Missing Higher Order Uncertainties and PDFs up to N3LO

Lucian Harland-Lang, University College London

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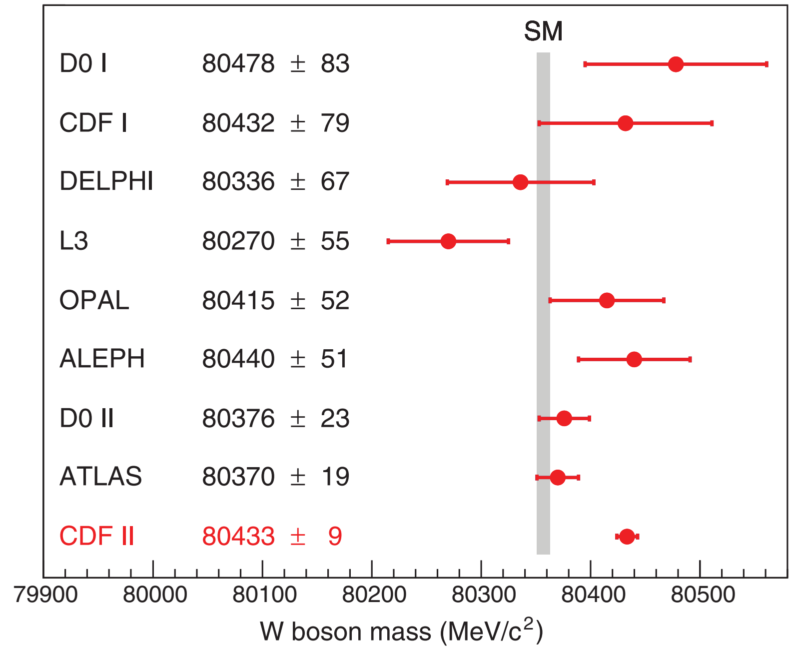
In collaboration with Tom Cridge, Jamie McGowan and Robert Thorne

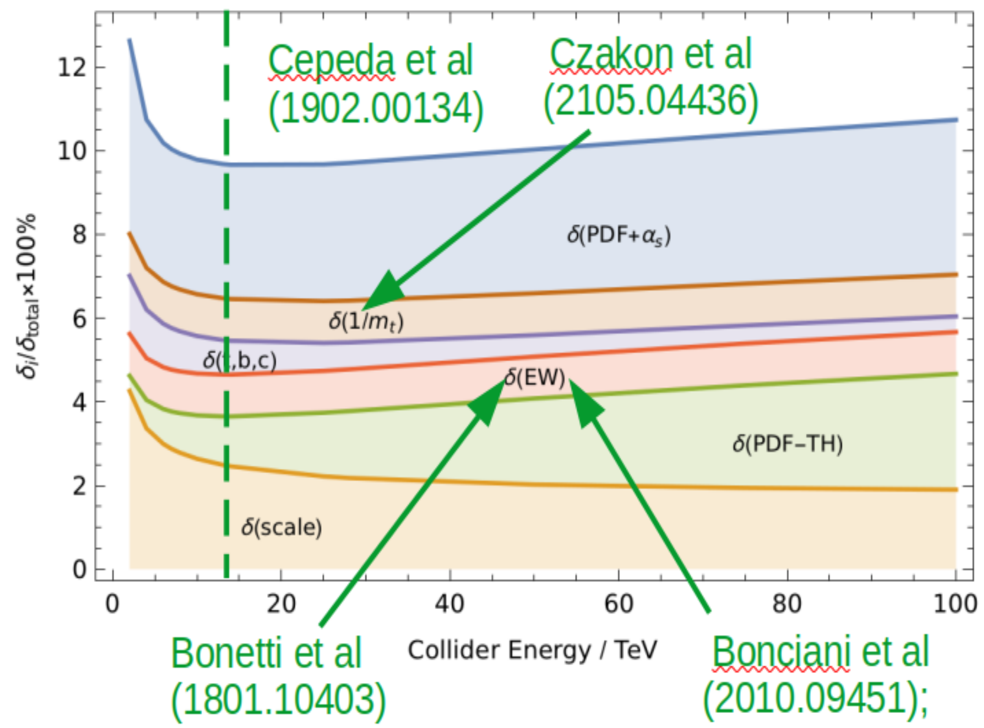
Motivation

- Accurate account of PDF uncertainties key bottleneck in LHC physics analyses:

SM Precision



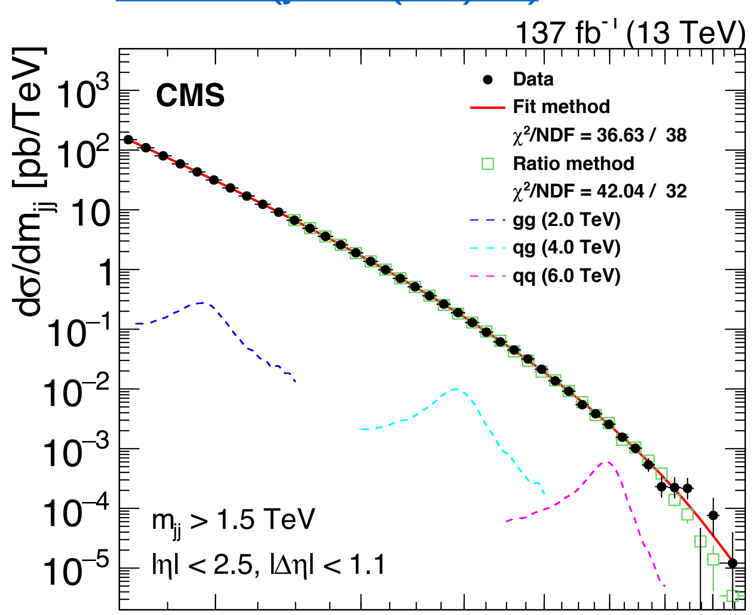
Higgs



LHC Higgs XSWG 2019

BSM searches

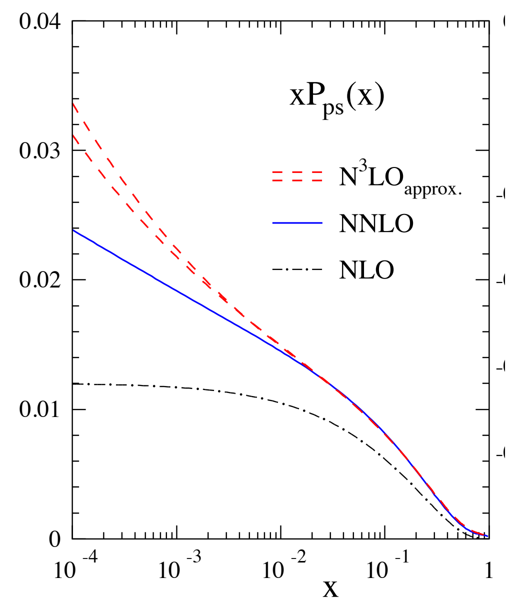
1911.03947 (JHEP05 (2020) 033)



$\longrightarrow$ Must include all sources of PDF uncertainty. Key element due to **missing higher orders** (MHOs) in the PDF fit theory.

- State-of-the art for PDF fits is **NNLO** in QCD: all relevant PDF processes/theory known at this order. But much progress made at **N3LO**:

★ PDF evolution



$$
\begin{aligned}
\gamma_{ps}^{(3)}(N=2) &= -691.5937093\,n_f + 84.77398149\,n_f^2 + 4.466956849\,n_f^3\,,\\
\gamma_{ps}^{(3)}(N=4) &= -109.3302335\,n_f + 8.776885259\,n_f^2 + 0.306077137\,n_f^3\,,\\
\gamma_{ps}^{(3)}(N=6) &= -46.03061374\,n_f + 4.744075766\,n_f^2 + 0.042548957\,n_f^3\,,\\
\gamma_{ps}^{(3)}(N=8) &= -24.01455020\,n_f + 3.235193483\,n_f^2 - 0.007889256\,n_f^3\,,\\
\gamma_{ps}^{(3)}(N=10) &= -13.73039387\,n_f + 2.375018759\,n_f^2 - 0.021029241\,n_f^3\,,\\
\gamma_{ps}^{(3)}(N=12) &= -8.152592251\,n_f + 1.819958178\,n_f^2 - 0.024330231\,n_f^3\,,\\
\gamma_{ps}^{(3)}(N=14) &= -4.840447180\,n_f + 1.438327380\,n_f^2 - 0.024479943\,n_f^3\,,\\
\gamma_{ps}^{(3)}(N=16) &= -2.751136330\,n_f + 1.164299642\,n_f^2 - 0.023546009\,n_f^3\,,\\
\gamma_{ps}^{(3)}(N=18) &= -1.375969240\,n_f + 0.960873318\,n_f^2 - 0.022264393\,n_f^3\,,\\
\gamma_{ps}^{(3)}(N=20) &= -0.442681568\,n_f + 0.805745333\,n_f^2 - 0.020918264\,n_f^3\,.
\end{aligned}
$$

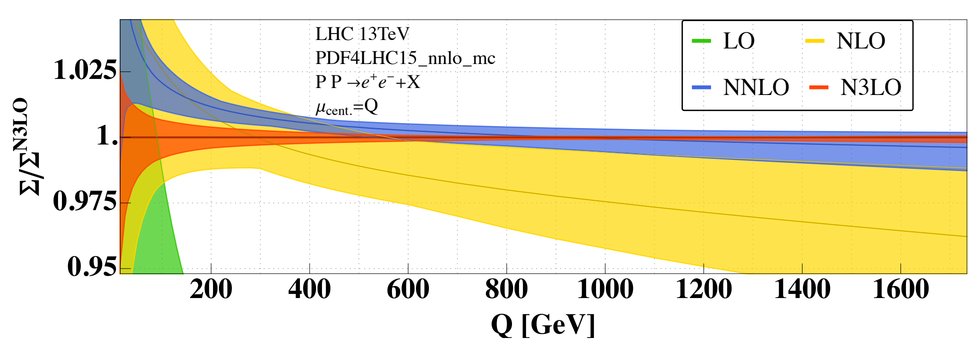
G. Falcioni et al., *Phys.Lett.B* 842 (2023) 137944

See F. Herzog's talk

- Can we make use of this information already in PDF fits?

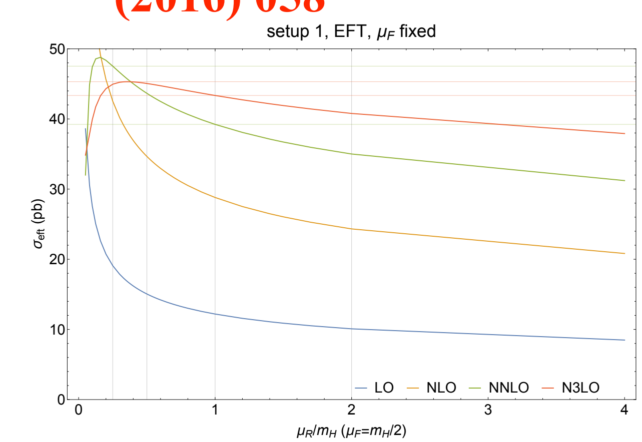
★ Cross sections:

C. Duhr and B. Mistleberger, *JHEP* 03 (2022) 116



Drell Yan

C. Anastasiou et al., *JHEP* 05 (2016) 058



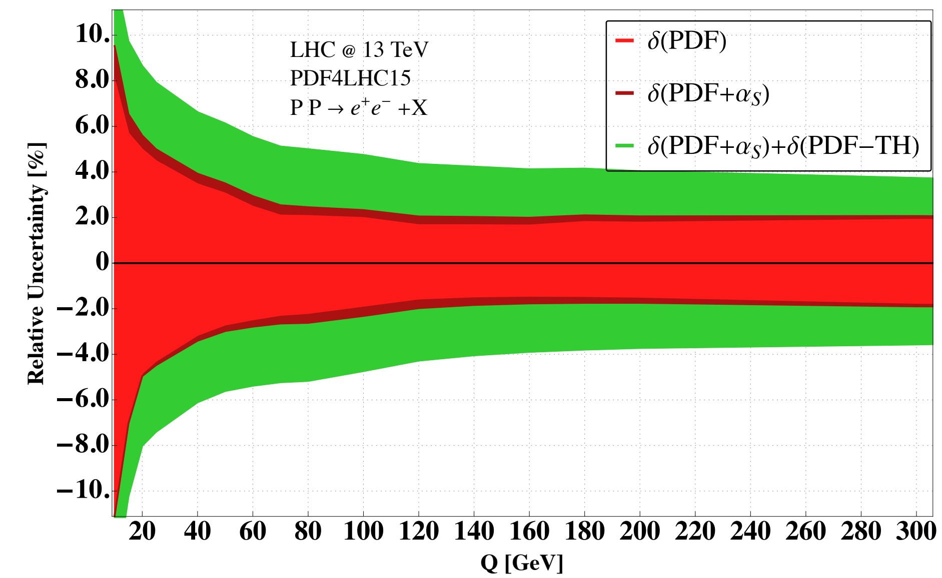
Higgs

- **N3LO** cross section predictions $\longleftrightarrow$ **N3LO** PDFs?

✦ N3LO cross section predictions $\leftrightarrow$ N3LO PDFs?

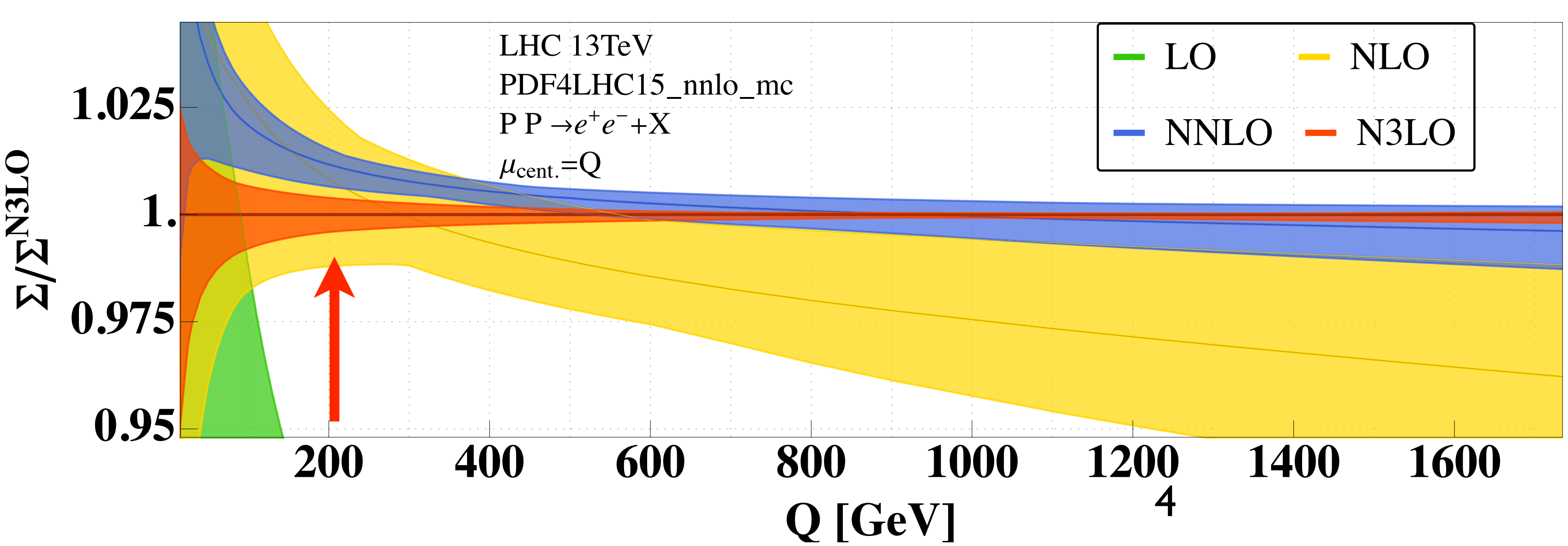
- For N3LO calculations of DY, Higgs (...) cross sections to be truly N3LO accurate requires N3LO PDFs.
- Not available, estimate uncertainty from using NNLO PDFs:

$$\delta(\text{PDF-TH}) = \frac{1}{2}\left|\frac{\Sigma^{\text{NNLO, NNLO-PDFs}}(Q^2) - \Sigma^{\text{NNLO, NLO-PDFs}}(Q^2)}{\Sigma^{\text{NNLO, NNLO-PDFs}}(Q^2)}\right| .$$



Clearly, rather approximate!

- Moreover, for DY the NNLO and N3LO (+ NNLO PDFs) results do not always overlap in uncertainty bands. Could this change with N3LO PDFs?



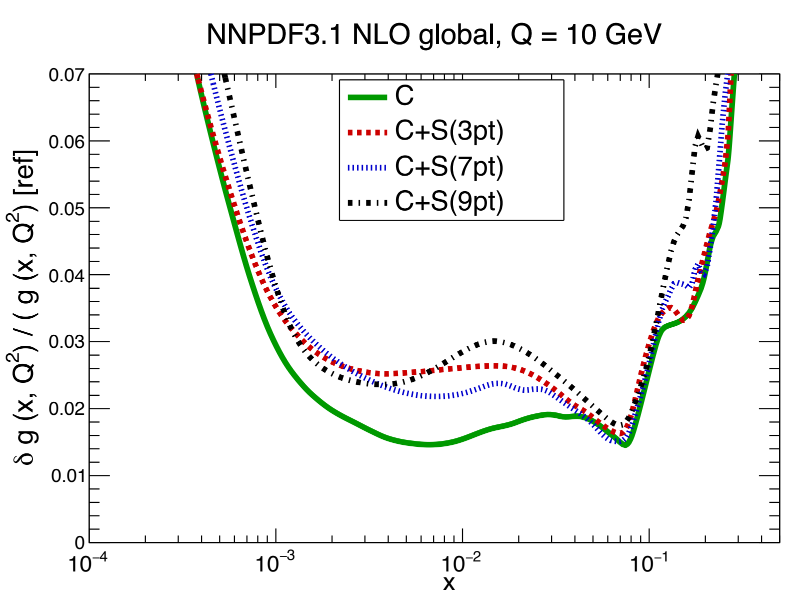
$\longrightarrow$ Motivation to work towards N3LO PDFs

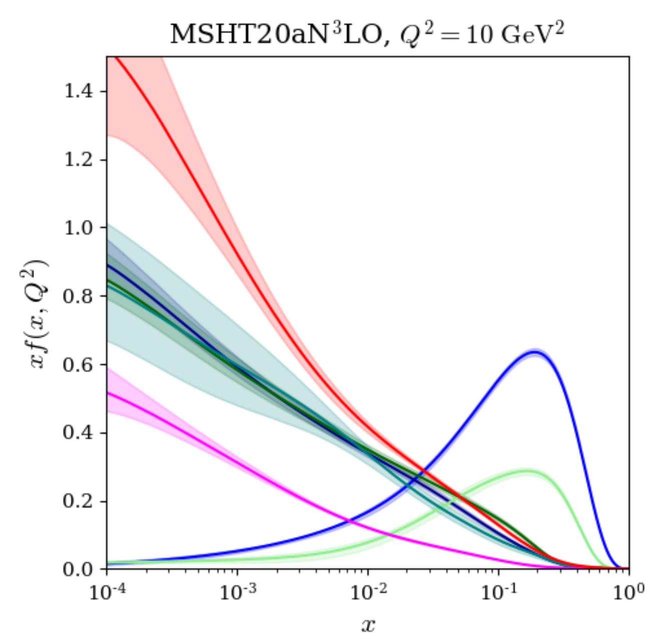
- To summarise: in high (1%) precision LHC era, and precision/accuracy of PDFs need to match this! Two key, and related, elements to consider:

Uncertainties due to missing higher orders in theory

Making use of available N3LO theory in PDF fit

- For **accuracy** and **precision**: combine both of these in global PDF fit.





Approximate N3LO and PDFs

How Close to N3LO?

- How close are we to a N3LO PDF fit?

Splitting functions:

Low and high x limits. Significant Mellin moment information. Further progress underway!

See F. Herzog's talk

DIS:

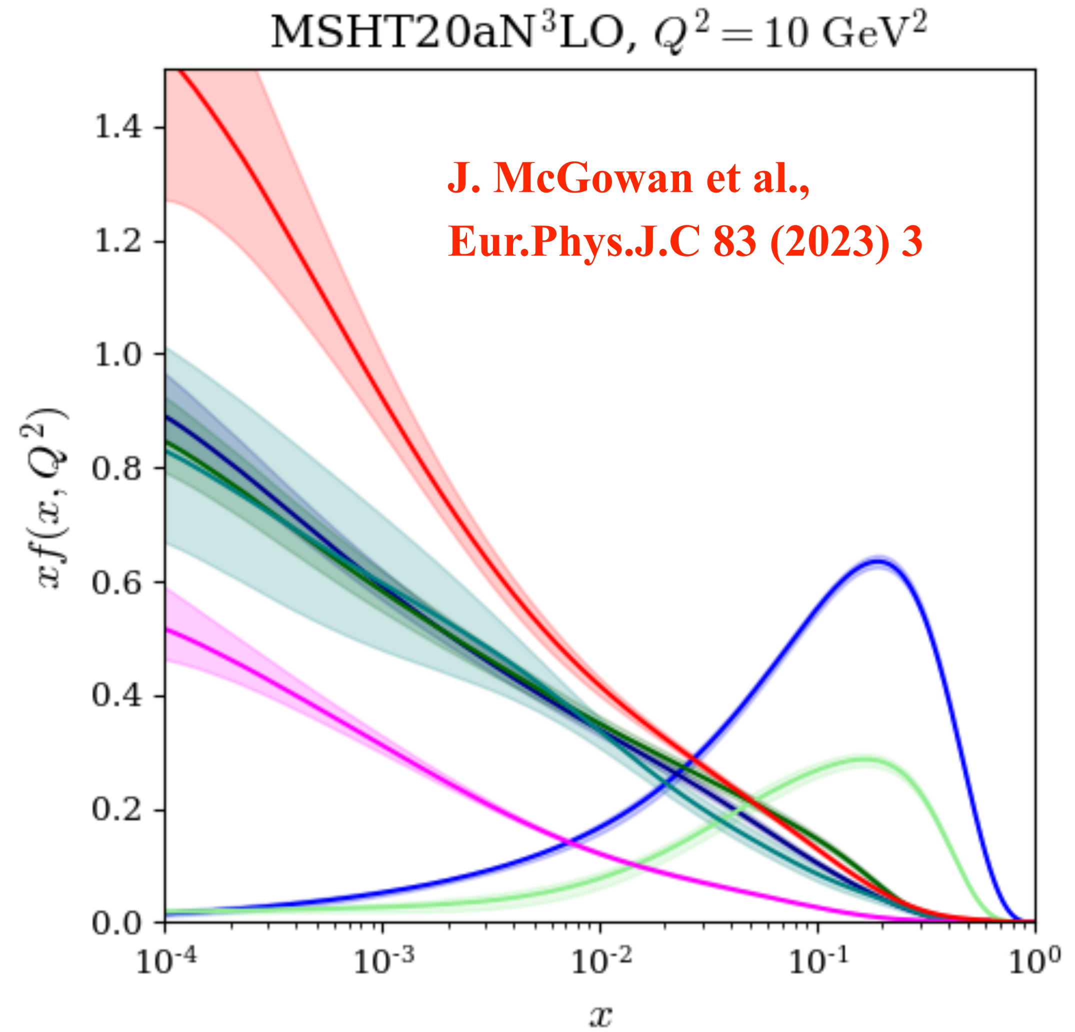
Massless coefficient functions known. Partial information on massive case and much information on transition matrix elements.

Hadronic cross sections:

Handful of (important) results. Little useable for a PDF fit: e.g. Drell-Yan in theory but not currently in practice.

- How to deal with in an approximate N3LO fit?

- First public approximate N3LO PDF set: **MSHT20aN3LO**.
    - Will focus on this as case study for now, but work is ongoing by other group(s)!



- Basic idea – perform a global PDF fit where:

    ★ When N3LO theory is **known** it is used.

    ★ When it is **unknown**, suitable account of residual uncertainty is included, but with any known information used.

