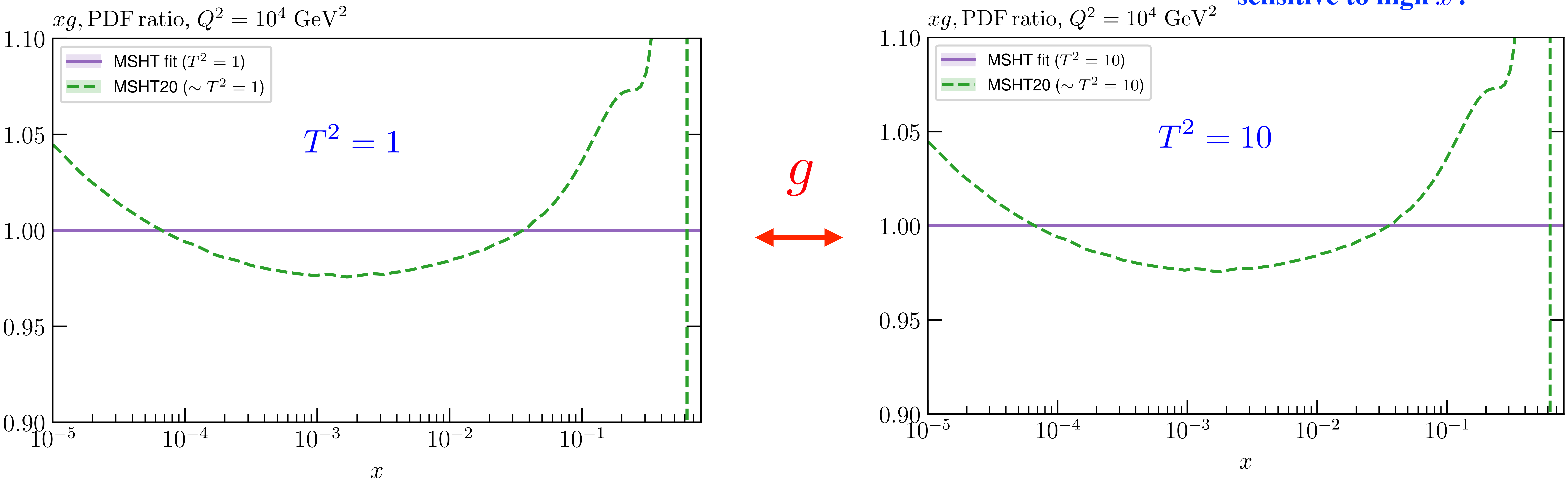


One source of difference: Deuteron Corrections

Tolerance (and Again)

- Final indication here. Perform fit to real NNPDF4.0 data + theory but with MSHT20 parameterisation.
- Compare to public MSHT20 fit: only difference due to differing data + theory.

One source of difference: LHC data sensitive to high x .



- Results arguably speak for themselves!
- Aside: MSHT parameterisation also performs very well vs. NN one. NNPDF uncertainties broadly $\sim T = 1$.

Stay tuned for more!

See LHL, DIS2024

MSHT at Approximate N3LO:

MSHT20aN3LO

Motivation

- **N3LO:**

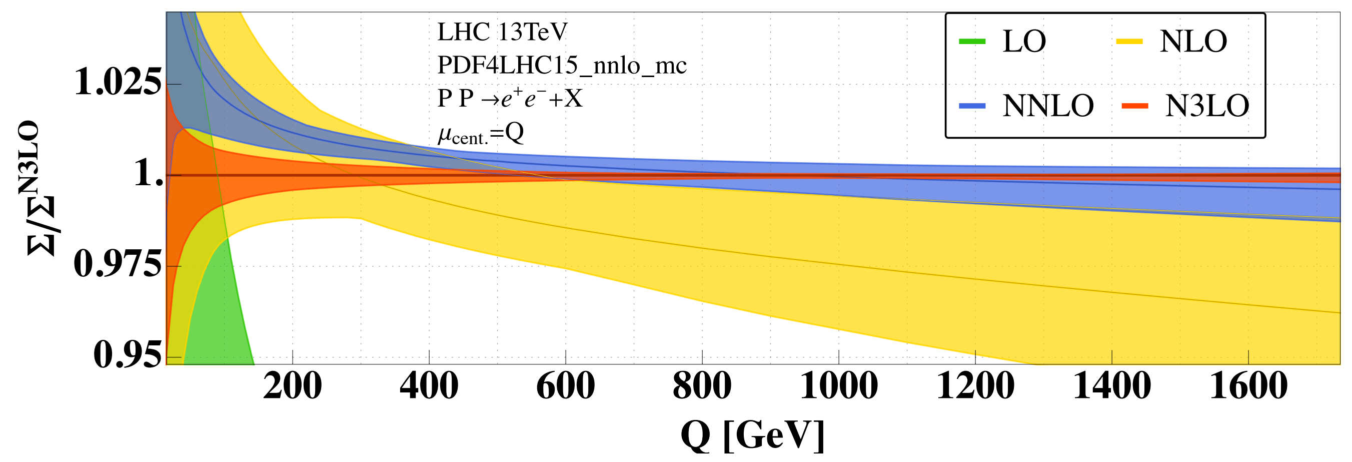
  ★ State of the art is NNLO for PDF fits but a lot known at N3LO about DGLAP evolution and DIS (light + heavy flavours). Why not use this?

  ★ For hadron colliders less is known but already quite a bit

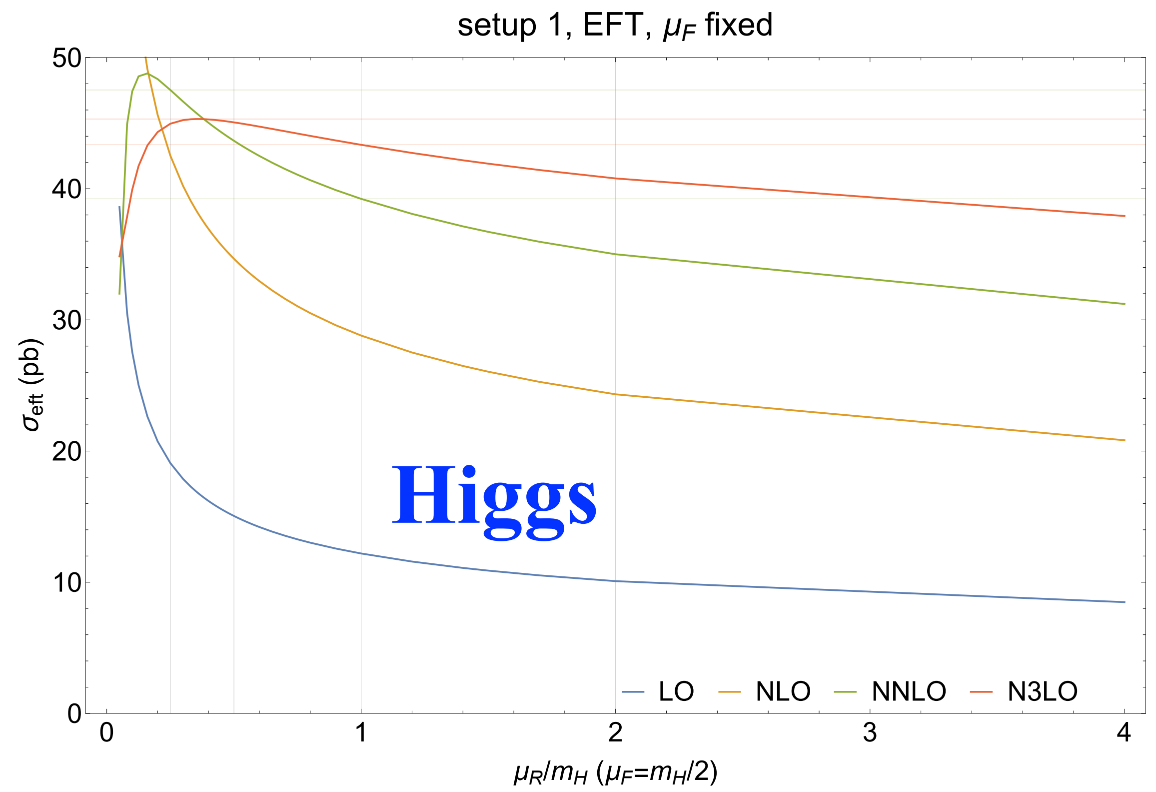
  - **Uncertainty** due to lack of N3LO PDFs a key factor $\Rightarrow$ need to - and can - go to N3LO!

$$\delta(PDF-TH) = \frac{1}{2}\left|\frac{\sigma^{(2)}_{\rm NNLO-PDFs} - \sigma^{(2)}_{\rm NLO-PDFs}}{\sigma^{(2)}_{\rm NNLO-PDFs}}\right|$$

Drell Yan



C. Duhr and B. Mistleberger, arXiv:2111.10379



C. Anastasiou et al., arxiv:1602.00695

- **Missing higher orders:**

  ★ As (LHC) data becomes ever more precise sensitivity to any data/theory mismatch increases.

$$\chi^2 \sim \sum \frac{(D-T)^2}{\sigma^2_{\rm exp}} \qquad T_{{\rm N}^x{\rm LO}} \neq D \Rightarrow \chi^2 \to \infty \text{ as } \sigma_{\rm exp} \to 0$$

  ★ Need to account for this missing higher order uncertainty:

  - More accurate PDF uncertainty.
  - Weight datasets correctly in fit (less well known $\Rightarrow$ larger uncertainty).

N3LO - What do we know?

- **Approximate** $\neq$ **poorly known**!

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

★ **Splitting functions:** a wealth of information. Moments & various limits, with much recent further progress. **G. Falcioni et al., arXiv:2307.04158, arXiv:2302.07593**

$$F_2(x,Q^2) = \sum_{\alpha\in H,q,g;\beta\in q,H} (C^{VF,n_f+1}_{\beta,\alpha} \otimes A_{\alpha i}(Q^2/m_h^2) \otimes f_i^{n_f}(Q^2))$$

★ **DIS:** massless coefficient functions known (+ massive high Q^2). Massive low Q^2 approx. known.

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

★ **Heavy Flavour:** again wealth of information. Moments & various limits, with much recent progress.

$$\sigma = \sigma_0 + \sigma_1 + \sigma_2 + \sigma_3 + \ldots \equiv \sigma_{N3LO} + \ldots$$

★ **Hadronic Cross Sections:** while much progress made, thus far not useable in PDF fits.

- First three ingredients now largely known with sufficient precision to give close to a N3LO fit. Final ingredient clearly the bottleneck for that - approximation + uncertainty required.

Emanuele Nocera, Forward Physics and QCD at the LHC and EIC, Bad Honnef 23

Splitting Functions

Singlet (P_{qq}, P_{gg}, P_{gq}, P_{qg})
- large-n_f limit [NPB 915 (2017) 335; arXiv:2308.07958]
- small-x limit [JHEP 06 (2018) 145]
- large-x limit [NPB 832 (2010) 152; JHEP 04 (2020) 018; JHEP 09 (2022) 155]
- 5 (10) lowest Mellin moments [PLB 825 (2022) 136853; ibid. 842 (2023) 137944; ibid. 846 (2023) 1

Non-singlet ($P_{NS,v}$, $P_{NS,+}$, $P_{NS,-}$)
- large-n_f limit [NPB 915 (2017) 335; arXiv:2308.07958]
- small-x limit [JHEP 08 (2022) 135]
- large-x limit [JHEP 10 (2017) 041]
- 8 lowest Mellin moments [JHEP 06 (2018) 073]

Including N3LO information - Evolution

- Two (brief) examples. Splitting functions, e.g. P_{qg} :
- Allows for uncertainty from remaining unknown pieces, via nuisance parameter ρ_{qg} .
- Since original MSHT20aN3LO release has been further progress on these.

$$P^{(3)}_{ab}(x) = \sum_{i=1}^{k} A_i f_i(x) + f_e(x, \rho_{ab})$$

Construct from known Mellin moments.

Variational parameter as unknown coefficient.

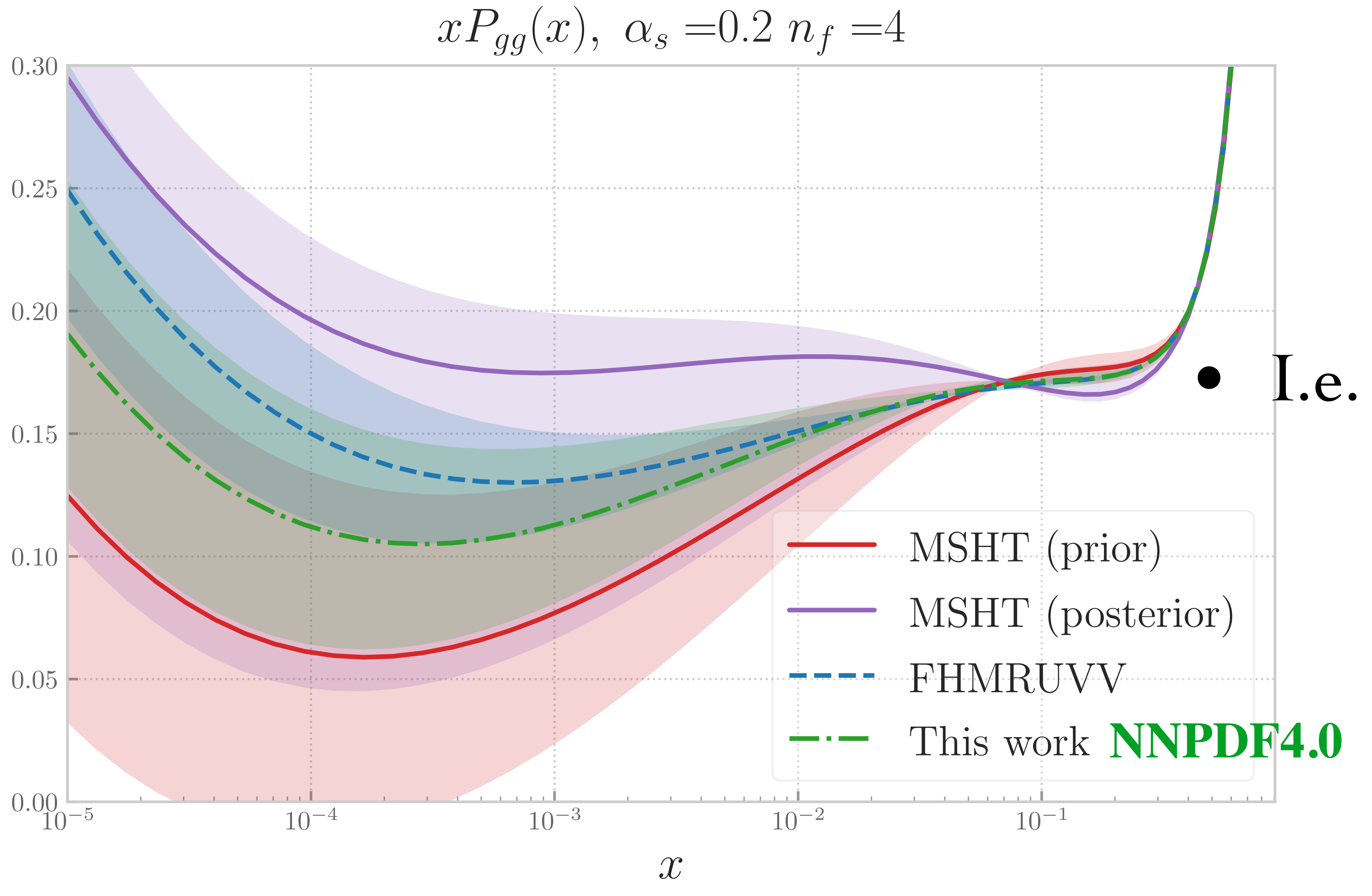
Contains exact small (and high) x info e.g. from resummation.

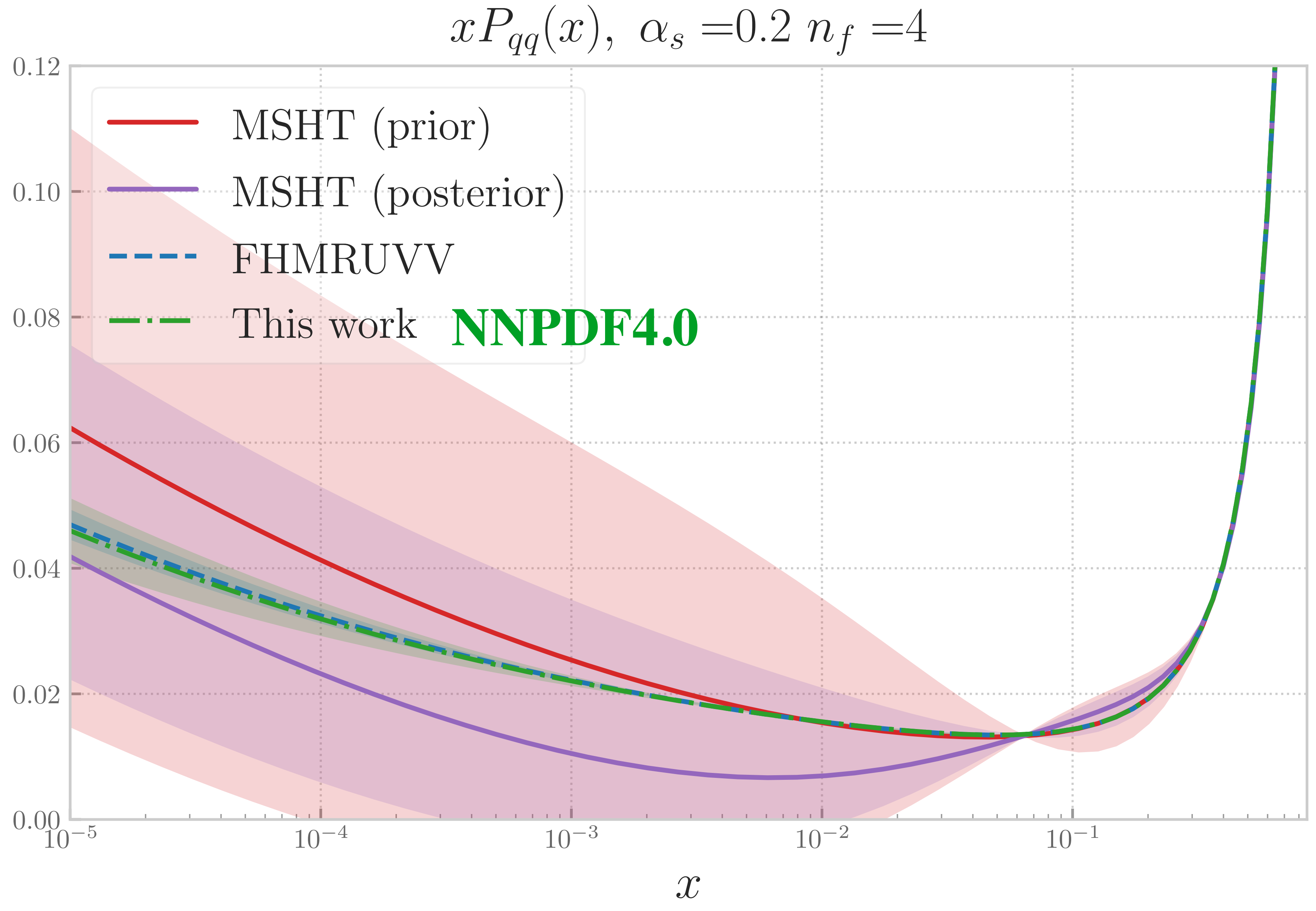
Known structure

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

R. D. Ball et al., arXiv:2402.18635

- Compare to more recent NNPDF release and recent FHMRUVV study:

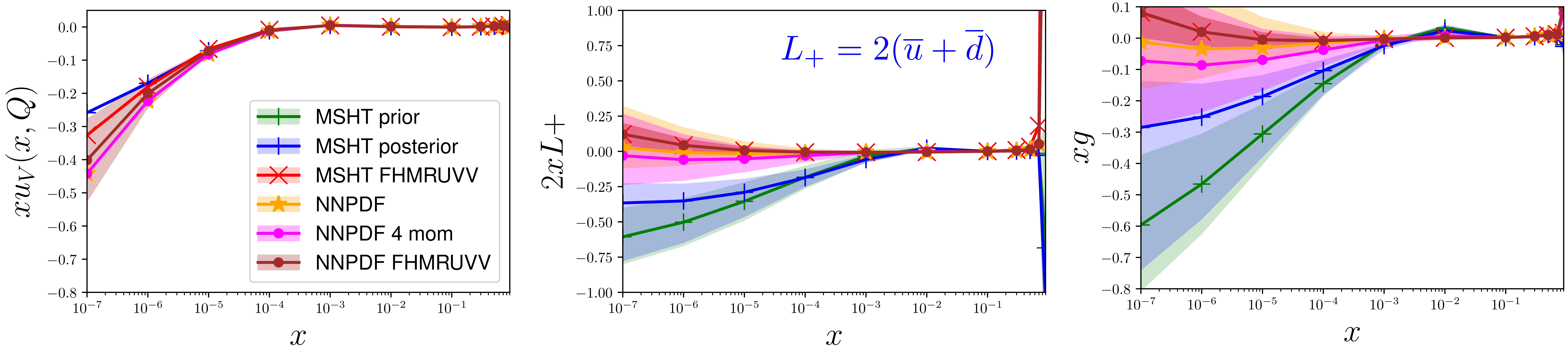




- I.e. quite some progress. Though new results within MSHT uncertainty band - validates approach.
- But what about impact on PDFs?