- Maximal use of available information. As more N3LO results appear, can be included in future updates $\longrightarrow$ no need to wait for entire N3LO!

In More Detail...

- 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

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

- Then we model N3LO theory via: $T' = T'_0 + \theta' u$

aN3LO theory (T')

central value ~ known N3LO (T'_0)

Allowed variation ~ unknown N3LO ($\theta' u$)

- With shift given by **prior** probability:

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

- Question: How do we determine **prior**?

Splitting Functions

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

  ★ Form at low x:
  $$P_{qg}^{(3)}(x) \to \frac{C_A^3}{3\pi^4}\left(\frac{82}{81}+2\zeta_3\right)\frac{1}{2}\frac{\ln^2 1/x}{x} + \rho_{qg}\frac{\ln 1/x}{x},$$

  ★ Even Mellin moments up to $N \geq 8$ $\int_0^1 \mathrm{d}x\, x^{N-1} P(x)$

  $\Rightarrow$ intermediate to high x constraints.

  ★ Other (high x and n_F) limits.

See backup for more details!

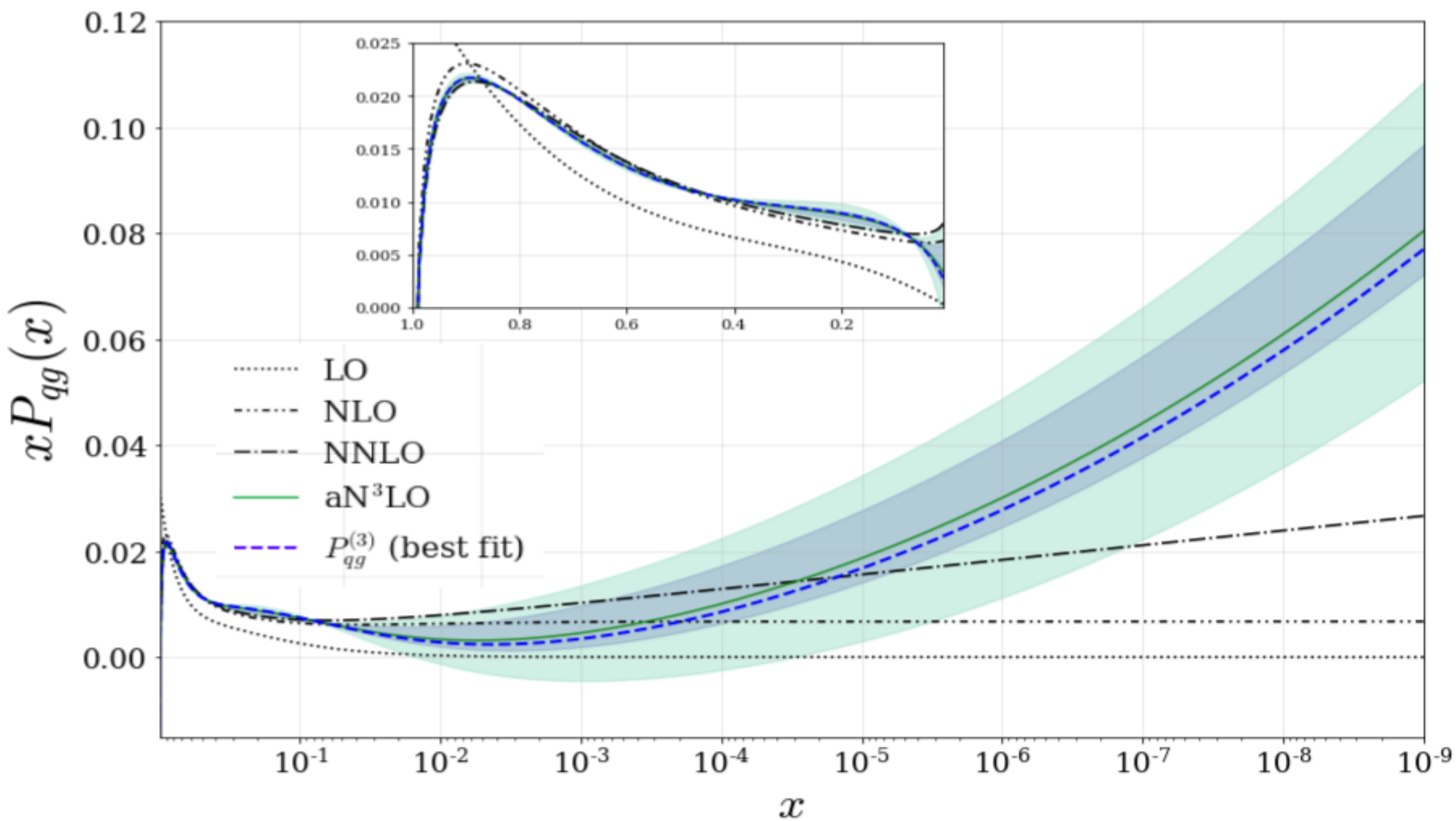
- Parameterise $P(x)$ using set of basis functions, $f_i(x)$, e.g.:

<u>Overall:</u>

$$P_{qg}^{(3)}(x) = A_1 \ln^2 x + A_2 \ln x + A_3 x^2 + A_4 \ln(1-x) + \frac{C_A^3}{3\pi^4}\left(\frac{82}{81}+2\zeta_3\right)\frac{1}{2}\frac{\ln^2(1/x)}{x} + \rho_{qg}\frac{\ln 1/x}{x}$$

- With: A_i : **Fixed by Mellin moments** ρ : **Nuisance parameter. Prior range set to cover different choices of and require reasonable behaviour.**

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

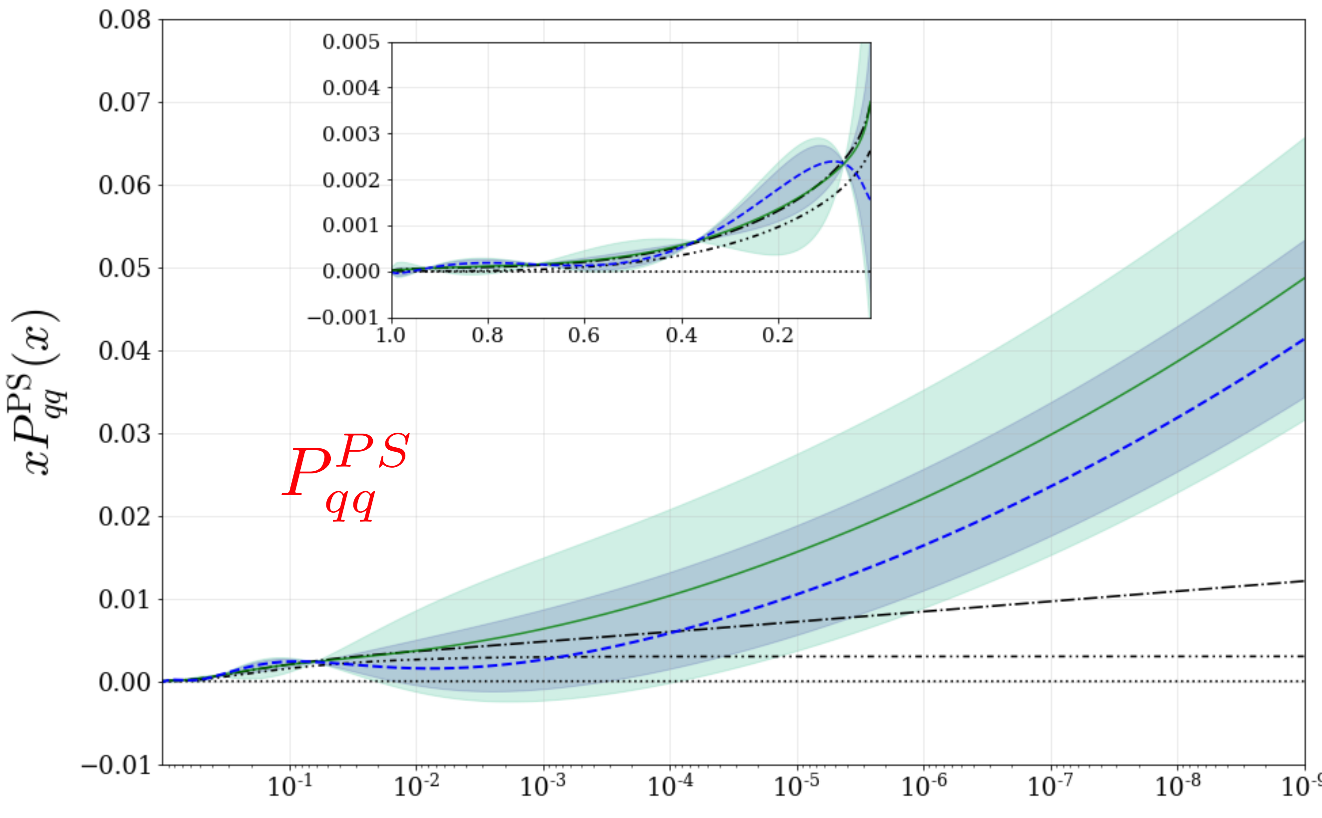


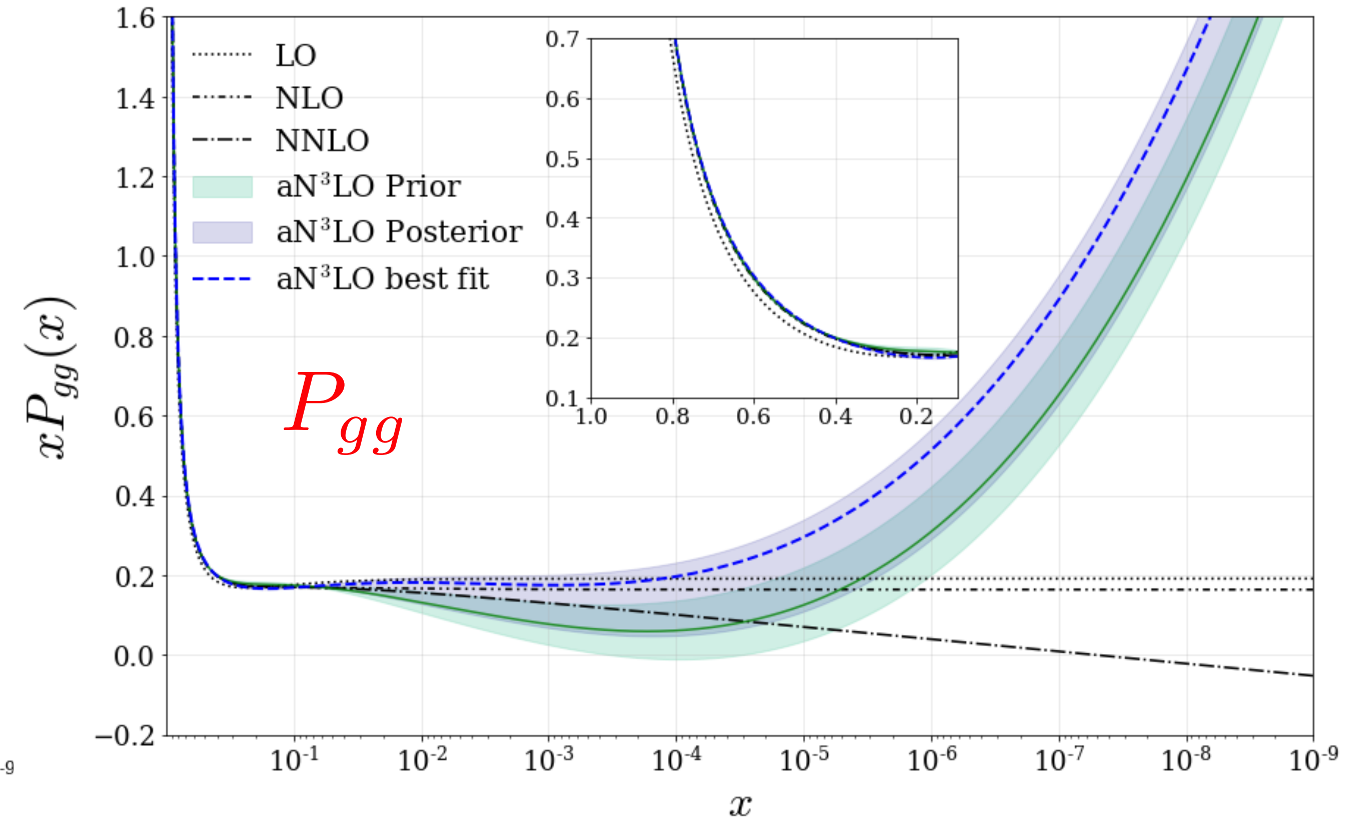
aN3LO

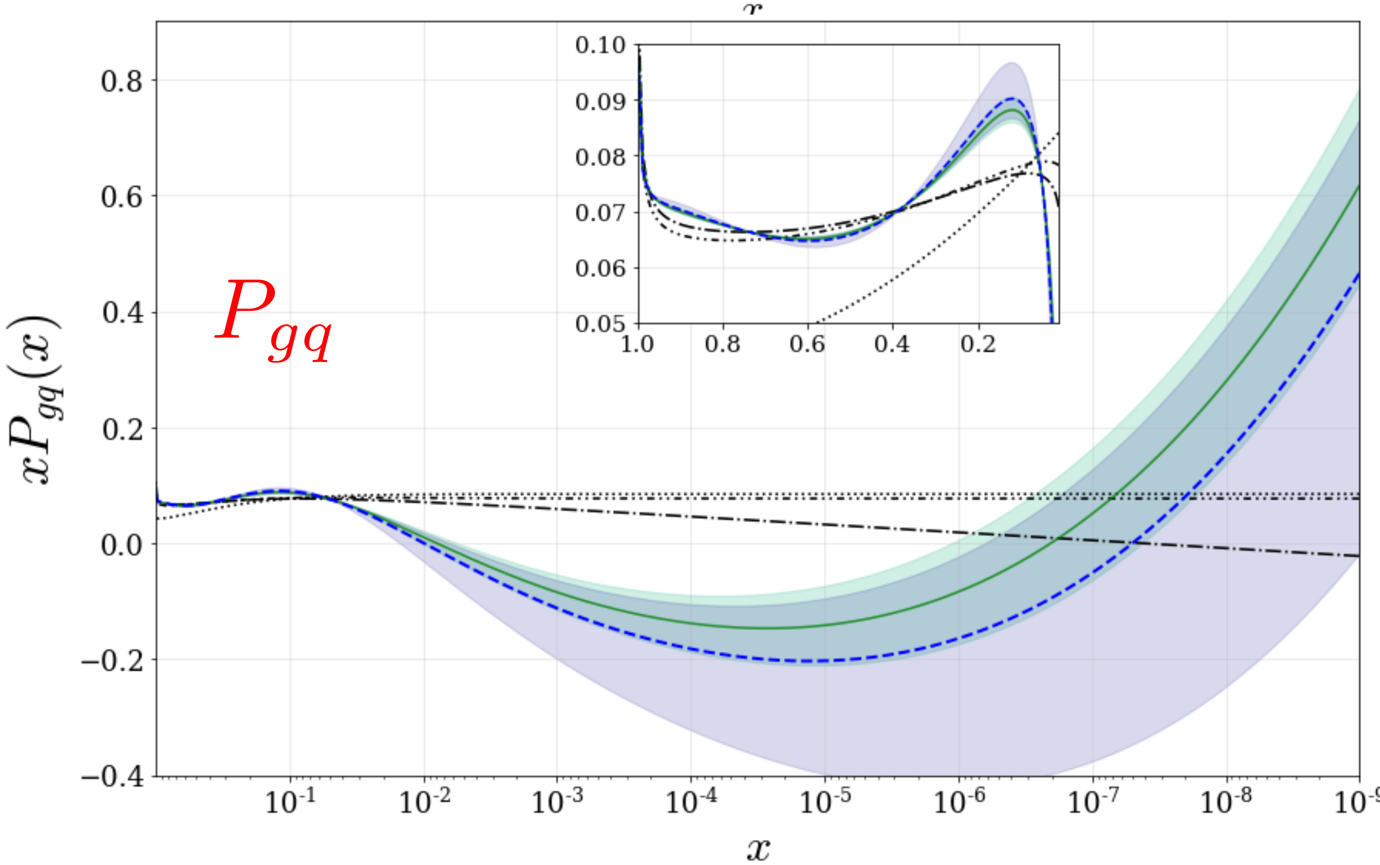
NNLO

NLO

- Similar trends for other splitting functions



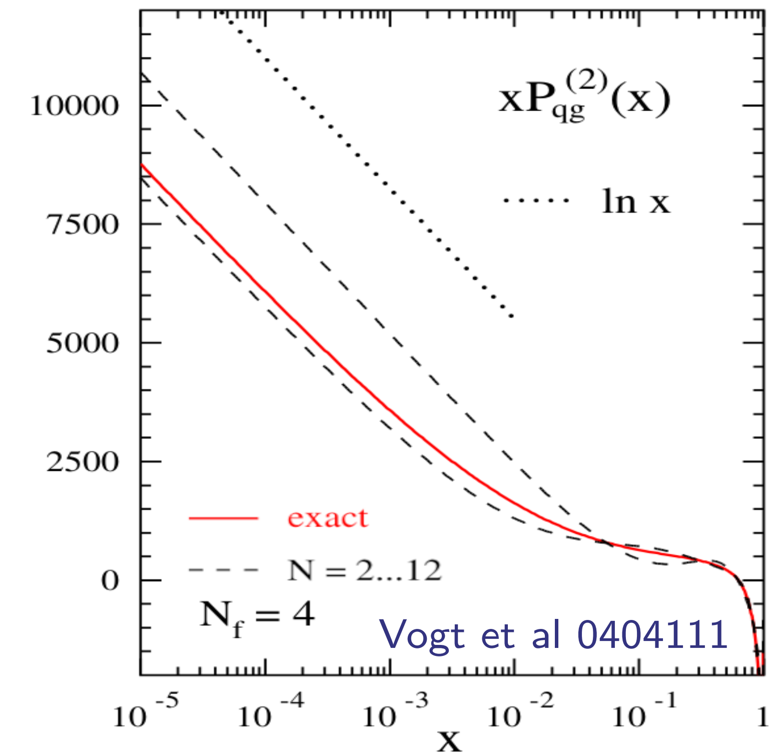


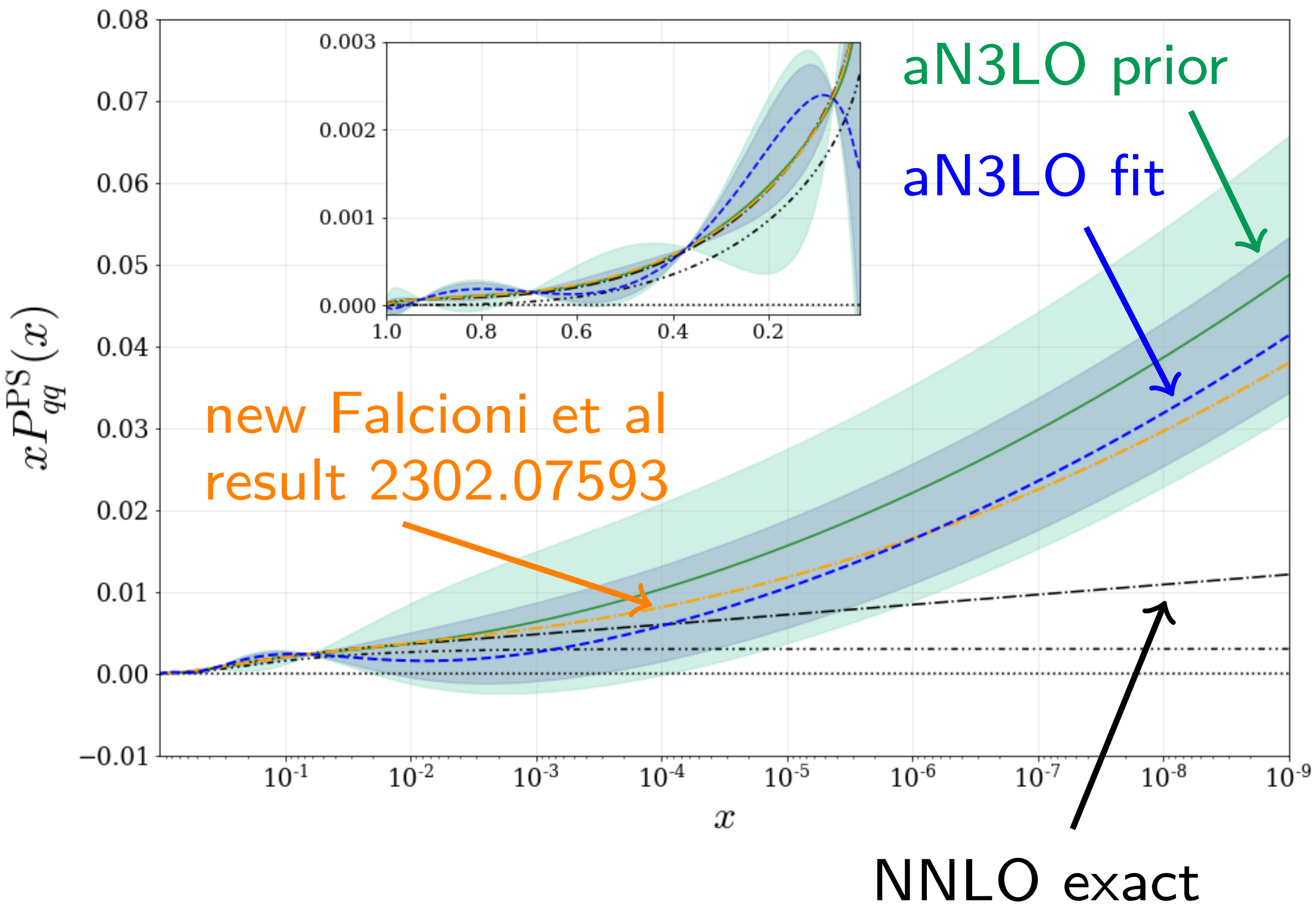


Validation

- Overall approach of using small x limits and Mellin moments already successfully used in other higher order calculations.

- Of particular note: used for NNLO splitting functions before full results were known. Matched eventual full calculation well!





- Validate/update continuously as more information comes in.

- Already done - new information on P_{qq}^{PS} available post-MSHTaN3LO. New result agrees well!

DIS Coefficient Functions

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

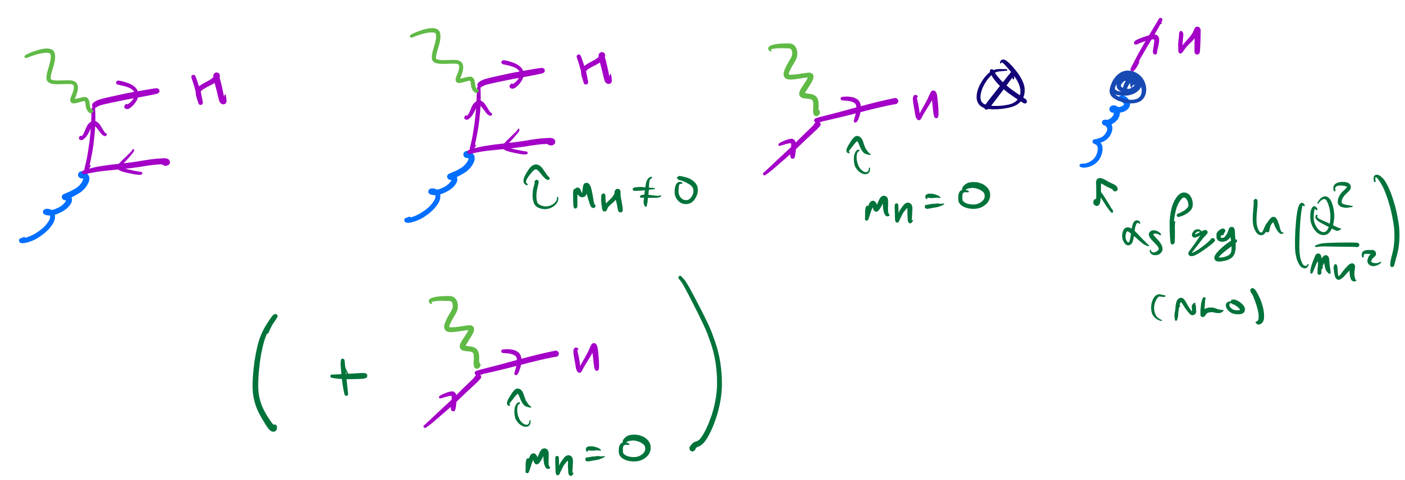
- DIS coefficient functions C_i known at N3LO for the massless quarks.
- Is this enough? Not quite - heavy quark contributions ($m_{c,b} \neq 0$) play important role. Here some information is known but not everything.
- Expressions for heavy flavour in low and high Q^2 limits:

★ High $Q^2 \gg m_h^2$: Zero Mass case known exactly.

★ Low $Q^2 \sim m_h^2$: massive (FFNS) unknown, with some information (LL small x and mass threshold).

- Impact of heavy flavour on PDF evolution controlled by **transition matrix elements** $A_{\alpha i}$.
- Some information at N3LO, but not all.
- Can follow similar procedure to approximate these (and massive coefficient functions). **(Backup)**

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



Hadronic Collisions

- For purpose of PDF fit assume nothing is known about this, and instead include a MHO uncertainty (= aN3LO K-factor) on cross sections.
- Do not use scale variations, rather base on known NLO and NNLO:

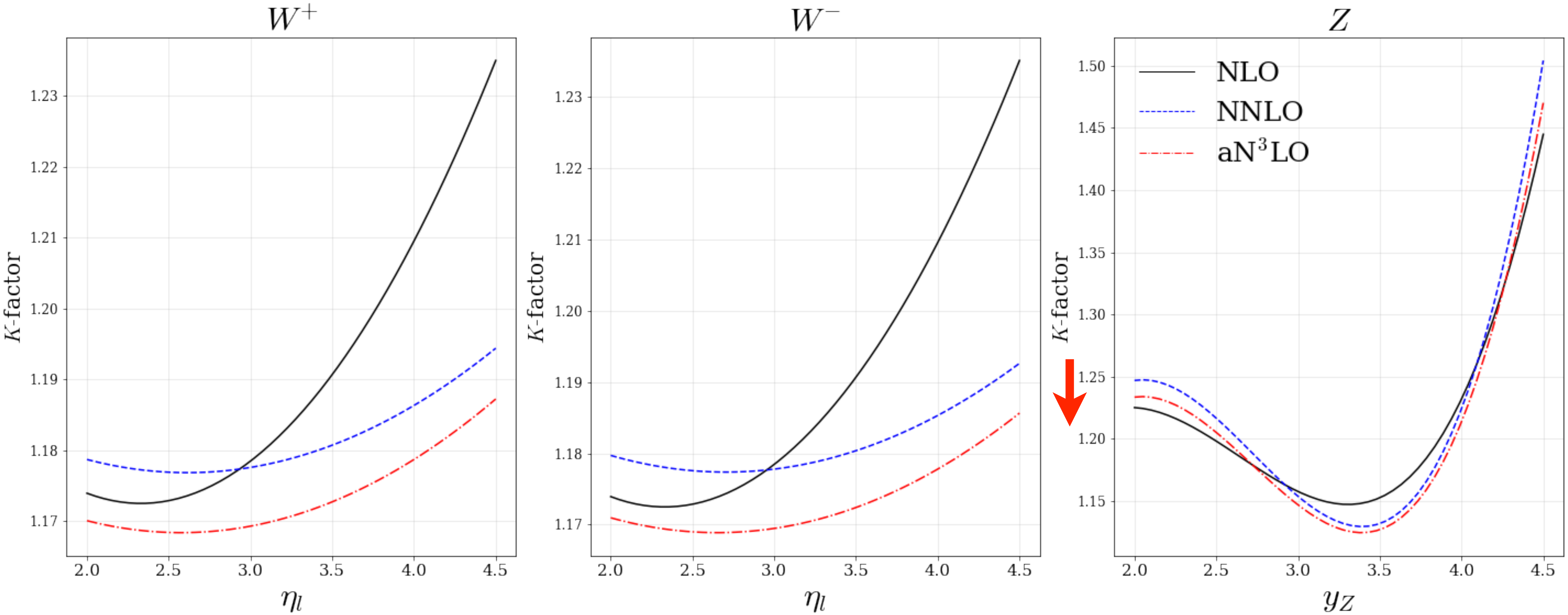
$$K^{\mathrm{N^3LO/LO}} = K^{\mathrm{NNLO/LO}} \left(1 + a_1(K^{\mathrm{NLO/LO}} - 1) + a_2(K^{\mathrm{NNLO/NLO}} - 1)\right)$$

i.e. form of aN3LO K-factor driven by lower order known K-factors.

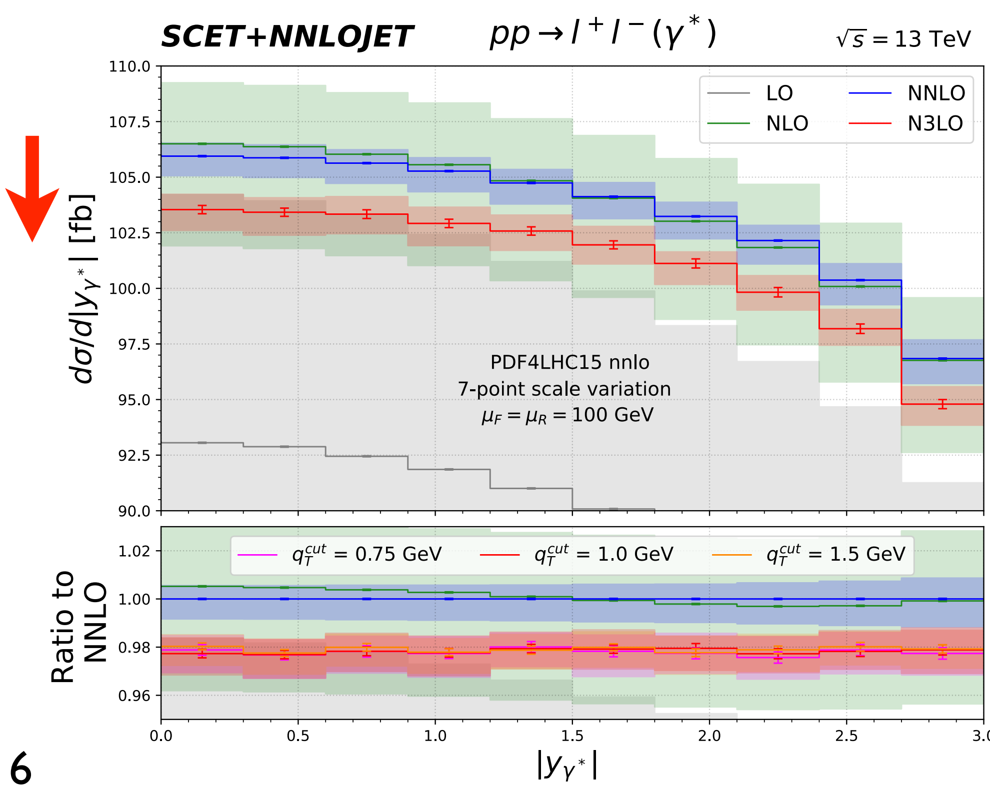
- Two nuisance parameters $a_{1,2}$ allowing freedom to determine preferred K-factor in fit. Normalization set so that prior distribution is $a_{1,2}^{\mathrm{cent}} = 0$ with 1σ variation corresponding to trend with lower orders.
- As expect K-factors to behave ~ similarly between similar processes, 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**.

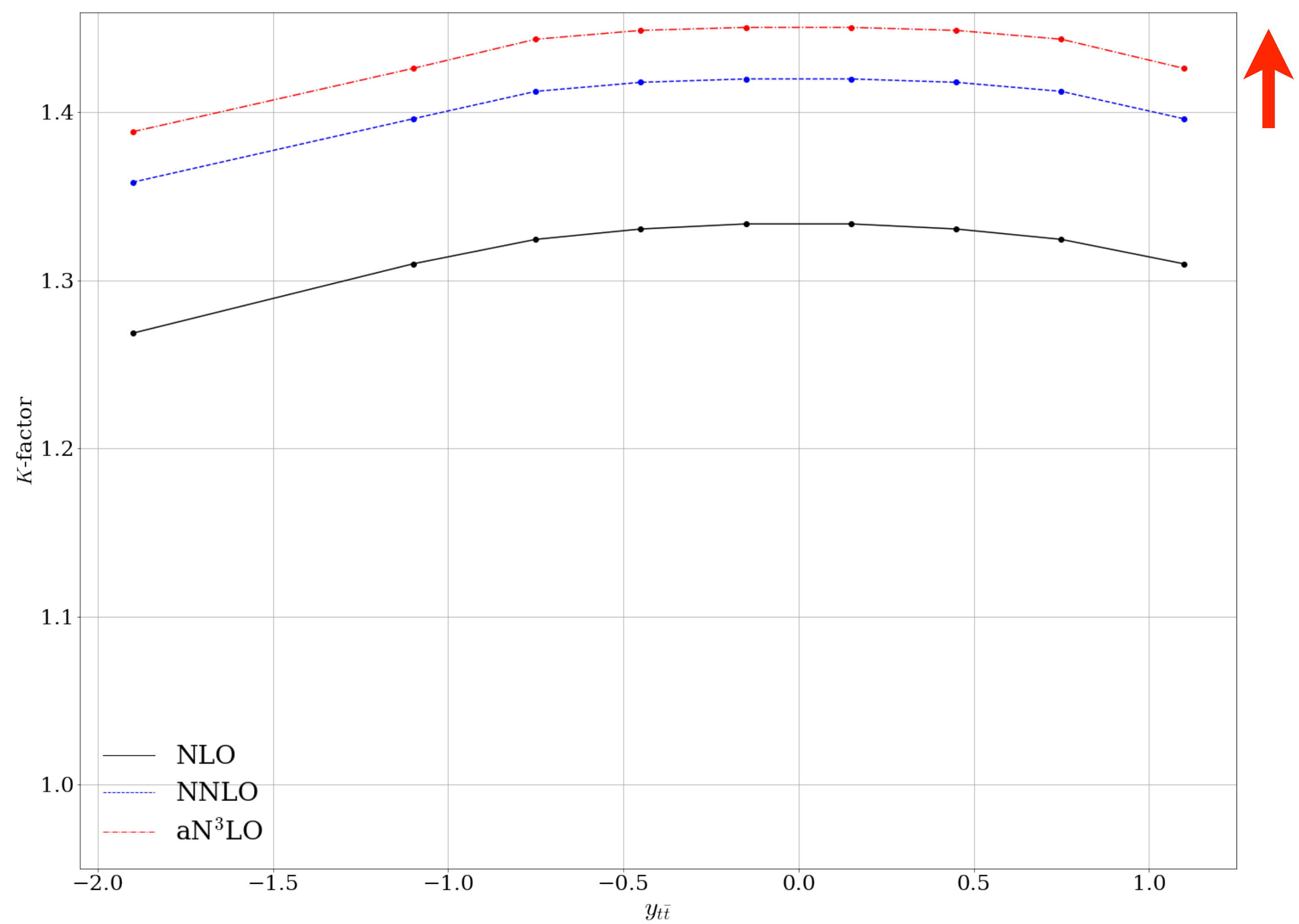


- Fit prefers a ~ 1% decrease from NNLO to aN3LO.
- This is in nice agreement with expectations from exact N3LO calculations!
- Implies improved perturbative convergence with aN3LO PDFs.

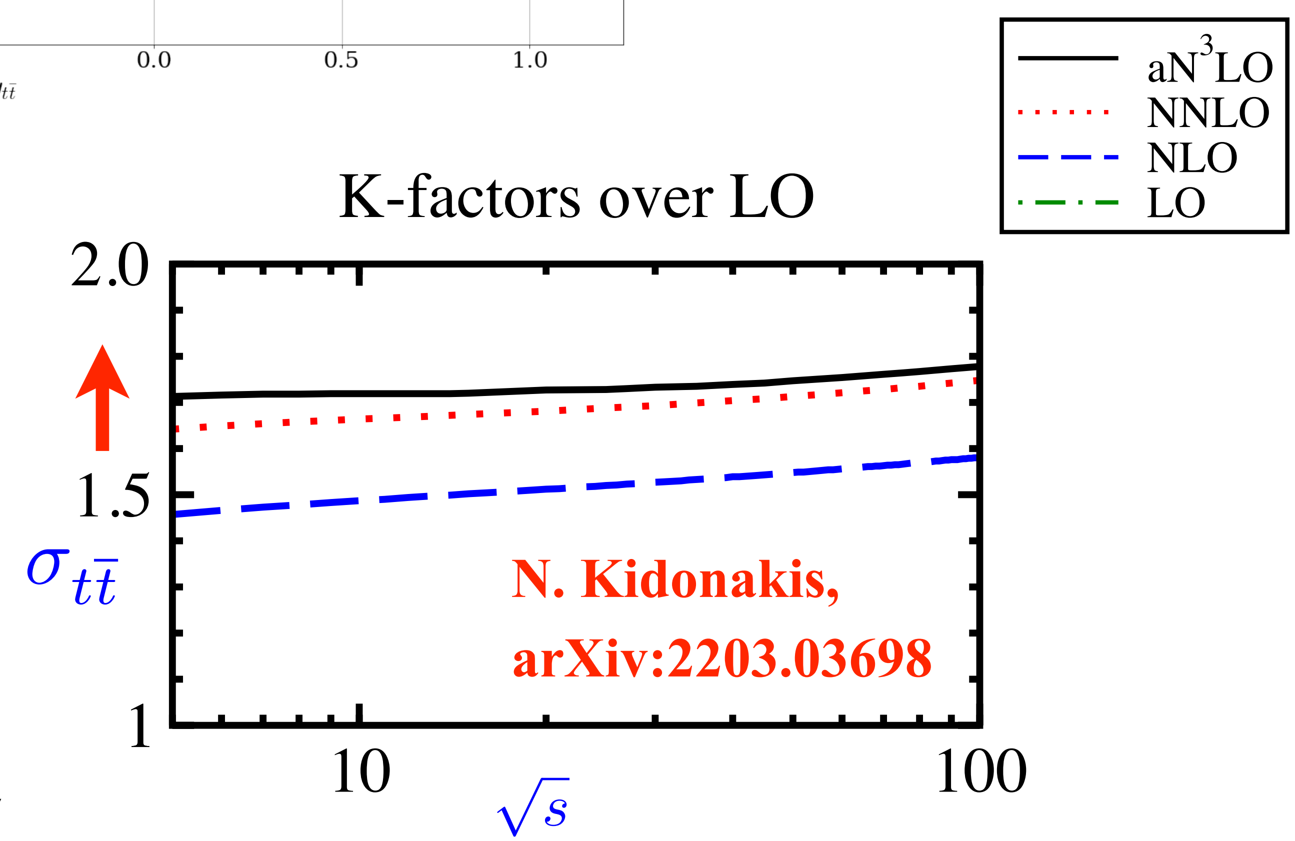


X. Chen et al., Phys.Rev.Lett. 128 (2022) 5, 052001

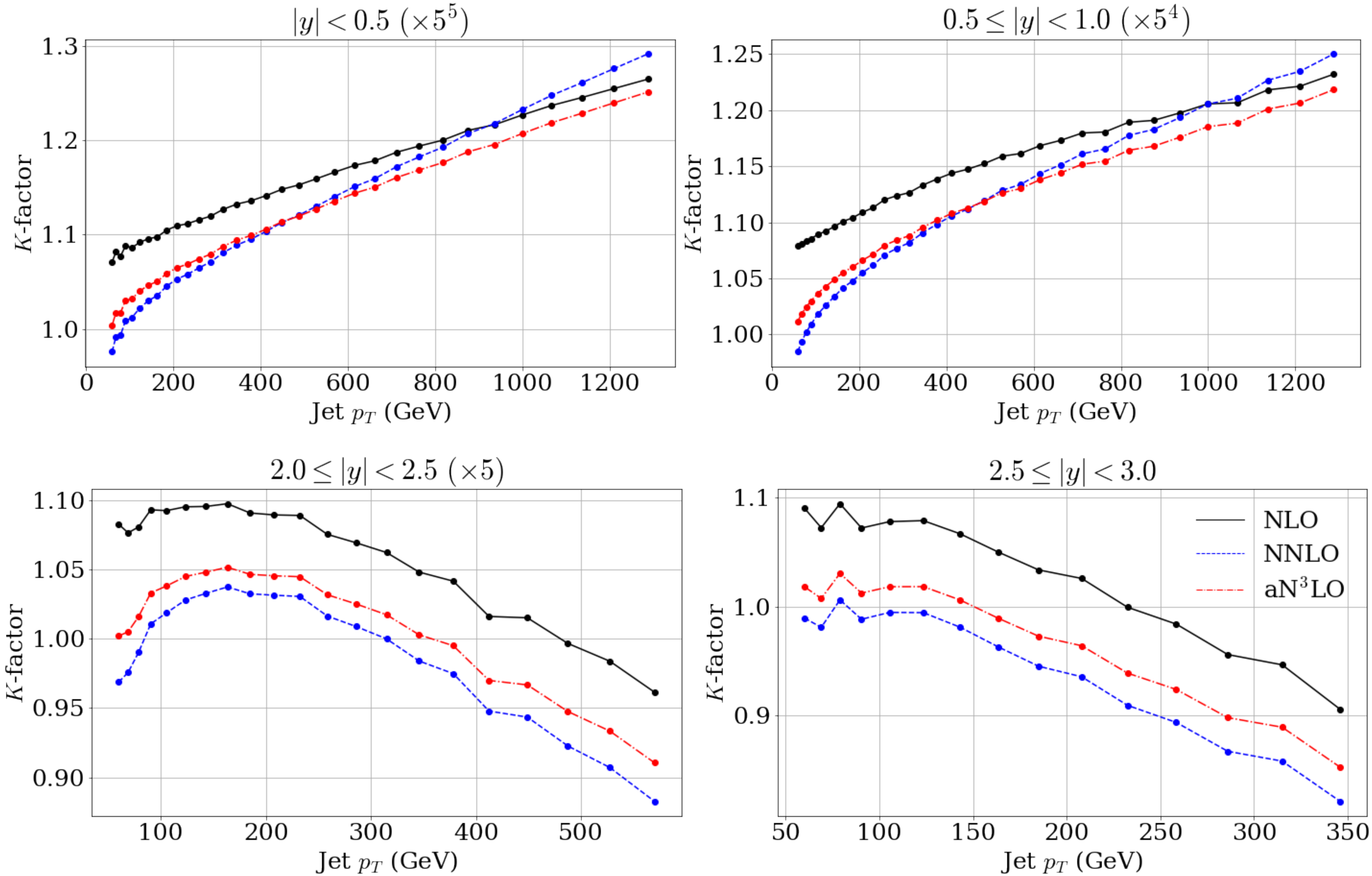
★ Resulting K-factors: $t\bar{t}$.



- 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.

Dimuon and Z $p_\perp$: backup.

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:

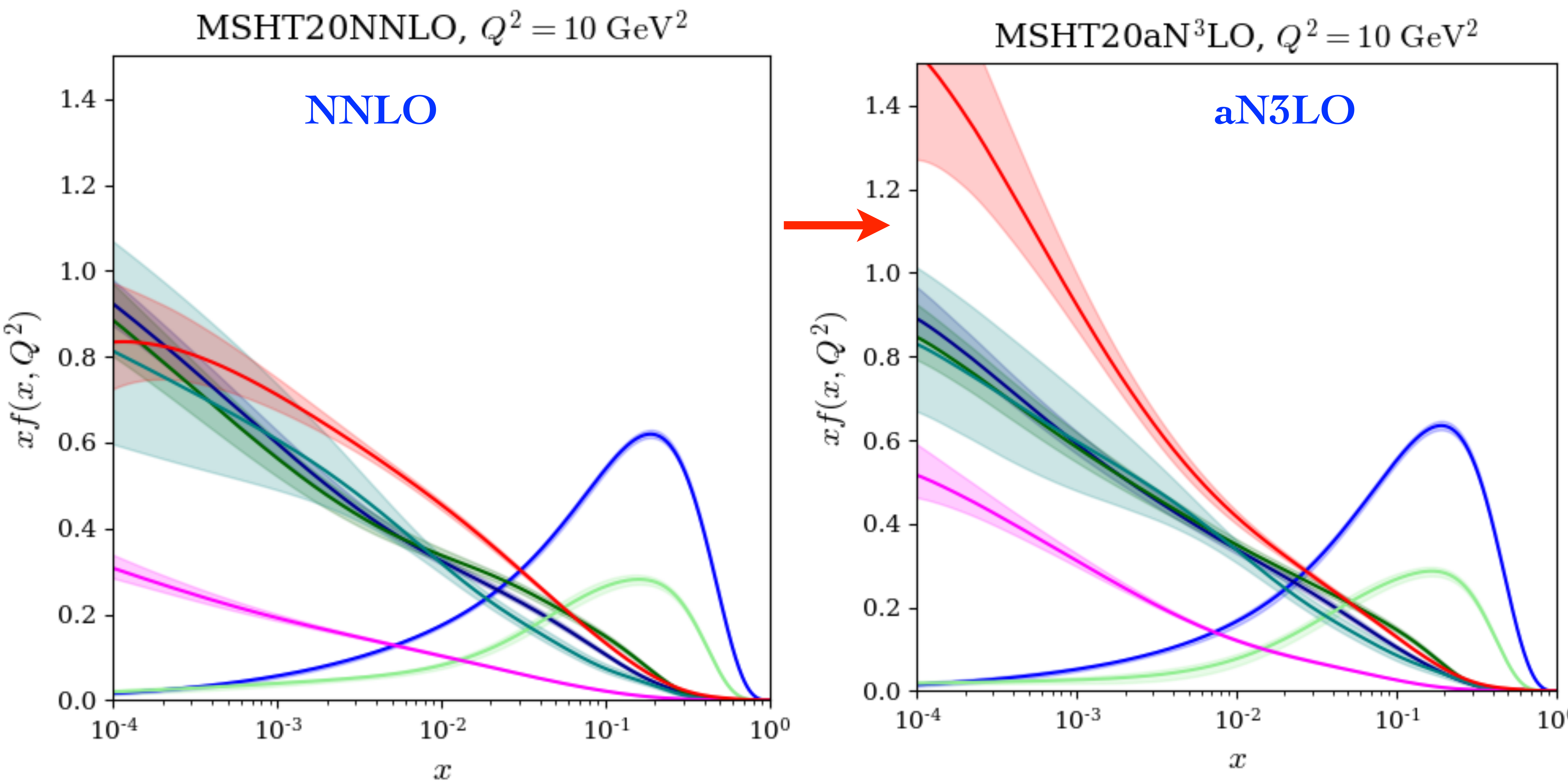
Dataset	N_{pts}	χ^2	$\Delta\chi^2$ from
DY data Total	864	1069.4	-18.5
Top data Total	71	75.1	-4.2
Jets data Total	739	963.6	$+21.5$
p_T Jets data Total	144	138.0	-77.2
Dimuon data Total	170	125.0	-1.2
DIS data Total	2375	2580.9	-90.8
Total	4363	4961.2	-160.1

- 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?

See my talk yesterday!