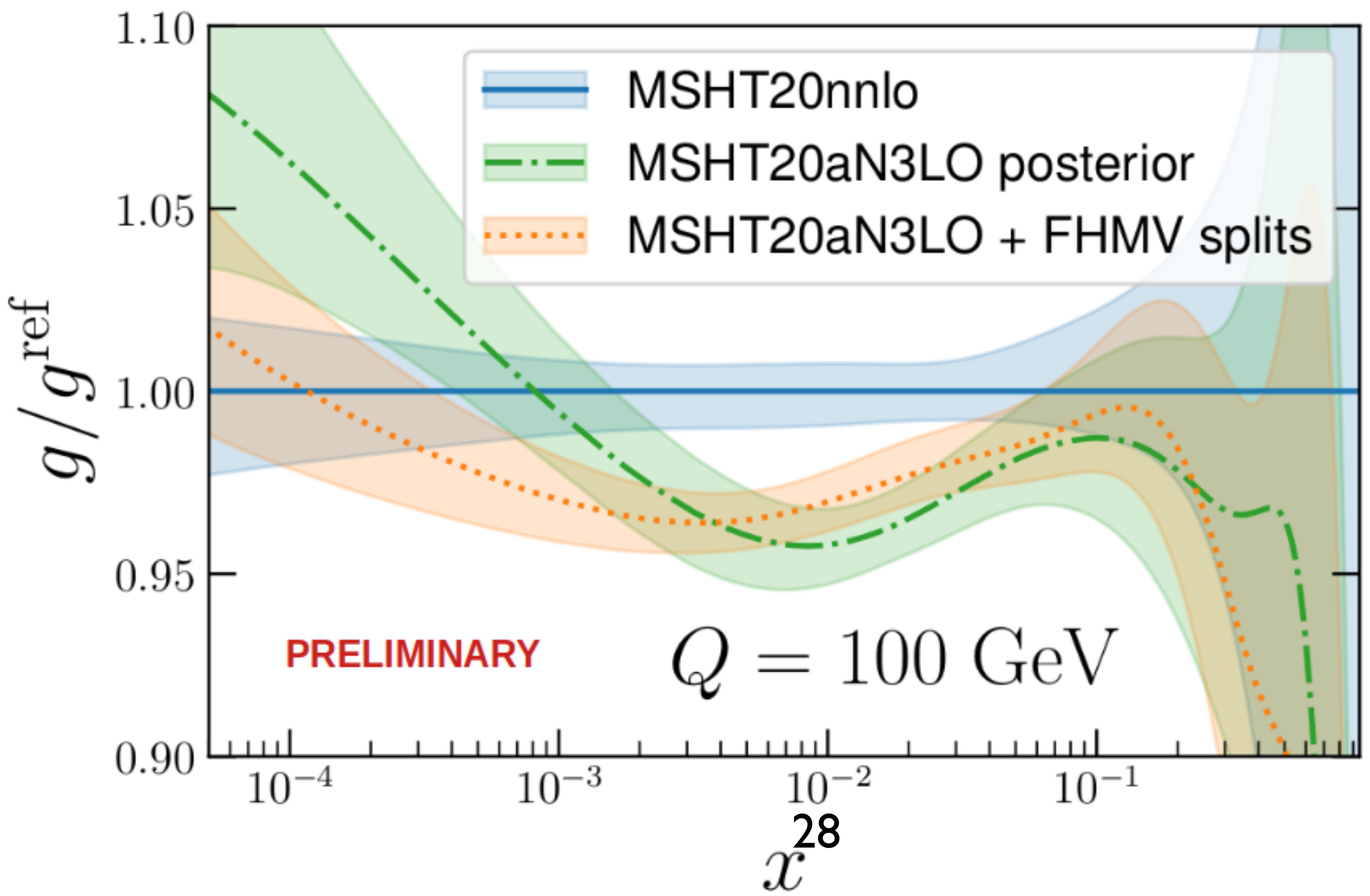
To appear on arXiv on next week

- Recent **benchmarking** exercise - consider impact of evolution on toy set of PDFs.



- Impact of new information at most at level of $\lesssim$ few percent in data region. At low x rather larger.

- Largely accounted for within MSHT uncertainties, e.g. most significant change in data region, on gluon:



- However in future release these updates can readily be included (in progress). Ability to do this built in to approach.

Including N3LO information - Hadronic K-Factors

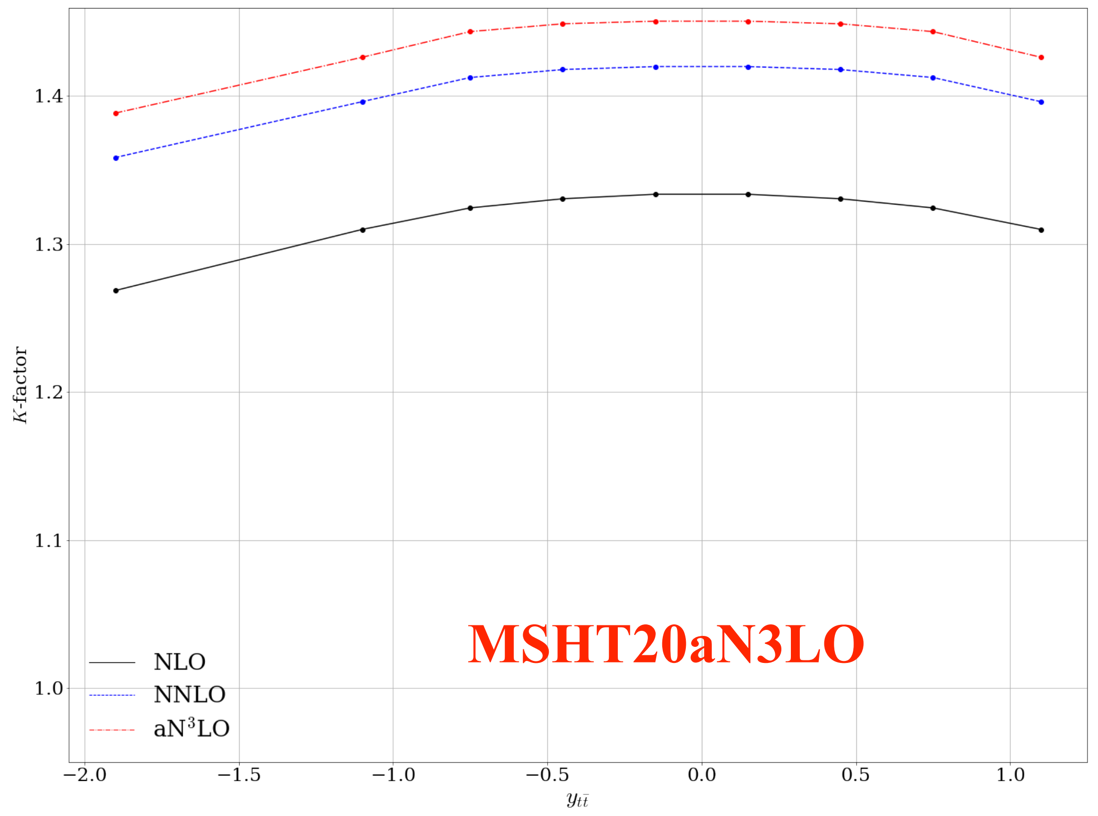
- Second, hadronic K-factors. Much less known than is currently useable for a fit. We simply allow N3LO K-factor to be free in fit within reasonable prior.
- Could e.g. use scale variations. We instead use known lower order results to guide this:

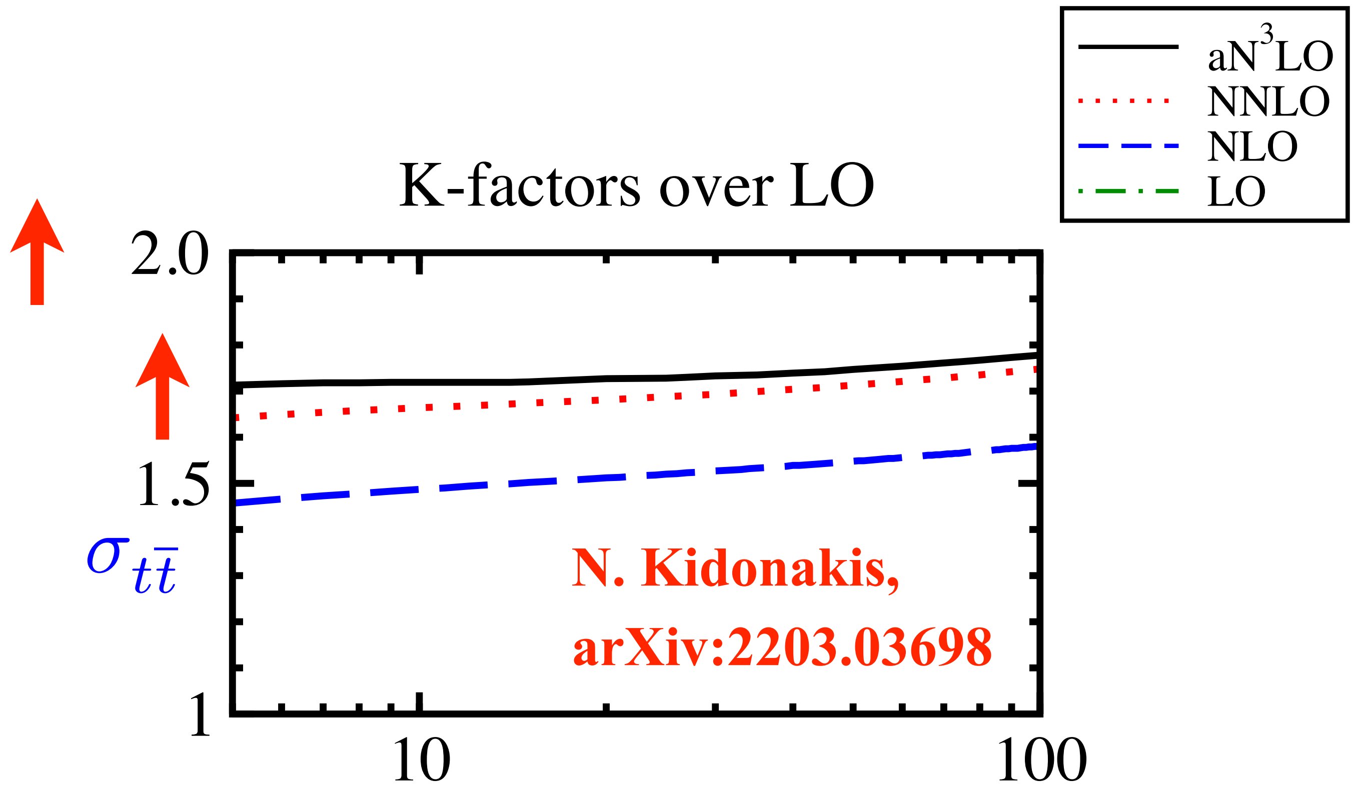
$$K^{\mathrm{N^3LO/LO}} = K^{\mathrm{NNLO/LO}}\left(1 + a_1(K^{\mathrm{NLO/LO}} - 1) + a_2(K^{\mathrm{NNLO/NLO}} - 1)\right)$$

- Divide datasets into subsets, with nuisance parameters correlated across these.
- Provides uncertainty from missing higher orders in hadronic cross sections.

Hadronic K-factors -	
Drell-Yan	DY_{NLO}, DY_{NNLO}
Top	Top_{NLO}, Top_{NNLO}
Jets	Jet_{NLO}, Jet_{NNLO}
p_T Jets	$p_T Jet_{NLO}$, $p_T Jet_{NNLO}$
Dimuon	$Dimuon_{NLO}$, $Dimuon_{NNLO}$

- Interestingly preferred values in fits qualitatively similar to known results:
- But as results come in (e.g. DY), can and would replace with these!





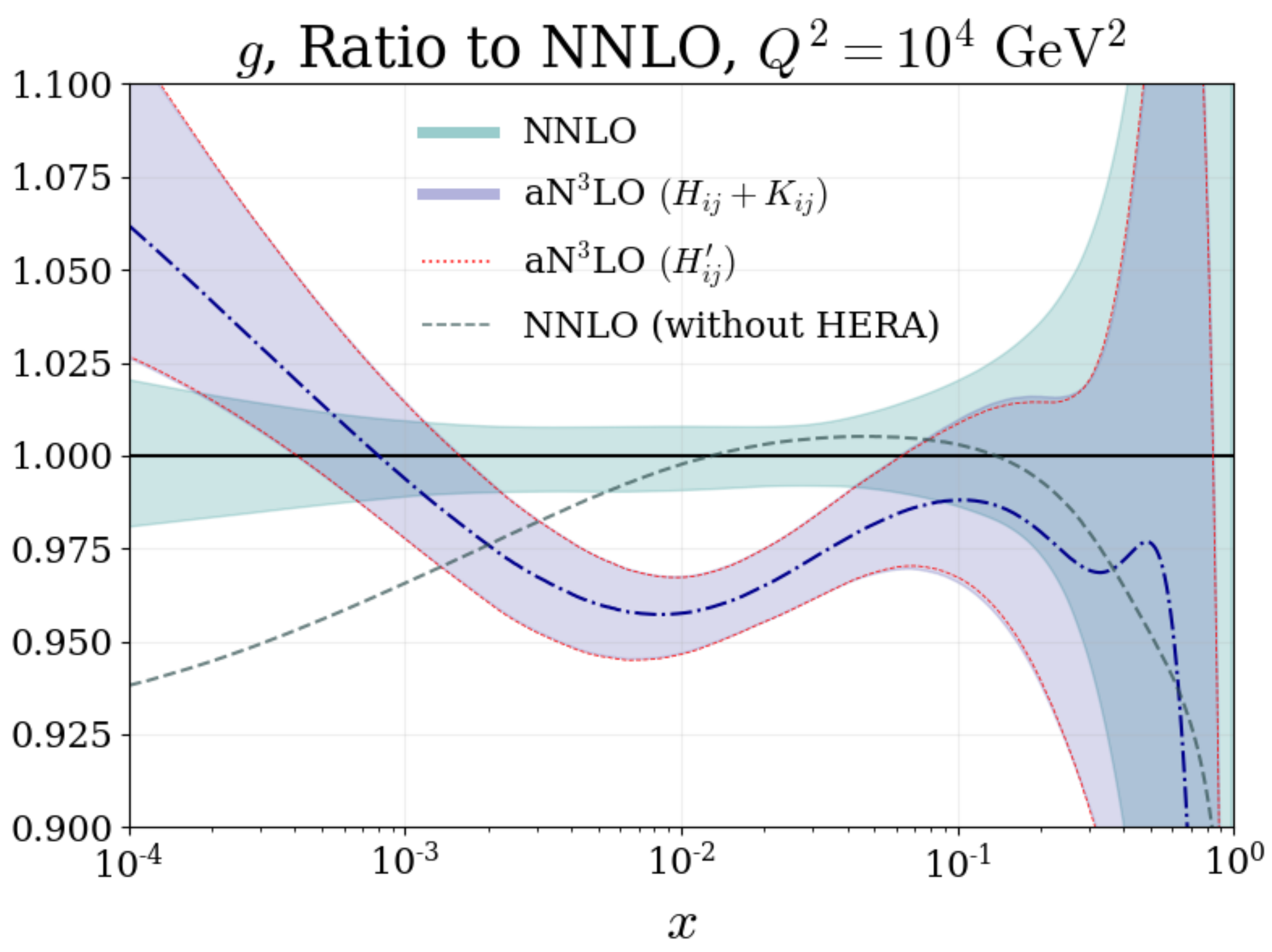
Results

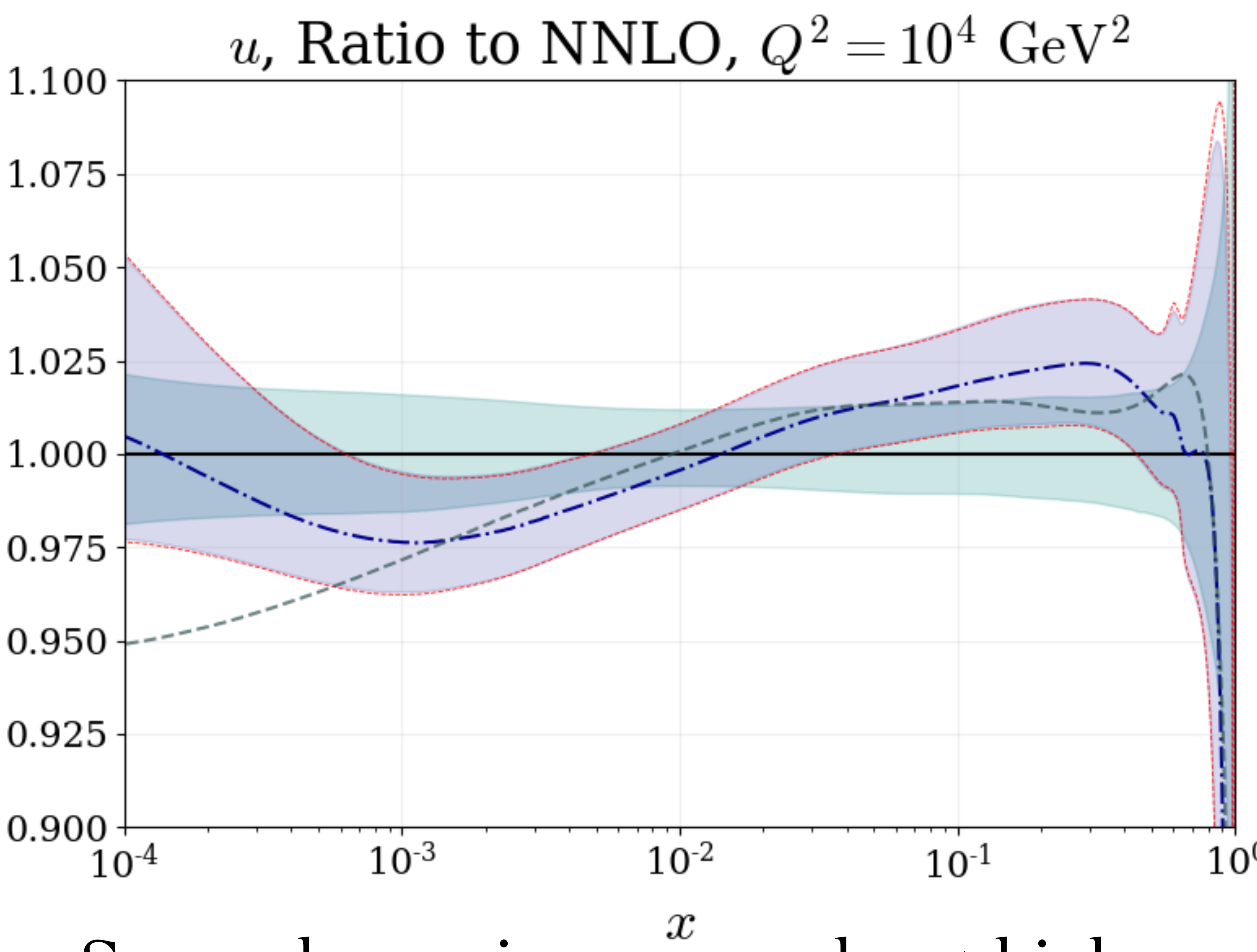
- Clear improvement in fit quality. Going from NNLO to aN3LO find $\Delta\chi^2 = -154.4$ (4363 points). Roughly half due to new aN3LO theory alone (not hadronic K-factors).