PDFs

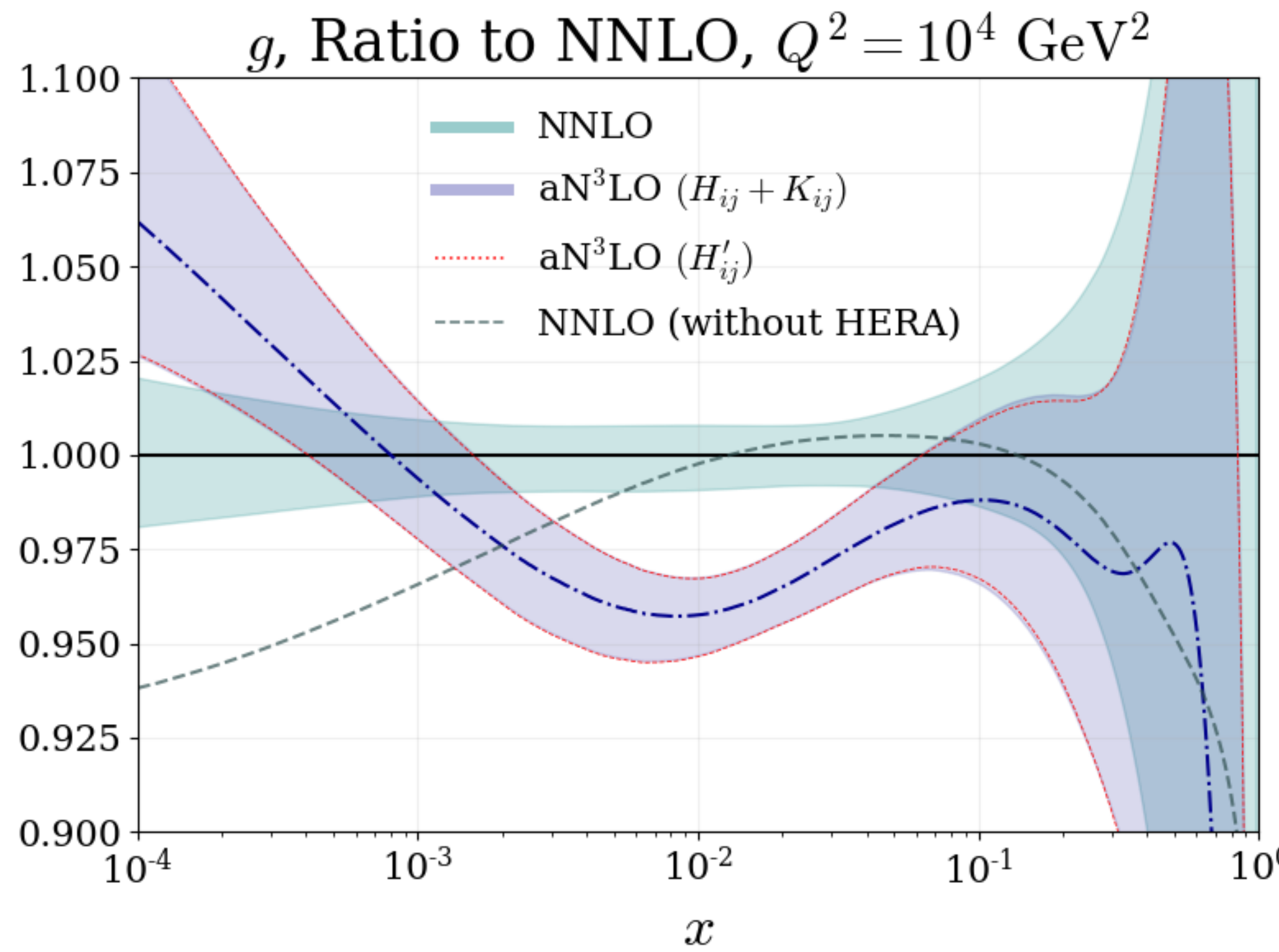
- Broad picture:



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

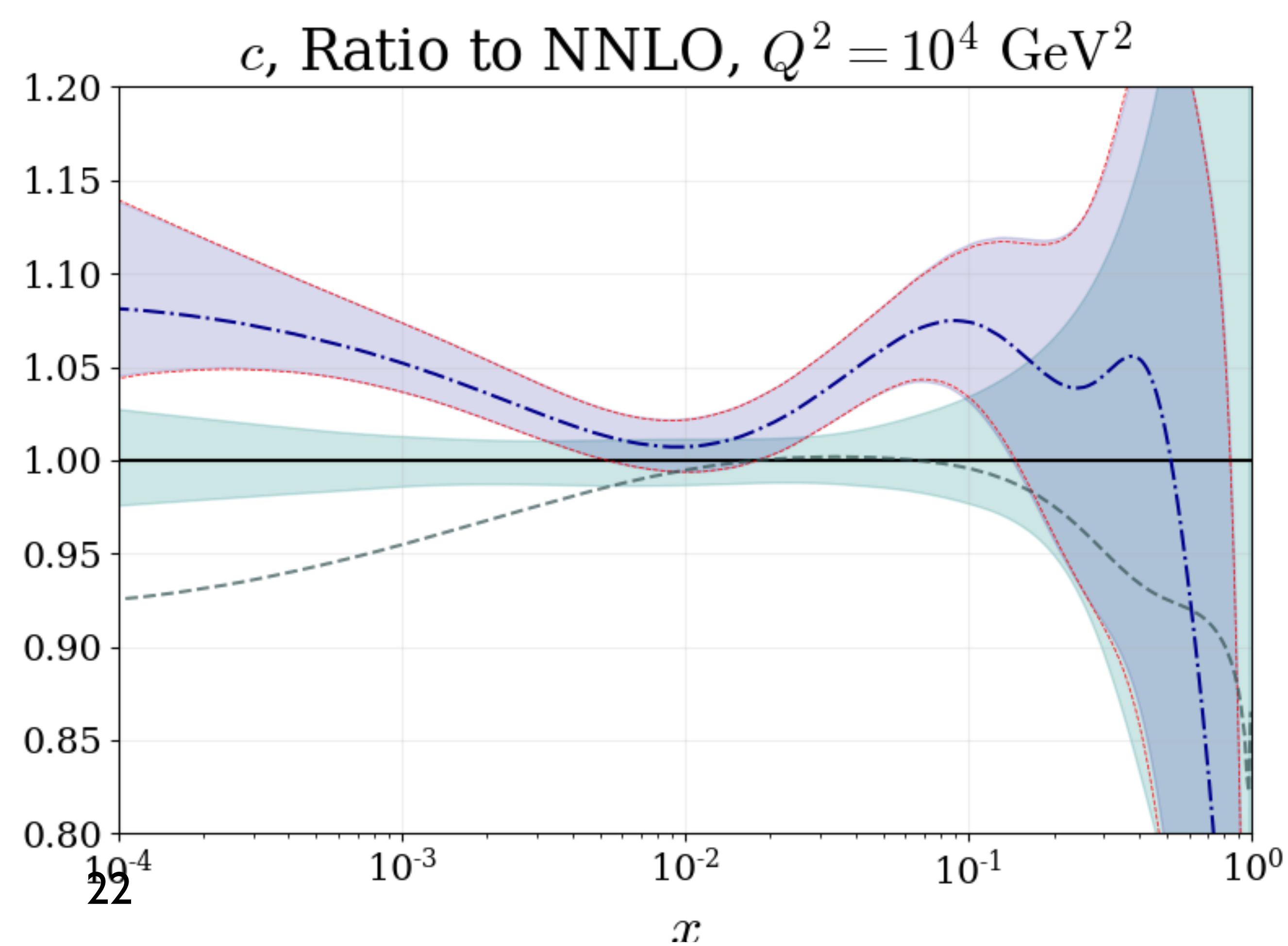
- Gluon enhanced at low x due to large logs in splitting functions.
- But also reduced at $x \sim 10^{-2}$ due to reduction in P_{qg} and compensation for increased gluon at low x .

See Backup for more.



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

Other PDFs: backup



PDFs - theoretical uncertainty

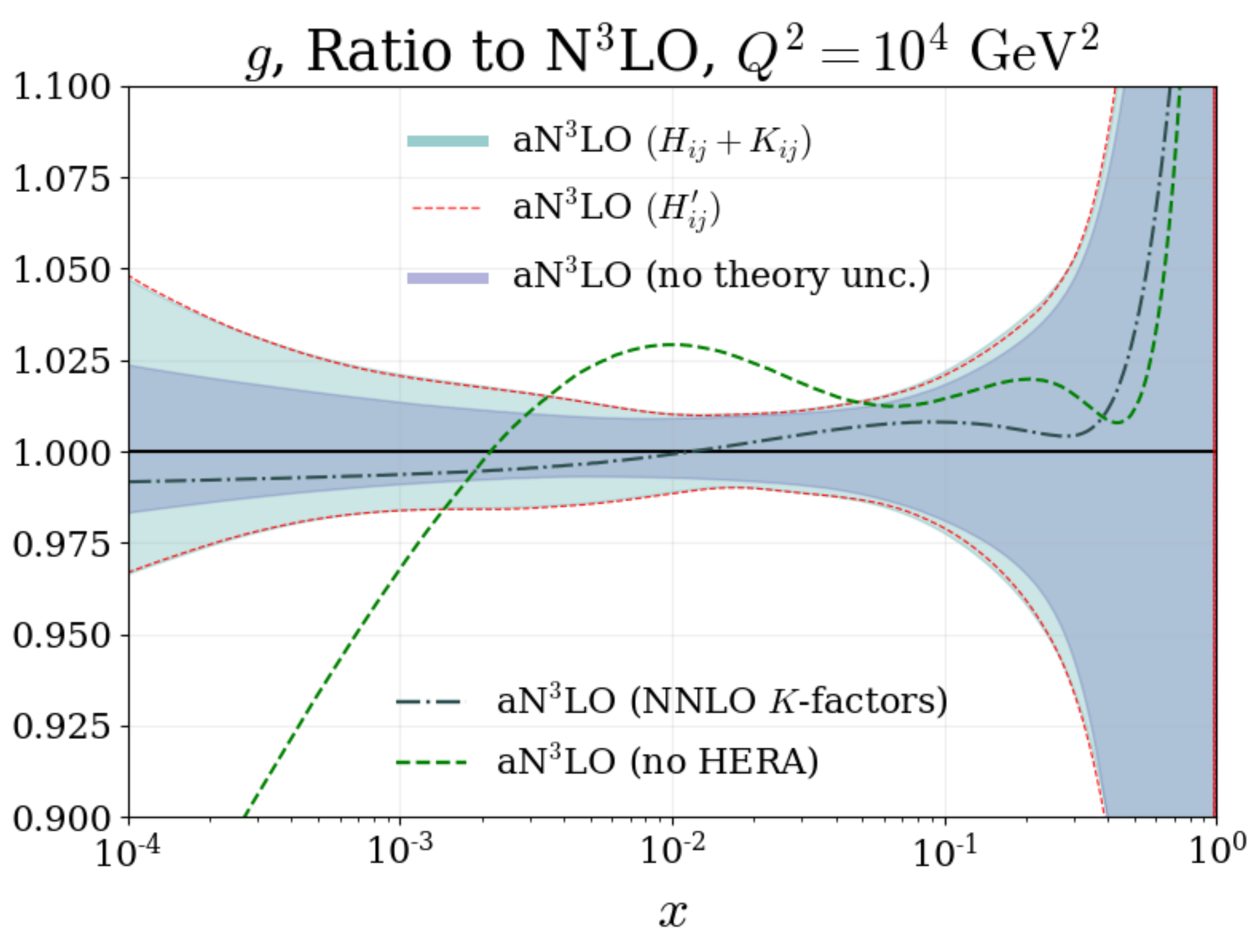
- Compare to results with aN3LO theory fixed to best fit value, i.e. no MHO 'theory' uncertainty. Impact relatively mild but not negligible.

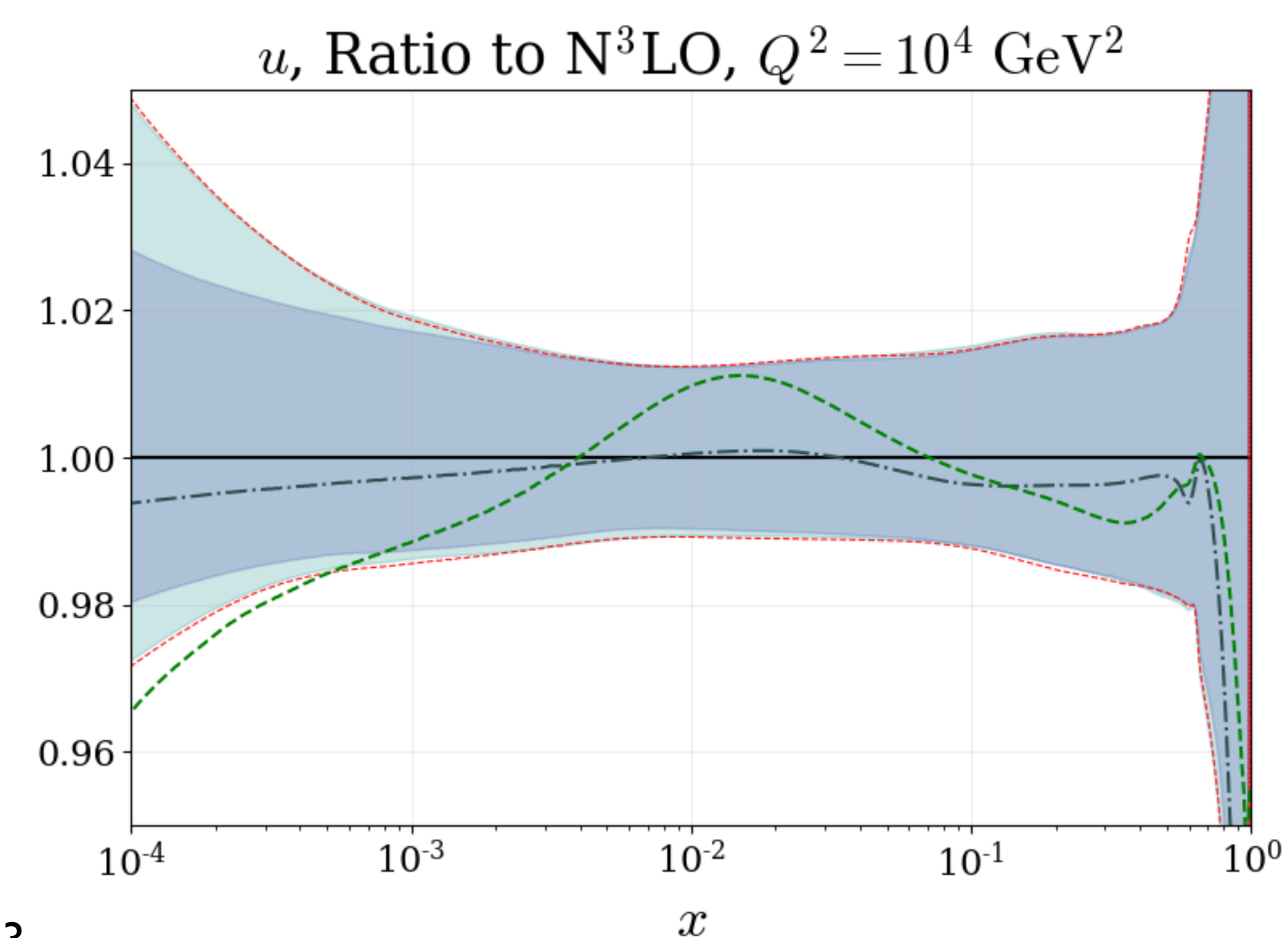
★ Gluon uncertainty most affected - increased at low x due to larger uncertainty in splitting functions.

★ Some increase in light quarks at low x.

★ But at high x impact tiny - much more known here and uncertainty lower.

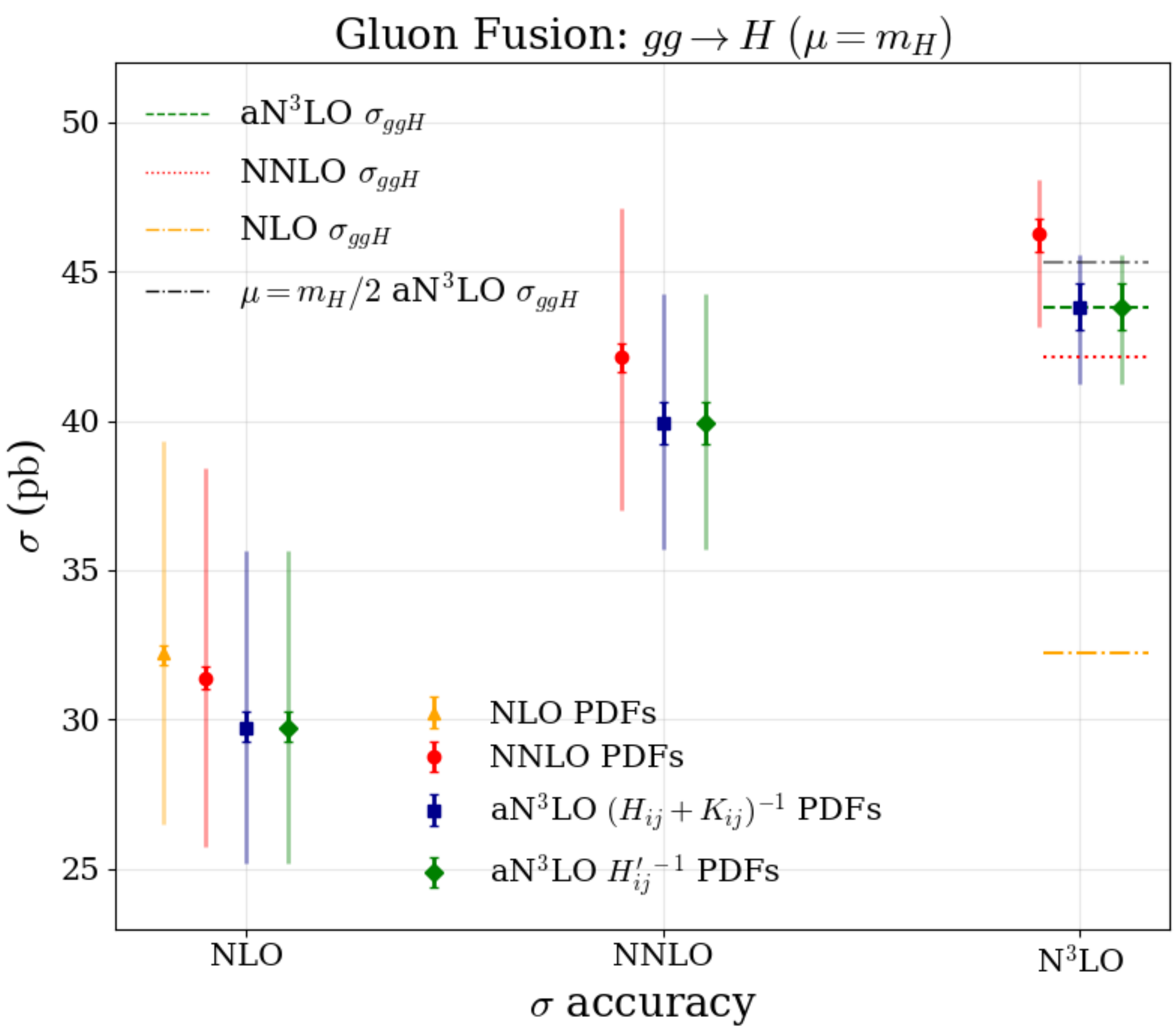
★ Impact of MHOs also on central value e.g. if NNLO K-factors used. **Backup**





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}).



Ongoing Study: NNPDF

- Have so far focussed on MSHT20aN3LO: so far only published result at this order.
- But NNPDF have been also presented results along similar (but not identical) lines.
- How are these results different/similar to MSHT and what does this tell us about overall aN3LO picture?
- Basic idea/motivation the same:

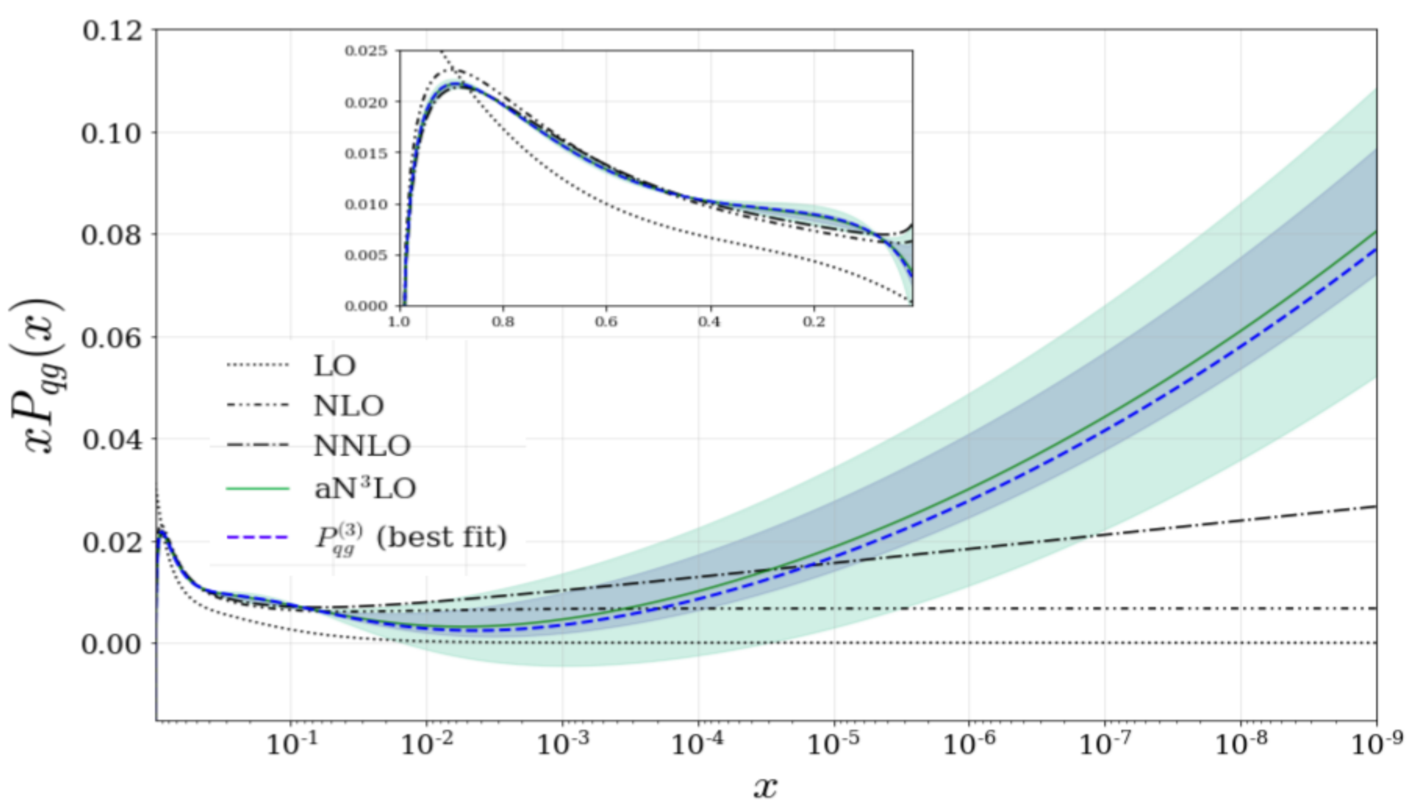
> Requirements for the next generation of PDFs are threefold:
>
> - To exploit the impressive progress in N3LO calculations we require PDFs of the same order
> - Missing higher order uncertainties (MHOUs) for some observables are larger than the experimental uncertainty and can thus no longer be neglected

R. Stegeman, this workshop

- Construction of aN3LO fit is similar in overall approach, but differing in key elements.

- Start with **splitting functions**. Basic approach as with MSHT: construct approx. $P(x)$ using known information. Differs in:
  - ⋆ Exact N3LO information used (e.g. NNPDF use high x limits).
  - ⋆ MSHT is x space, NNPDF Mellin space.
  - ⋆ Treatment of $P(x)$ uncertainty band in fit.

- Latter most important distinction.
- Recall MSHT constructs a prior uncertainty band but final posterior band determined by fit.



$\Rightarrow$ Information from global fit quality effectively included in aN3LO estimate.

- NNPDF take a different approach: set of P^i constructed, one for each functional basis f_i with certain cases discarded according to chosen quality criteria.

$i \sim O(100)$

$$f_1 = \frac{S_1(N)}{N} \qquad f_3 = \{\frac{1}{(N-1)}, \frac{1}{N}\}$$

$$f_2 = \frac{1}{(N-1)^2} \qquad f_4 = \{\frac{1}{(N-1)}, \frac{1}{N^4}, \frac{1}{N^3}, \frac{1}{N^2}, \frac{1}{N}, \frac{1}{(N+1)^3}, \frac{1}{(N+1)^2}, \frac{1}{N+1}, \frac{1}{N+2}, \mathscr{M}[\ln(1-x)], \mathscr{M}[(1-x)\ln(1-x)], \frac{S_1(N)}{N^2}\}$$

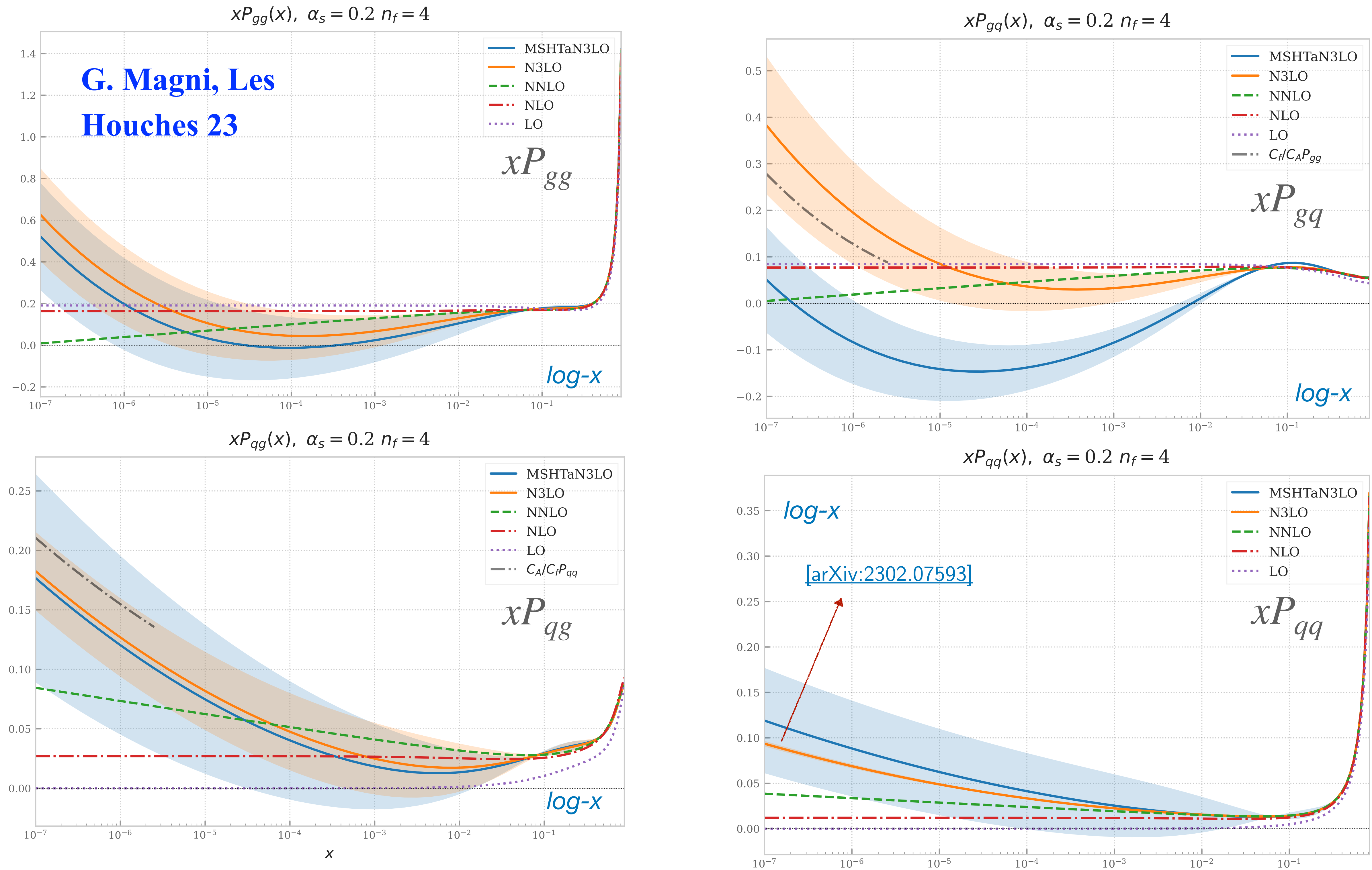
- Each of these is use independently in PDF fit, and final result is constructed democratically from all i fits.

$\Rightarrow$ Information from global fit quality not included in aN3LO estimate.

- Genuine choice in how fitting splitting functions is approached:

	Pro	**Con/Caveat**
⋆ MSHT:	Information from global fit on aN3LO used!	Sensitivity to higher orders/other issues in fit.
⋆ NNPDF:	Arguable 'Cleaner' aN3LO uncertainty	Information from global fit on aN3LO not used!

- Personal view: including information from global fit well motivated. But differences should be explored more in future.



- General consistency but difference in P_{gq} . Less pheno relevance and one where highest power of log ($\ln^2(1/x)/x$) unknown. Under investigation!
- Difference in P_{qq} as Falcioni et al. came after MSHT20.
- N.B. the MSHT20 results here are the prior (not posterior) bands.

- What about hadronic cross sections? Scale variation approach taken, studied in detail in earlier works. **NNPDF, *Eur.Phys.J.C* 79 (2019) 11, 931**

- Basic idea well known - `rule of thumb' variation of $\mu_{f,r}$ by factor of 2:

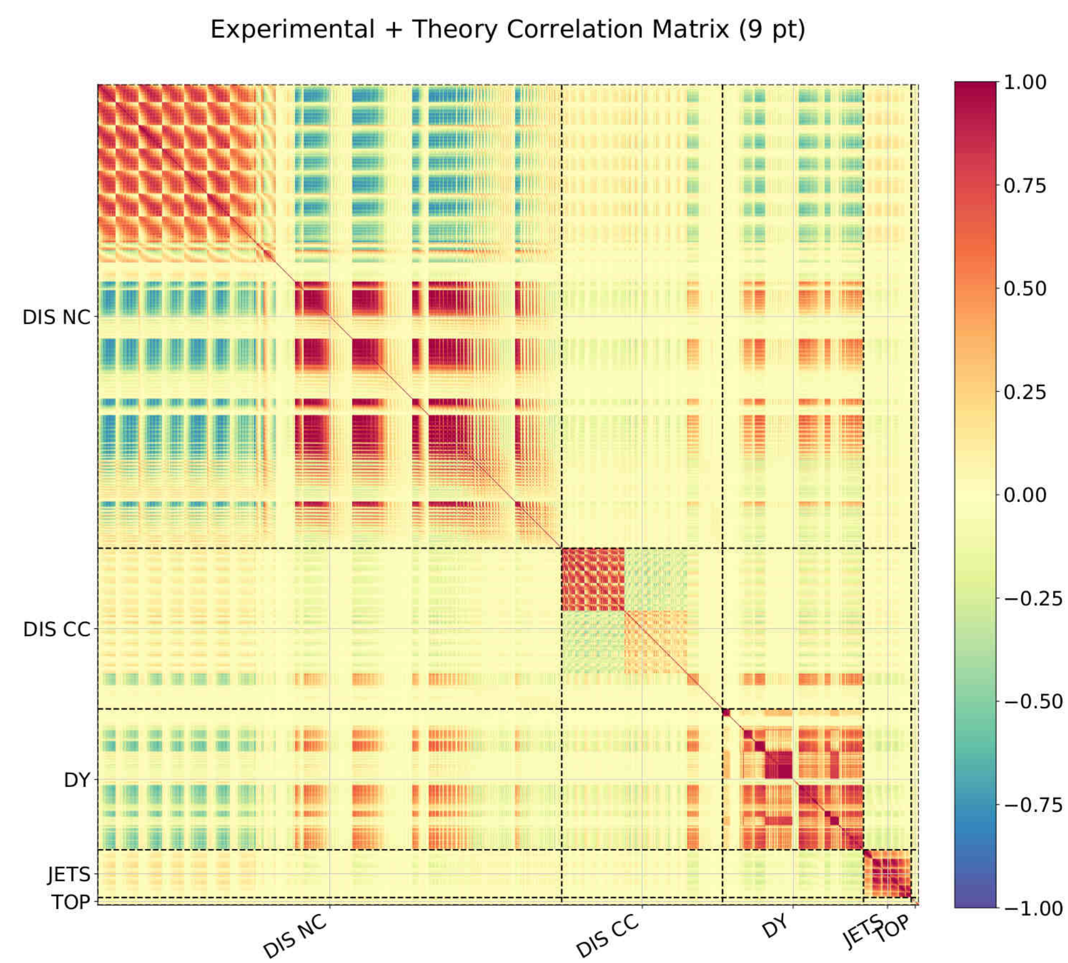
$$\sigma = \sigma_0\,(1 + c_1\alpha_S + \cdots c_n\alpha_S^n) \qquad \frac{\mathrm{d}\sigma}{\mathrm{d}\mu} = O(\alpha_S^{n+1}) \qquad \delta\sigma = \sigma(2\mu_0) - \sigma(\mu_0/2)$$

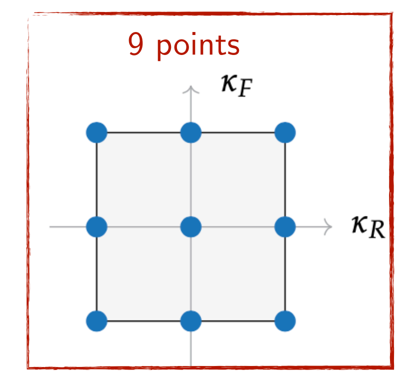
gives ~ MHOU on σ .

NNPDF, *Eur.Phys.J.C* 79 (2019) 11, 931

- This is used to construct theory covariance matrix - MHO uncertainty + correlations between/within processes.

- Full results with this presented at NLO only so far. NNLO/N3LO ongoing.





- How does this compare to MSHTaN3LO approach? **See A. Barontini's talk for more results!**

- ⋆ MSHT: aN3LO MHO given by **nuisance parameters** and $\propto$ NLO, NNLO K-factors.

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

- ⋆ NNPDF: **covariance matrix** constructed from scale variations.

- Will certainly give different results, but in fact achieve similar things:
  - For NNPDF (MSHT) uncertainty implicitly (explicitly) at next order.

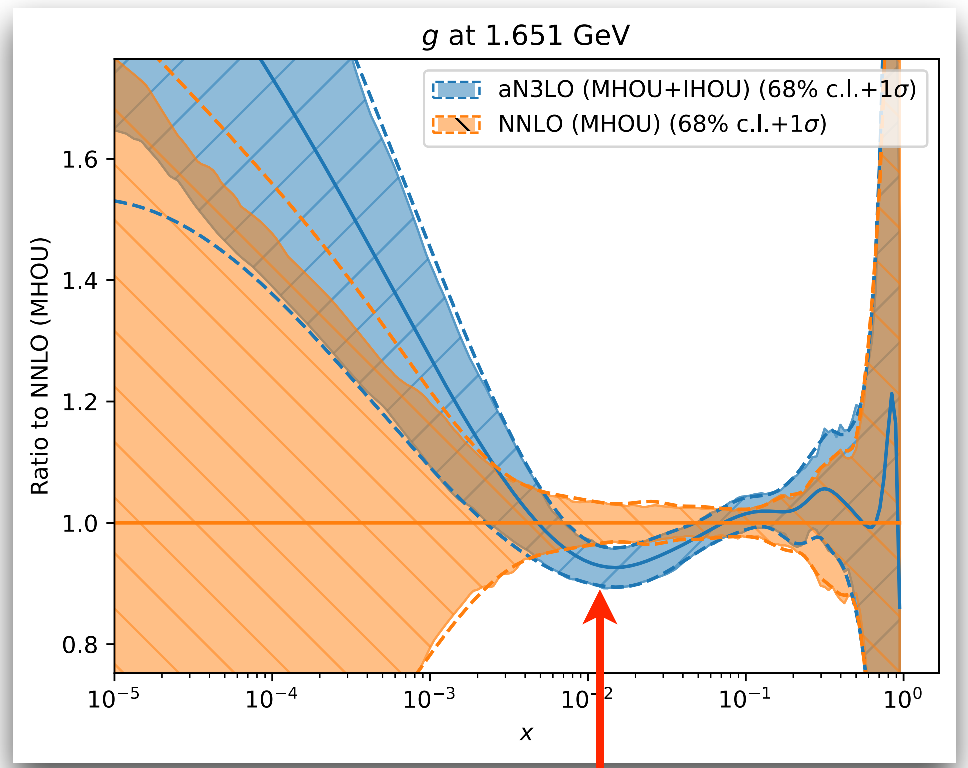
$$\frac{\mathrm{d}\sigma}{\mathrm{d}\mu} = O(\alpha_S^{n+1})$$

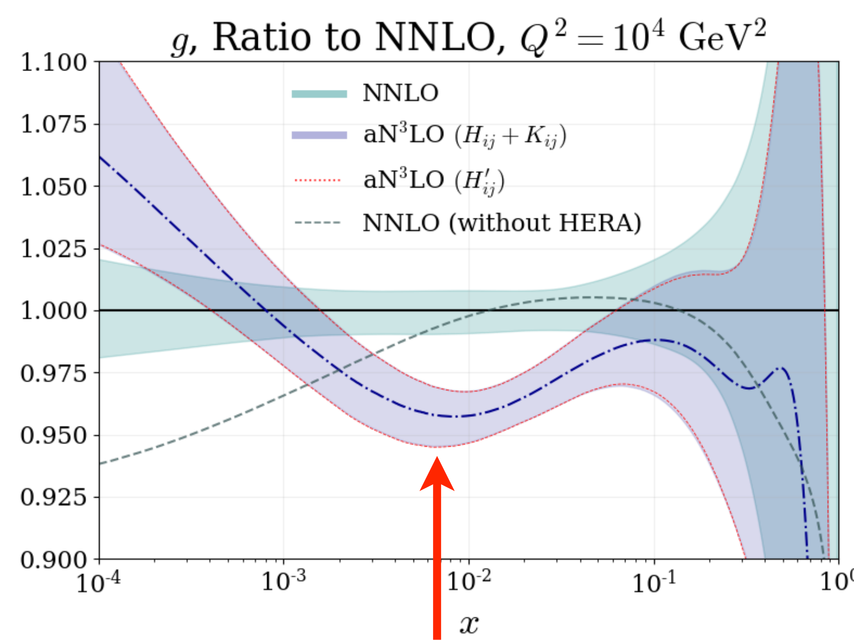
  - Correlations between classes of processes qualitatively similar.
  - Nuisance parameter vs. covariance matrix difference superficial - these are equivalent. Covariance matrix does not avoid fit picking a preferred scale.

- But not to overstate: approaches are different!

(Very) Initial Comparison

- First indication is that impact on gluon at aN3LO is more significant for MSHT, though trend the same.





- In region relevant to ggH - important to clarify!
- Reason for this unclear (differing P_{ij}, Q^2 cuts, MHOs…).
- Benchmarking needed, and underway!

Fit/Prediction Correlations

- Final subtlety: for predicted cross sections ($\hat{\sigma}$ + PDF) also require MHO uncertainty. Risk of double counting? Typically scale variations used…

LHL and R. S. Thorne, EPJC79 (2019), no.1, 39

Fit $\quad O_{\text{fit}} \sim f_i(\mu^2) \otimes \sigma_i(\mu^2) \sim f_i(\mu^2) \otimes \left(\sigma_i^{(0)}(\mu^2) + \alpha_S\, \sigma_i^{(1)'}(\mu^2) + \cdots\right)$

$\downarrow$ **A**

$\downarrow$ **B**

f_i

$\downarrow$ **C**

$i:$ PDF type

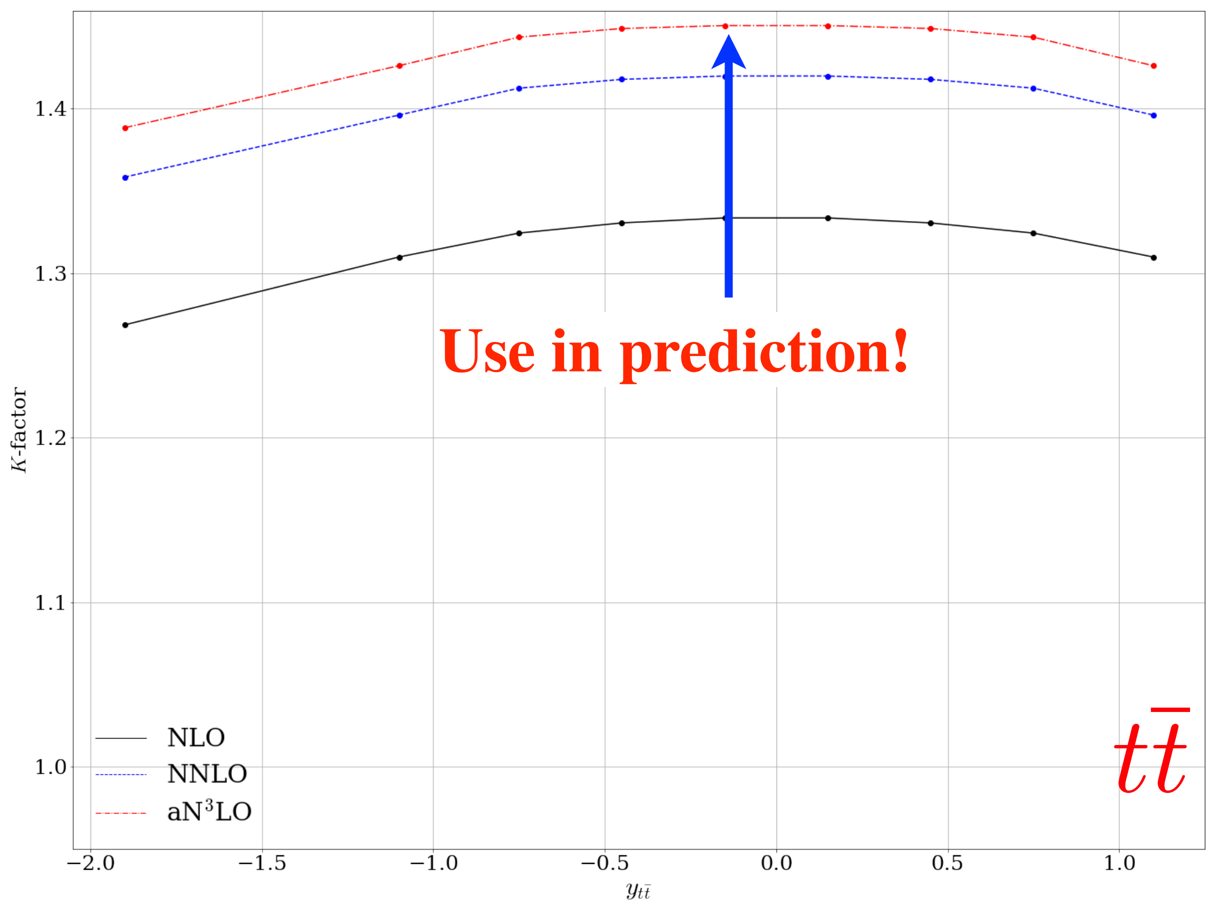
Prediction $\quad O_{\text{pred}} \sim f_i(\mu^2) \otimes \sigma_i'(\mu^2) \sim f_i(\mu^2) \otimes \left(\sigma_i^{(0)'}(\mu^2) + \alpha_S\, \sigma_i^{(1)'}(\mu^2) + \cdots\right)$

- ★ Simplified study: recast PDF fit as direct relationship between fit and predicted observables. Find clear risk of **overestimating** errors due to factorization scale variation in certain regions (low/high x).

R. Ball an R. Pearson, *Eur.Phys.J.C* 81 (2021) 9, 830

- How this translates to full fit is non-trivial, but in some cases possible/desirable to keep track of correlations…

- For processes (top, jets, DY…) in fit where NNLO + MHOUs are used, can/should keep track of the aN3LO K-factor preferred by fit and their uncertainty.
- MSHT provides theses as 'decorrelated' eigenvectors to use.

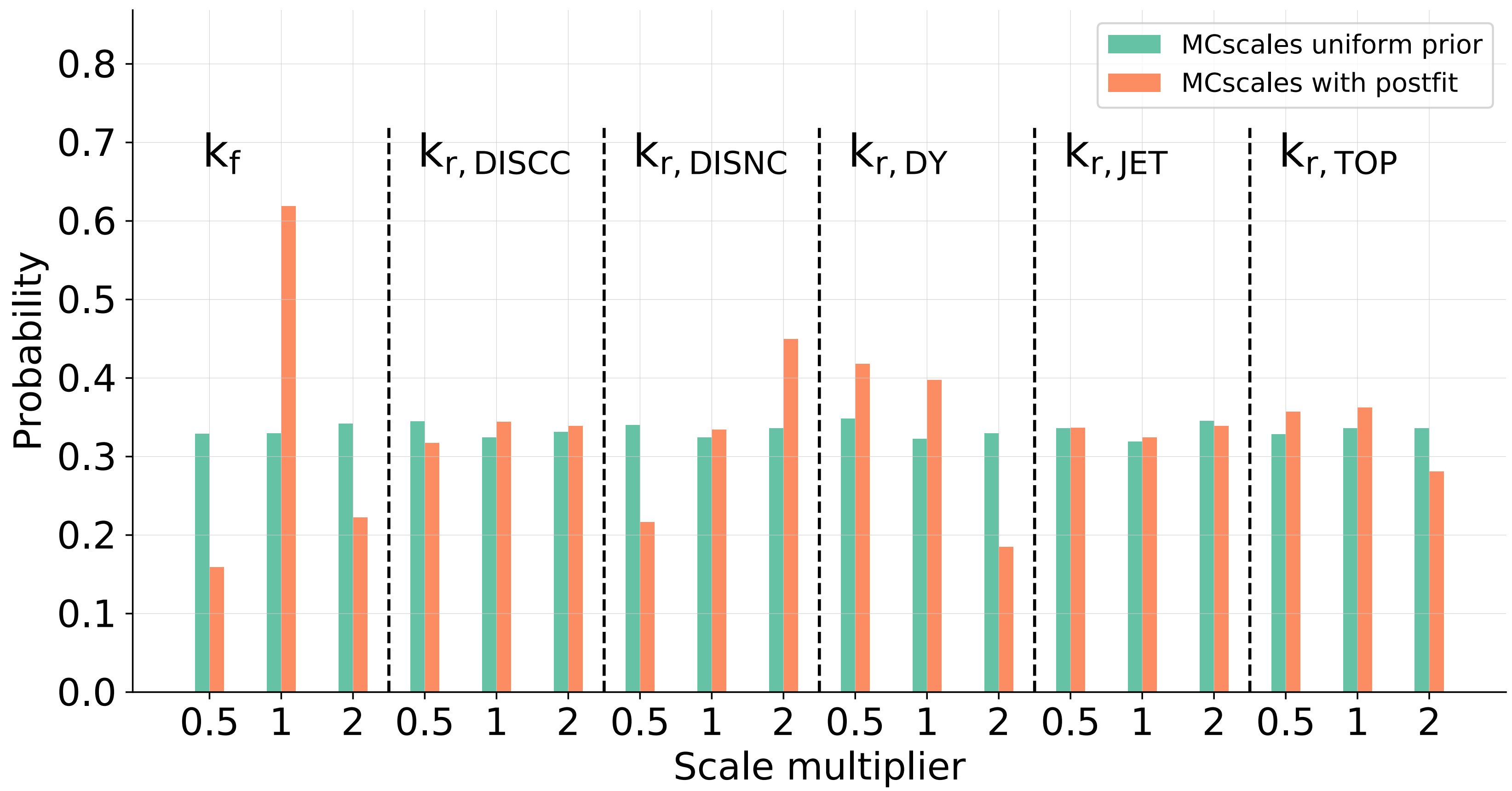


Matrix	Central Values		Eigenvector	+ Limit		- Limit	
	$a_{\rm NLO}$	$a_{\rm NNLO}$		$a_{\rm NLO}$	$a_{\rm NNLO}$	$a_{\rm NLO}$	$a_{\rm NNLO}$
$K_{ij}^{\rm DY}$	-0.282	0.079	43	-0.378	0.062	-0.145	0.103
			44	-0.334	0.374	-0.256	-0.071
$K_{ij}^{\rm Top}$	0.041	0.651	45	-0.564	0.455	0.692	0.862
			46	0.026	1.210	0.070	-0.456

- Allows MHOU (in MSHT approach) in predictions to be consistently propagated through, including PDF correlation.
- Also in principle possible in scale variation (NNPDF) approach, with first study in this direction performed…

Z. Kassabov, M. Ubiali, C. Voisey, *JHEP* 03 (2023) 148

- MCscales study: replica PDF fits performed with different $\mu_{r,f}$ choices.
- Postfit selection made so that larger χ^2 values dropped: effectively profiling over $\mu_{r,f}$.