χ^2/N_{pts}	LO	NLO	NNLO	aN3LO
	2.57	1.33	1.17	1.14

Smooth fit improvement with order and amount of improvement reducing with order - as we might hope.

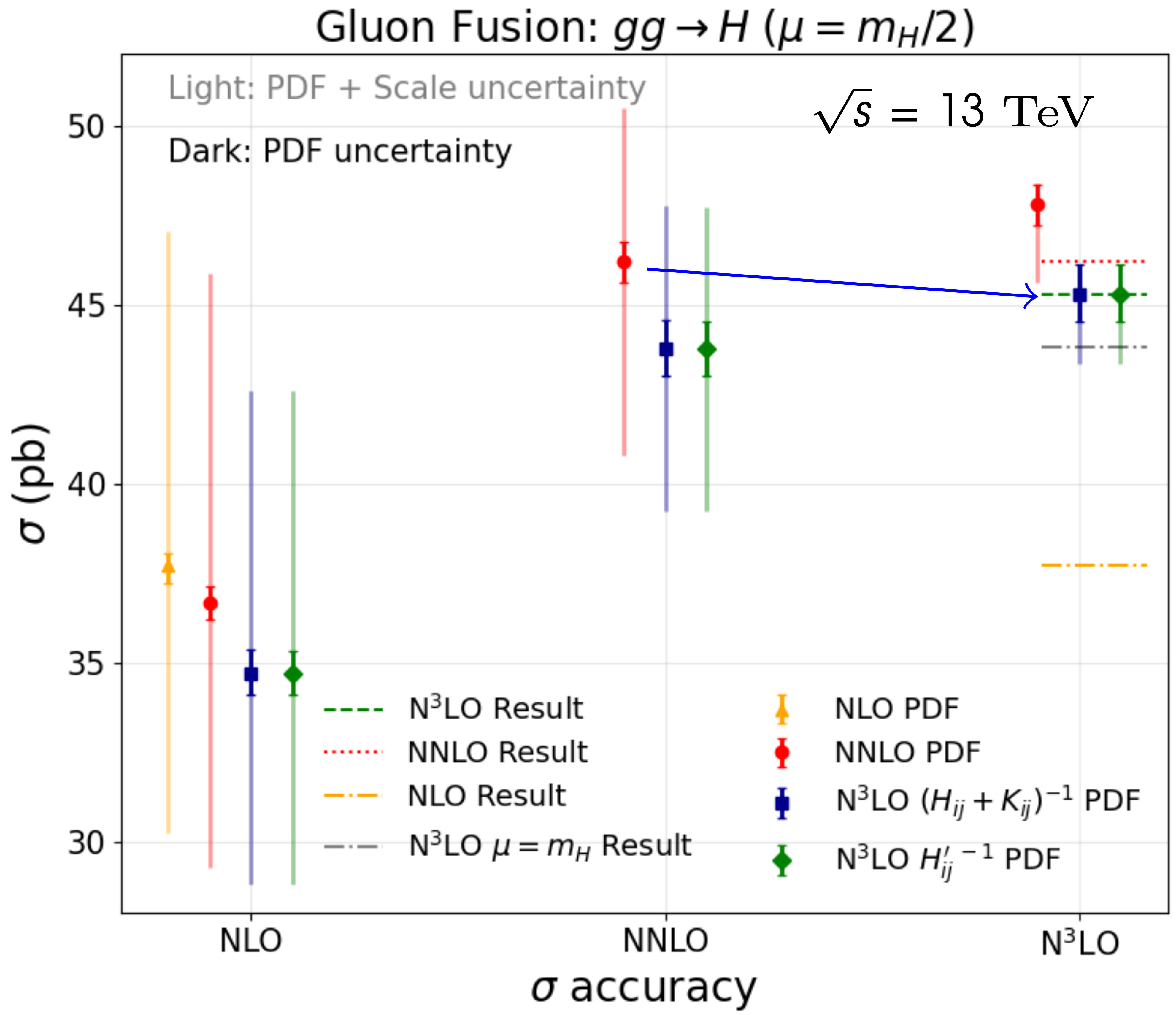
- Evidence that aN3LO reduces tensions between low and high x regions. Impact on PDFs…



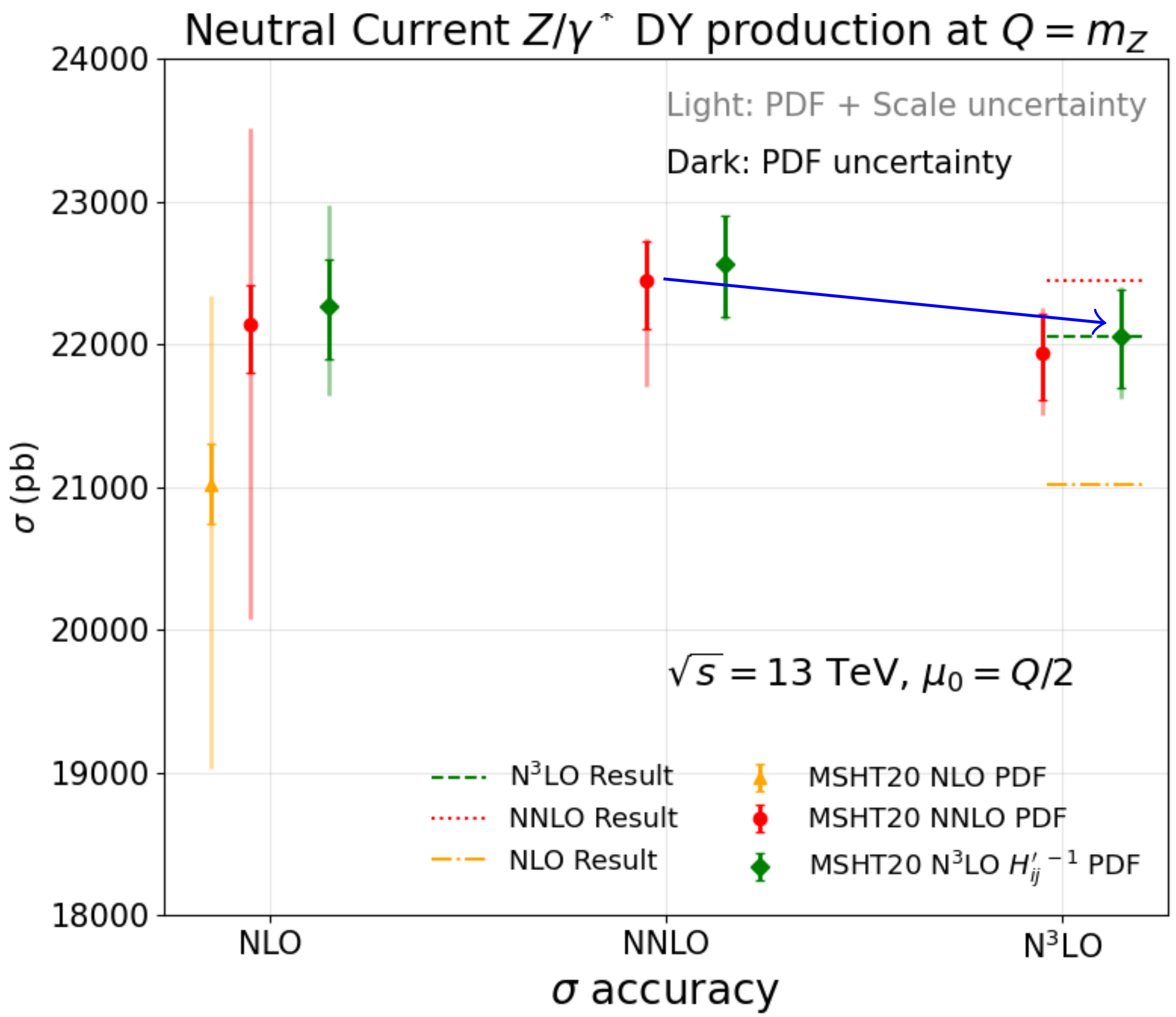


- Largest change is in gluon at low and intermediate x. Some change in e.g. quarks at high x .

- Change in gluon corresponds to reduction in e.g. ggH at N3LO - improves stability.



- Some increase in NC DY - again mild improvement in stability.



Determination of the Strong Coupling at aN3LO

Extracting the strong coupling in a PDF fit

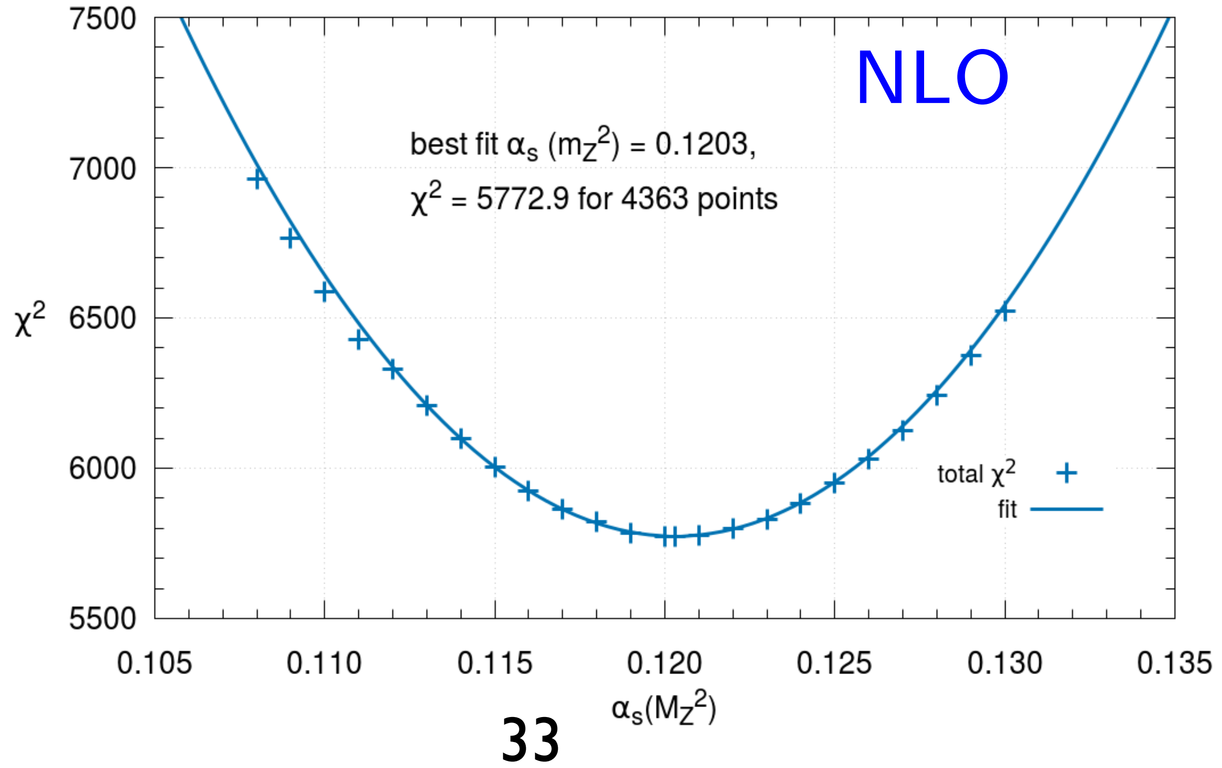
$$P(x,\alpha_s) = \alpha_S P^{(0)}(x) + \alpha_S^2 P^{(1)}(x) + \alpha_S^3 P^{(2)}(x) + \alpha_S^4 P^{(3)}(x) + \ldots$$

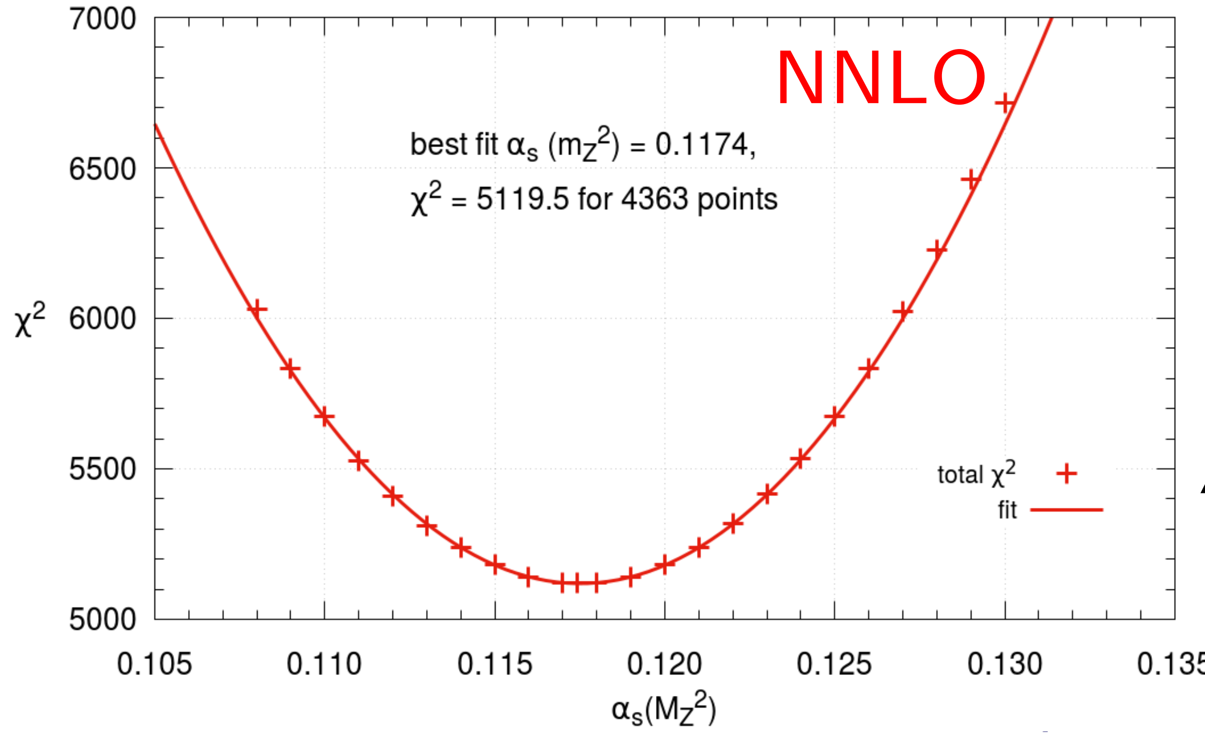
- Global PDF fit sensitive to value of strong coupling through impact on **evolution** and **cross sections**.
- While baseline sets often provided with $\alpha_S = 0.118$, can allow it be to free parameter and see what we find.
- Individual datasets have different α_S dependencies, but **global** determination provides robust fit.
- Determination of α_S and PDFs highly correlated. Only completely consistent way to include impact of a (PDF sensitive) hadronic measurements is via full refit. **S. Forte and Z. Kassabov, arXiv: 2001.04896**

$\alpha_{S,\mathrm{NNLO}}(M_Z^2) < \alpha_{S,\mathrm{NLO}}(M_Z^2)$
as NNLO corrections +ve, so
fitting same data $\Rightarrow$ lower α_S.

$$\alpha^{prev}_{S,\mathrm{NLO}}(M_Z^2) = 0.1203 \qquad \alpha^{prev}_{S,\mathrm{NNLO}}(M_Z^2) = 0.1174$$

- In original (up to) NNLO MSHT20 fit, the best fit values were found to be:
- What about aN3LO?





Nice Quadratic χ^2 profile ✓

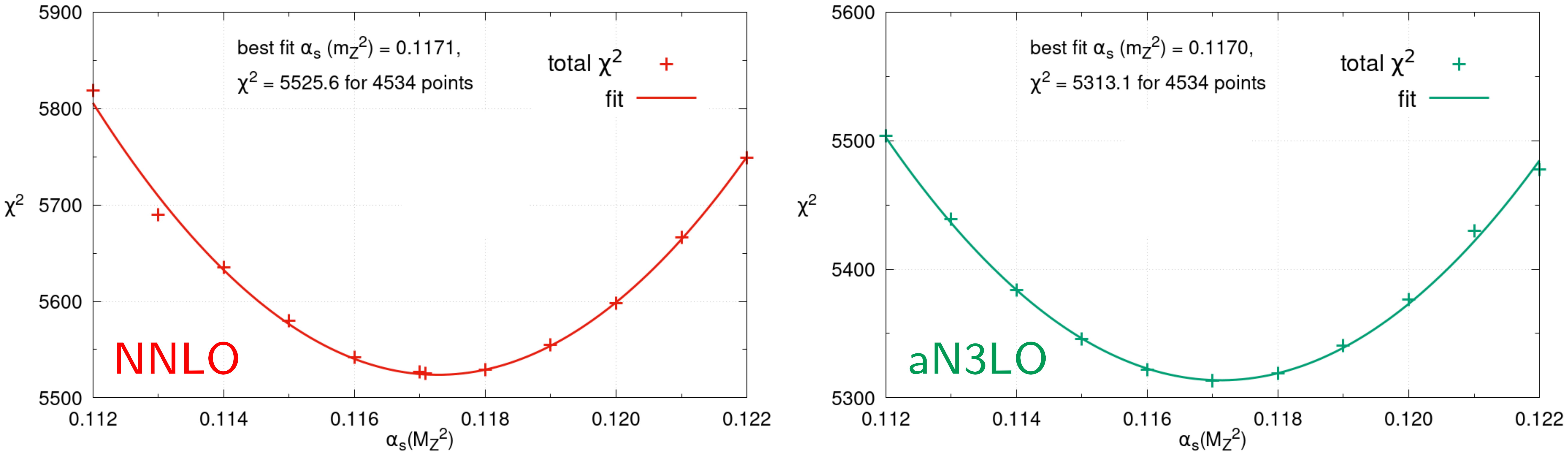
Note we provide the $\Delta\chi^2$ changes with α_S $\Rightarrow$ can use this info!

The strong coupling at aN3LO

Minor updates + ATLAS 8 TeV jets

- Can now extend this analysis to aN3LO. Baseline very similar (not identical) to MSHT20. Find:

$$\alpha^{new}_{S,\mathrm{NNLO}}(M_Z^2) = 0.1171 \qquad \alpha^{new}_{S,\mathrm{aN3LO}}(M_Z^2) = 0.1170$$

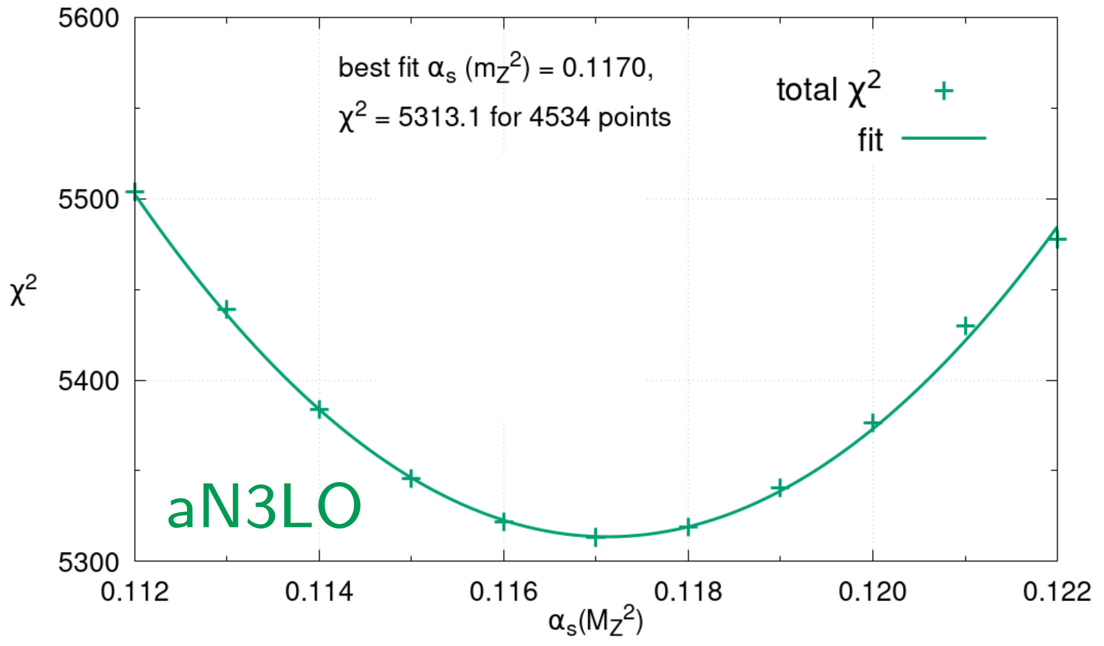


Nice Quadratic χ^2 profile ✓

0.1180 ± 0.0009

- NNLO: similar to previous result (0.1174).
- Very good perturbative convergence to aN3LO, and both consistent with world average.
- Confirmed that more recent aN3LO splitting function information gives v. similar result ($\ll$ uncertainty)
- Looking in more detail…

- Find that global χ^2 profile built up of different competing pulls…



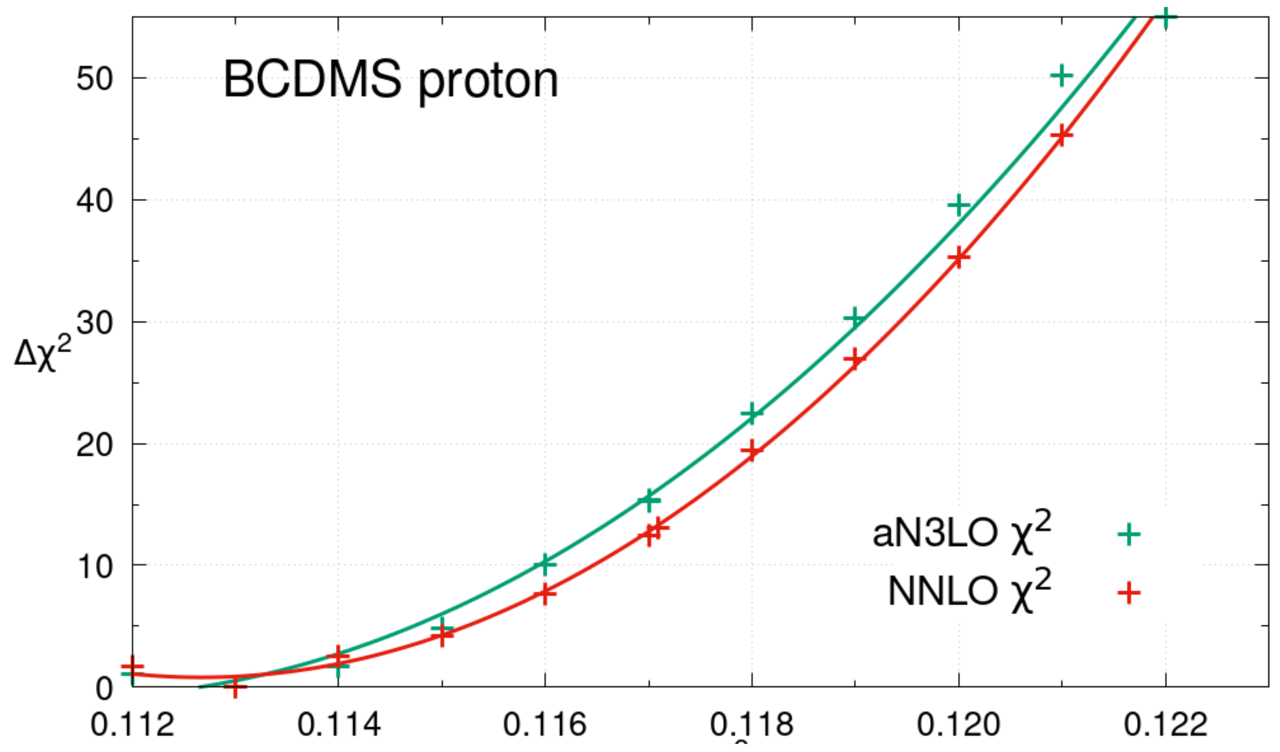
★ **Fixed target data**. DIS in particular sensitive through impact on evolution

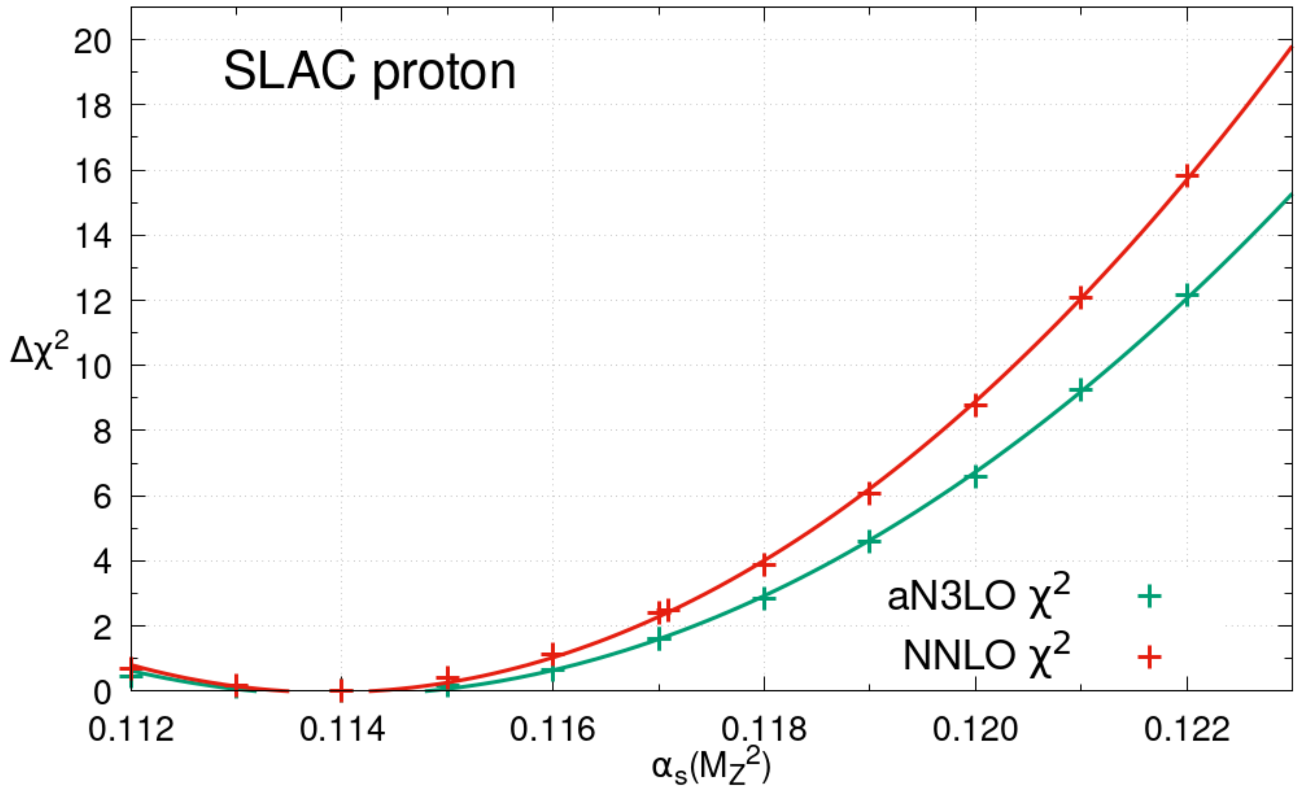
★ **LHC DY**. Due to high precision provide reasonable constraints

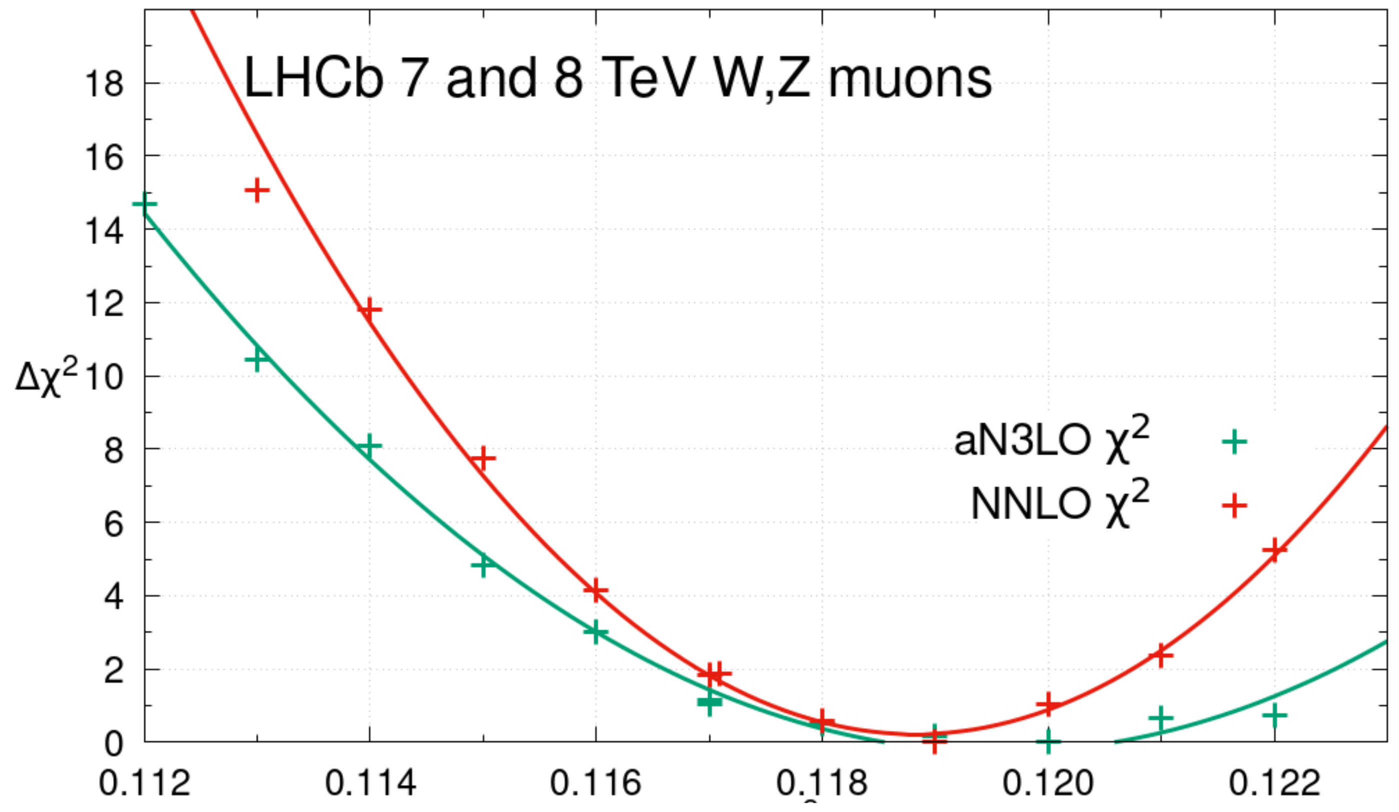
★ **LHC Jets**. Clear direct constraints. Some difference between datasets…

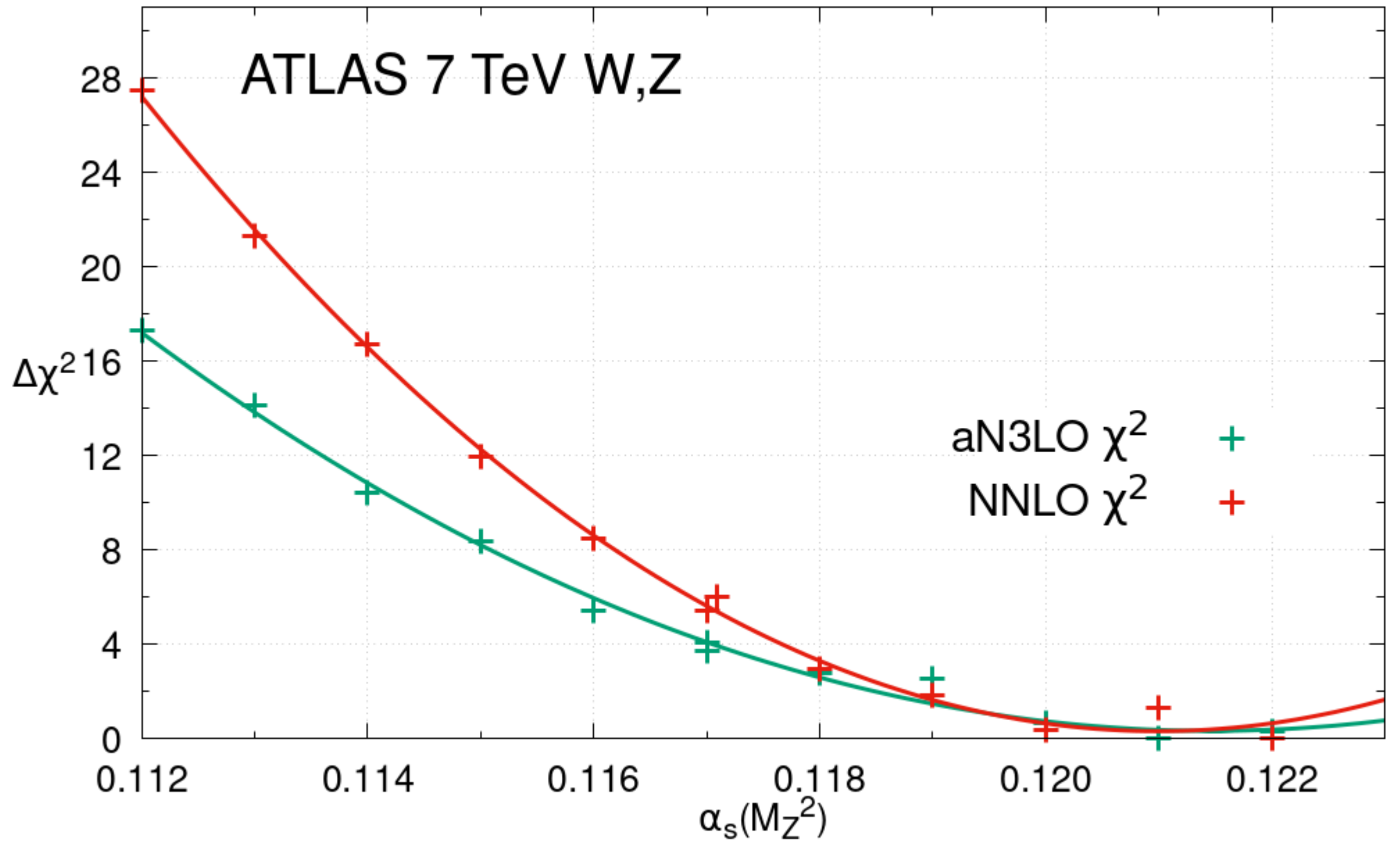
NNLO
aN3LO

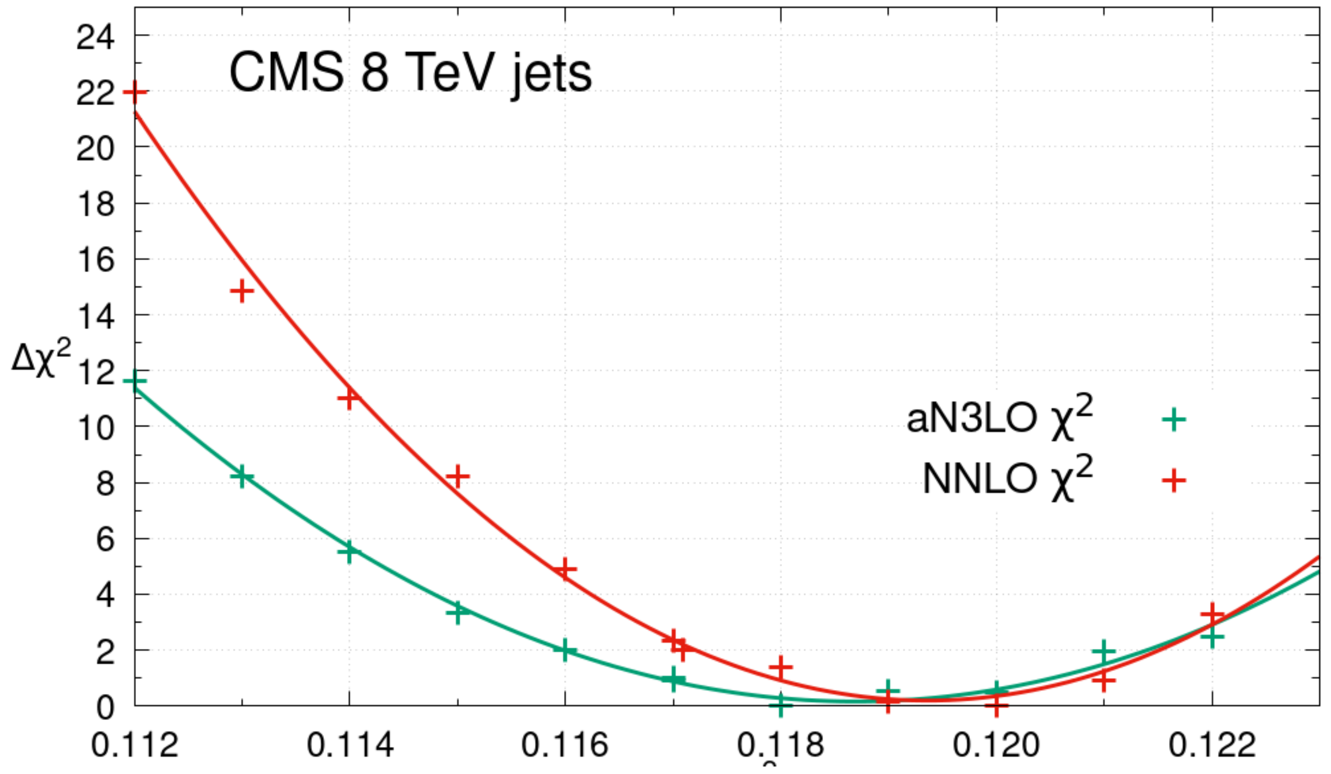
BCDMSp prefers lower α_S to slow fall of structure function with Q^2.