- The mcscales_v1 replicas made available, so that $\mu_{r,f}$ variation can again be consistently propagated through to predictions.

Interpretation/Usage

- ★ If N3LO cross sections are known, use aN3LO PDF + their theoretical uncertainties. No need for:

$$\cancel{\delta(\text{PDF-TH}) = \frac{1}{2}\left|\frac{\Sigma^{\text{NNLO, NNLO-PDFs}}(Q^2) - \Sigma^{\text{NNLO, NLO-PDFs}}(Q^2)}{\Sigma^{\text{NNLO, NNLO-PDFs}}(Q^2)}\right|}.$$

- ★ For DIS processes advised to use aN3LO PDF with aN3LO coefficient functions.
- ★ When predicting processes included in fit, can keep track of aN3LO information to provide consistent aN3LO result.
- ★ For processes not included in fit, the change between using NNLO and N3LO can be taken as a corresponding uncertainty.

$$\delta(\text{PDF} - \text{TH}) = \frac{1}{2}\left|\frac{\sigma^{(2)}_{\text{aN}^3\text{LO}} - \sigma^{(2)}_{\text{NNLO}}}{\sigma^{(2)}_{\text{aN}^3\text{LO}}}\right|$$

Final Remarks

- ★ Though full N3LO is a way off, we already have more than enough information to provide a genuine description of N3LO PDF, with an associated uncertainty.
- ★ Not 'just' NNLO + uncertainty - known N3LO information requires central value to be systematically different.
- ★ To get as much as possible out of PDF arsenal, these aN3LO sets will be crucial - can't afford to wait for full N3LO.
- ★ Will require continuous updating - MSHT work underway to include (already significant) new information.
- ★ Futher benchmarking underway - lots more work to do!

Thank you for listening!

Backup

DIS Coefficient Functions

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

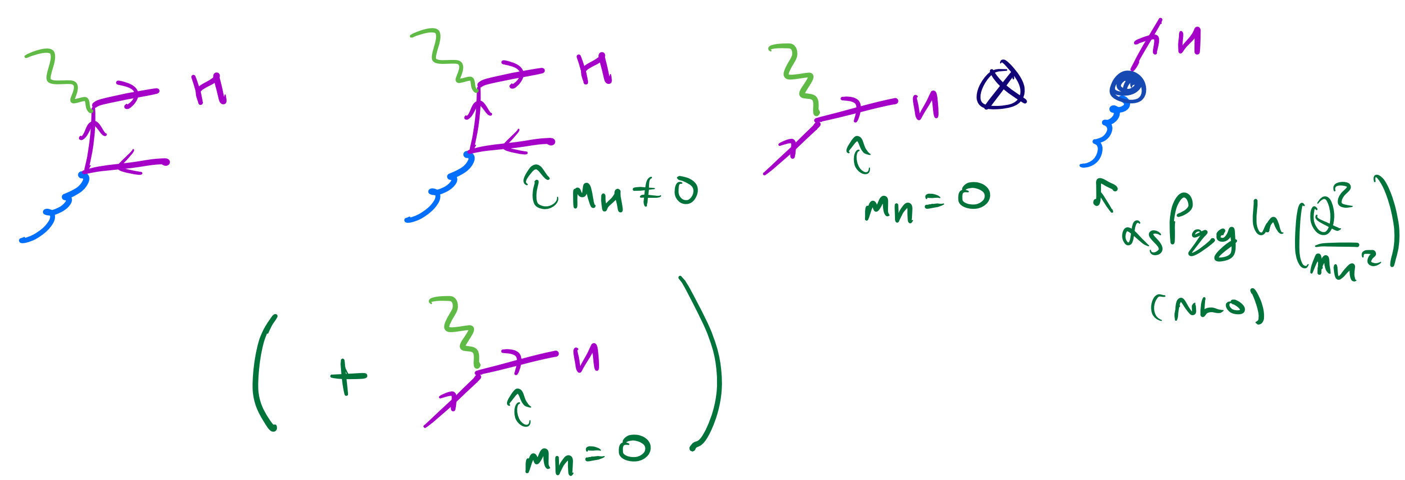
- DIS coefficient functions C_i known at N3LO for the massless quarks.
- Is this enough? Not quite - heavy quark contributions ($m_{c,b} \neq 0$) play important role. Here some information is known but not everything.
- Expressions for heavy flavour in low and high Q^2 limits:

★ High $Q^2 \gg m_h^2$: Zero Mass case known exactly.

★ Low $Q^2 \sim m_h^2$: massive (FFNS) unknown, with some information (LL small x and mass threshold).

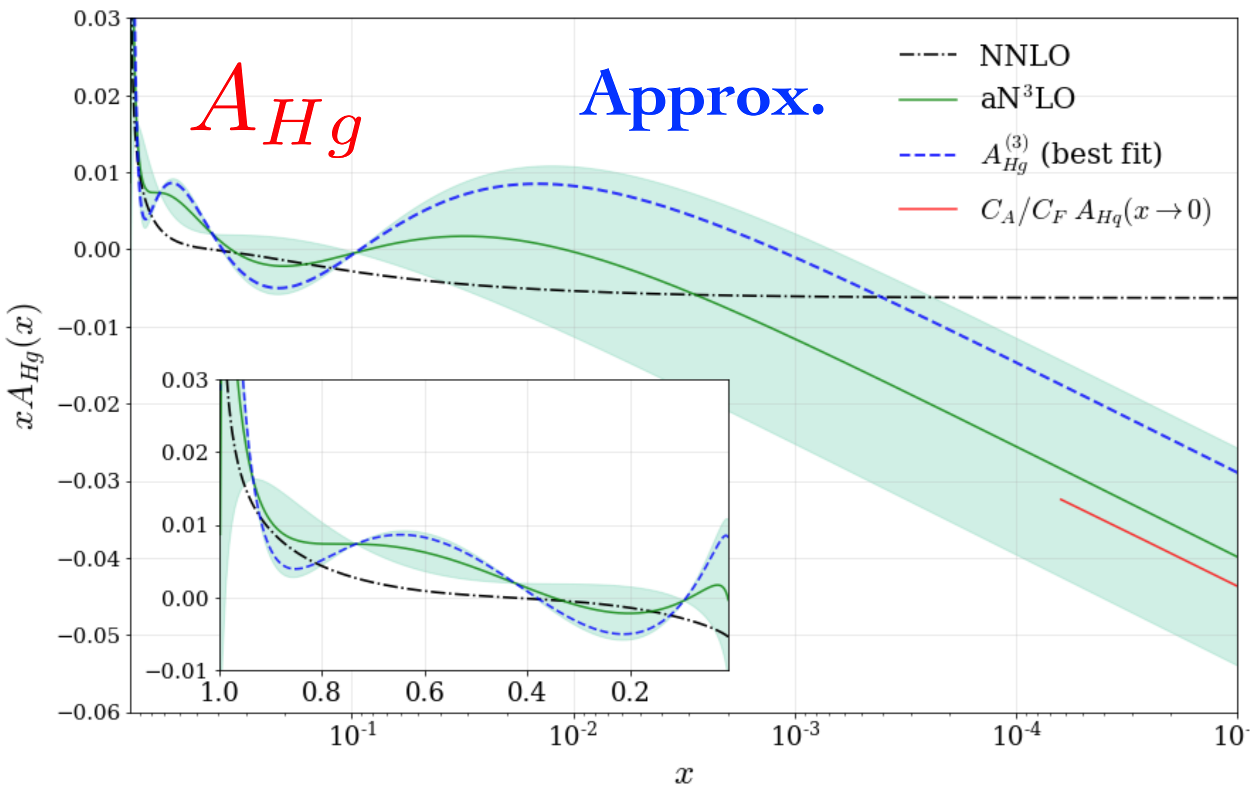
- General Mass Variable Flavour Number scheme interpolates between limits.
- Impact of heavy flavour on PDF evolution controlled by **transition matrix elements** $A_{\alpha i}$.
- Some information at N3LO, but not all.

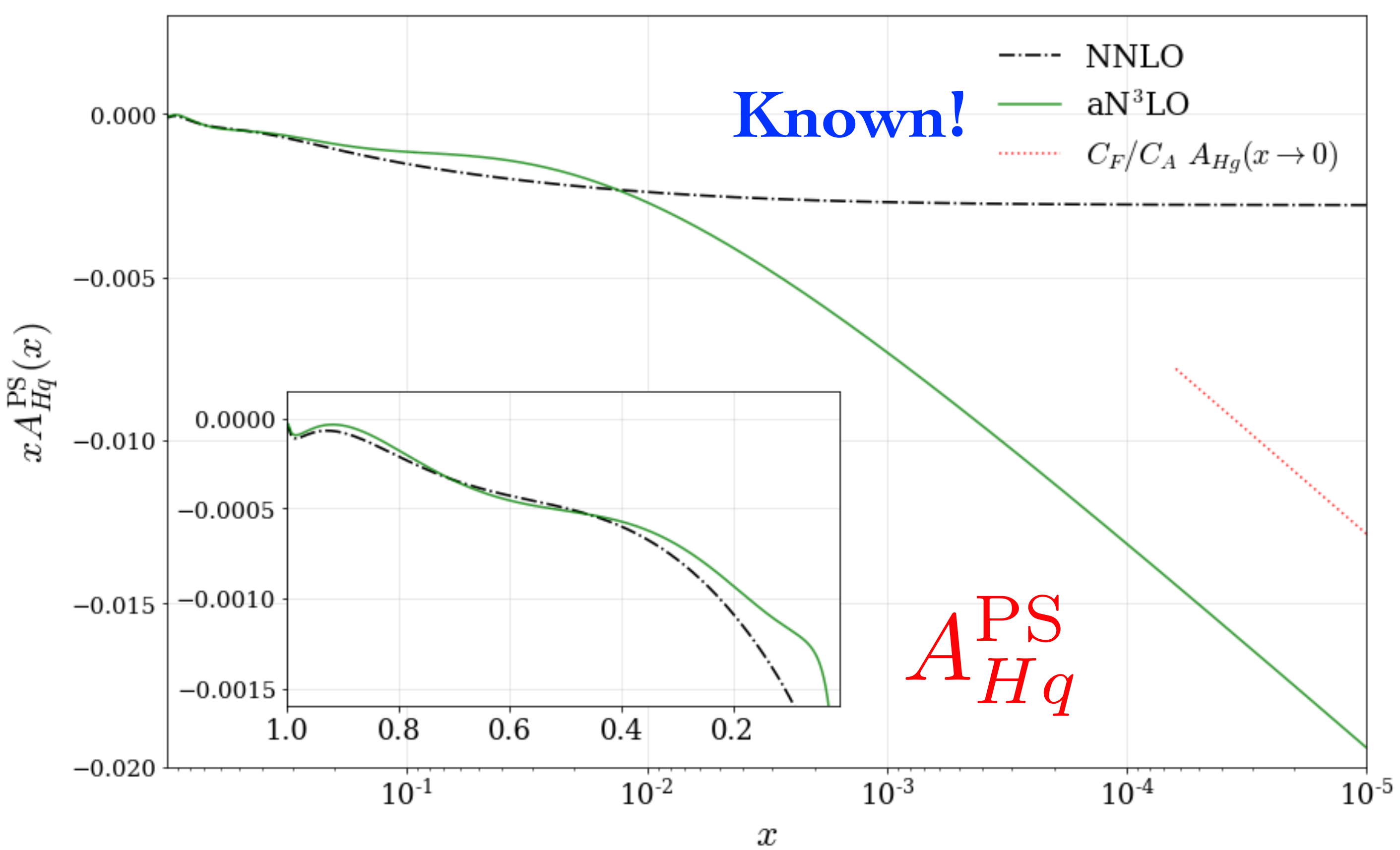
$$C^{VF}_{H,g} = C^{FF,(1)}_{H,g} - C^{VF,(0)}_{H,H} \otimes A^{(1)}_{Hg}$$



Transition Matrix Elements

- Situation similar to P_{ij}. In some cases (e.g. $A^{(3)}_{Hg}$) we know low x and Mellin information $\Rightarrow$ follow similar procedure to buid up approximation.
- For other cases ($A^{(3)}_{gq,H}, A^{\mathrm{PS},(3)}_{Hq}$) exact results are known - simply use these.

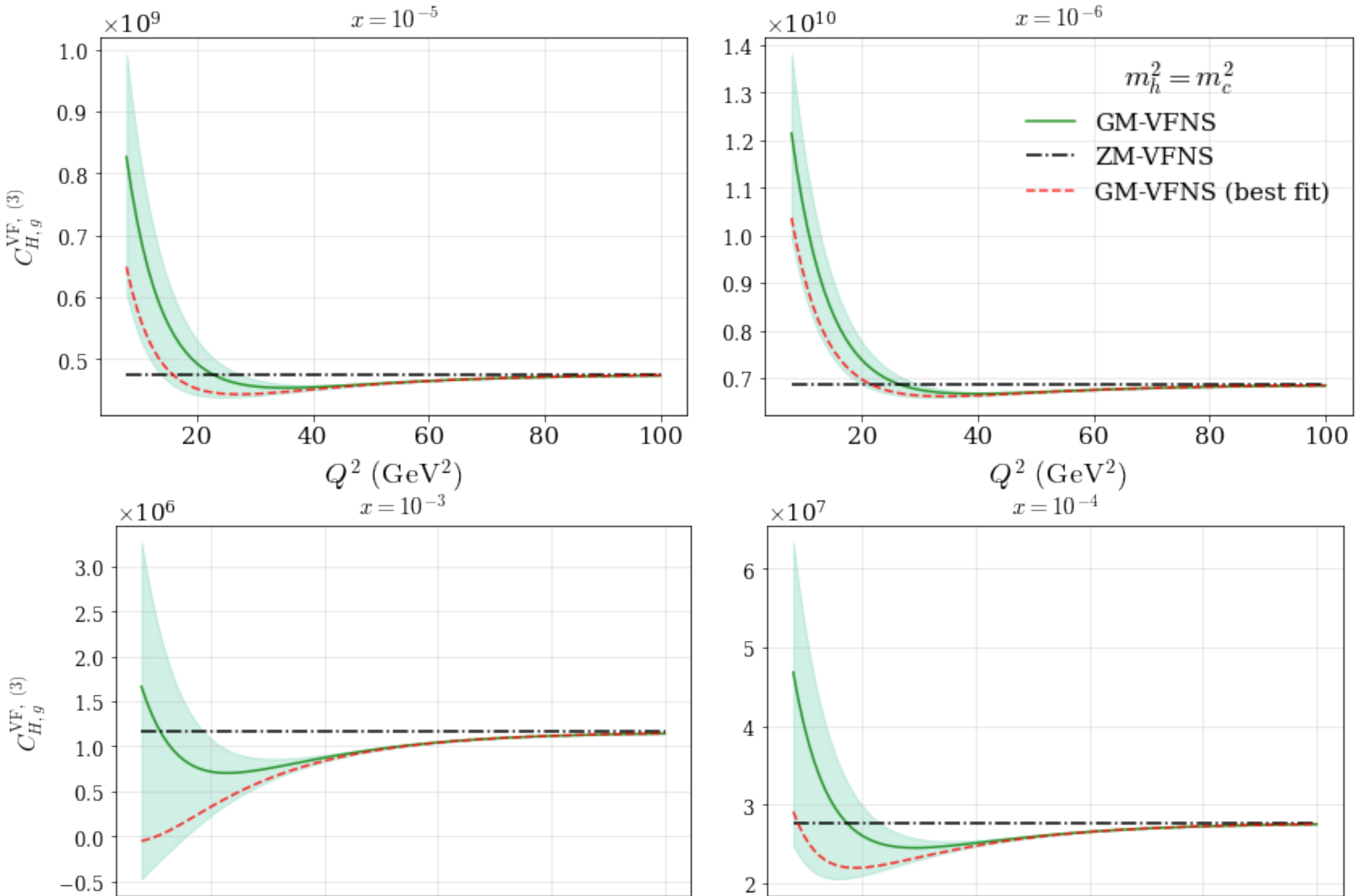




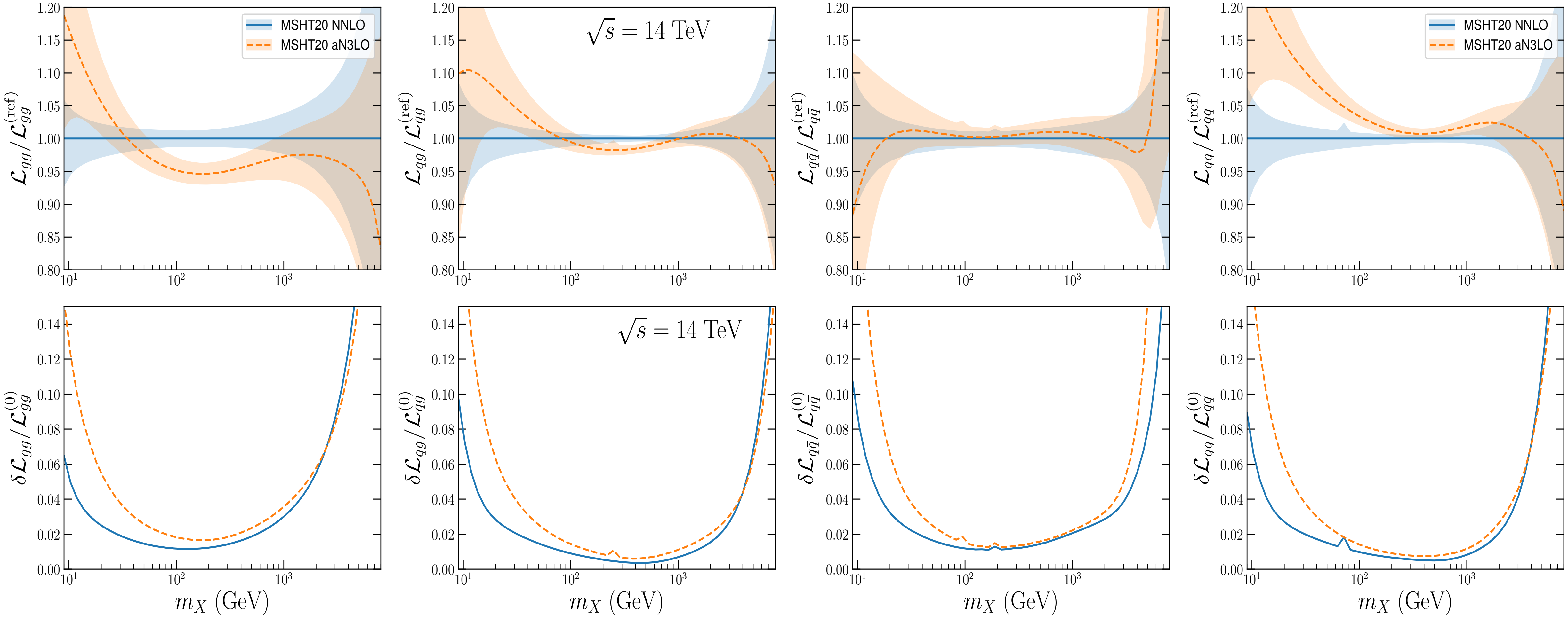
Coefficient Functions

- 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 GM-VFNS prediction.

$C_{H,g}$



aN3LO PDF luminosities:

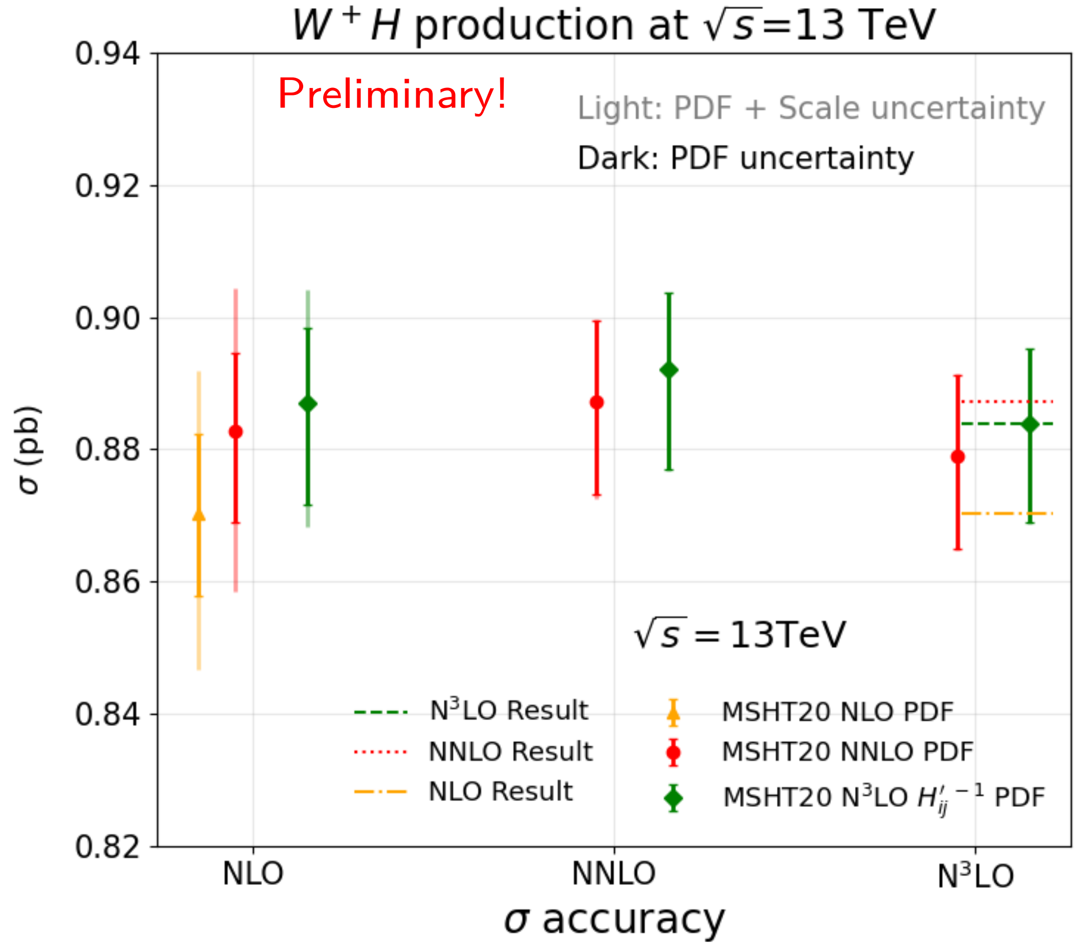


- PDF changes have implications for PDF luminosities for phenomenology.
- *gg* luminosity reduced around 100GeV and increased at 10GeV, *gg* uncertainty grows with inclusion of aN3LO and theoretical uncertainties.
- *qq* luminosity raised at low invariant masses from enhanced charm.
- Luminosity uncertainties enlarged (and more so at lower invariant masses) due to inclusion of aN3LO and PDF theory uncertainties.

Impact on VH cross-sections:

Preliminary!

- Consider impact of our aN3LO PDFs on VH associated production (Higgsstrahlung) at LHC, e.g. W^+H at 13 TeV:



N.B. For scale variations - do μ_R and μ_F at NNLO but only μ_R at aN3LO as PDF uncertainty from MHOs already in PDF eigenvectors.

Results obtained using the `n3loxs` code[28].

- Result with aN3LO PDFs raised slightly, reflects increased quarks at high x, antiquarks at low x and strange and charm.
- N3LO σ + aN3LO PDF result very close to NNLO σ + NNLO PDF result, increased stability in predictions.