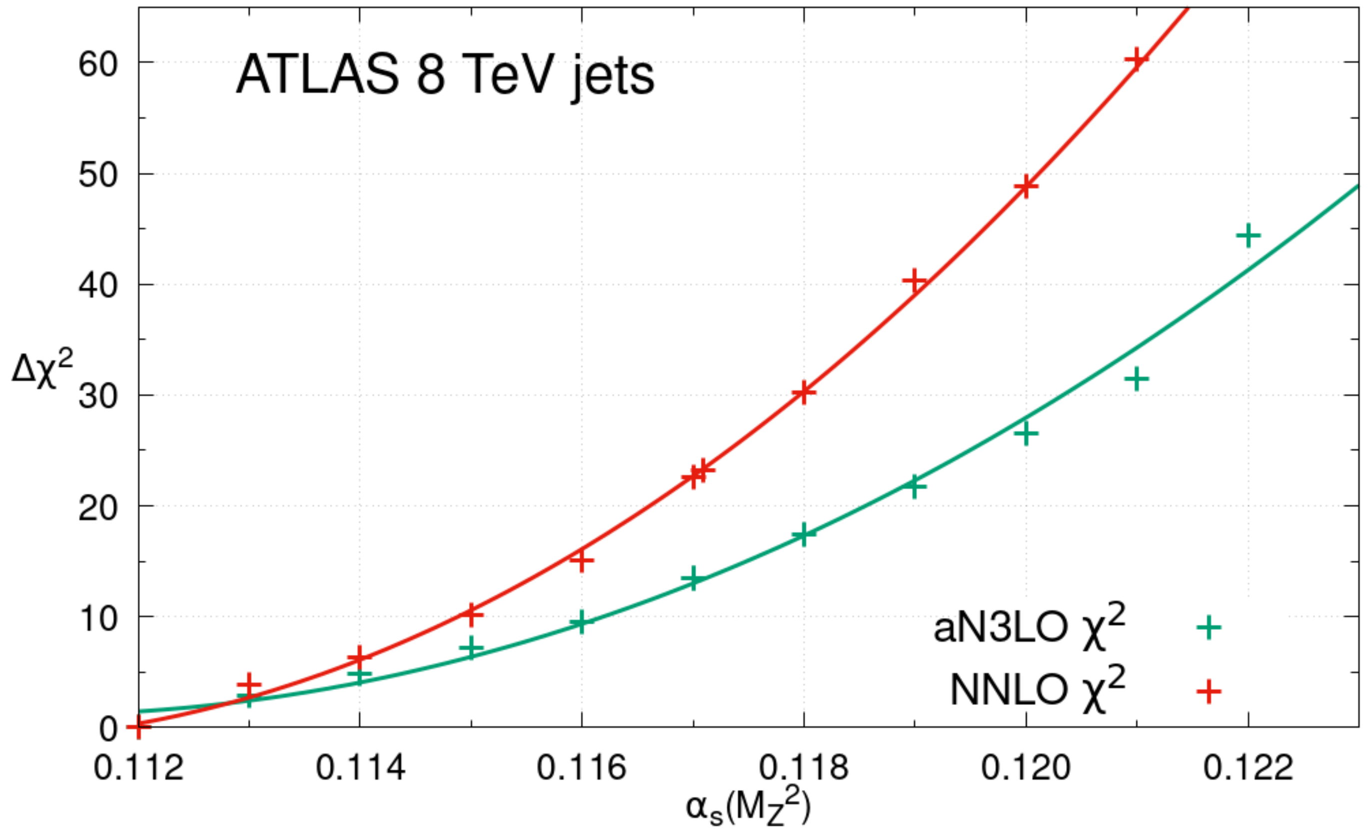












- Trends all rather similar between NNLO and aN3LO (i.e. convergence).

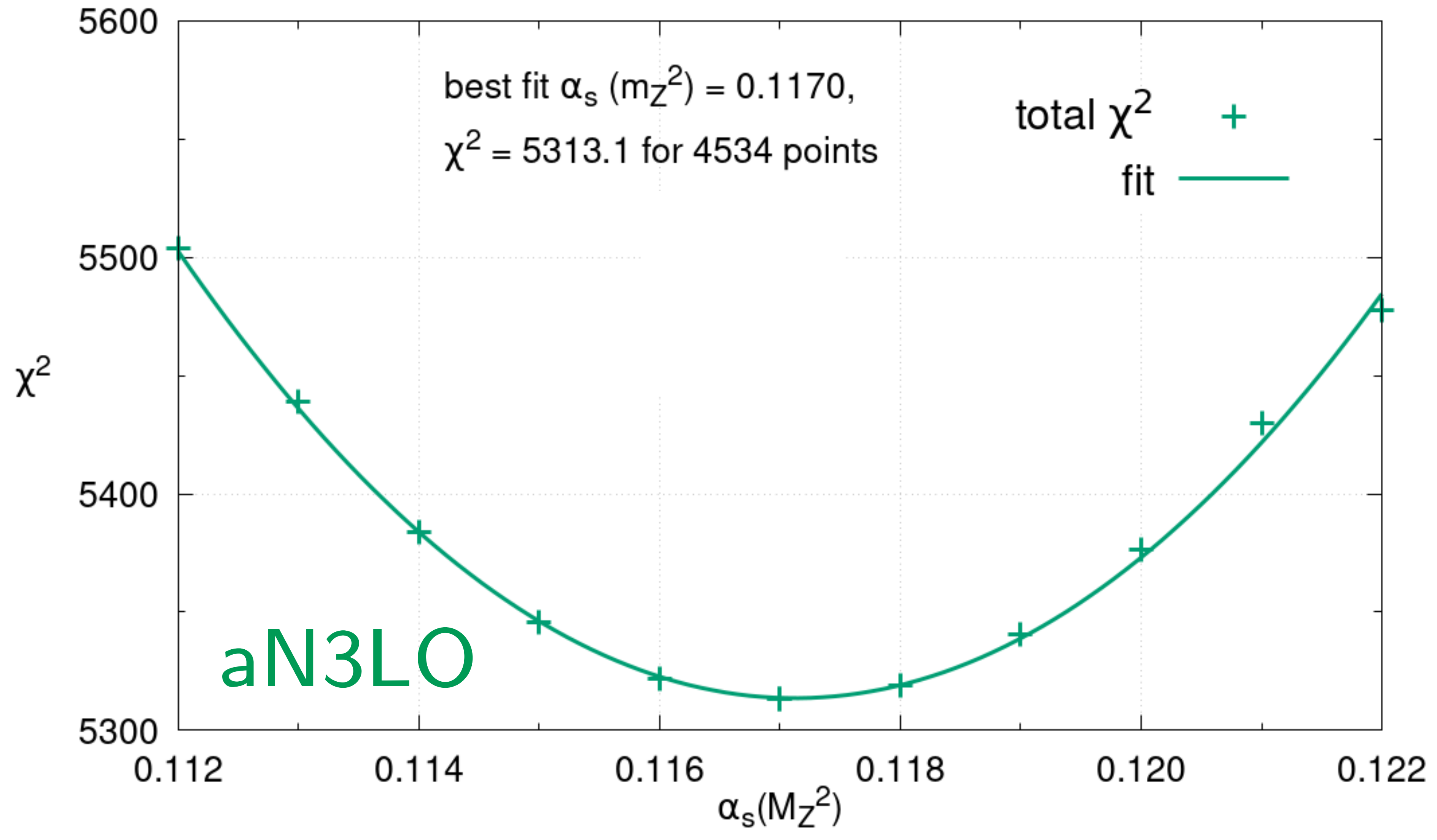
Uncertainty Evaluation

- In textbook case, would simply take $\Delta\chi^2 = 1$ from minimum, to give (roughly):

$$\alpha_S = 0.1170 \pm 0.0005$$

- However from discussion before, expect to be too aggressive. Enlarged tolerance needed.

- In MSHT apply `dynamic tolerance' criterion. Briefly:
  - ★ Evaluate individual χ^2 profile for each dataset
  - ★ Deviation with α_S increasing/decreasing monitored and limited such that this does not exceed 'hypothesis testing' criterion $\Delta\chi^2 \lesssim \sqrt{2N}$ i.e. remains good according to this measure.
  - ★ In toy model can show given two datasets in tension that PDF uncertainty $\propto$ difference (unlike $T = 1$).
  - ★ Will result in one dataset setting most stringent upper/lower limits, but find many others with similar limits, i.e. uncertainty not driven by a single (potentially problematic) dataset.
  - ★ Broadly corresponds to $T \sim 3$.



Backup

***For experts: in reality, limit is rescaled by best fit value:** $\Delta\chi^2 \lesssim \chi^2_{n,0}\left(\frac{\xi_{68}}{\xi_{50}} - 1\right)$

T. Cridge and M. Lim, arXiv:2306.14885

Though reasons to suggest we could…

F_2^c provides upwards bound of: $\Delta\alpha_S(M_Z^2) = +0.0020$.

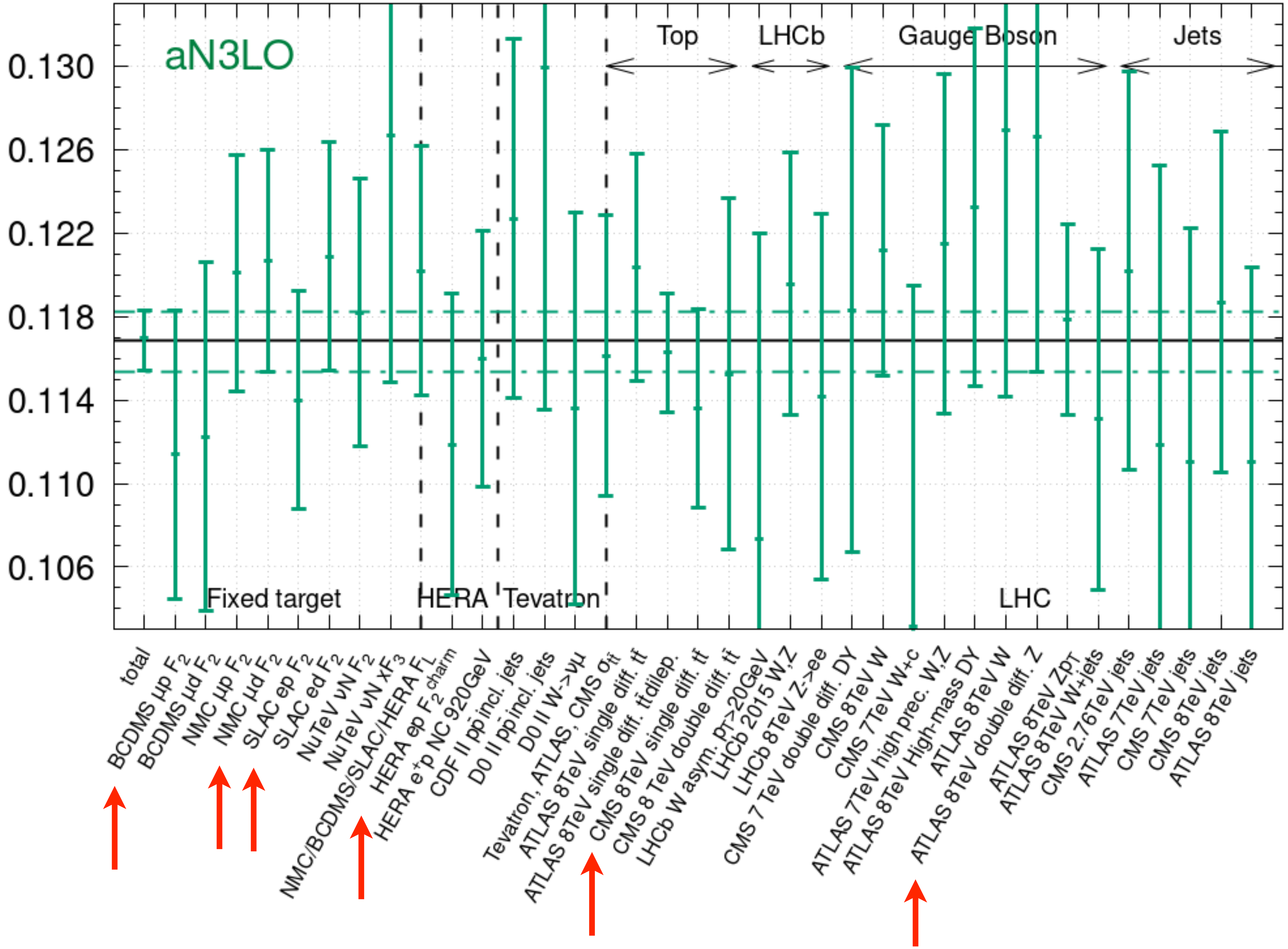
CMS and ATLAS (dilepton) $t\bar{t}$ single diff. would give slightly higher upper α_S bounds, but not used.

(Consistent with other fixed target DIS (p), and ~ known N3LO)

BCDMSp data strongest constraint upwards: $\Delta\alpha_S(M_Z^2) = +0.0013$.

NMC deuteron, ATLAS 8 TeV Z both give lower bounds of $\Delta\alpha_S(M_Z^2) = -0.0017$.

SLAC deuteron data gives lower bound: $\Delta\alpha_S(M_Z^2) = -0.0016$.



- Putting together and suitably symmetrising, we quote:

$$\alpha_{S,\mathrm{aN3LO}}(M_Z^2) = 0.1170 \pm 0.0016$$

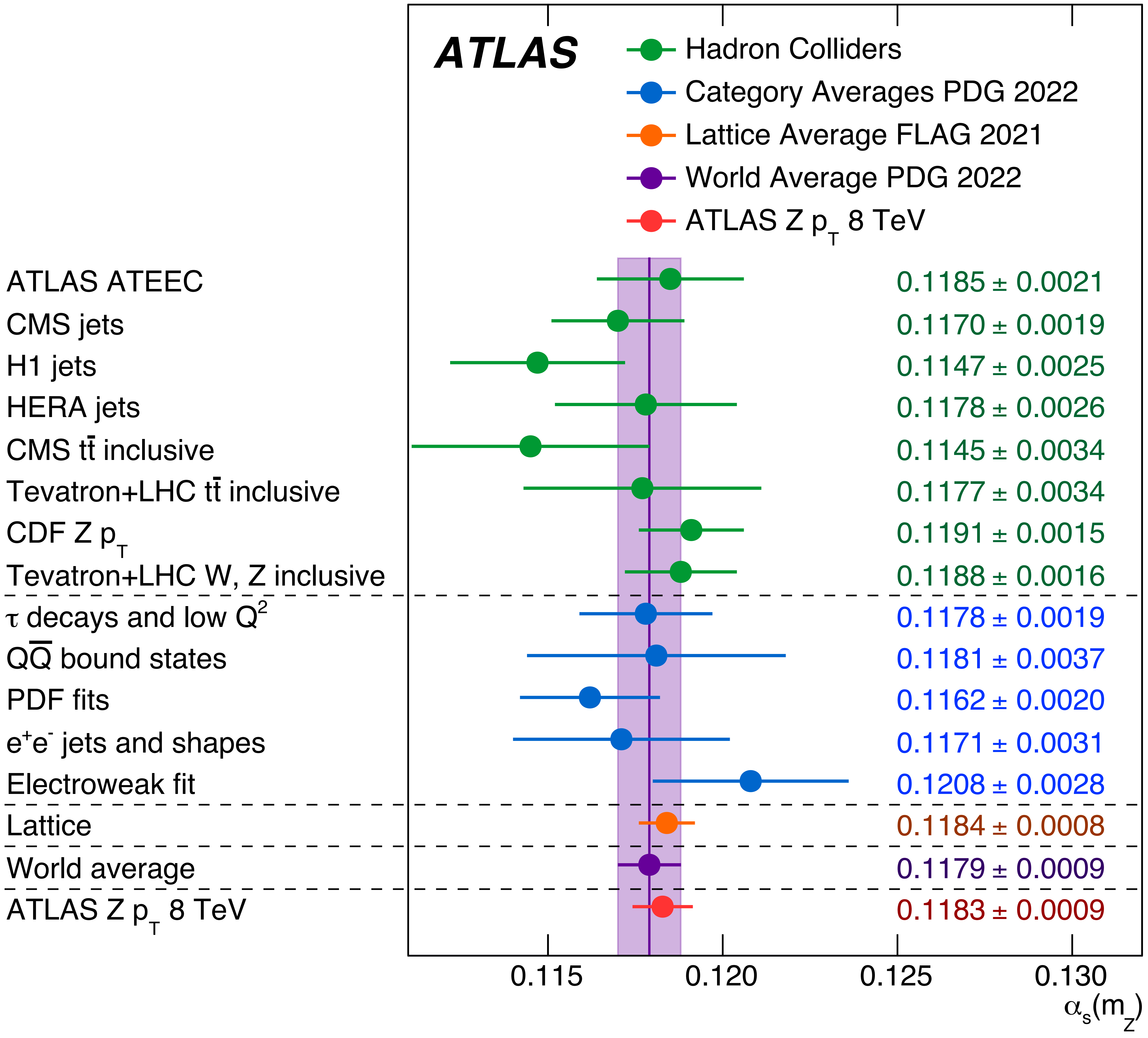
Consistent with (NNLO) World Average of 0.1180 ± 0.0009.

With thanks to T. Cridge

Comparison to other results

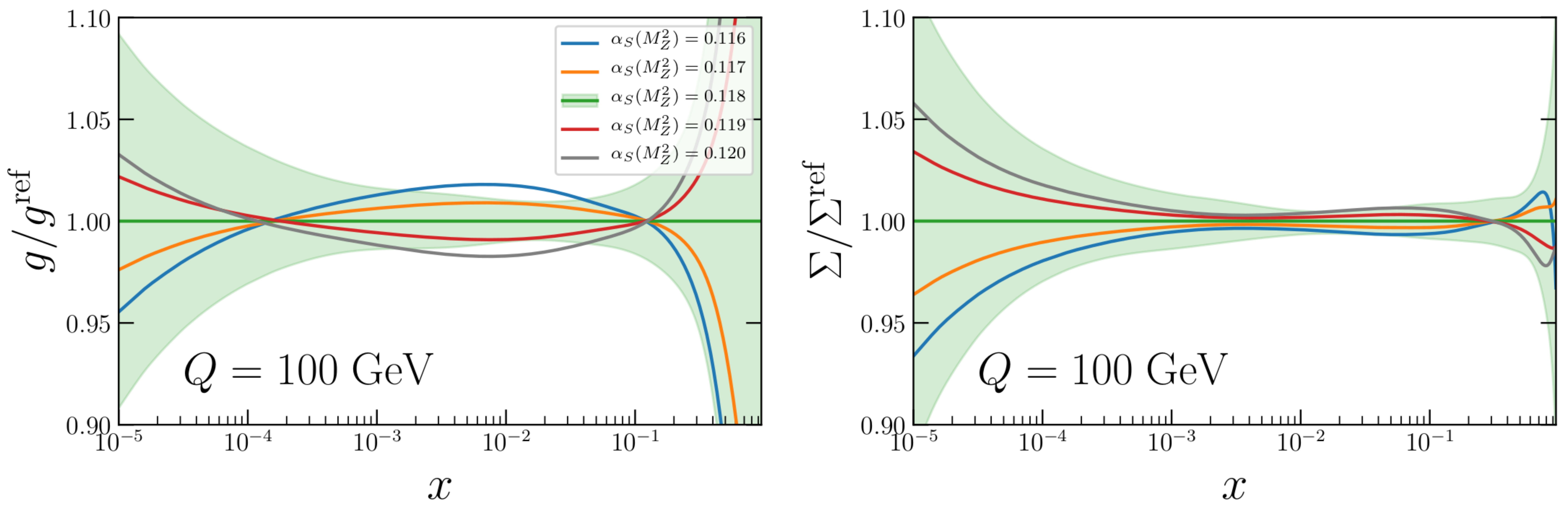
$$\alpha_{S,\mathrm{aN3LO}}(M_Z^2) = 0.1170 \pm 0.0016$$

- Consistent with world average and recent ATLAS measurement.
- Uncertainty larger but similar order.
- Again, if we took $\Delta\chi^2 = 1$ would be factor of ~ 2 smaller, but v. good reasons to believe that is too agressive. $\alpha_S = 0.1170 \pm 0.0005$

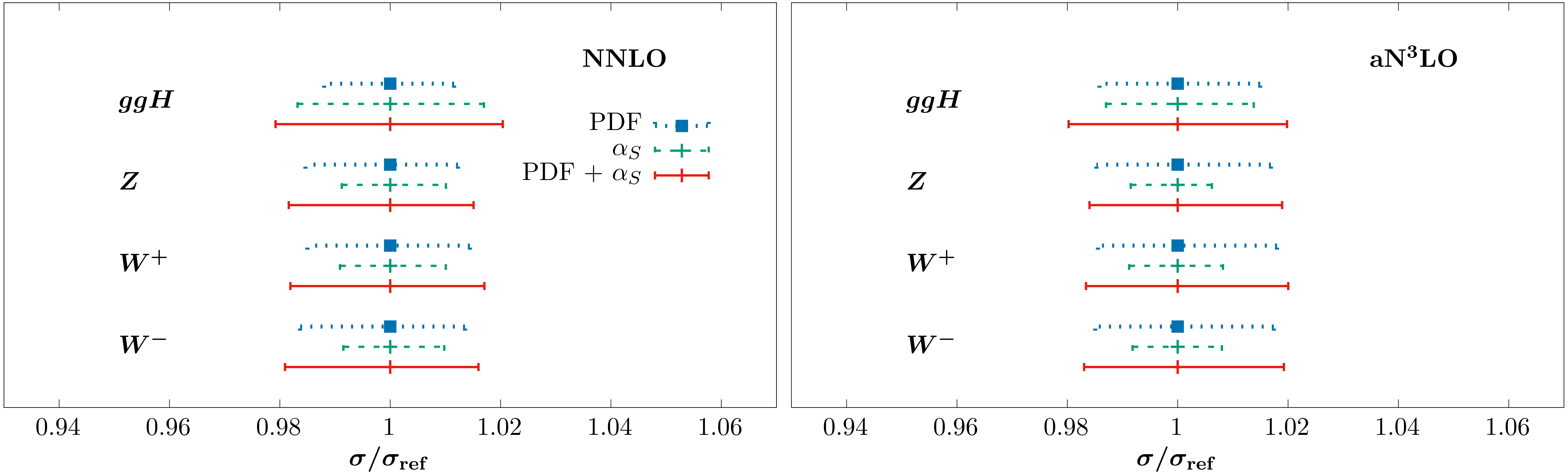


PDFs

- ★ Clear correlation between PDFs and α_S, as expected.
- ★ Change generally within PDF uncertainties for $\Delta\alpha_S = \pm 0.001$ though close to edge for gluon.
- ★ **Gluon** anticorrelated with α_S for $x \lesssim 0.1$ to maintain $\mathrm{d}F_2/\mathrm{d}Q^2 \sim \alpha_S g$. Correlation at high $x \gtrsim 0.1$ from sum rule.
- ★ Less impact on **quarks** - reduced/increased at high/low x from splitting.



Cross Sections



★ Impact on cross sections includes α_S variation in matrix elements + PDFs - non-trivial interplay to get final result. Important to treat these together!

★ For LHC **Higgs** the anticorrelation between gluon and α_S compensates larger direct uncertainty.

★ For **DY** direct α_S uncertainty small, and largest effect from change in PDF.

★ Combined PDF + α_S broadly leads to at most moderate increase over PDF uncertainty alone.

Jets vs. Dijets?

T.C., L.A. Harland-Lang,
R.S. Thorne 2312.12505.

- Studied in detail in recent paper. Worth briefly mentioning here. Bottom line:

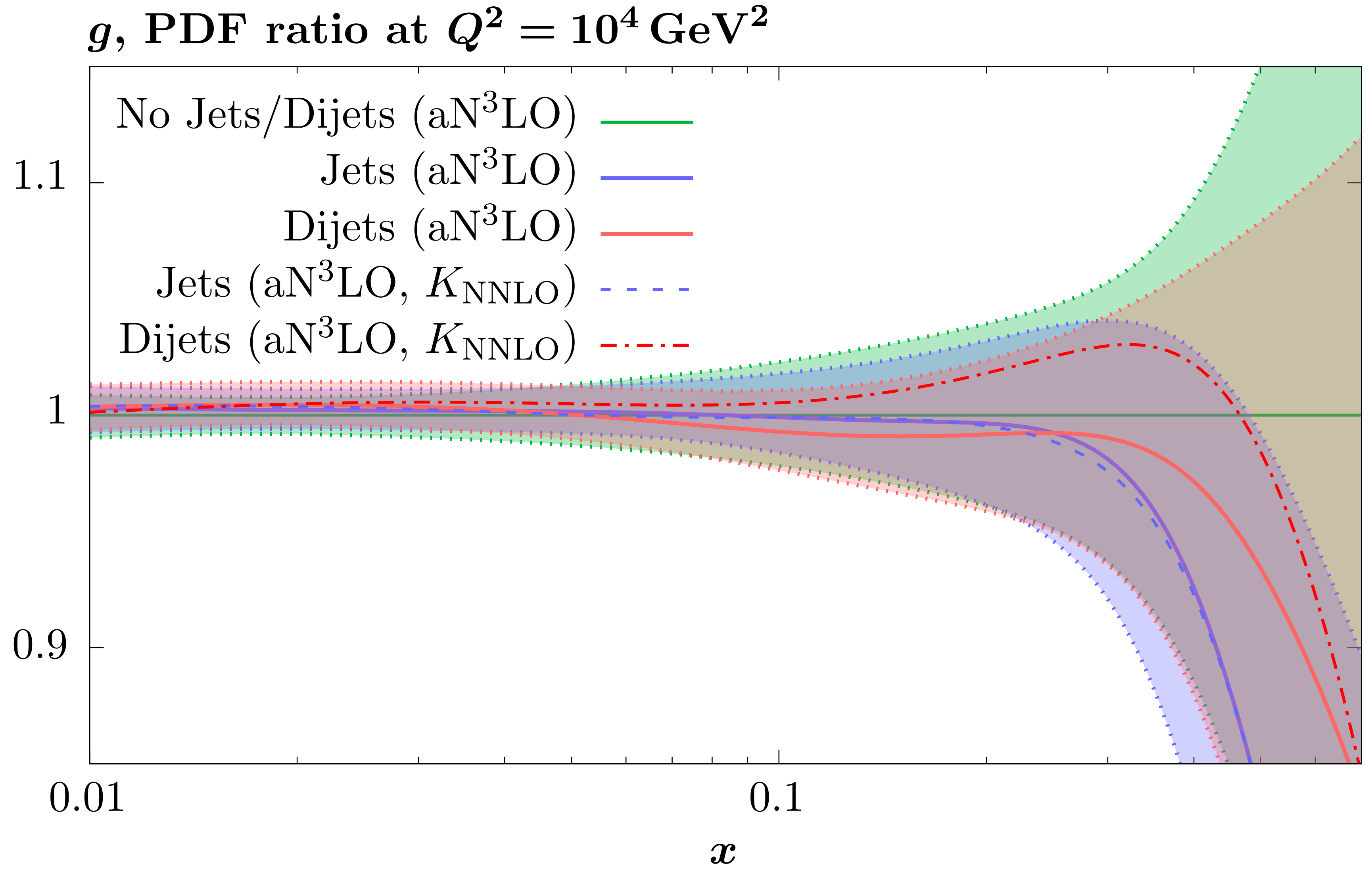
Note inclusive jets are fit in results so far!

★ Potentially general reasons to prefer dijet data: non-unitary nature of inclusive jets, and potential for 3D distributions in dijets (more constraining!).

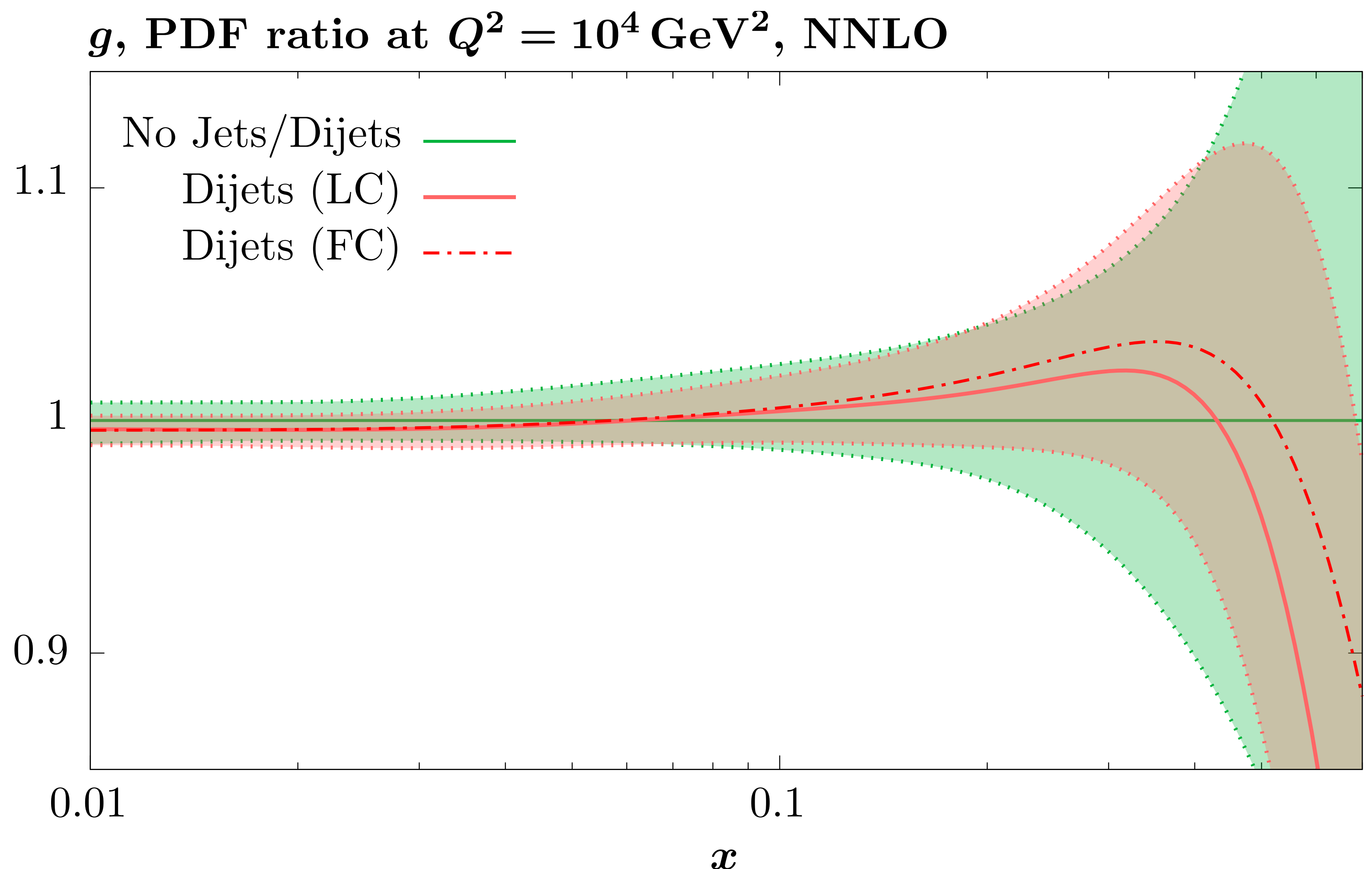
★ Supported by our study: fit quality better in dijet case at both NNLO and aN3LO

★ Some difference in pull on gluon at NNLO, better consistency at aN3LO.

Inclusive Jets	N_{pts}	χ^2/N_{pts} NNLO	χ^2/N_{pts} aN3LO	Dijets	N_{pts}	χ^2/N_{pts} NNLO	χ^2/N_{pts} aN3LO
Total	472	1.39	1.43	Total	266	1.12	1.04
Total (+ATLAS 8 TeV jets)	643	1.67	1.61	Total	266	1.12	1.04



★ Impact of full colour mild...

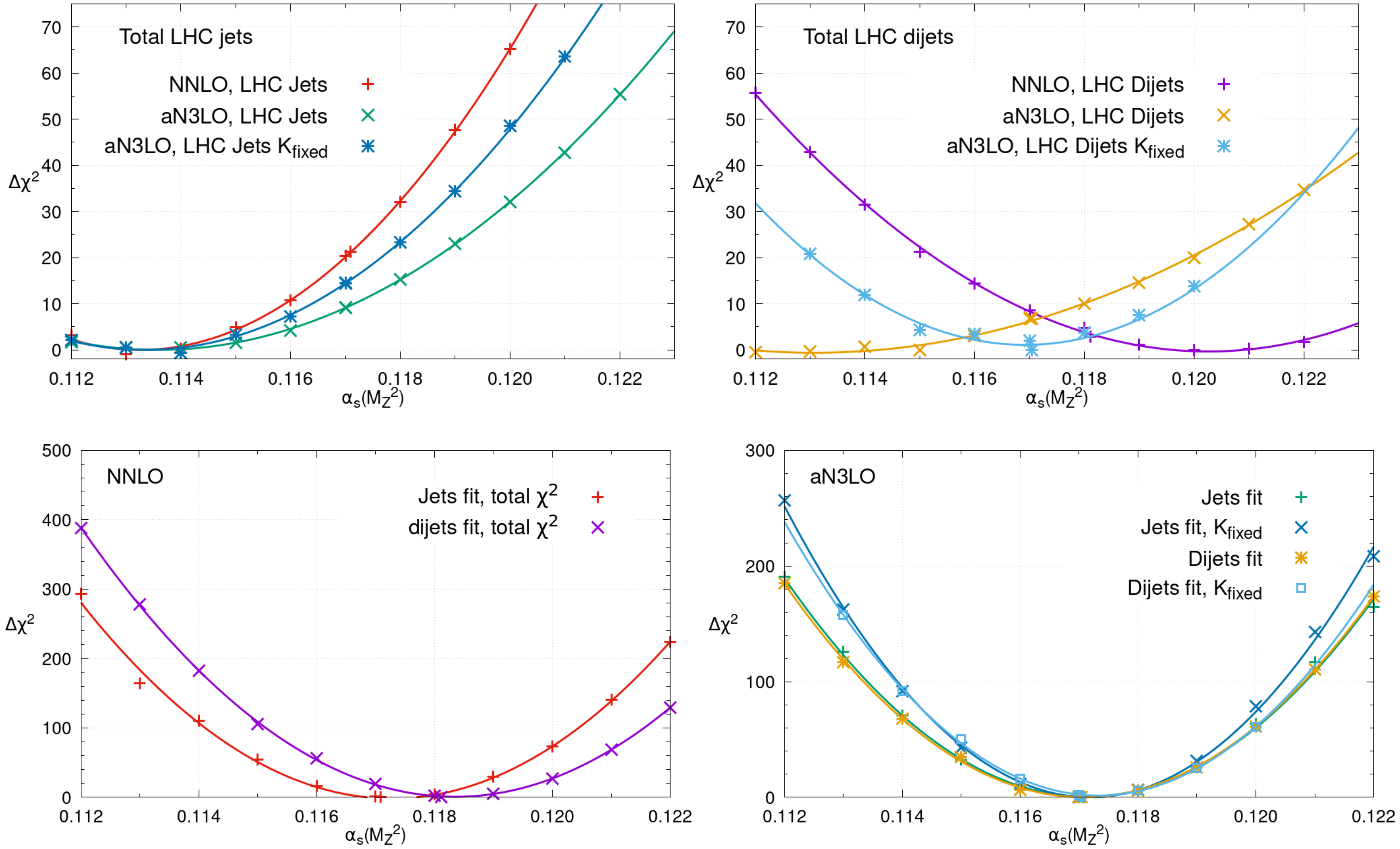


- What about α_S ?