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.

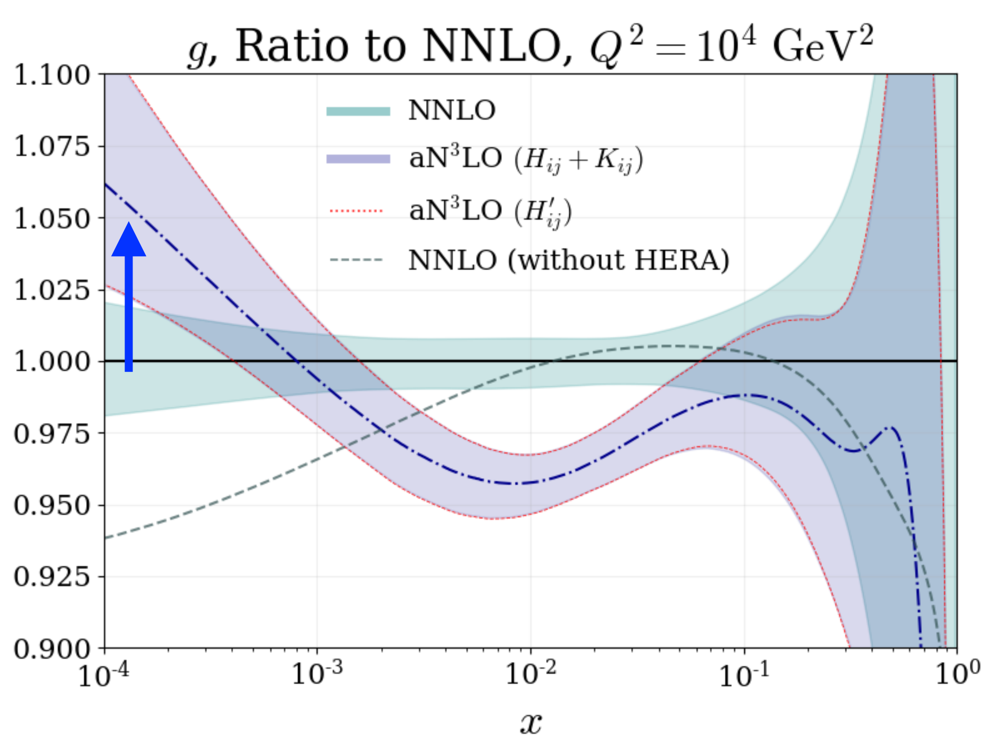
aN3LO

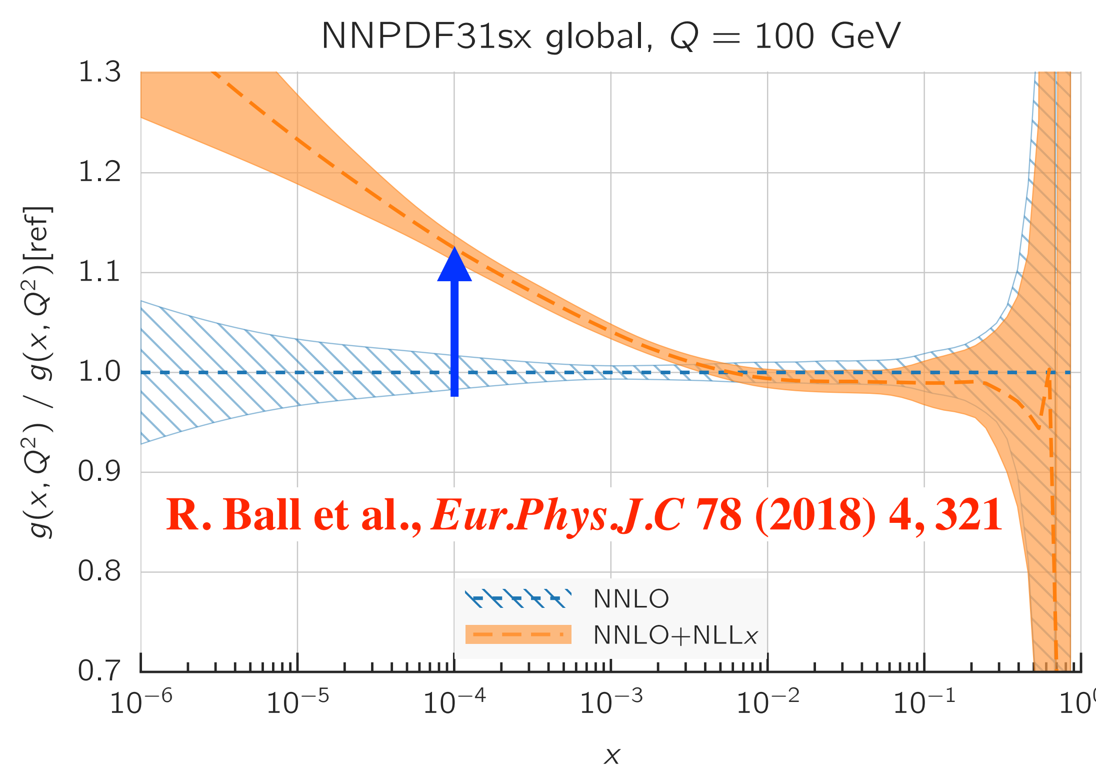
DIS Dataset	χ^2	$\Delta\chi^2$ from NNLO
HERA e^+p NC 820 GeV [144]	84.3 / 75	-5.6
HERA e^-p NC 460 GeV [144]	247.7 / 209	-0.6
HERA e^+p NC 920 GeV [144]	474.0 / 402	-38.7
HERA e^-p NC 575 GeV [144]	248.5 / 259	-14.5
HERA e^-p NC 920 GeV [144]	243.0 / 159	-1.4
Total	2580.9 / 2375	-90.8

Resummation

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

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





Preliminary

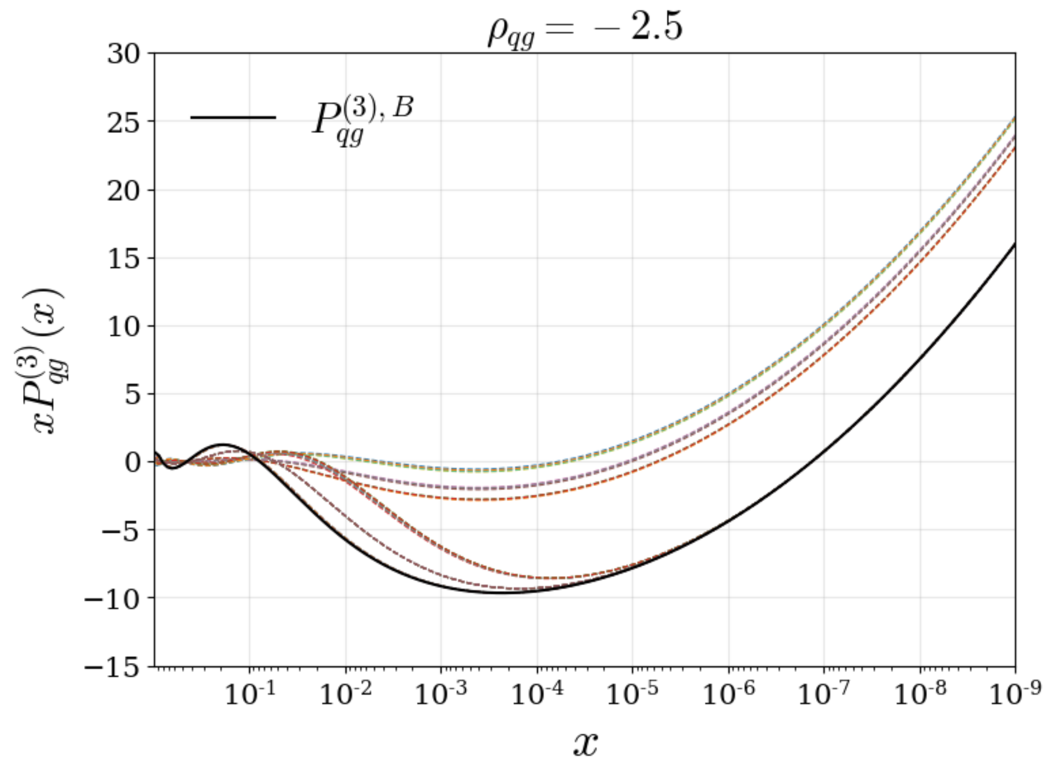
Dijet Data

- 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.



- 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.

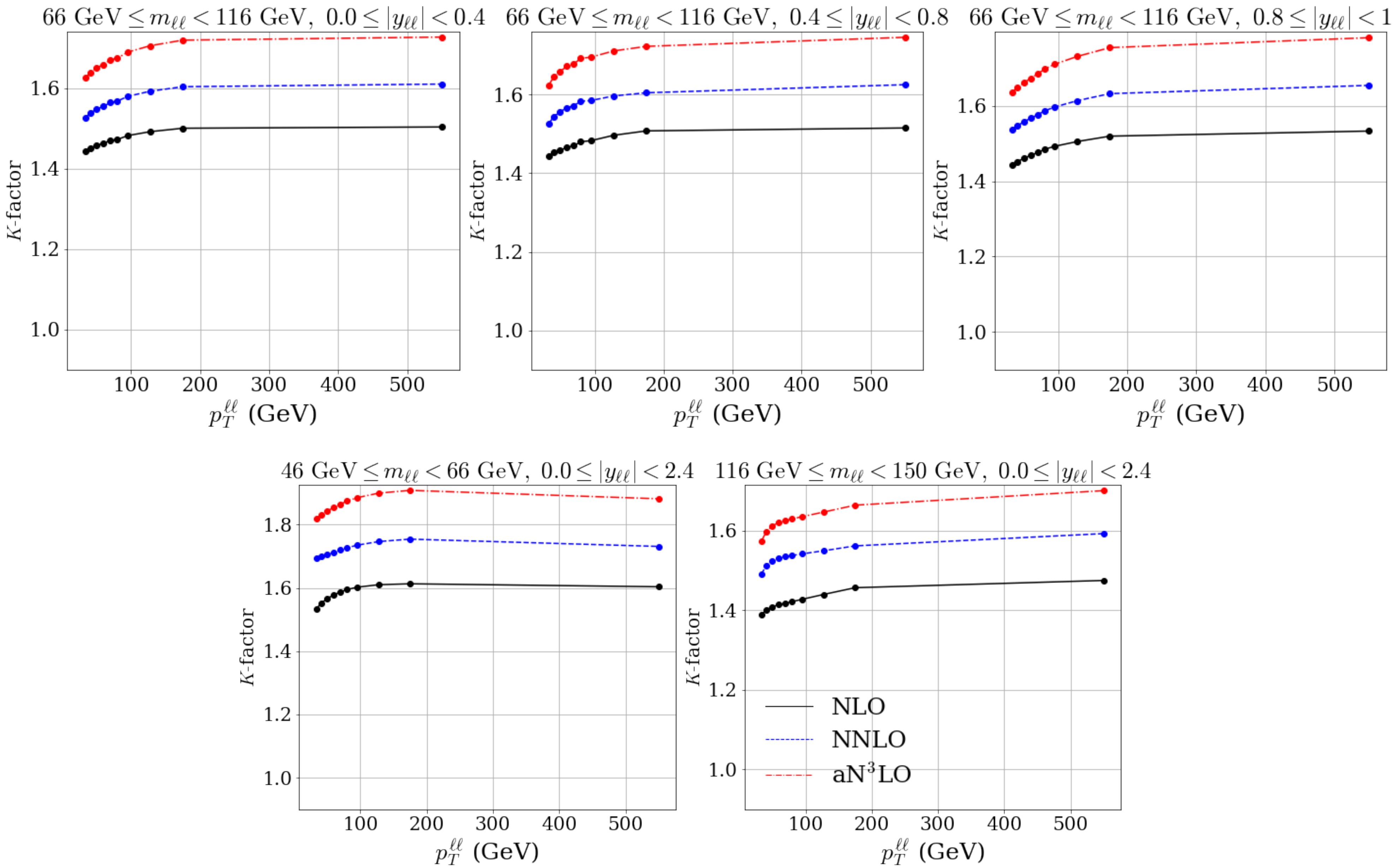
- In the end choose one set of $f_i(x)$ and range of ρ to satisfy this.

- 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!

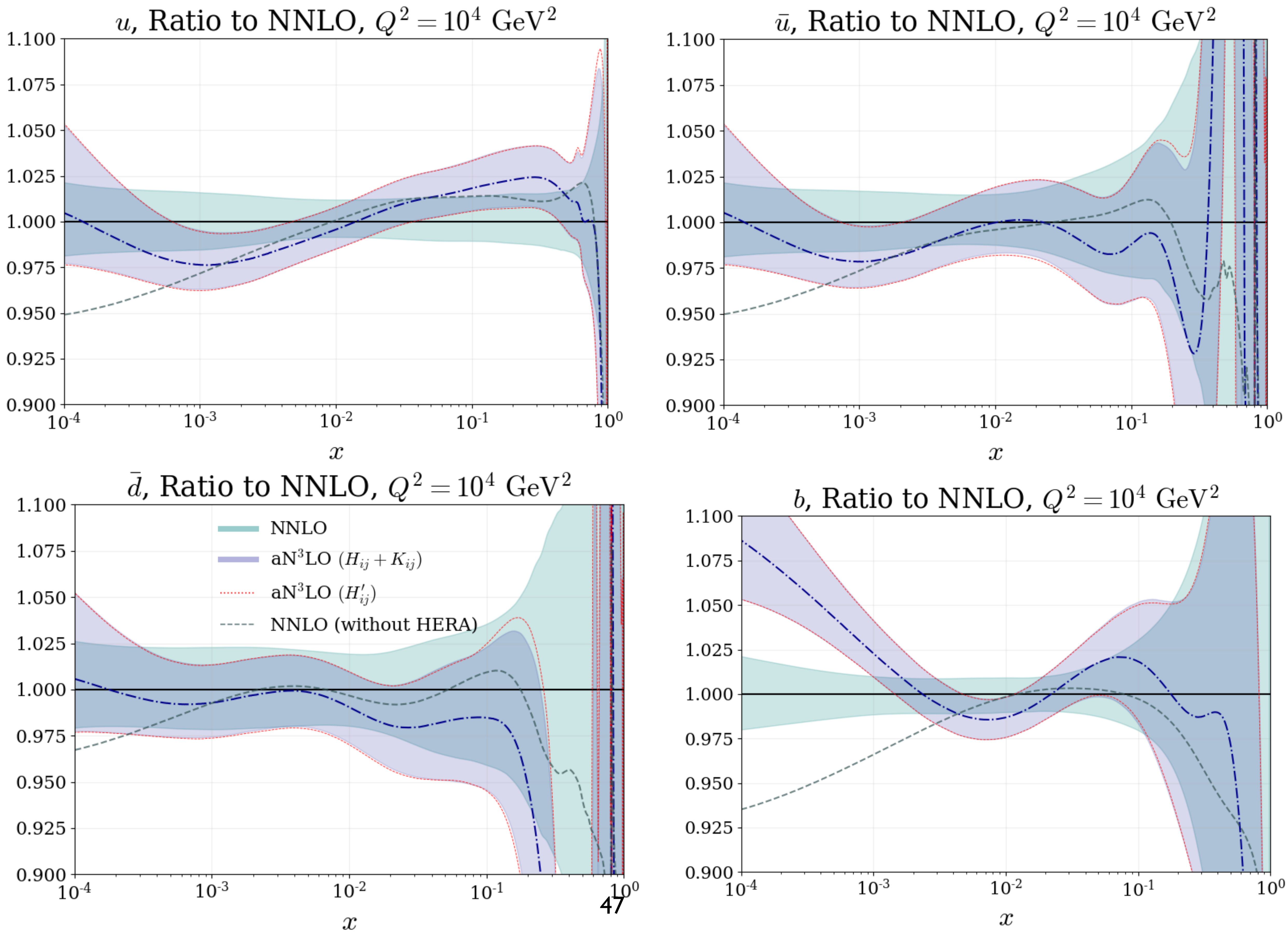
W. L. van Neervan and A. Vogt,
***Nucl.Phys.B* 588 (2000) 345-373,**
***Nucl.Phys.B* 568 (2000) 263-286**

★ Resulting K-factors: $Z\ p_\perp$

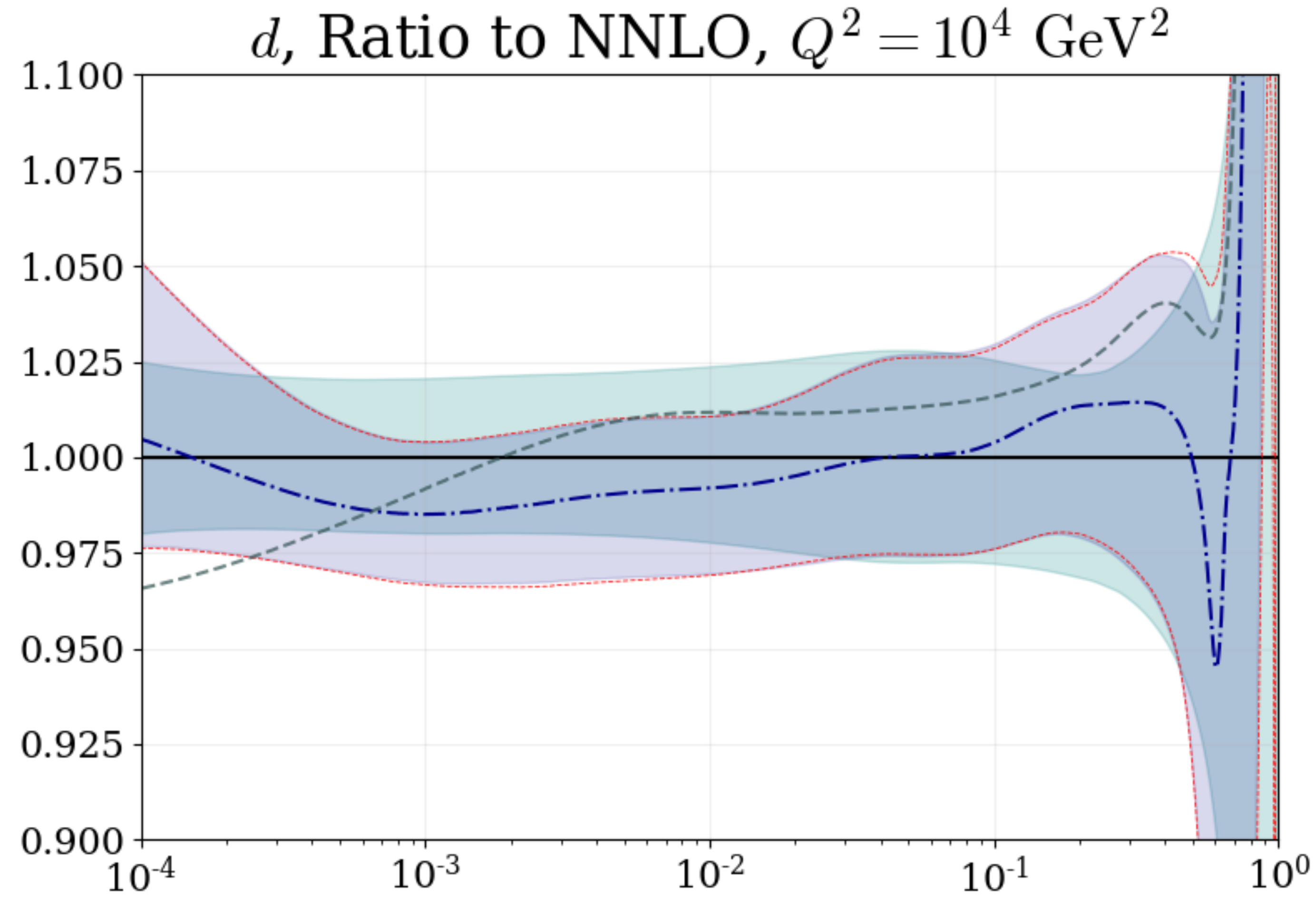


- Somewhat larger shift here. Arguably consistent with rather larger lower order corrections.
- **Note**: here (and elsewhere) K-factor is one preferred by fit $\Rightarrow$ may be tendency for this to lie towards 'all orders' result. Important when interpreting wrt perturbative stability.

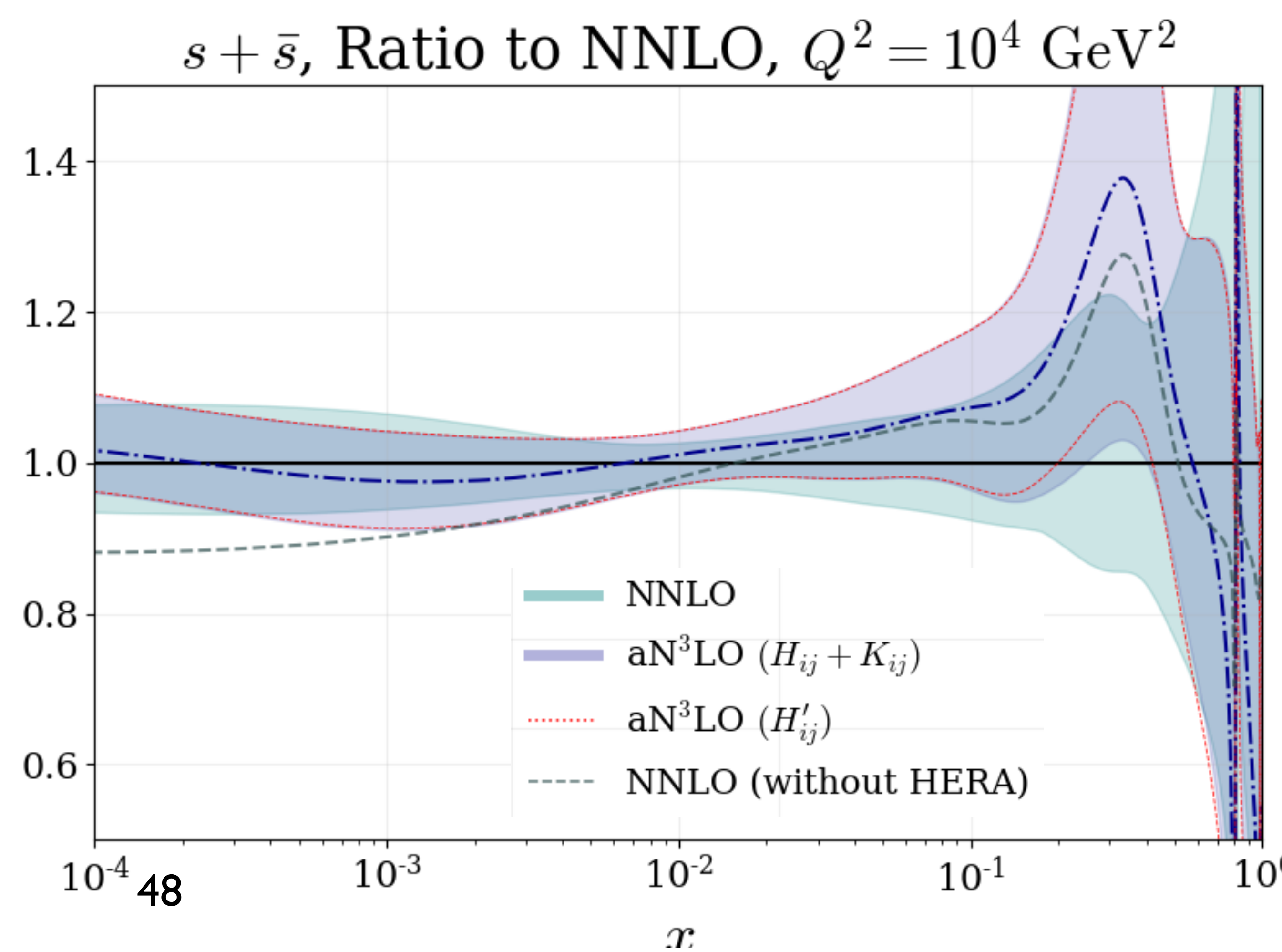
• Other PDFs…


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)

- Some enhancement in light quarks at high x .



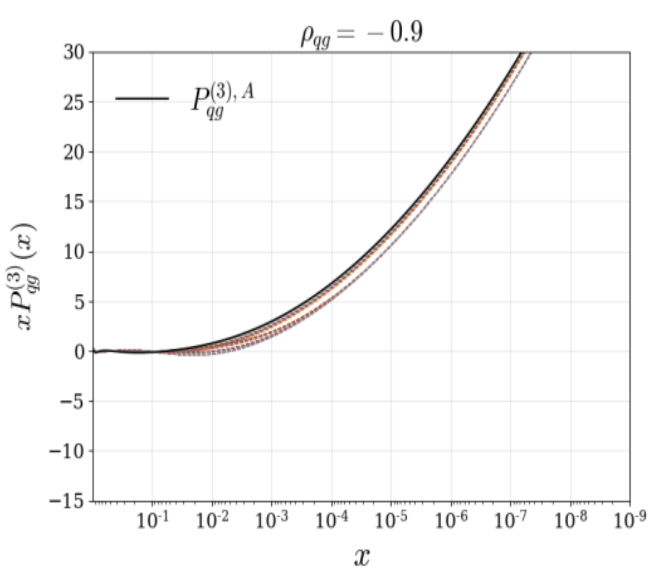
- Strange quark enhanced at high x .
- Follows the NNLO (no HERA) rather closely - reduced tensions.

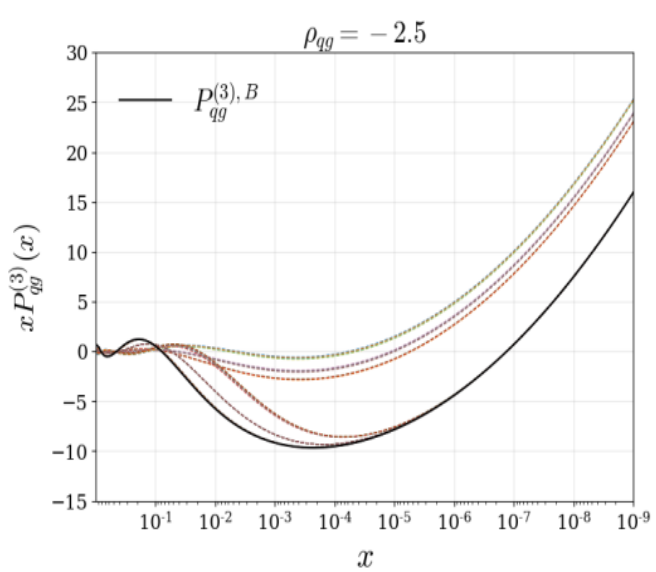


Other PDFs: backup

How to determine the priors:

- Key part of the theoretical nuisance parameter framework for missing N3LO pieces is setting up the priors and penalties on their variations.
- Q. How do we do this? A. Conservatively!
- Set ρ_{ab} prior variation by requiring:
  1. At low x bound set once exact expression $f_e(x, \rho_{ab})$ exits range of results from different (larger) x functional forms, e.g. see lower plots.
  2. At high x bound set if N3LO correction becomes too large (rare).
  3. Once functional form fixed, check range of prior and extend as necessary to incorporate different functional form variation.



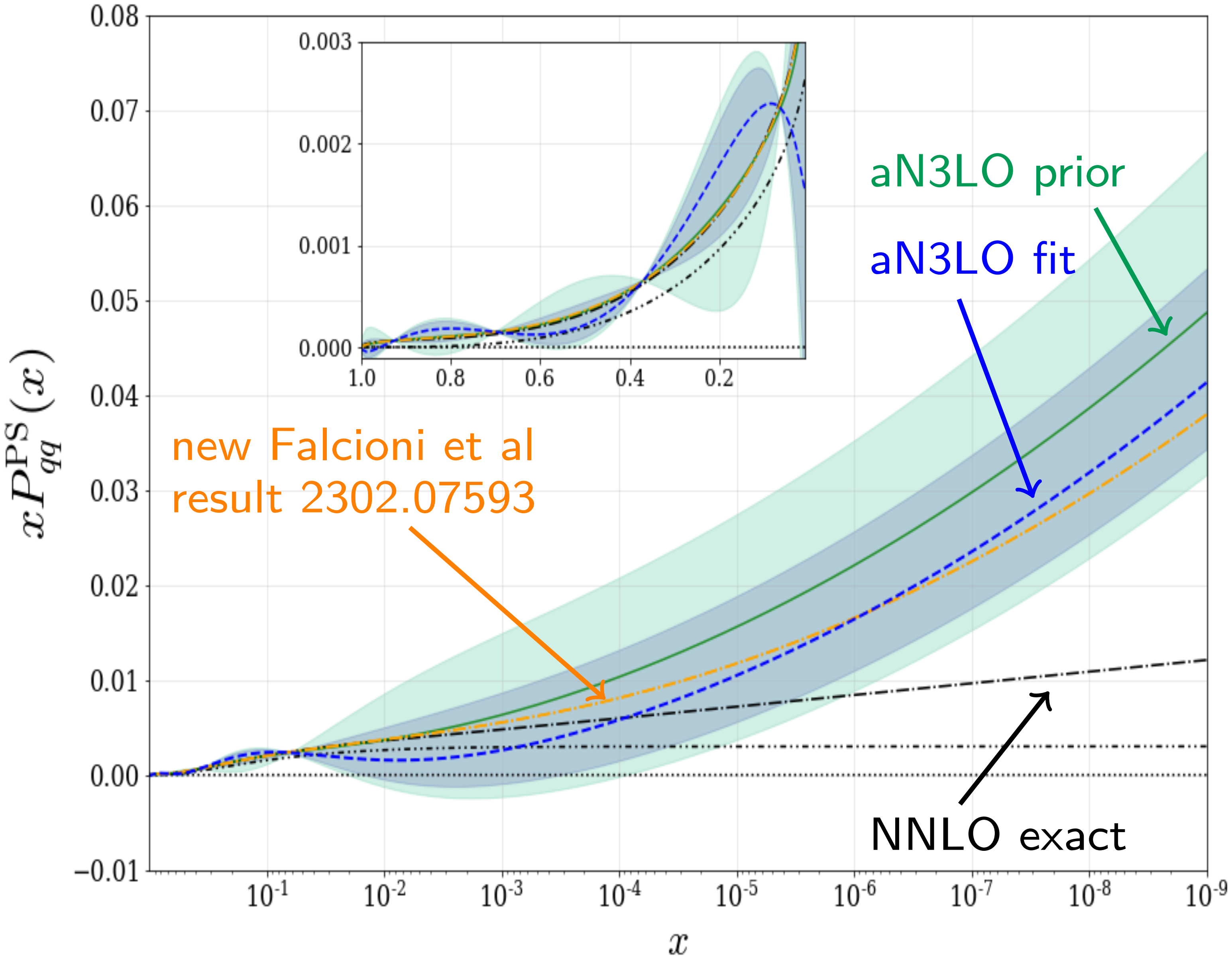


- Find penalties on theory nuisance parameters after fit are small and posterior errorbands reduced relative to prior $\Rightarrow$ prior set conservatively.

Further aN3LO information?:

What else could be added?:

- More information on high-x behaviour from threshold resummations.
- Cusp/virtual anomalous dimensions for P_{gg}, P_{qq}^{NS}.
  $\Rightarrow$ very high-x.
- N3LO k-factors as they become available for PDFs.
- $A_{gg,H}^{(3)}$ recently calculated. J. Ablinger et al 2211.05462.
- New info on P_{qq}^{PS}:
  - more moments
  - further low and high x log coefficients and fitting remaining logs.

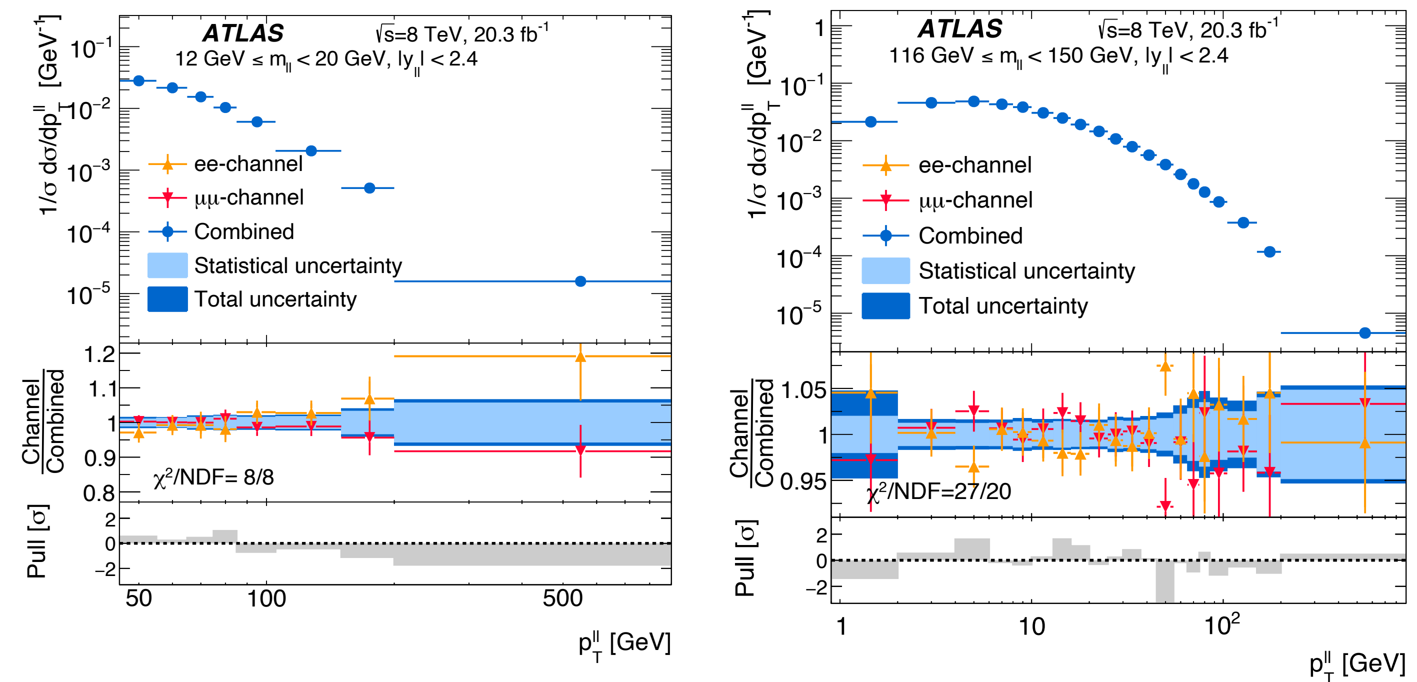


- Good agreement with our aN3LO result! Much better than NNLO!

ATLAS, G. Aad et al., Eur. Phys. J. C 76, 291 (2016)

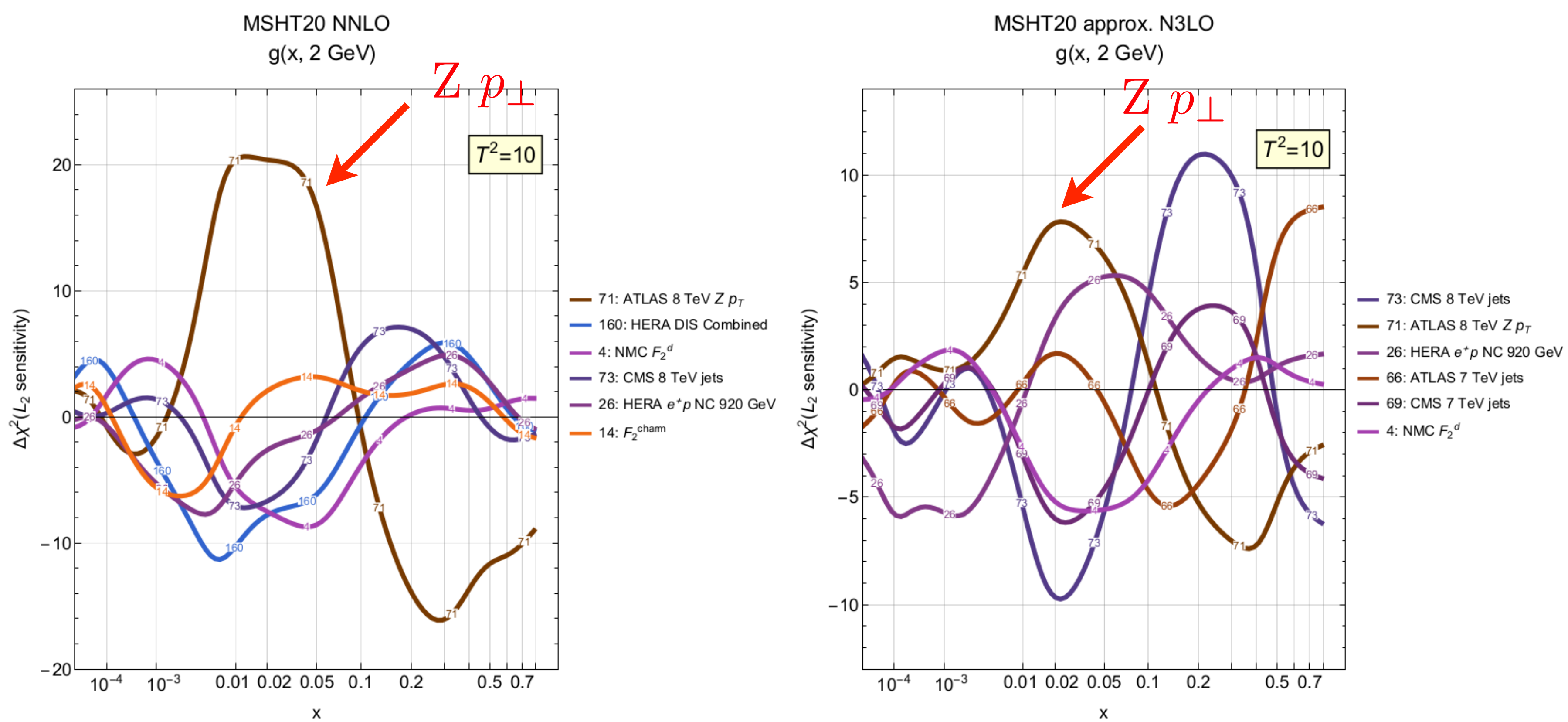
- ATLAS $Z\,p_\perp$ (more properly dilepton $p_\perp$) data presented double differentially in $m_{ll}, p_\perp^{ll}$

$12 < m_{ll} < 150\,\text{GeV} \quad p_\perp^{ll} > 30\,\text{GeV}$



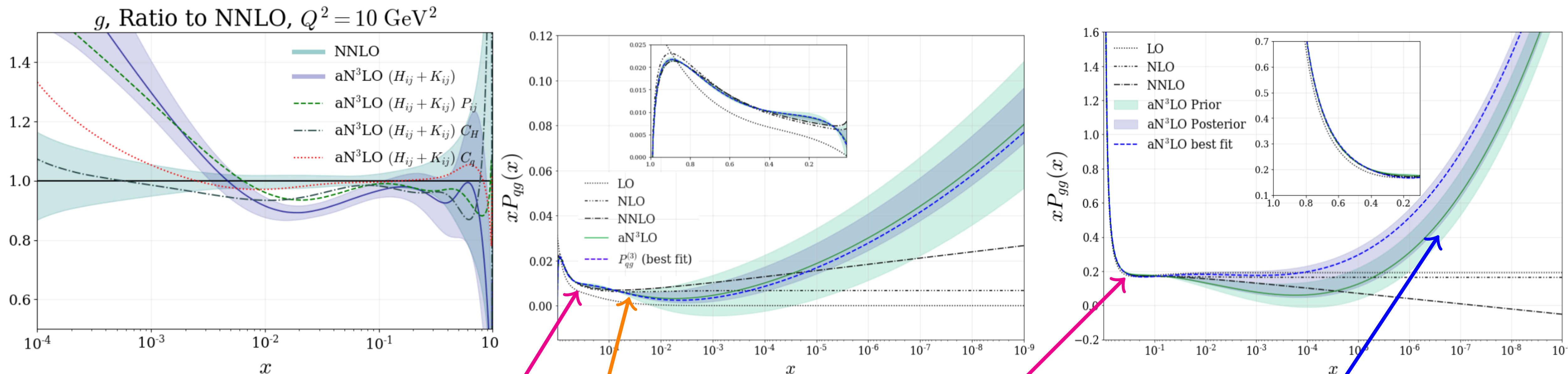
- Treatment of this dataset rather different between groups.
- Fit quality v. poor in default NNLO fit, with dramatic improvement at aN3LO (1.86 vs. 1.04), and highly sensitive to other data in fit (jets vs. dijets).

- Reduced **tension** at aN3LO also backed up by L2 sensitivities (reduced scale).



aN3LO PDFs - What causes the changes in the gluon?:

- Around $10^{-2} \lesssim x \lesssim 10^{-1}$ P_{ij}, C_H contribute $\approx$ equally. Also some C_q.
- At low x P_{ij} dominate, this contains much known N3LO information.



- Known Mellin moments tightly constrain high x splitting functions.
- At intermediate x increased P_{qg} and momentum sum rule affect gluon.
- At small x, LL and NLL (latter for P_{gg}) resummed pieces dominate.
- P_{gq} (not shown) has largest power of unknown log: $\log^2(1/x)/x$.
- Most singular NNLO term at small x in P_{gg} $(\alpha_S^3/x \log^2(1/x))$ is 0, so expect new N3LO piece $(\alpha_S^4/x \log^3(1/x))$ to cause significant change.

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.

Splitting Functions

- Start with QCD splitting functions:

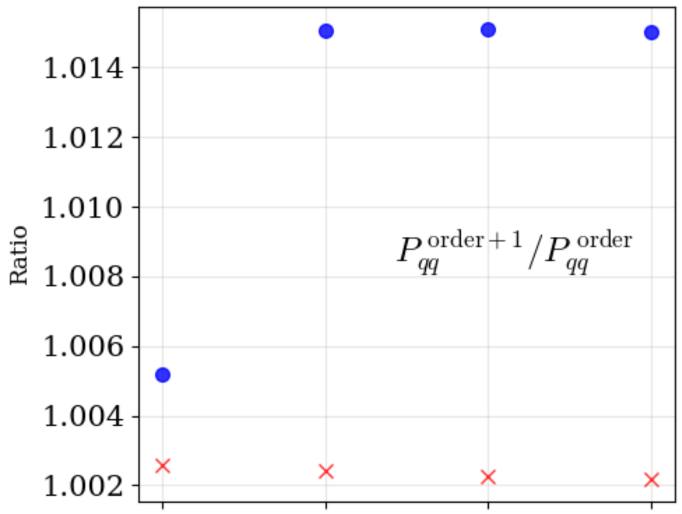
$$\boldsymbol{P}(x,\alpha_s) = \alpha_s \boldsymbol{P}^{(0)}(x) + \alpha_s^2 \boldsymbol{P}^{(1)}(x) + \alpha_s^3 \boldsymbol{P}^{(2)}(x) + \alpha_s^4 \boldsymbol{P}^{(3)}(x) + \ldots$$

- 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 $N \geq 8$
$$\int_0^1 \mathrm{d}x\, x^{N-1} P(x)$$
$\Rightarrow$ 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 $\boldsymbol{P}_{qg}^{(3)}(x)$:

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

Coefficient known

Form known
Coefficient unknown

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

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

- Pick one set of functions, with prior range in ρ set such that full $f_i(x)$ variation is covered and overall behaviour is reasonable, e.g.:

Overall:

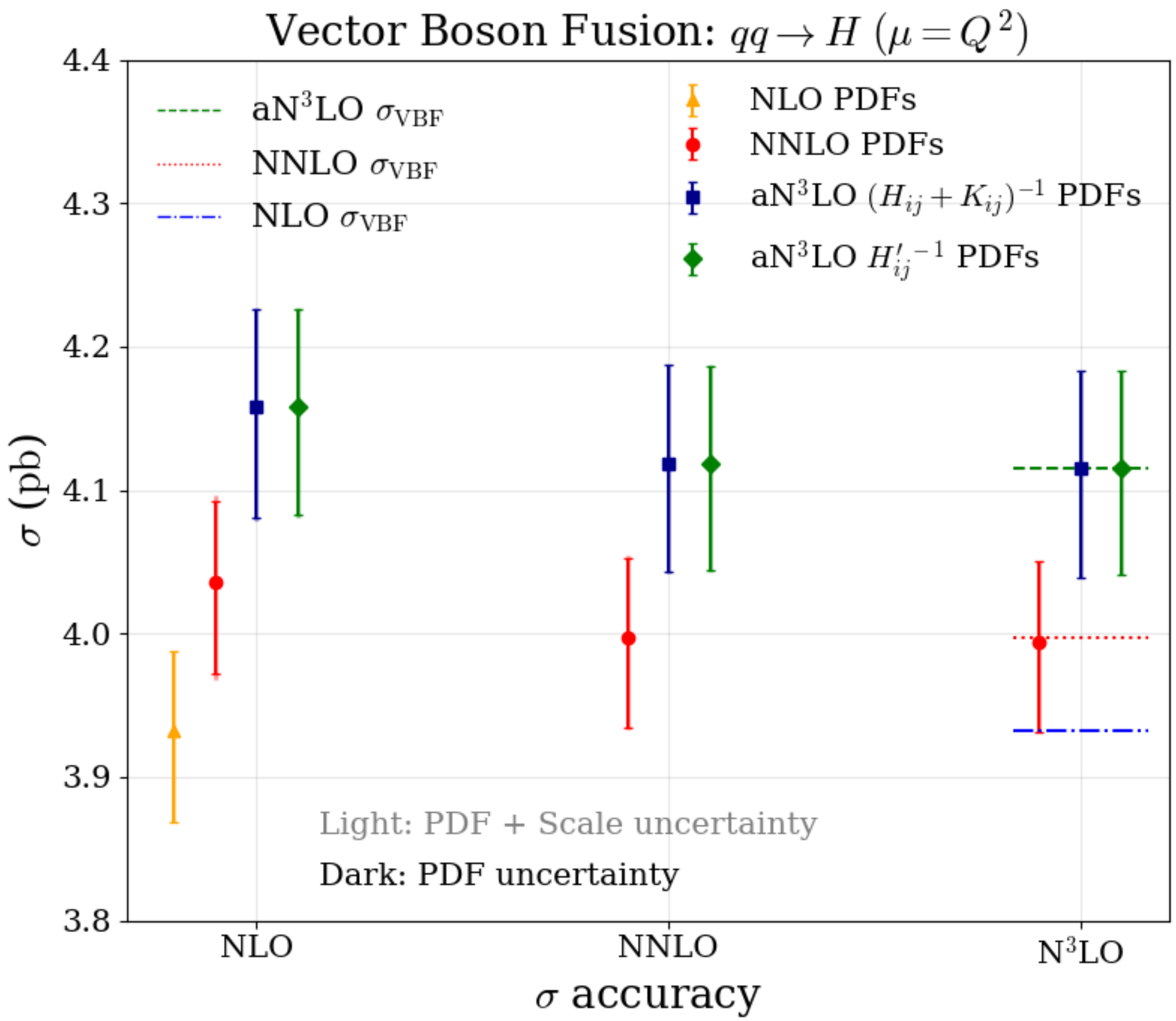
$$P_{qg}^{(3)}(x) = A_1 \ln^2 x + A_2 \ln x + A_3 x^2 + A_4 \ln(1-x) + \frac{C_A^3}{3\pi^4}\left(\frac{82}{81} + 2\zeta_3\right)\frac{1}{2}\frac{\ln^2(1/x)}{x} + \rho_{qg}\frac{\ln 1/x}{x}$$

- Some subjectivity in precise prior range of ρ / choice of $f_i(x)$, but:

  ⋆ Band of allowed $P(x)$ rather well constrained by known N3LO information (c.f. comparison to NNPDF later).

  ⋆ We allow ρ to vary as nuisance parameter $\Rightarrow$ reduced sensitivity to prior, with posterior range decided by fit.

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



NNLO K-factors - PDFs