  ★ NNLO: pull very different between jets and dijets.

  ★ aN3LO: this stabilises!

★ Translates into difference in global profiles:



★ Much better consistency at aN3LO, though at NNLO consistent within (dynamic tolerance) uncertainties:

$$\alpha_S(M_Z^2)(\text{Dijet, NNLO}) = 0.1181 \pm 0.0012 \qquad \alpha_S(M_Z^2)(\text{Jet, NNLO}) = 0.1171 \pm 0.0015$$

★ But in tension with $T^2 = 1$: ~ 0.0004 ~ 0.0005

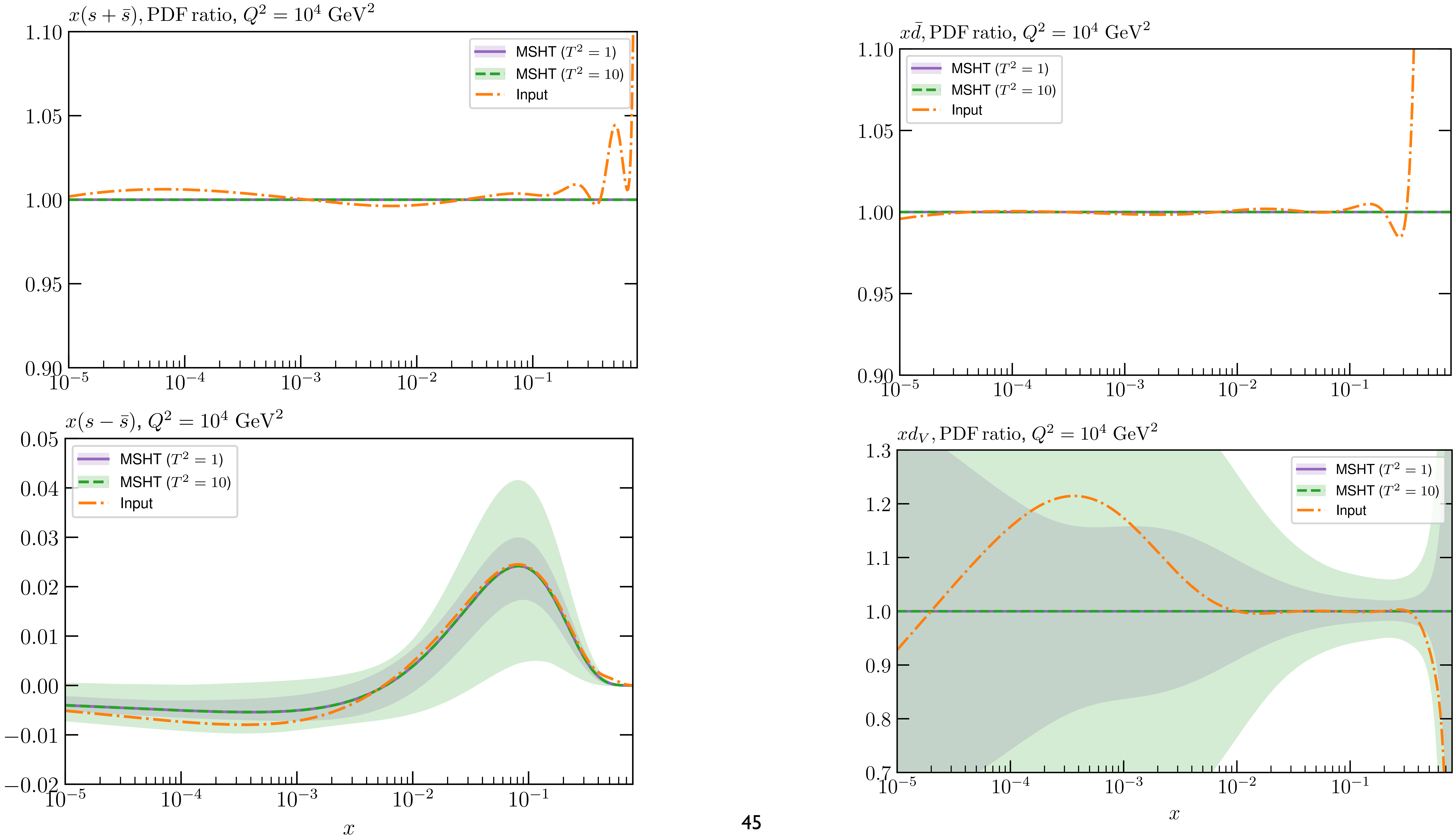
Summary/Outlook

- ★ Parton Distribution Functions a key input in the LHC precision physics programme.
- ★ Precise and accurate PDF determination crucial. Global PDF fits currently the best way to achieve this.
- ★ Have presented here the first global closure test of the MSHT fitting approach: parameterisation inflexibility not observed to be major contribution to error budget.
- ★ But I have tried to motivate why an enlarged error definition is nonetheless needed in the complex environment of a global PDF fit.
- ★ Approximate N3LO PDFs very well advanced - a lot is known and these improve accuracy of results along with missing higher order uncertainties.
- ★ First strong coupling determination at aN3LO - perturbative convergence has been reached.

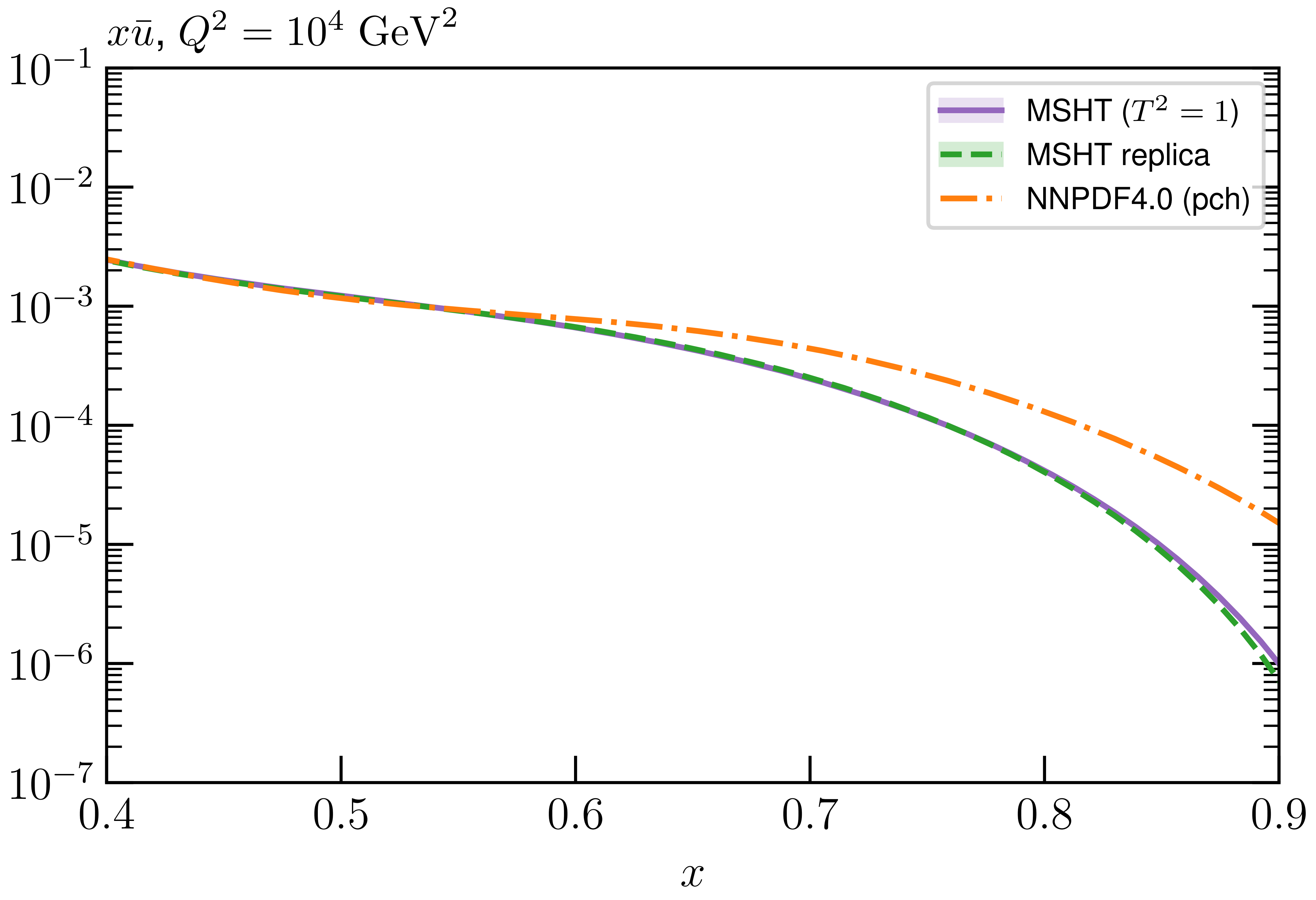
Thank you for listening!

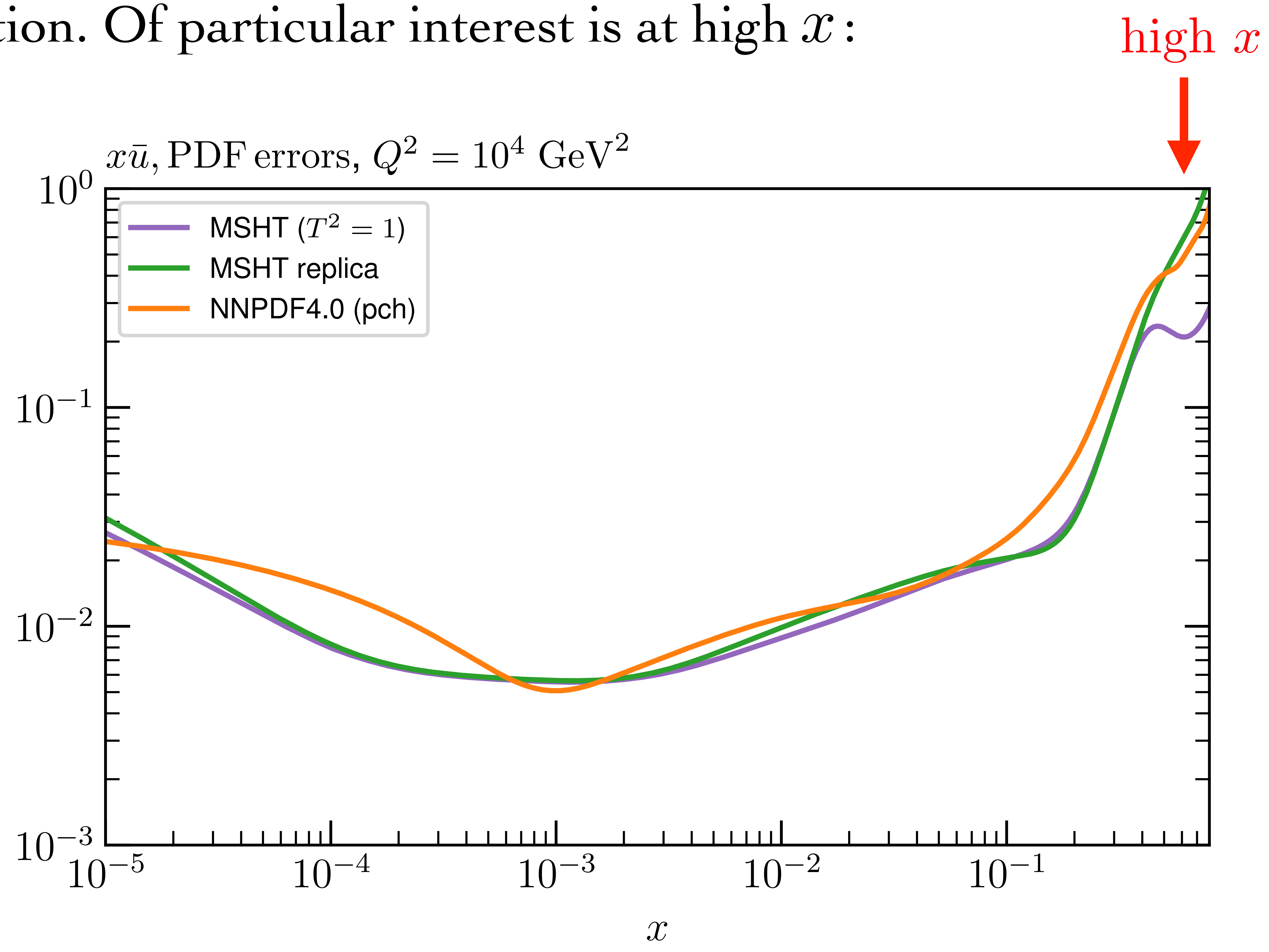
Backup

Global Closure PDFs



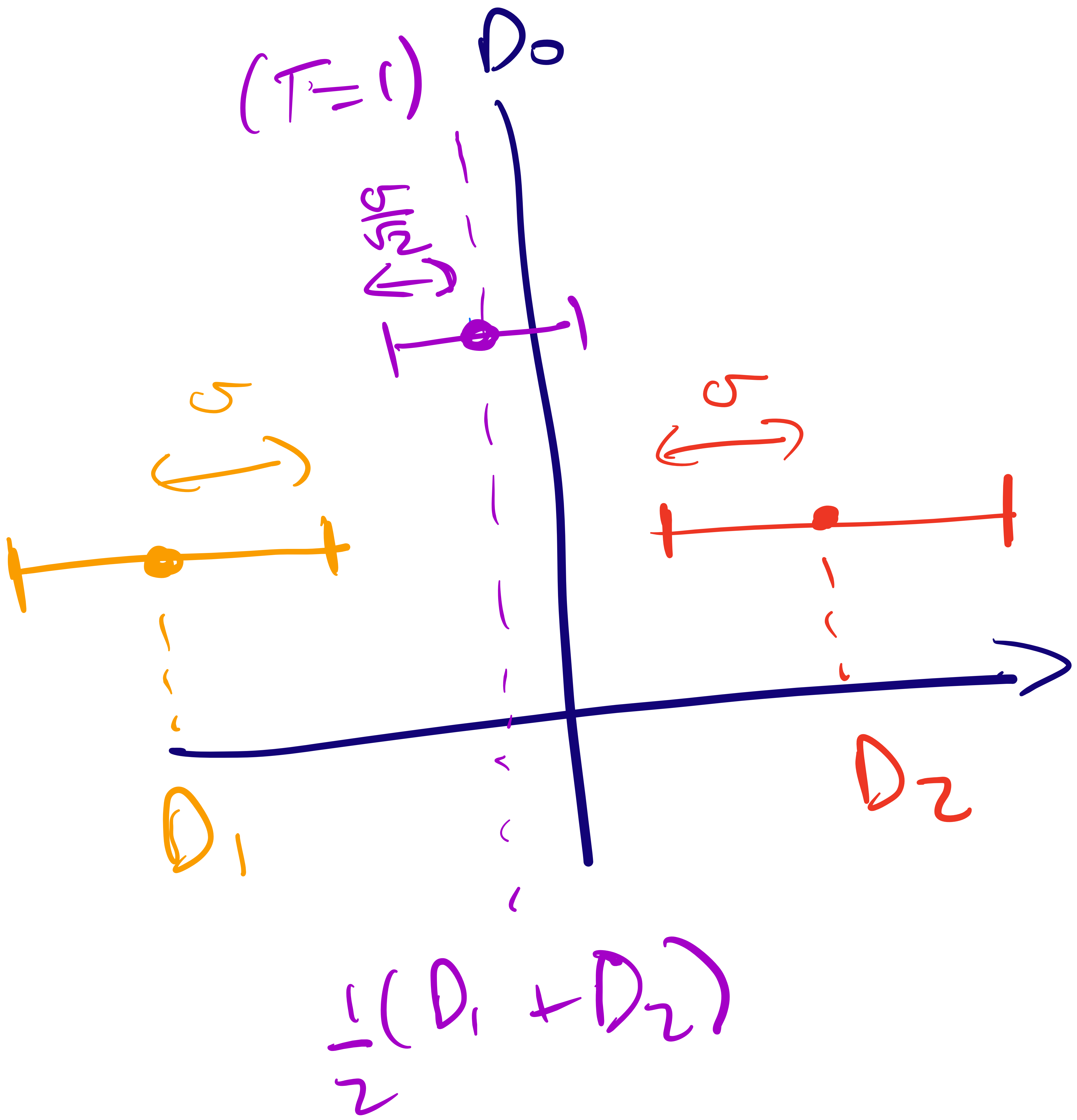
- However exact agreement between Hessian and MC replica approach only expected in exact Gaussian approximation. Away from this can see some deviation. Of particular interest is at high x:





- MC replica uncertainty much larger here - helps improve matching with input set.
- Much more in line with NNPDF uncertainty. Perhaps MC replica propagation (rather than NN) playing (most?) significant role here?

Tolerance: Toy Model



$$t_0 = \frac{1}{2}(D_1 + D_2)$$

$$t = t_0 + \Delta t$$

$$\Delta t = \pm\frac{\sigma}{\sqrt{2}}$$

Independent of particular values of $D_{1,2}$

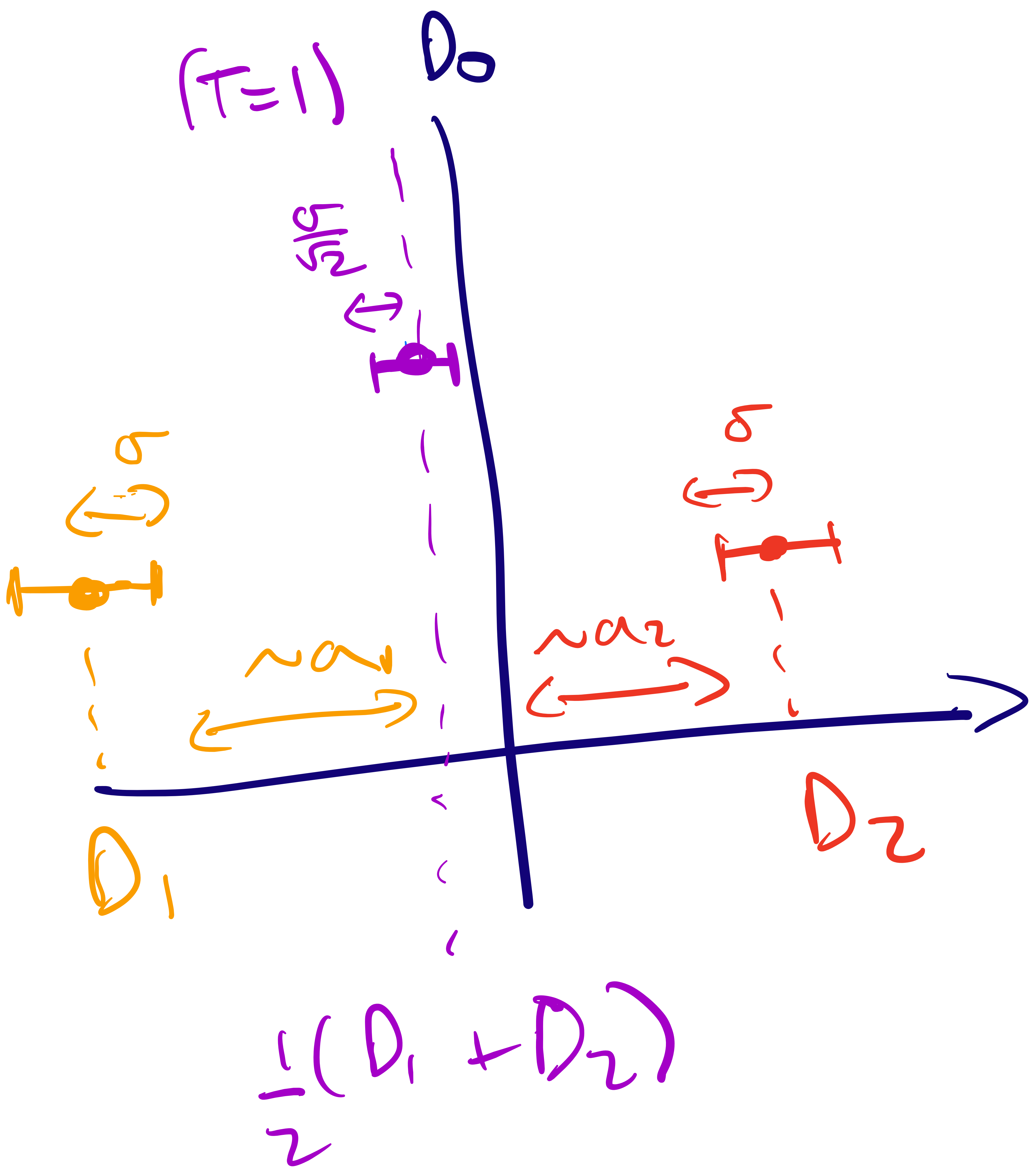
For **consistent** case

$$D_{1,2} = D_0 + \sigma\delta_{1,2} \ ,$$

this is **correct**.

$\delta_{1,2}$: univariate Gaussian

Tolerance: Toy Model



$$t_0 = \frac{1}{2}(D_1 + D_2)$$

$$t = t_0 + \Delta t$$

$$\Delta t = \pm\frac{\sigma}{\sqrt{2}}$$

Independent of particular values of $D_{1,2}$

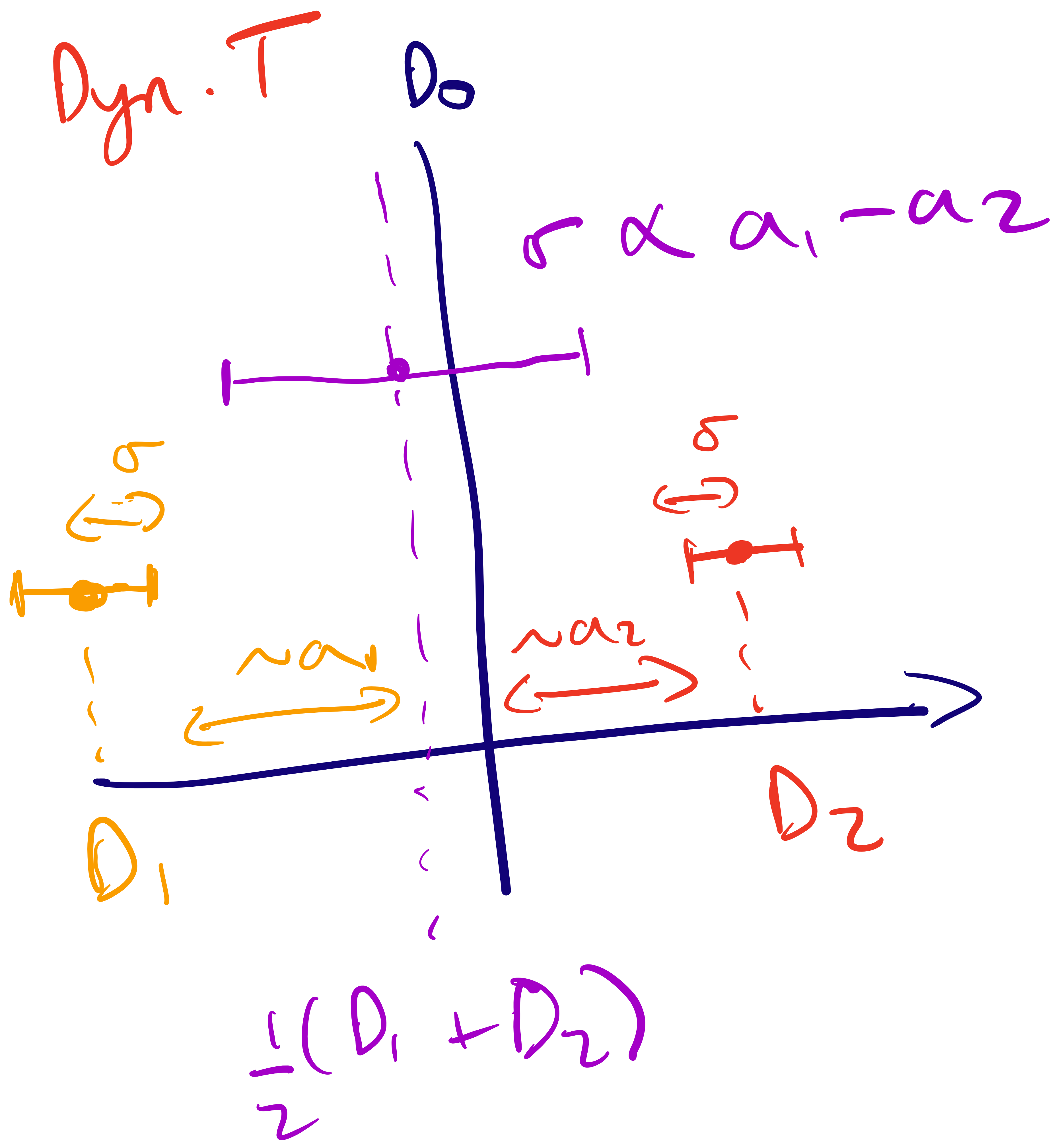
For **inconsistent** case

$$D_{1,2} = a_{1,2} + (D_0 + \sigma\delta_{1,2})\ ,$$

this is **incorrect**.

$\delta_{1,2}$: univariate Gaussian

Tolerance: Toy Model



$$t_0 = \frac{1}{2}(D_1 + D_2)$$

$$t = t_0 + \Delta t$$

Applying **dynamic tolerance instead** find

$$\Delta t \propto a_1 - a_2$$

i.e. larger spread to account for tension.

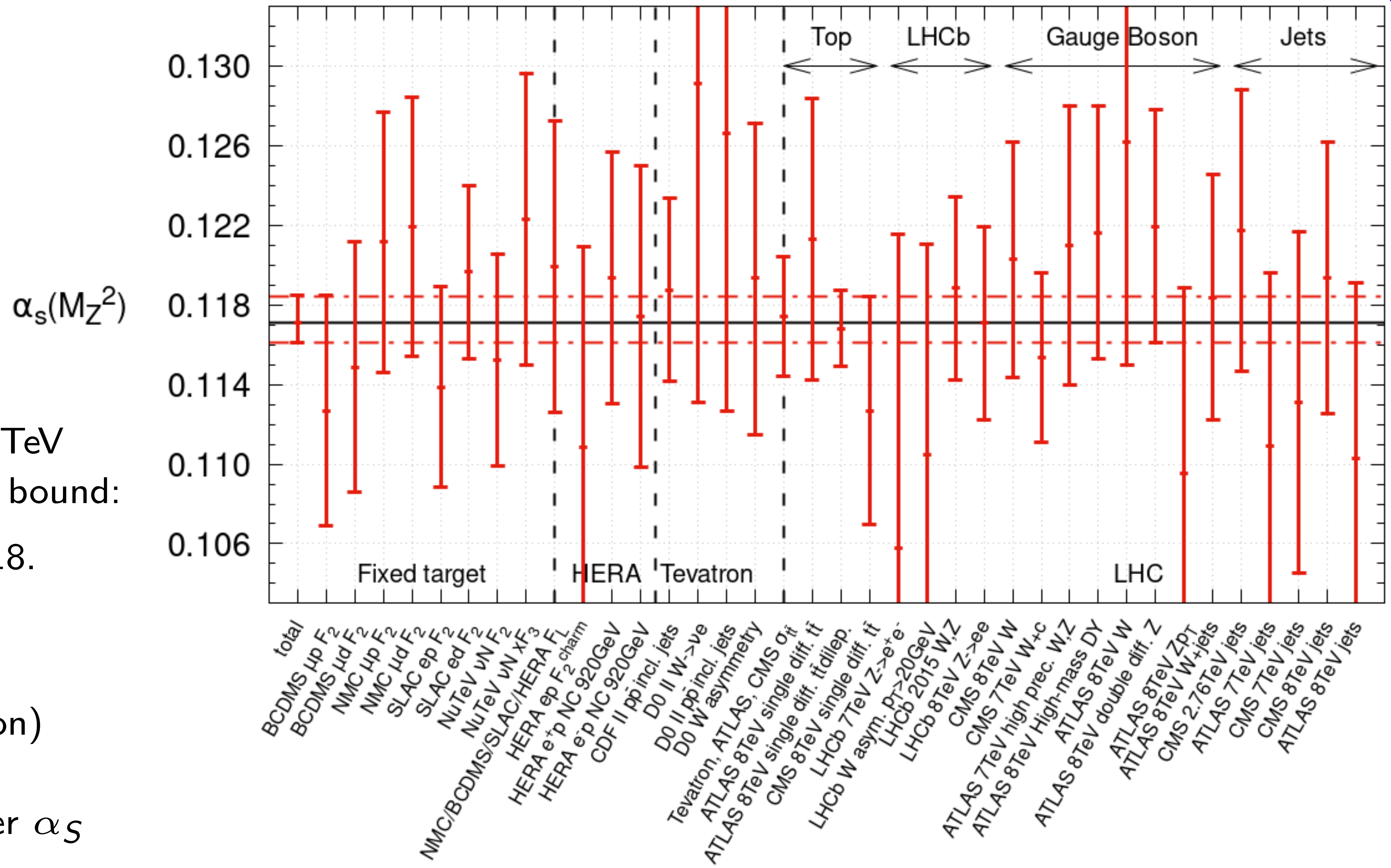
MSHT20 α_S bounds - NNLO

Consistent with α_S bounds seen in previous studies, and between orders (NNLO and aN3LO).

BCDMSp data strongest constraint upwards: $\Delta\alpha_S(M_Z^2) = +0.0014$.

SLACp and ATLAS 8TeV Zp_T both give upper bound: $\Delta\alpha_S(M_Z^2) = +0.0018$.

CMS/ATLAS (dilepton) $t\bar{t}$ single diff. would give lower/same upper α_S bound, but not used.



ATLAS 8 TeV Z data gives lower bound: $\Delta\alpha_S(M_Z^2) = -0.0010$.

NMC deuteron, ATLAS 8 TeV High Mass DY give lower bounds of $\Delta\alpha_S(M_Z^2)$ -0.0017, -0.0018.

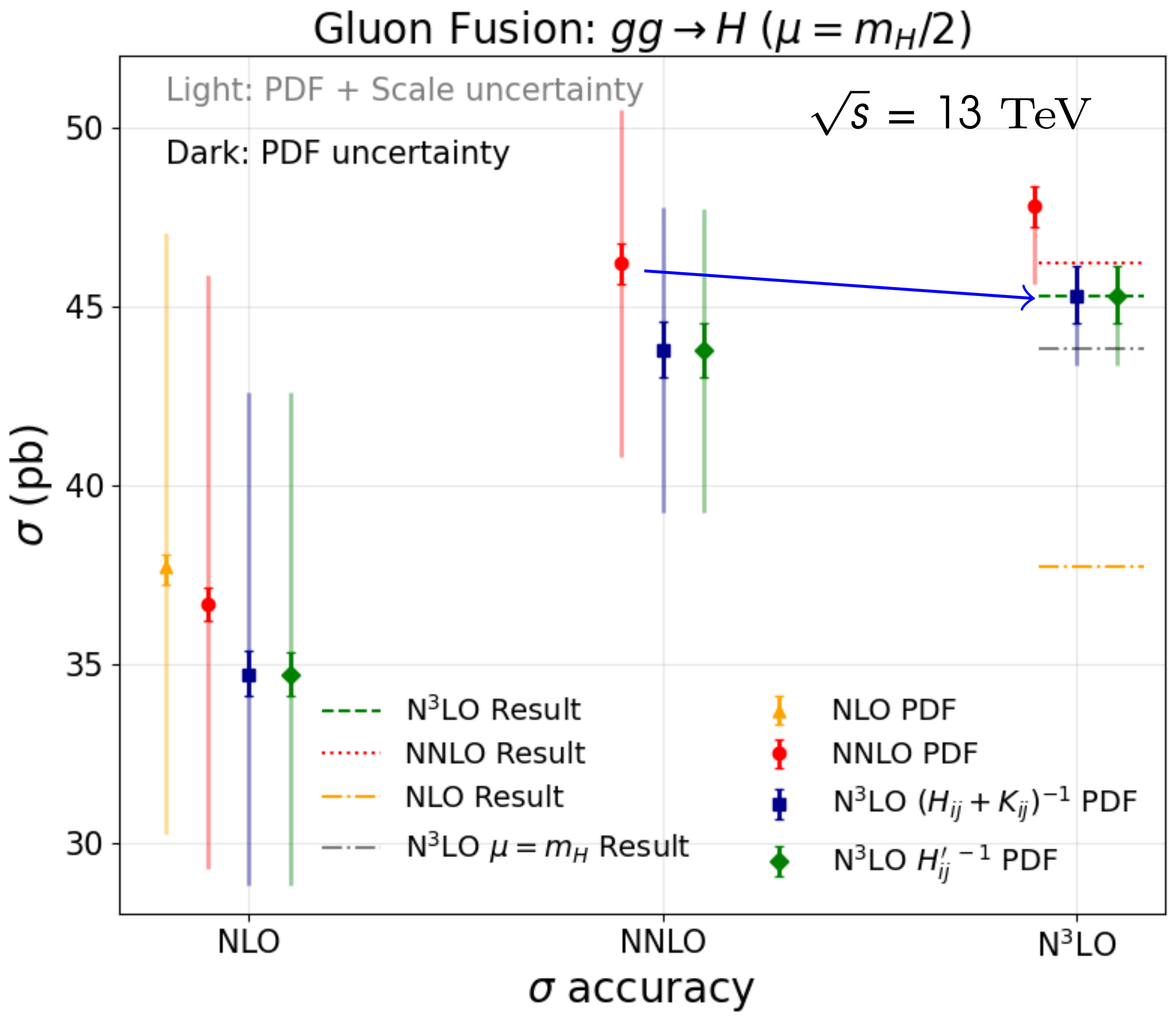
- Therefore upper/lower bounds are $+0.0014$/-0.0010 at NNLO.

$$\alpha_{S,\mathrm{NNLO}}(M_Z^2) = 0.1171 \pm 0.0014$$

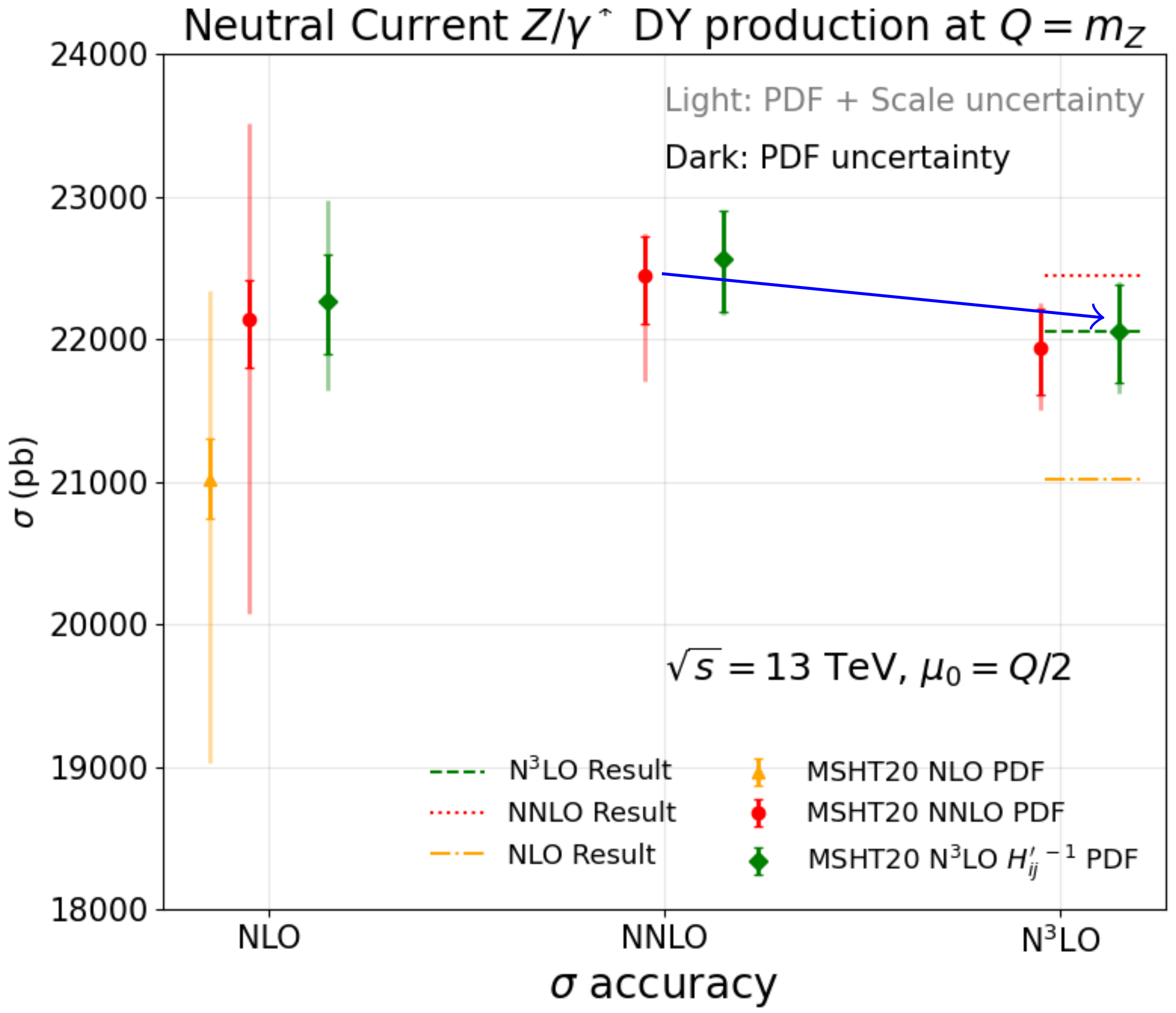
Consistent with World Average of 0.1180 ± 0.0009.

With thanks to T. Cridge

- Change in gluon corresponds to reduction in e.g. ggH at N3LO - improves stability.



- Some increase in NC DY - again mild improvement in stability.



Stay tuned!

- Has lead to detailed benchmarking of evolution. MSHT: updating to latest result has mild impact.

- NNPDF have also produced aN3LO fit. Gluon qualitatively similar, but change smaller: