Theoretical Uncertainties (and how to Tame them) at the LHC

The LHC Precision Program

Centro de Ciencias de Benasque, 3rd September 2023

Pedro Pascual Benasque Center for Science

Pedro Pascual
(academic grandfather)

Jose Ignacio Latorre
(academic father)

Founded in 1994, to provide Spain with an **Aspen-** or **Les Houches-like venue** for scientific gatherings

Almost **300 meetings**, with durations from a few days to several weeks, held since its foundation

Now covering **all areas of science** (from quantum information to cosmology) and beyond (wine-tasting!)

Pedro Pascual Benasque Center for Science

HEP group, University of Barcelona, 1984

Founde … gatherings

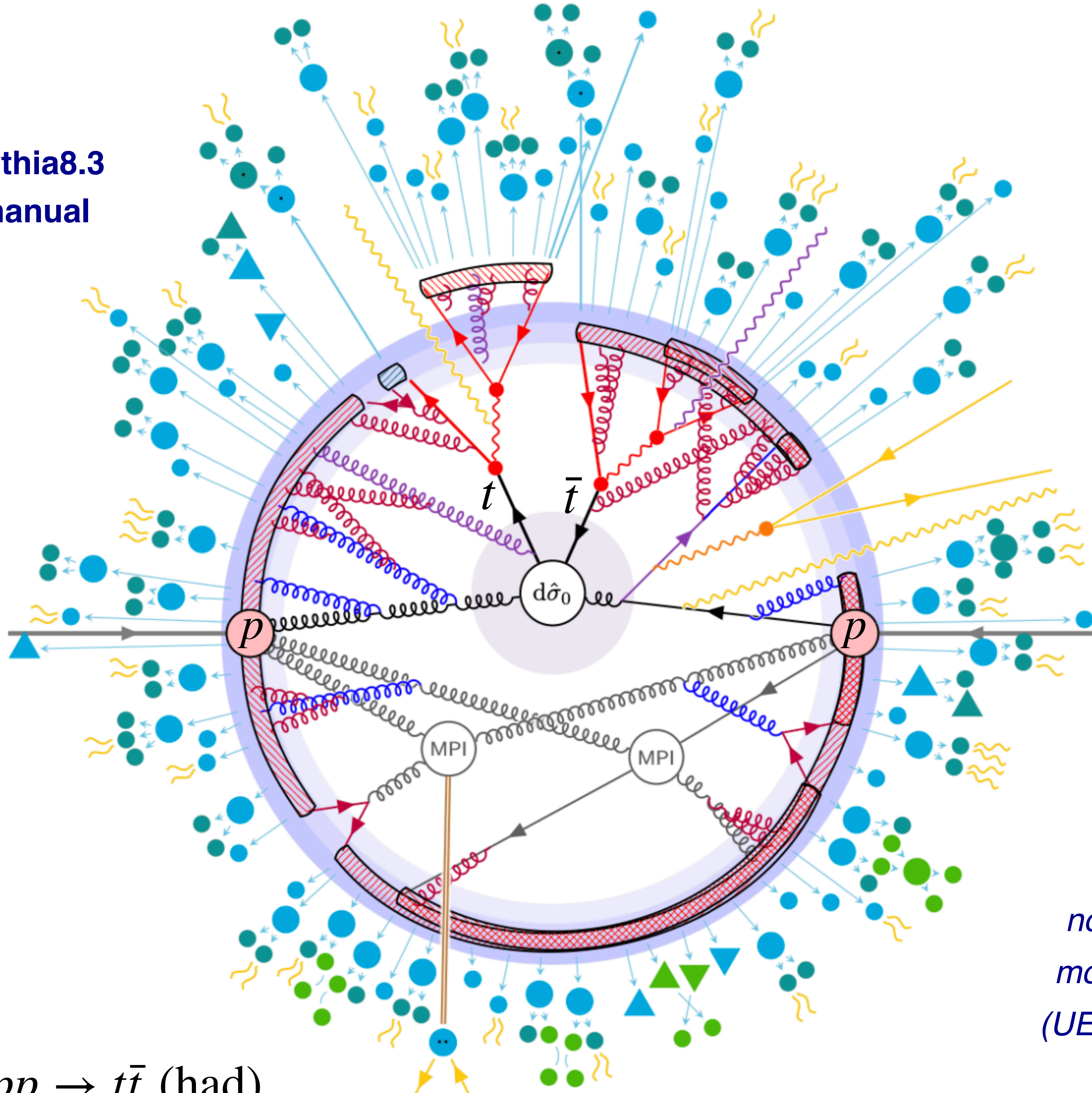
Almc … ndation

Now co … e-tasting!)

Theory Uncertainties at the LHC …

Modelling LHC collisions

Pythia8.3 manual



$pp \to t\bar{t}$ (had)

Theoretical predictions of LHC cross-sections involve:

- Proton structure: parton distributions
- Partonic matrix elements (QCD & EW)
- Parton shower (initial- and final-state)
- Hadronization & fragmentation
- Underlying event, MPI, pile up …..

Each of these ingredients comes with some **theoretical uncertainty**

note: some of these "theory" aspects of LHC modelling are often folded into measurements (UE, unfolding, acceptances, QED radiation ….)

specially parameters of MC models are under poor theoretical control!

Inclusive cross-sections

Inclusive processes (i.e. Drell-Yan) are theoretically the cleanest (experiment-independent).

$$\sigma_{\mathrm{LHC}}(M,s) \propto \sum_{ij} \int_{M^2}^{s} d\hat{s}\, \mathscr{L}_{ij}(\hat{s},s)\, \tilde{\sigma}_{ij}(\hat{s},\alpha_s(M)) \left[1+\mathcal{O}\,(\Lambda/M)^p\right]$$

Partonic luminosities (*non-perturbative, fit to data*)

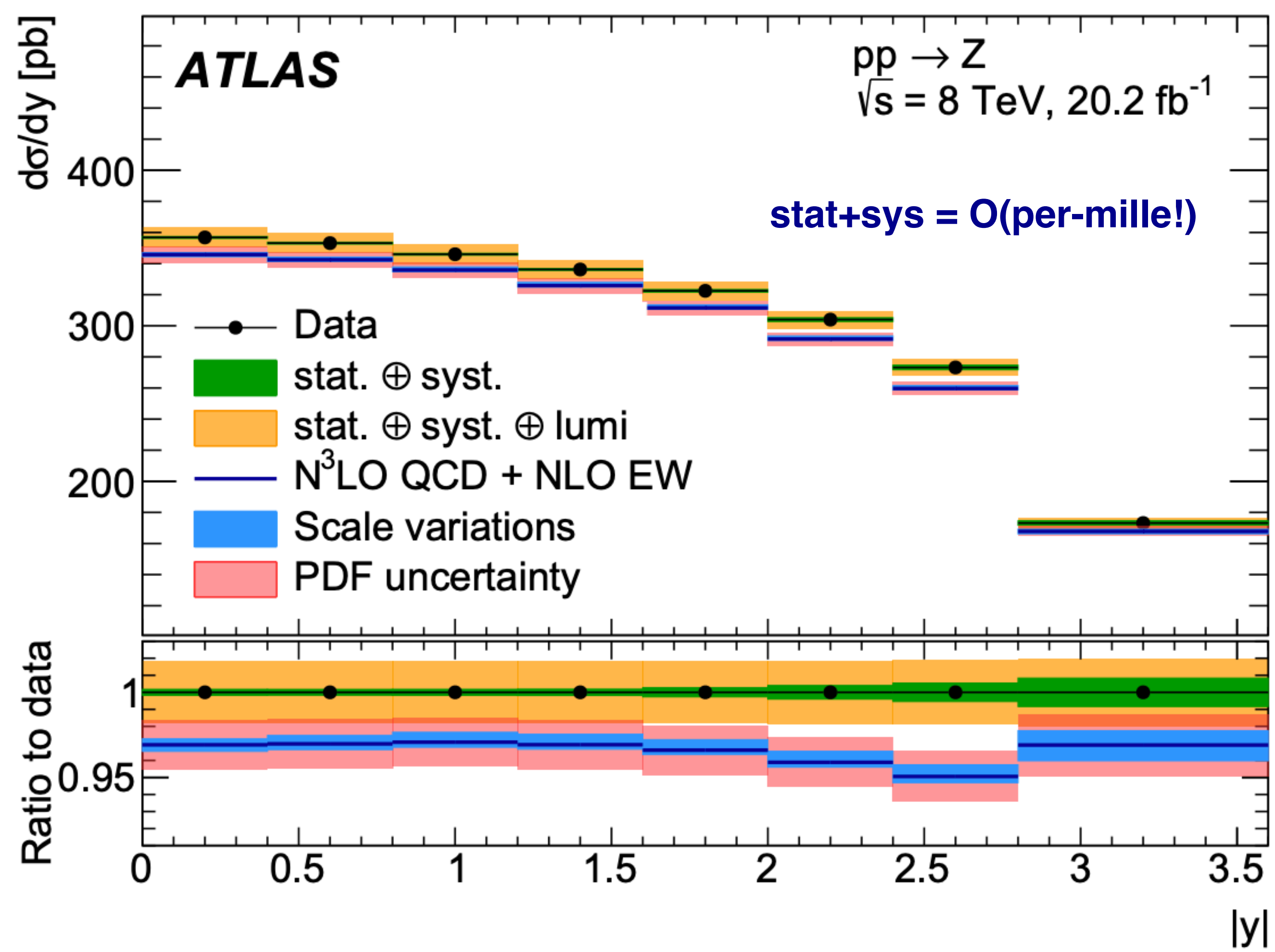
Hard-scattering cross-sections (*perturbative, from Feynman diagrams*)

low-scale QCD dynamics (*MC models, limited analytical understanding*)

At the **level of precision achieved by LHC experiments** (i.e. ATLAS Z pT 8 TeV) we'd better account for all theory errors in our predictions

theory & model uncertainties limiting factor for many LHC analyses

Of course, inclusive predictions do not match actual LHC measurements ….



Parton Distribution Functions

$$\sigma_{\rm LHC}(M,s) \propto \sum_{ij} \int_{M^2}^{s} d\hat{s}\; \mathcal{L}_{ij}(\hat{s},s)\, \tilde{\sigma}_{ij}(\hat{s},\alpha_s(M)) \left[1+\mathcal{O}\left(\Lambda/M\right)^p\right]$$

$$\mathcal{L}_{ij}(Q^2,s) = \frac{1}{s}\int_{Q^2/s}^{1} \frac{dx}{x} f_i\left(\frac{Q^2}{sx},Q\right) f_j\left(x,Q\right)$$

PDFs are **parametrised** at some low hadronic scale

$$xg(x,Q_0=1\ \mathrm{GeV},\{a\}) = f_g(x,a_g^{(1)},a_g^{(2)},\ldots)$$

then **constrained from global dataset**

$$\chi^2\left(\{\boldsymbol{a}^{(k)}\}\right) = \frac{1}{n_{\rm dat}} \sum_{i,j=1}^{n_{\rm dat}} \left(\sigma_{\rm i,th}(\{\boldsymbol{a}^{(k)}\}) - \sigma_{\rm i,exp}\right) \left({\rm cov}^{-1}\right)_{ij} \left(\sigma_{\rm j,th}(\{\boldsymbol{a}^{(k)}\}) - \sigma_{\rm j,exp}\right)$$

together with an estimate of the **associated uncertainties** (from the fitted data, methodology choices, input SM parameters, missing higher order QCD corrections…)

Several groups provide regular updates of their PDF determinations: NNPDF, CT, MSHT, ABM, ATLASPDFs, …

Results of LHC interpretations/measurements can depend sensitively of PDF treatment

Parton Distribution Functions

Reducing PDF uncertainties entering LHC predictions requires an **in-depth understanding of the differences between analysis**, i.e. differences between PDF sets do not ``go away" trivially when adding more data or using more precise theory calculations

ATLAS strong coupling extraction from Z pT data at 8 TeV

	PDF set	$\alpha_s(m_Z)$	PDF uncertainty	g [GeV^2]	q [GeV^4]
baseline	MSHT20 [37]	0.11839	0.00040	0.44	−0.07
	NNPDF4.0 [84]	0.11779	0.00024	0.50	−0.08
	CT18A [29]	0.11982	0.00050	0.36	−0.03
	HERAPDF2.0 [65]	0.11890	0.00027	0.40	−0.04

$$\Delta_{\mathrm{PDF}}\left(\mathrm{MSHT20\ only}\right) = 0.34\,\%$$

$$\Delta_{\mathrm{PDF}}\left(\mathrm{NNPDF4.0} - \mathrm{CT18A}\right) = 1.6\,\%$$

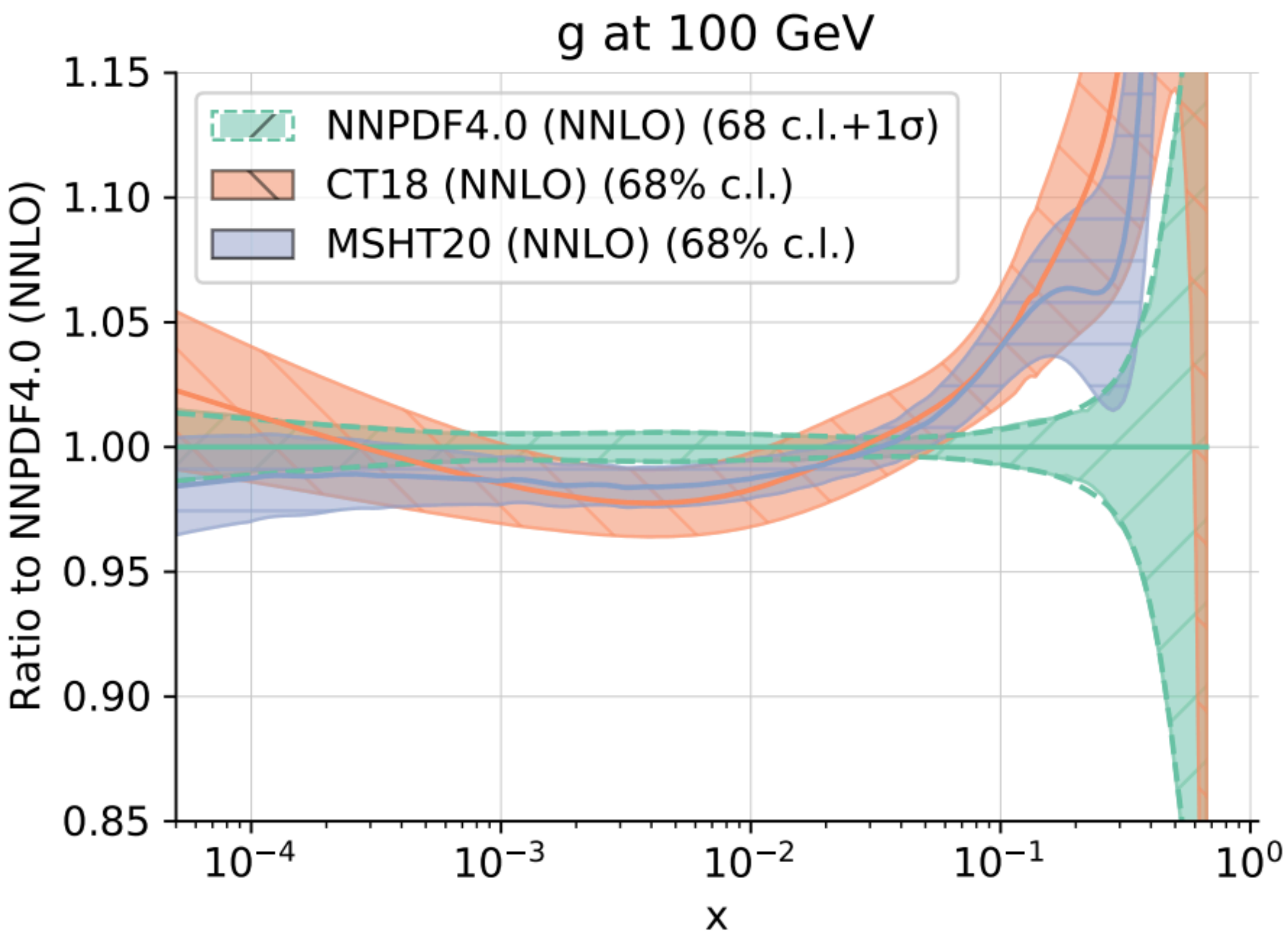
What is the ``true PDF uncertainty" that should be associated to this measurement?

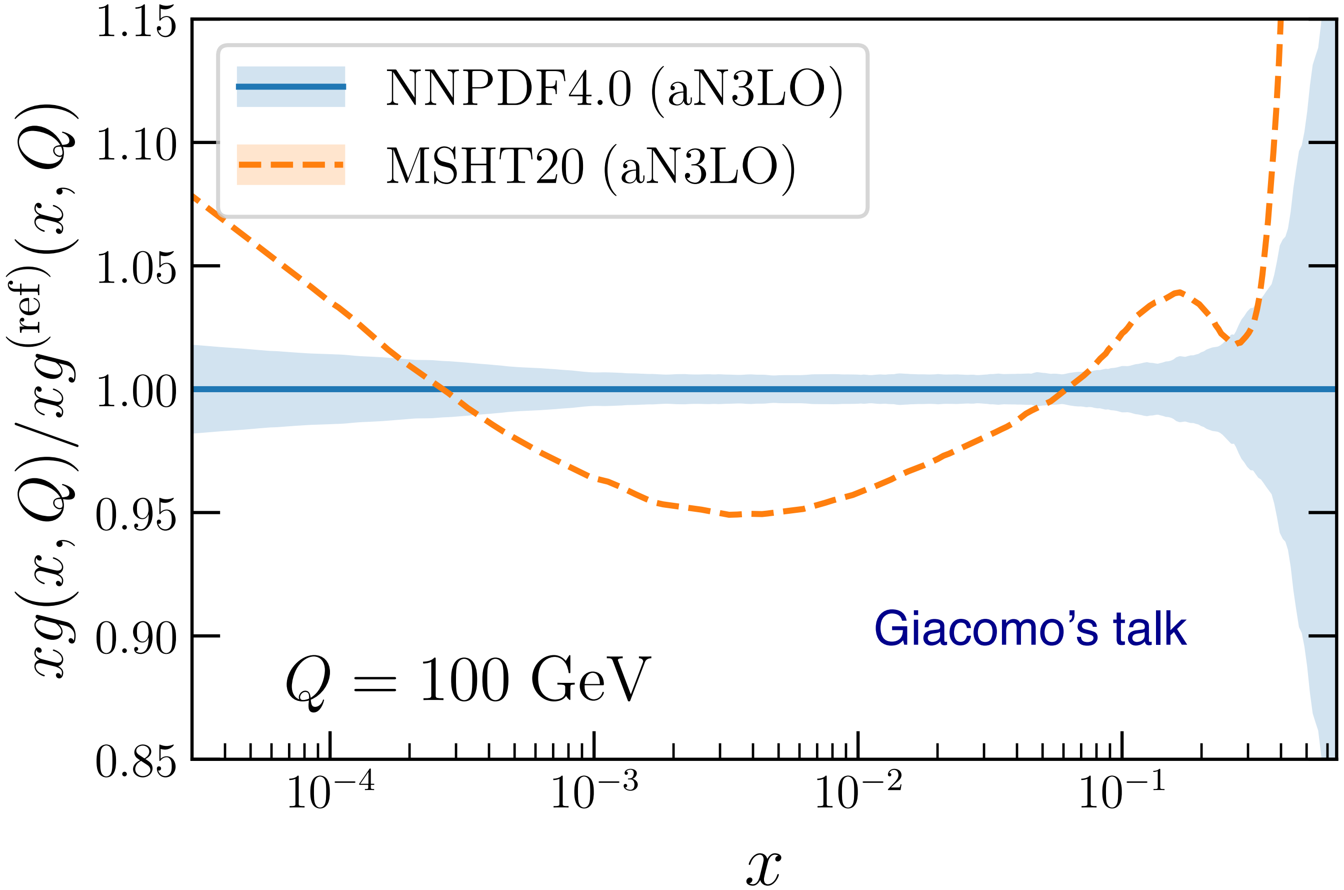
Even within the same experiment, the **baseline PDF is different** for each analysis i.e. ATLAS takes CT18 as central value for *W*-mass extraction …

is this a satisfactory situation?

Parton Distribution Functions

Maybe PDF differences are reduced as we improve our theory calculations by going to **N³LO QCD**?

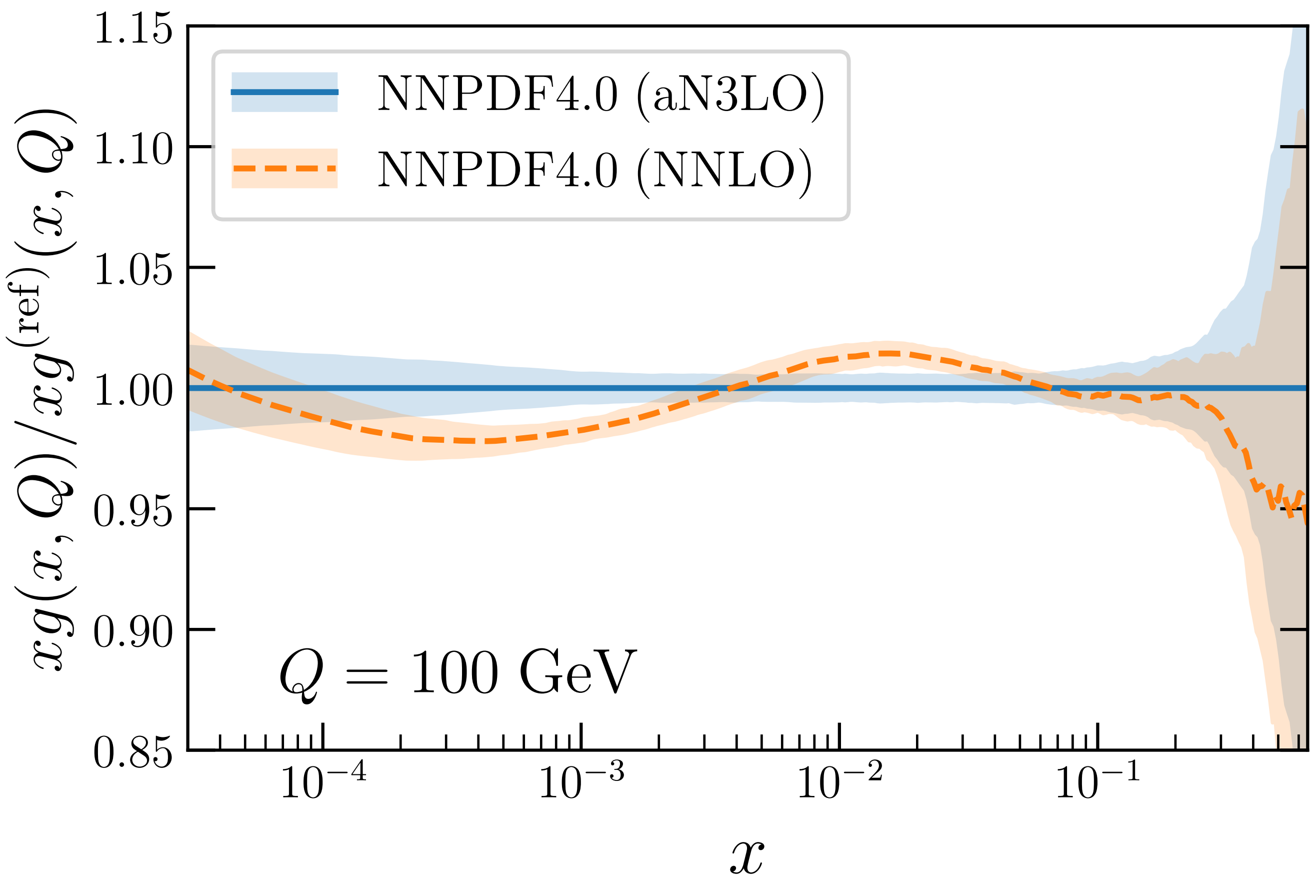


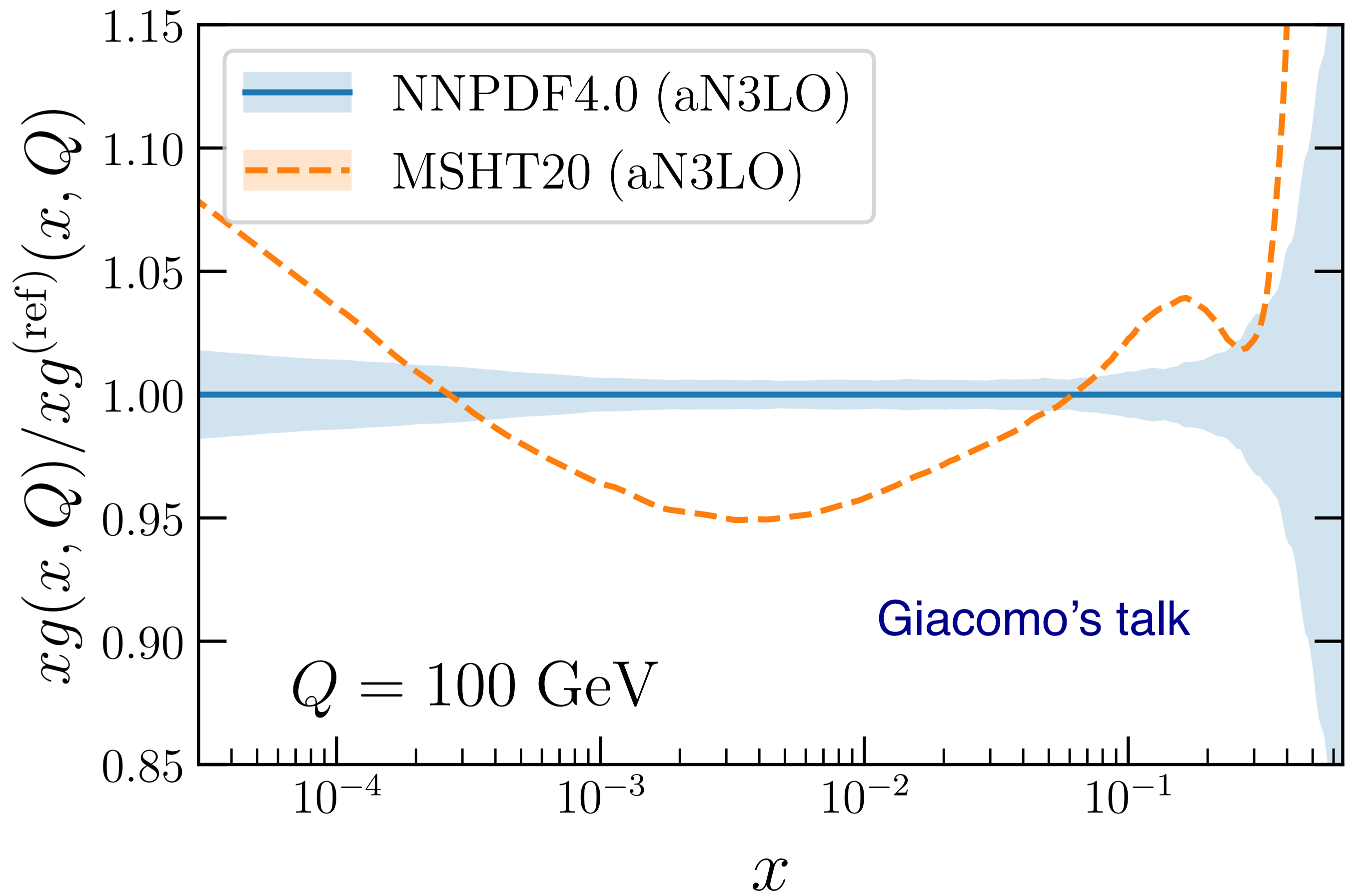


on the contrary, differences between MSHT20 and NNPDF4.0 increase in the **N³LO QCD fits**

Parton Distribution Functions

Maybe PDF differences are reduced as we improve our theory calculations by going to **N³LO QCD**?





on the contrary, differences between MSHT20 and NNPDF4.0 increase in the **N³LO QCD fits**

but no need to panic, we understand why this happens!

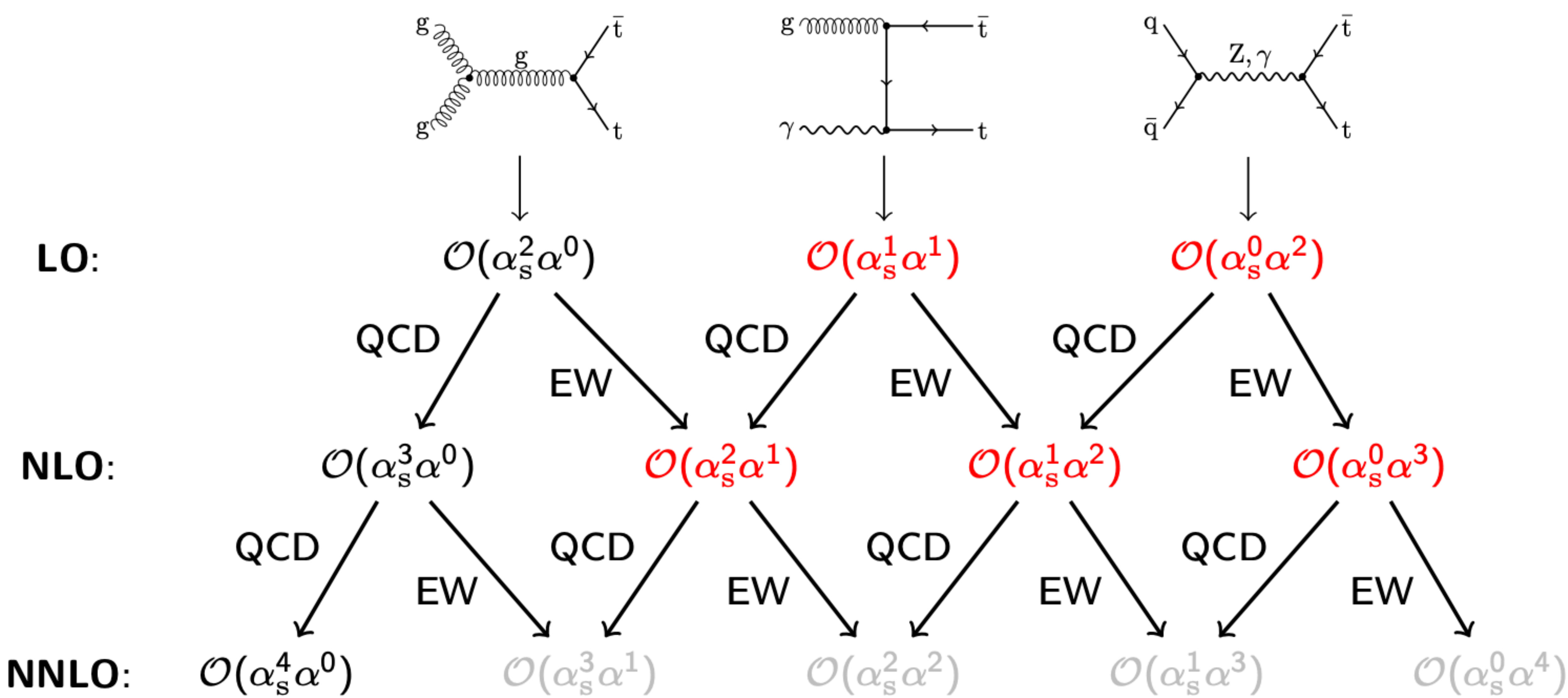
N³LO corrections to PDFs are moderate except for small-*x* physics

Take-away message: take seriously **differences in PDF sets,** don't hide them under the carpet

Hard-scattering cross-sections

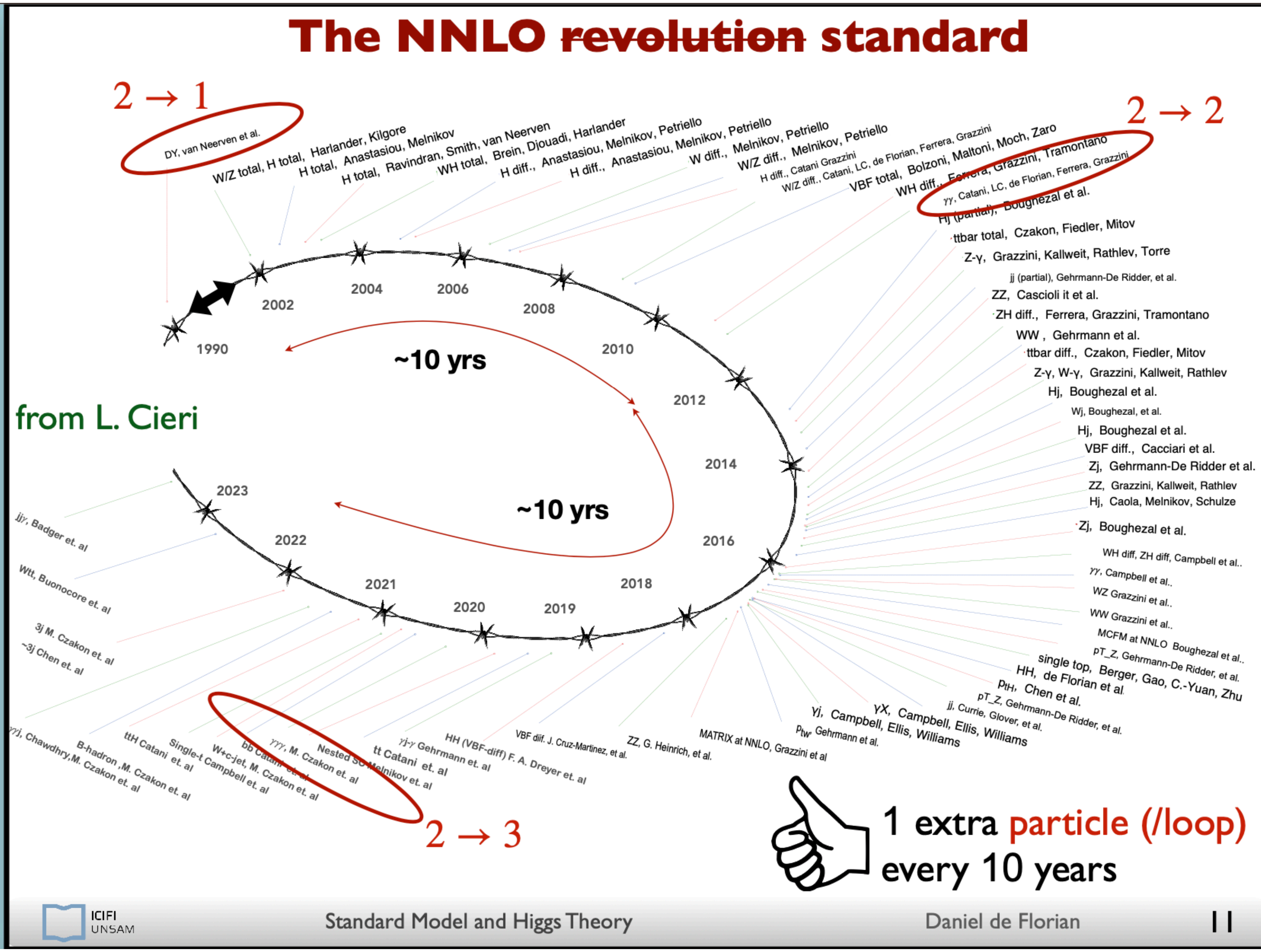
$$\sigma_{\mathrm{LHC}}(M,s) \propto \sum_{ij}\int_{M^2}^{s} d\hat{s}\; \mathscr{L}_{ij}(\hat{s},s)\; \tilde{\sigma}_{ij}(\hat{s},\alpha_s(M))\left[1+\mathcal{O}\left(\Lambda/M\right)^p\right]$$

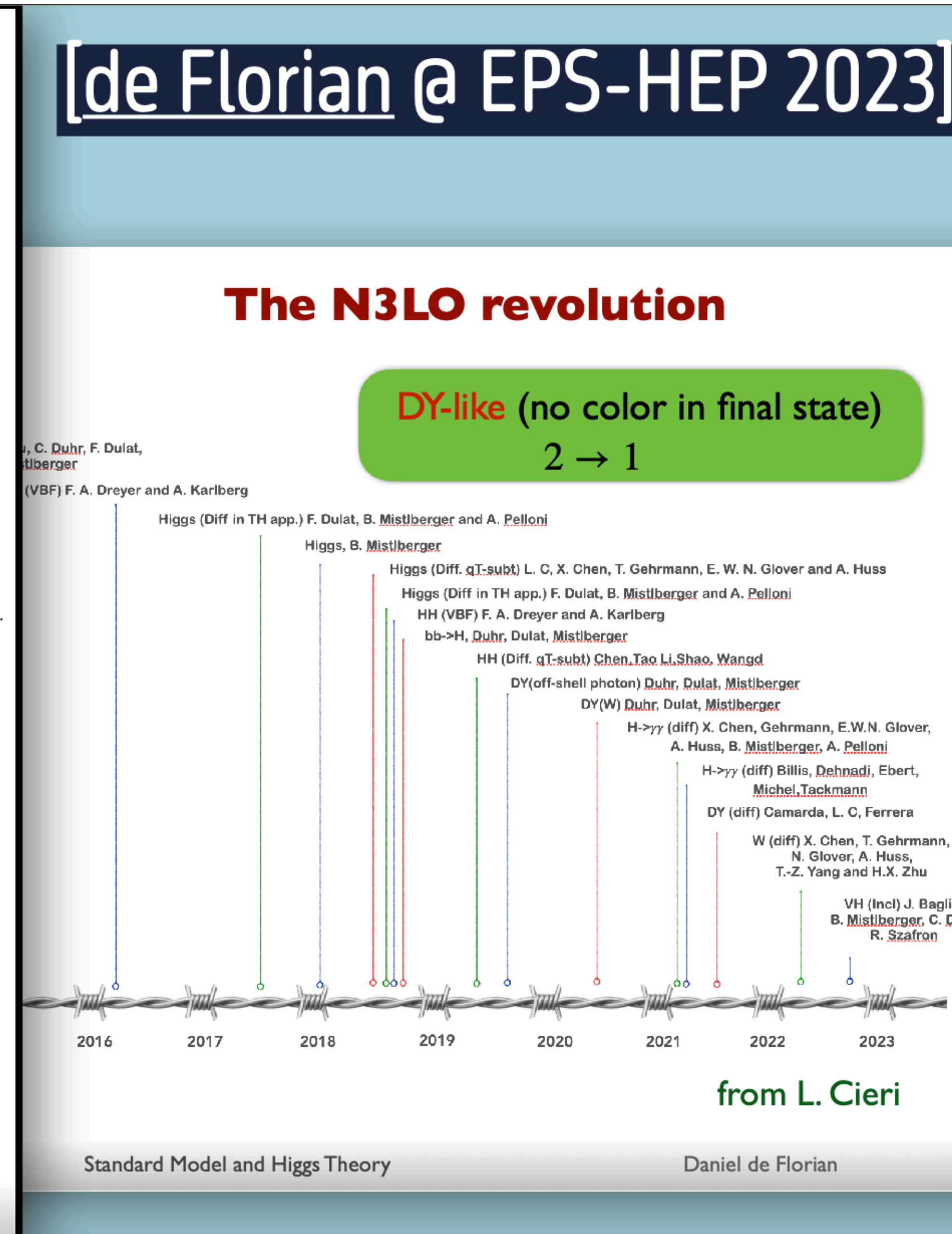
$$\tilde{\sigma}_{ij}(\hat{s},\alpha_s,\alpha = \sigma_{\mathrm{B}} \times \left(1+\sum_{i=1}\sum_{j=0}\alpha_s^i\alpha^j\tilde{\sigma}_{ij}\right)$$



Hard-scattering cross-sections

The higher the accuracy of the perturbative calculation,
the smaller the **missing higher order uncertainties (MHOUs)**



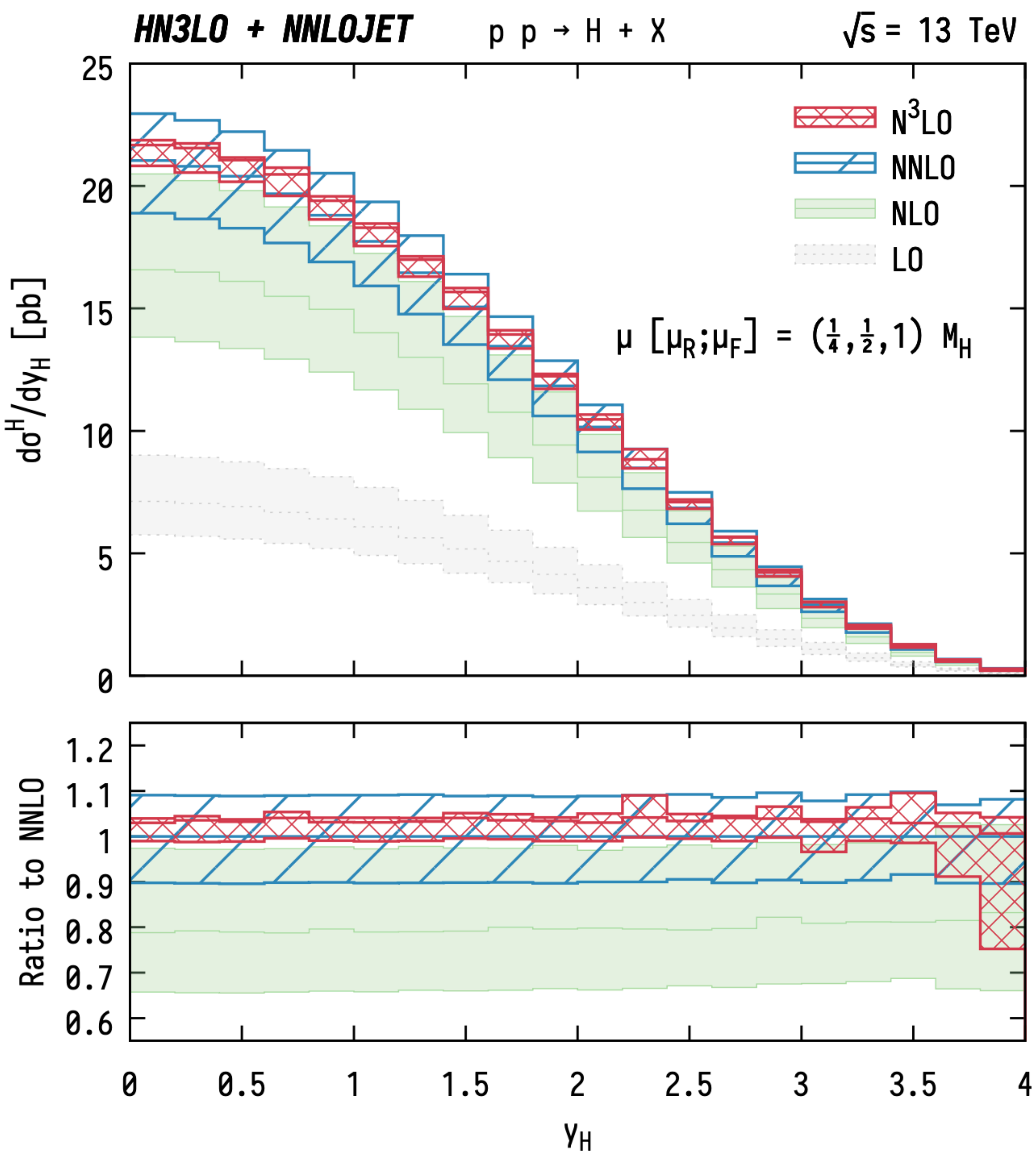


Immense progress in NNLO and N3LO calculations, NLO electroweak corrections, matching to showers …

However, increased accuracy may or may not result in improved precision

Hard-scattering cross-sections

Why **higher-order QCD calculations** are important?



Chen et al, 2102.07607

Fully differential N3LO **Higgs in gluon-fusion**

$$\widetilde{\sigma}(\alpha_s, \alpha) = \widetilde{\sigma}^{(0)} \left(1 + c_{1,0}\alpha_s + c_{2,0}\alpha_s^2 + c_{3,0}\alpha_s^3\right)$$

NLO *NNLO* *N3LO*

- Improved **precision & accuracy**: enhance physics reach of the same measurement
- Reliable estimate of **missing higher-order uncertainties** (MHOUs)
- Assess convergence of **perturbative expansion**

For Higgs rapidity distribution in gluon fusion:

- NLO: first sensible estimate of MHOUs
- NNLO: required for O(10%) precision
- N3LO: required for **few-percent** precision
- Good convergence of perturbative expansion

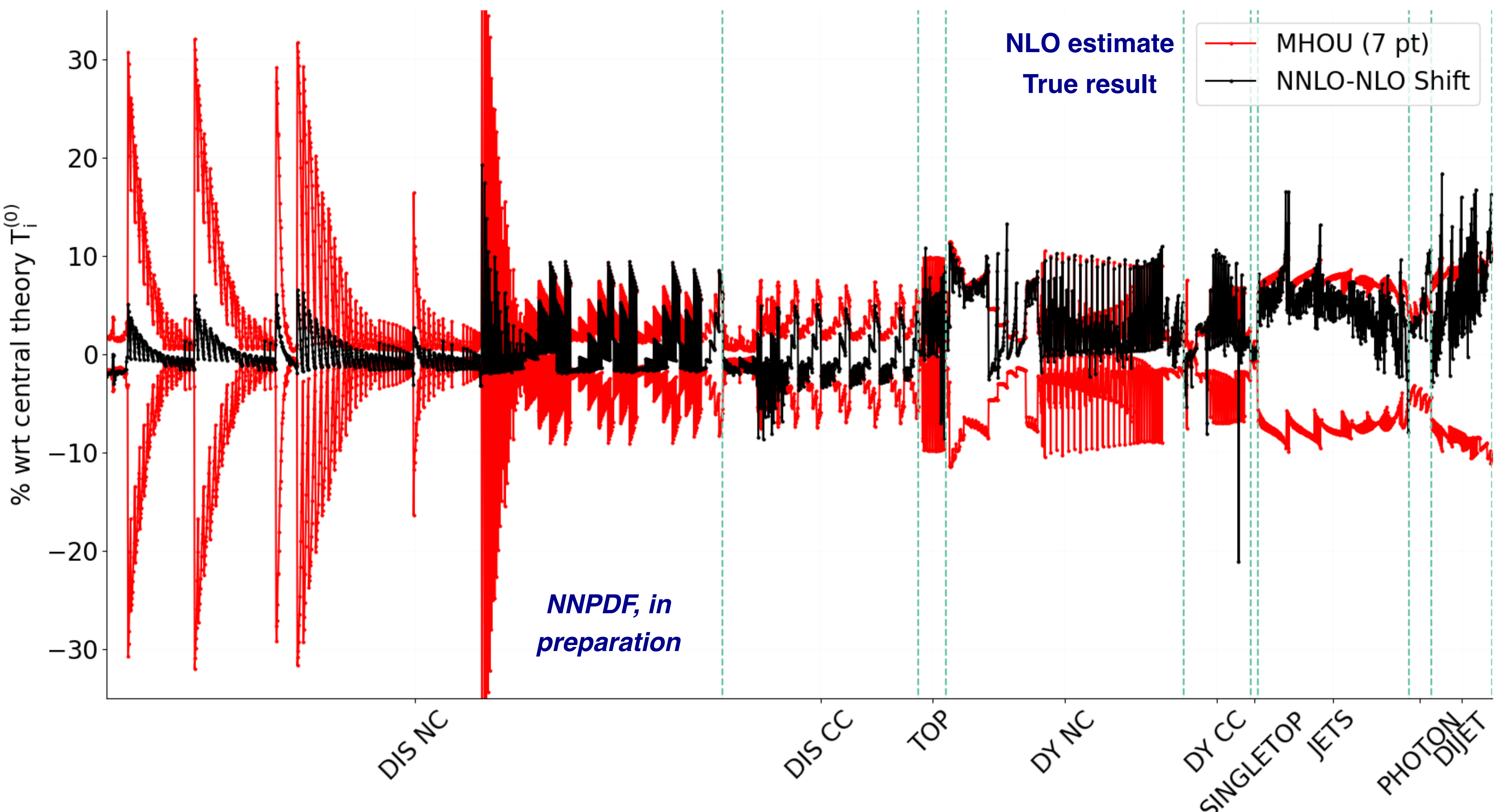
MHO uncertainties

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\mathcal{O}}(\mathcal{O},\xi_{\mathrm{R}},\xi_{\mathrm{F}}) = \sum_{a,b}\int_0^1 \mathrm{d}x_1 \int_0^1 \mathrm{d}x_2 \int_{Q^2_{\min}}^{Q^2_{\max}} \mathrm{d}Q^2\, f_a(x_1,\xi^2_{\mathrm{F}}Q^2) f_b(x_2,\xi^2_{\mathrm{F}}Q^2)\sigma_{ab}(x_1,x_2,Q^2,\xi_{\mathrm{R}},\xi_{\mathrm{F}})$$

LHC observables depend on arbitrary scales: the **factorisation** and **renormalisation scale**

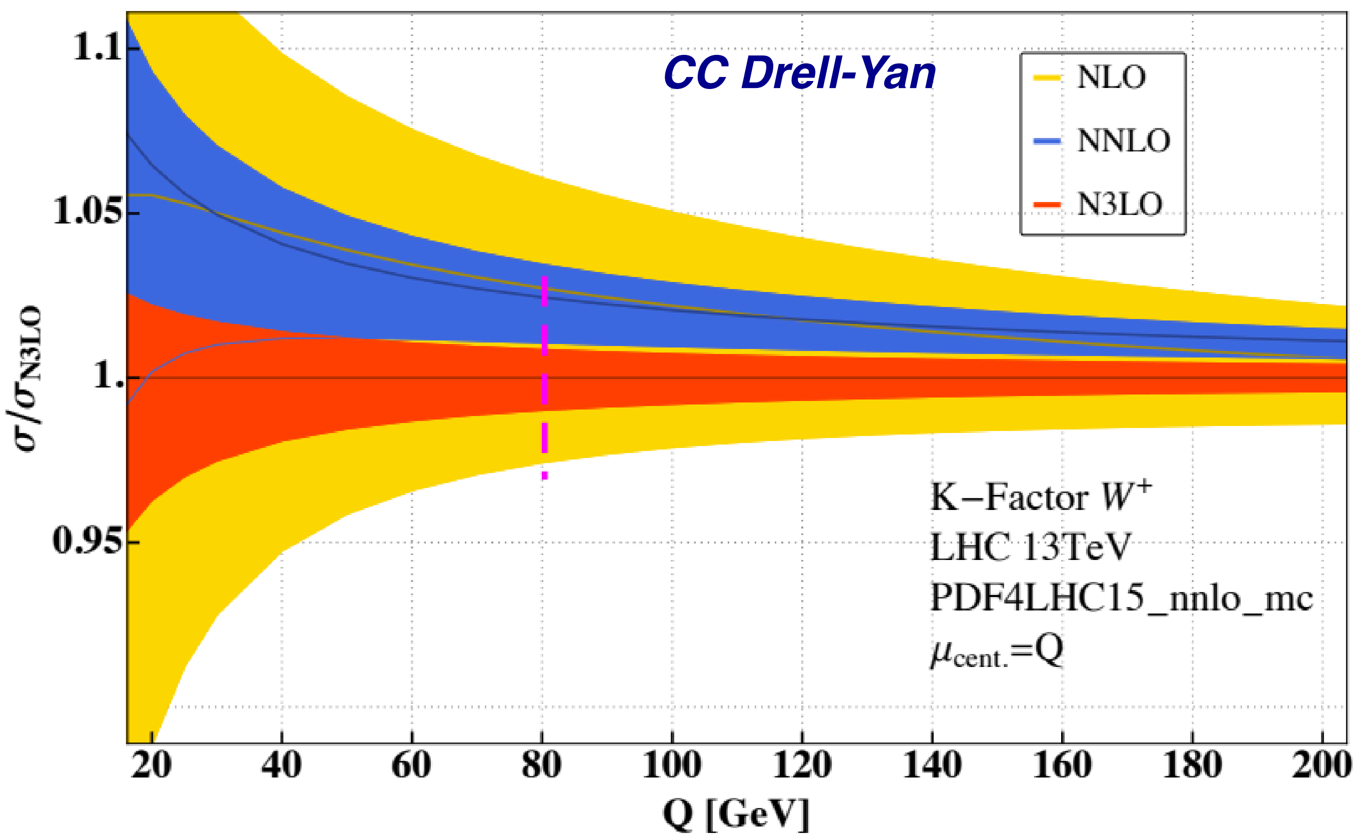
$$\mu_F = \xi_F Q \qquad \mu_R = \xi_R Q$$

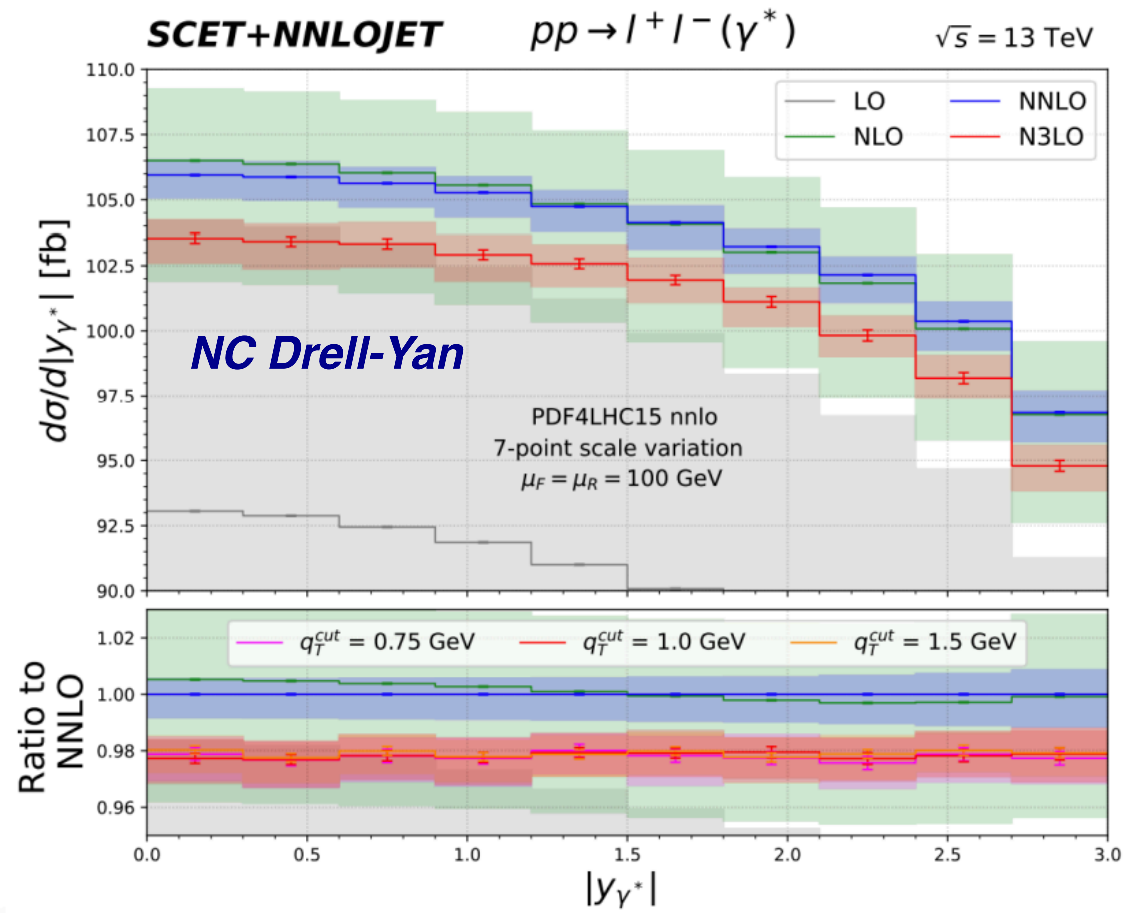
This dependence is artefact of perturbative series truncation: their variation **estimates the MHOUs**



Accuracy = Precision?

Several examples in which NNLO and N³LO calculations (for fixed PDFs) **do not overlap** within MHOUs





Ongoing studies with the theory community to understand this effect

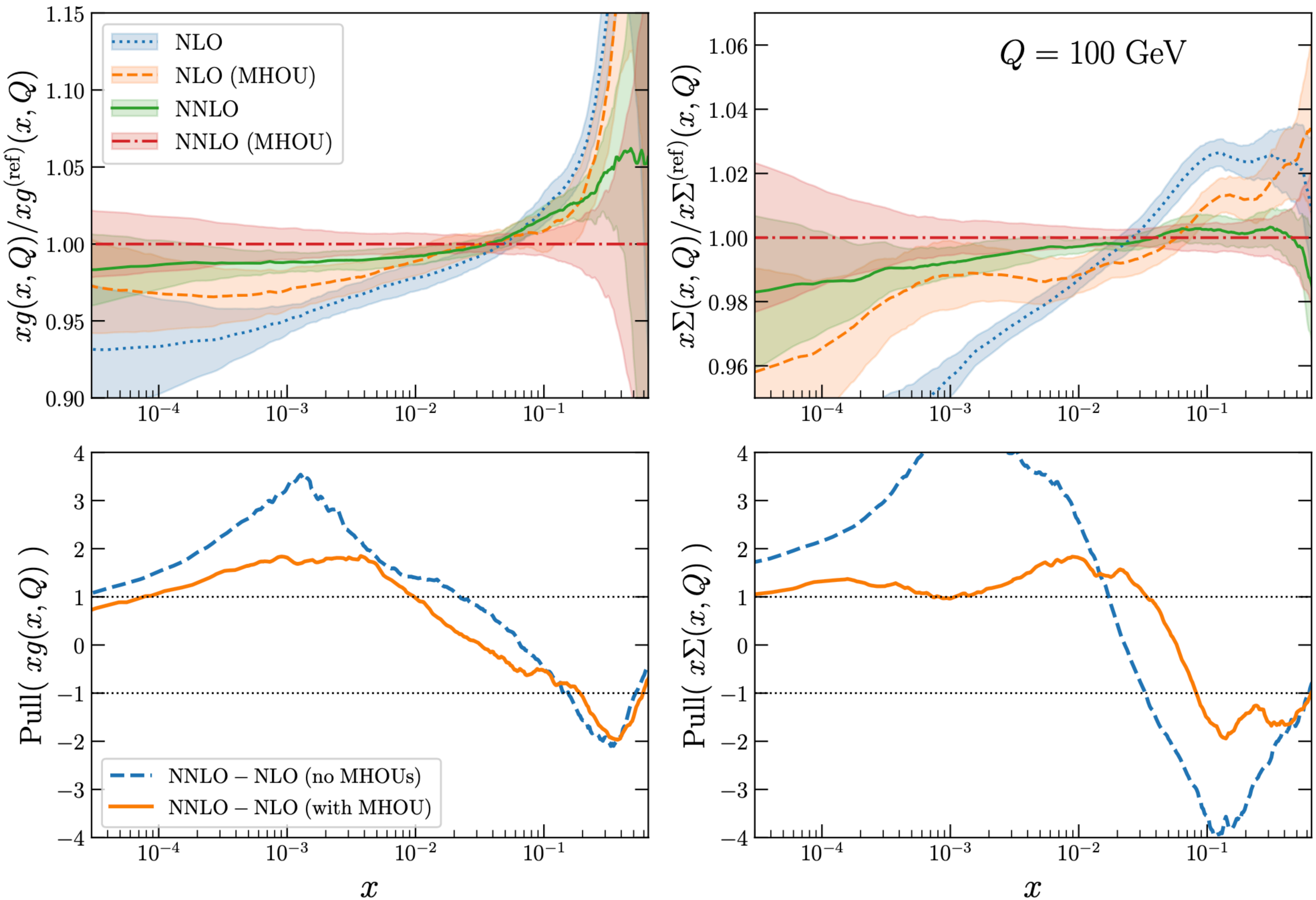
- Solved by aN³LO PDFs? By PDFs which include MHOUs in the fit?
- Different methods to estimate MHOU not based on scale variations? Bayesian approaches?
- Agreement improved or worsened once fiducial cuts are applied?

N³LO LHC phenomenology still in its infancy, a lot to learn still

PDF fits with MHOUs

PDF uncertainties **do not account for MHOUs**: NNLO PDFs not necessarily more precise than NLO

NNPDF: **global fits with MHOUs up to N³LO**, with improved perturbative convergence!



Non-perturbative power corrections

$$\sigma_{\rm LHC}(M,s) \propto \sum_{ij} \int_{M^2}^{s} d\hat{s}\, \mathscr{L}_{ij}(\hat{s},s)\, \widetilde{\sigma}_{ij}(\hat{s},\alpha_s(M)) \left[1 + \mathcal{O}\left(\Lambda/M\right)^p\right]$$

$$\mathcal{O}\left(\Lambda/M\right)^p \rightarrow p = 1,\ M = 100\ \text{GeV} \rightarrow 1\,\%\ \text{correction}$$

$$\mathcal{O}\left(\Lambda/M\right)^p \rightarrow p = 2,\ M = 10\ \text{GeV} \rightarrow 1\,\%\ \text{correction}$$

These non-perturbative effects can play a key role given precision of current LHC data

Recent progress in understanding the role of these effects from first-principle calculations

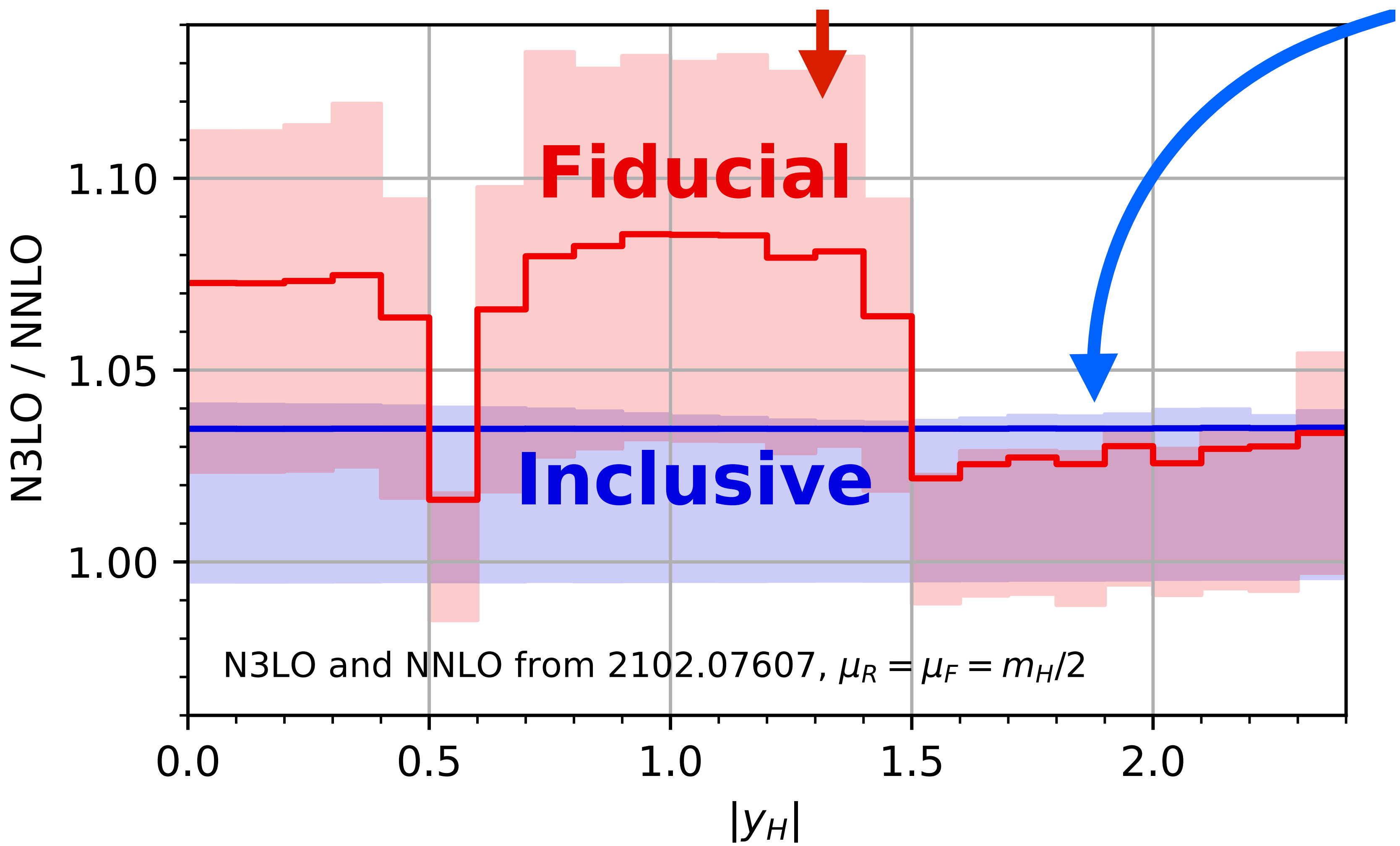
- Deep-Inelastic Scattering: ***p=2***
- Jet and dijet production: ***p=1***
- Inclusive cross-sections and rapidity distributions in Higgs and Drell-Yan : ***p=2***
- p_T distribution in Z production: ***p=2*** but log enhancement
- top pair production: ***p=1***

$$\Delta_{\rm NP} \sim \left(\frac{\Lambda}{p_T^Z}\right)^2 \ln\left(\frac{\Lambda}{p_T^Z}\right)$$

from G. Salam, NNPDF Collaboration meeting Sept 2023

Spurious non-perturbative effects can also be generated by cuts i.e. asymmetric cuts Higgs production

Non-perturbative power corrections



Chen, Gehrmann, Glover, Huss, Mistlberger & Pelloni, 2102.07607

N[3]LO corrections display **larger MHOUs in fiducial** than in inclusive cross-sections

can be traced back to **asymmetric selection cuts** sensitive to Higgs **low-p_T modelling**

$$p_{t,+} > 0.35 m_H$$
$$p_{t,-} > 0.25 m_H$$

Once product cuts are used for the fiducial cross-section, N[3]LO corrections behave ``as expected''

$$\sqrt{p_{t,+} p_{t,-}} > 0.35 m_H$$
$$p_{t,-} > 0.25 m_H$$

Improving theoretical predictions at the LHC is not just a matter of ``brute force'': **deep understanding of the underlying physical processes** is crucial!

from G. Salam, NNPDF Collaboration meeting Sept 2023

… and how to Tame them

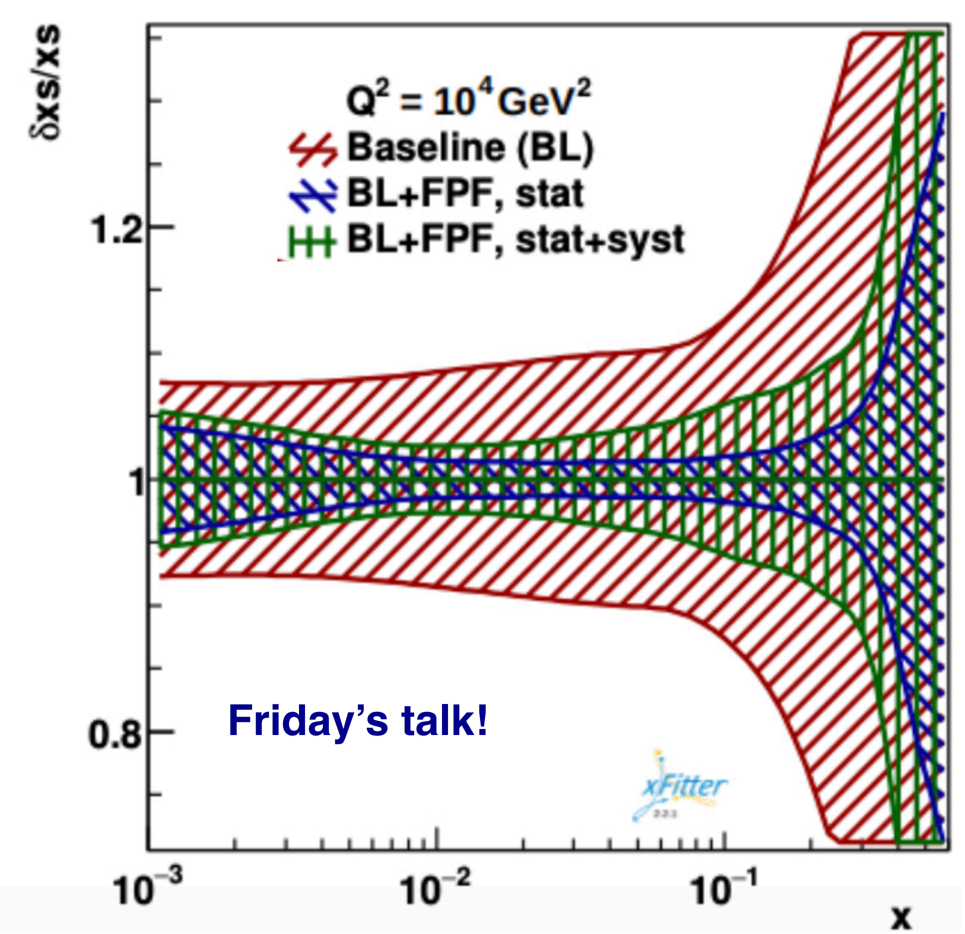
Towards 1% phenomenology at LHC

$$\sigma_{\rm LHC}(M,s) \propto \sum_{ij} \int_{M^2}^{s} d\hat{s}\; \mathscr{L}_{ij}(\hat{s},s)\, \widetilde{\sigma}_{ij}(\hat{s},\alpha_s(M)) \left[1+\mathcal{O}\left(\Lambda/M\right)^p\right]$$

Partonic luminosities (*non-perturbative, fit to data*)

- Include **more data**: LHC Run III now and in the next decade HL-LHC, EIC and FASER/FPF)
- Fully profit from N^3LO, resummed, and higher-order **QCD and EW calculations**
- **Develop novel methodologies** (ie NNPDFs from gaussian processes) and **validate existing ones** (Hessian fits with the NNPDF code)
- Extensive account for all possible **sources of uncertainty** in the PDFs

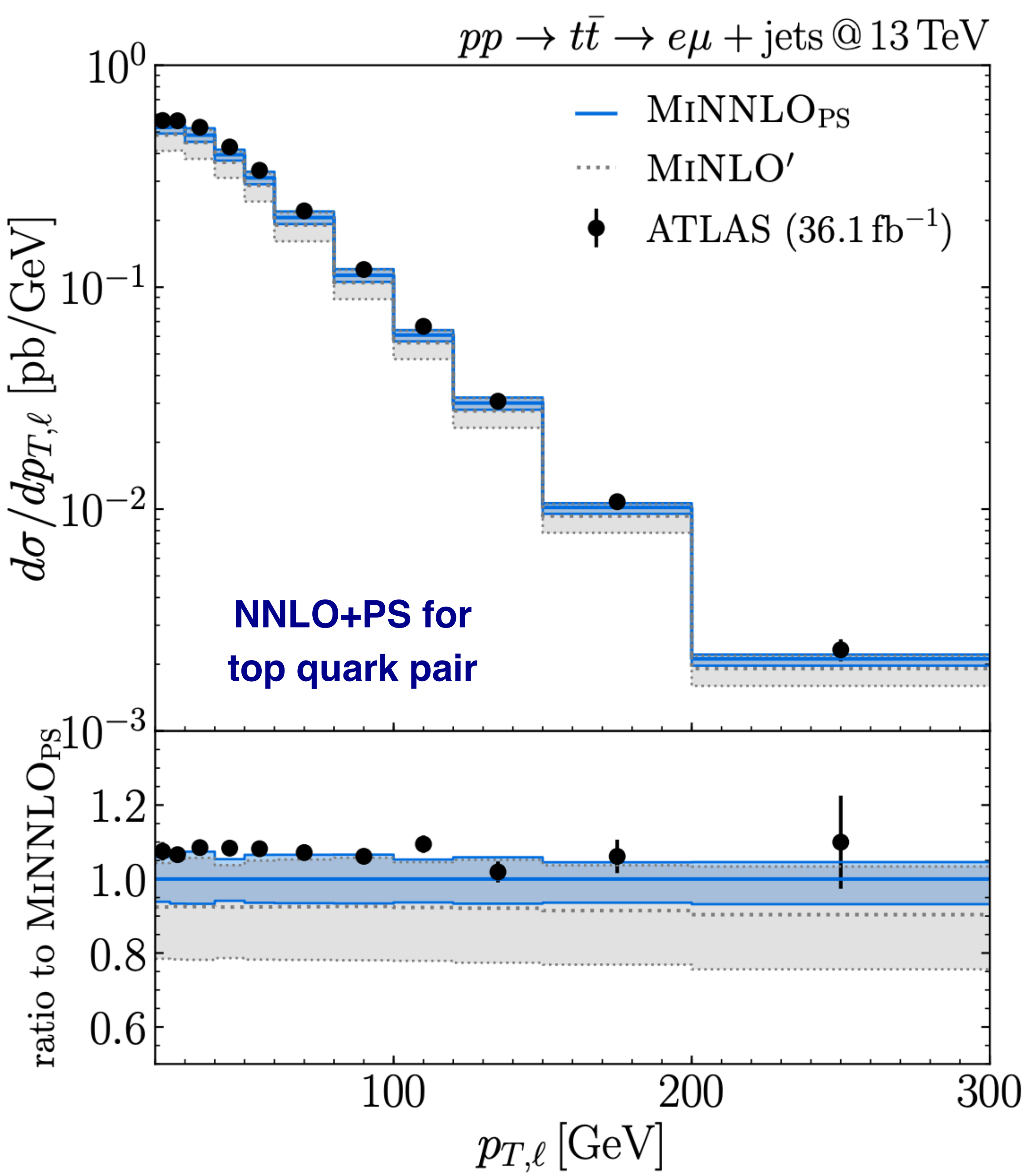
PDF constraints from LHC neutrinos



Towards 1% phenomenology at LHC

$$\sigma_{\rm LHC}(M,s) \propto \sum_{ij} \int_{M^2}^{s} d\hat{s}\ \mathscr{L}_{ij}(\hat{s},s)\ \widetilde{\sigma}_{ij}(\hat{s},\alpha_s(M))\left[1+\mathcal{O}\left(\Lambda/M\right)^p\right]$$

Hard-scattering cross-sections (*perturbative, from Feynman diagrams*)



- Continue **N³LO program** (coloured final states)
- Establish **NNLO+PS** as paradigm for LHC simulations
- Match fixed-order codes with **resummed calculations** (p_T distributions)
- Better estimates of MHOUs?
- Interface state-of-the-art QCD calculations to **fast grid evaluators** to facilitate phenomenology

Mazzitelli et al 2112.12135

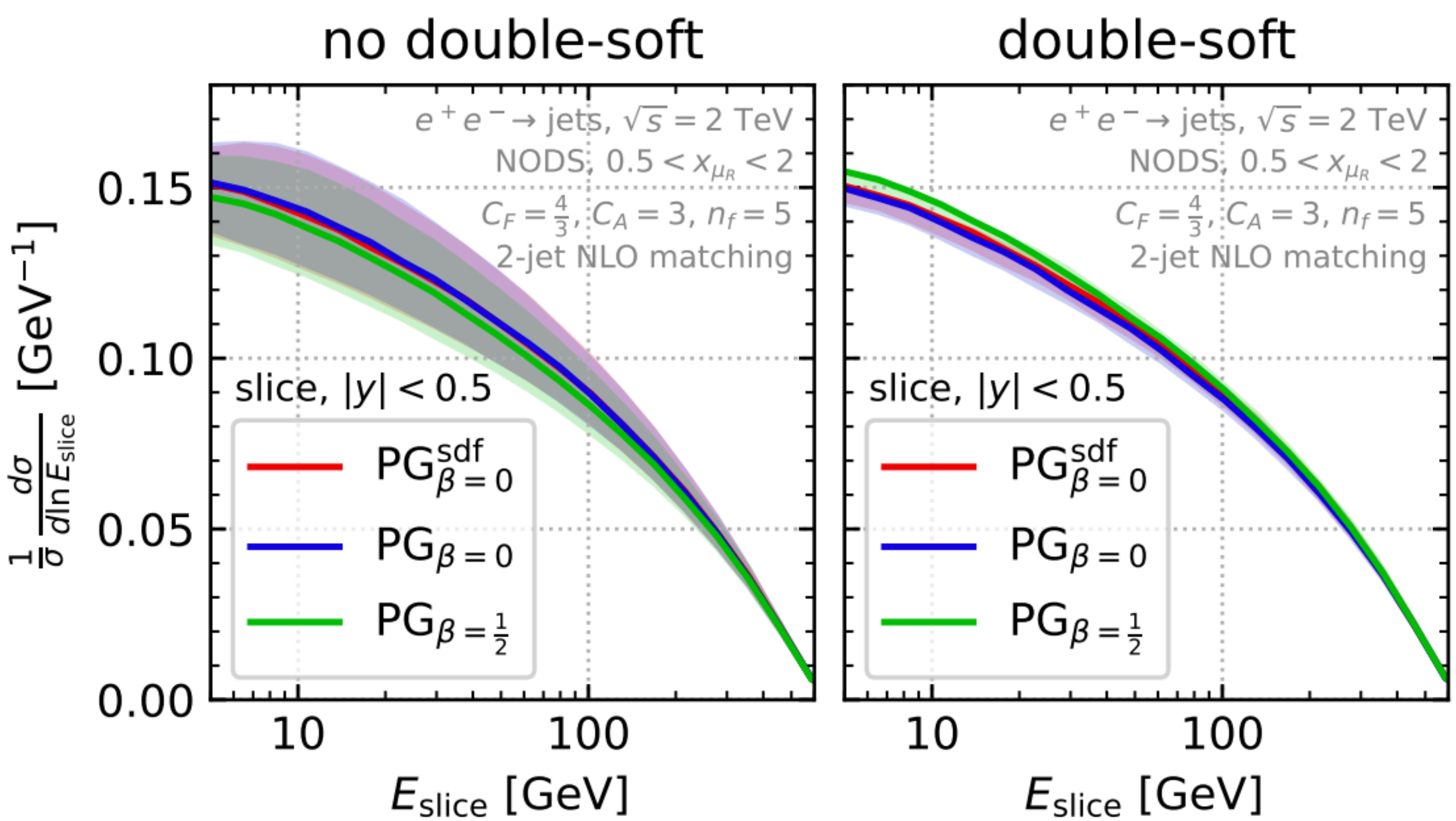
Towards 1% phenomenology at LHC

$$\sigma_{\mathrm{LHC}}(M,s) \propto \sum_{ij} \int_{M^2}^{s} d\hat{s}\; \mathscr{L}_{ij}(\hat{s},s)\, \tilde{\sigma}_{ij}(\hat{s},\alpha_s(M)) \left[1+\mathcal{O}\left(\Lambda/M\right)^p\right]$$

- **NLL parton showers** in general-purpose MCs (more accurate & reduce model dependence)
- Better analytical understanding of **power-corrections at the LHC**
- Experiment/theory cross-talk to avoid ``fitting away" **process-dependent corrections** into general-purpose MC tunes

PanScales shower with higher-order soft accuracy

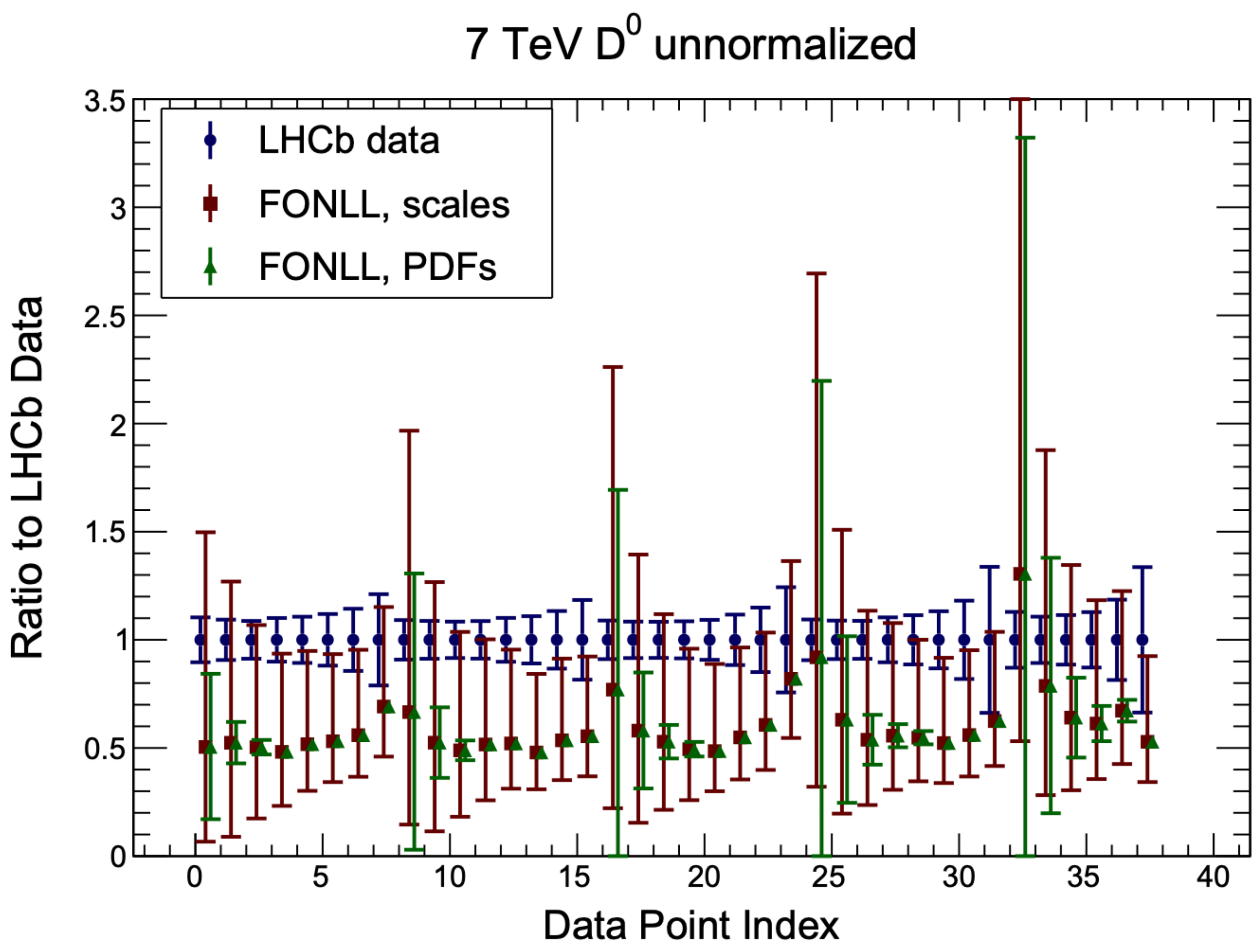
Ferrario Ravasio et al 23



Tailored observables

By cleverly **designing new observables**, we can reduce the sensitivity of theory predictions wrt to some source of uncertainty (i.e. MHOU) and **emphasise another** (i.e. PDFs)

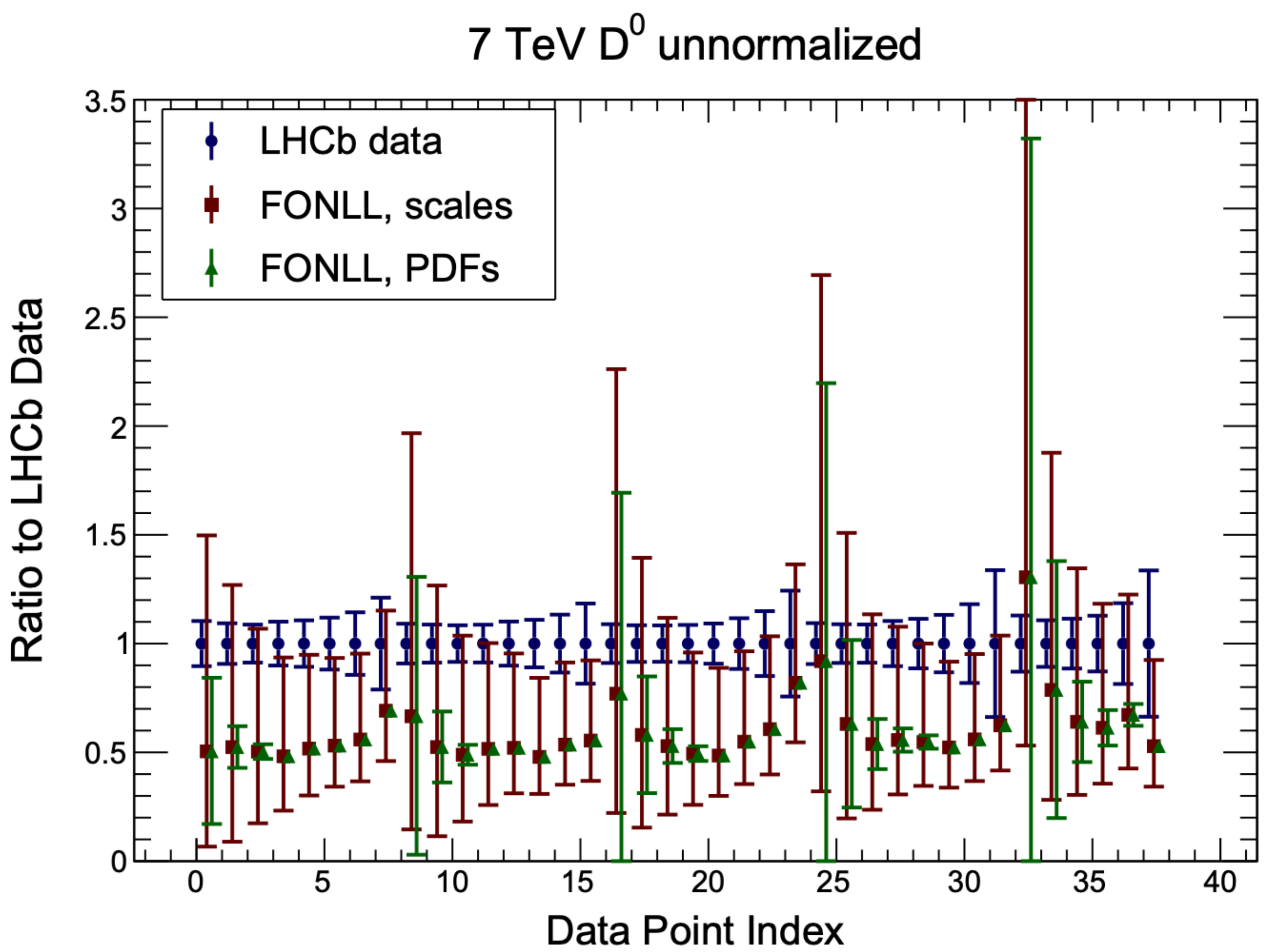
forward D-meson production has large MHOUs



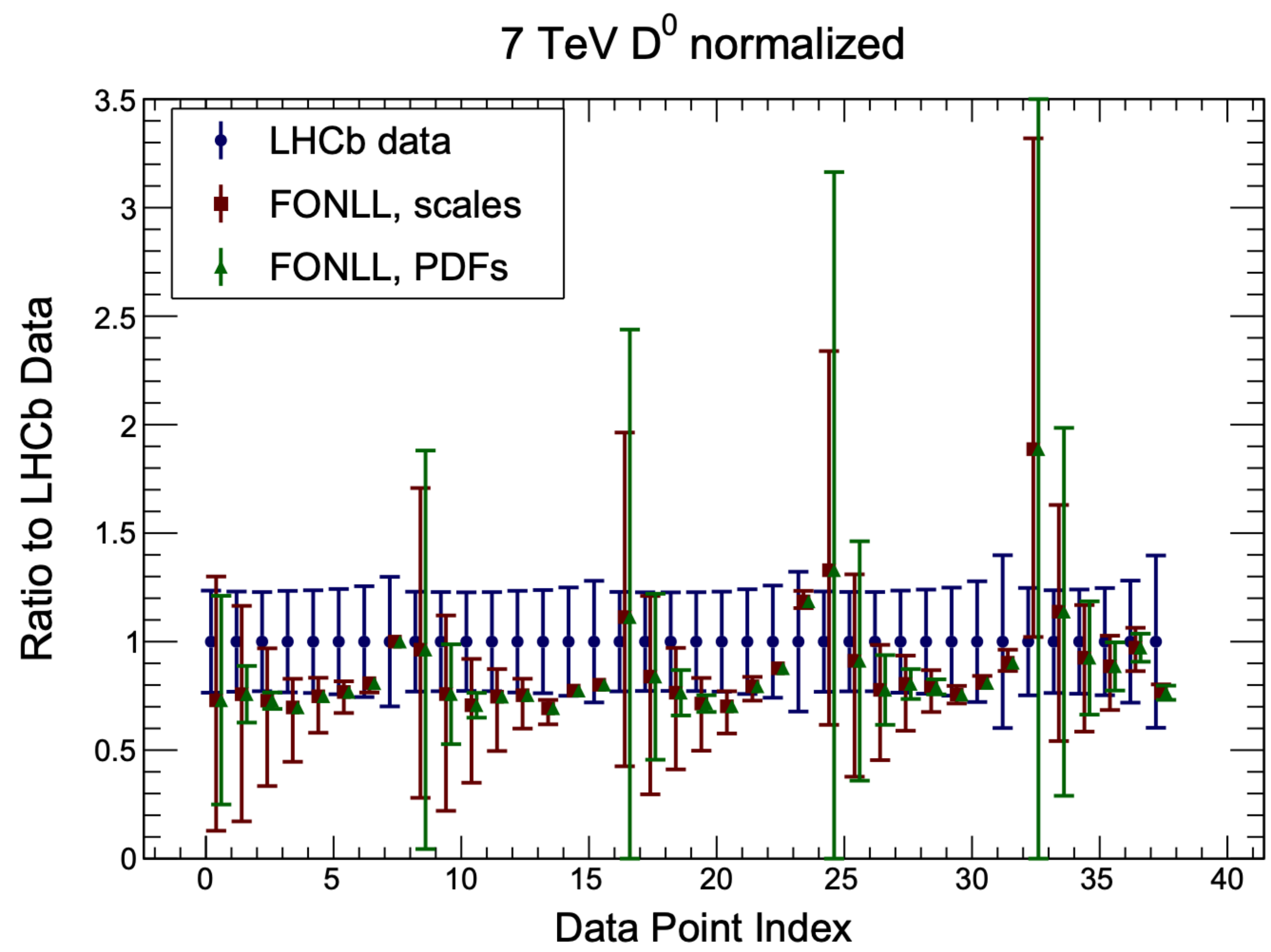
Tailored observables

By cleverly **designing new observables**, we can reduce the sensitivity of theory predictions wrt to some source of uncertainty (i.e. MHOU) and **emphasise another** (i.e. PDFs)

forward D-meson production has large MHOUs



markedly reduce when normalising to central rapidity bin



MHOUs are flat in *D*-meson rapidity, while PDF sensitivity is enhanced at forward rapidities

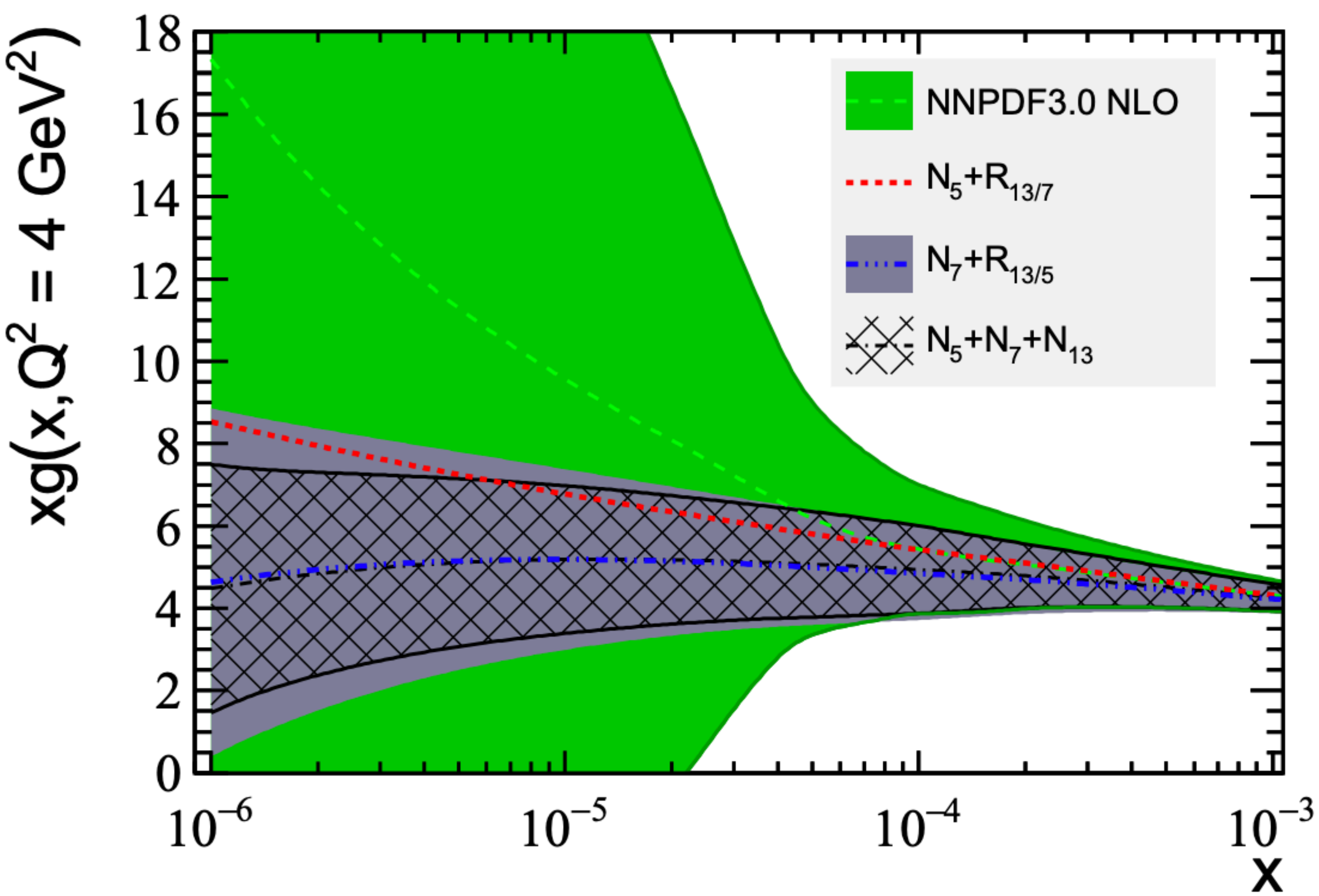
$$N_X^{ij} = \frac{d^2\sigma(\mathrm{X\ TeV})}{dy_i^D d(p_T^D)_j} \Big/ \frac{d^2\sigma(\mathrm{X\ TeV})}{dy_{\mathrm{ref}}^D d(p_T^D)_j}$$

Gauld et al 15

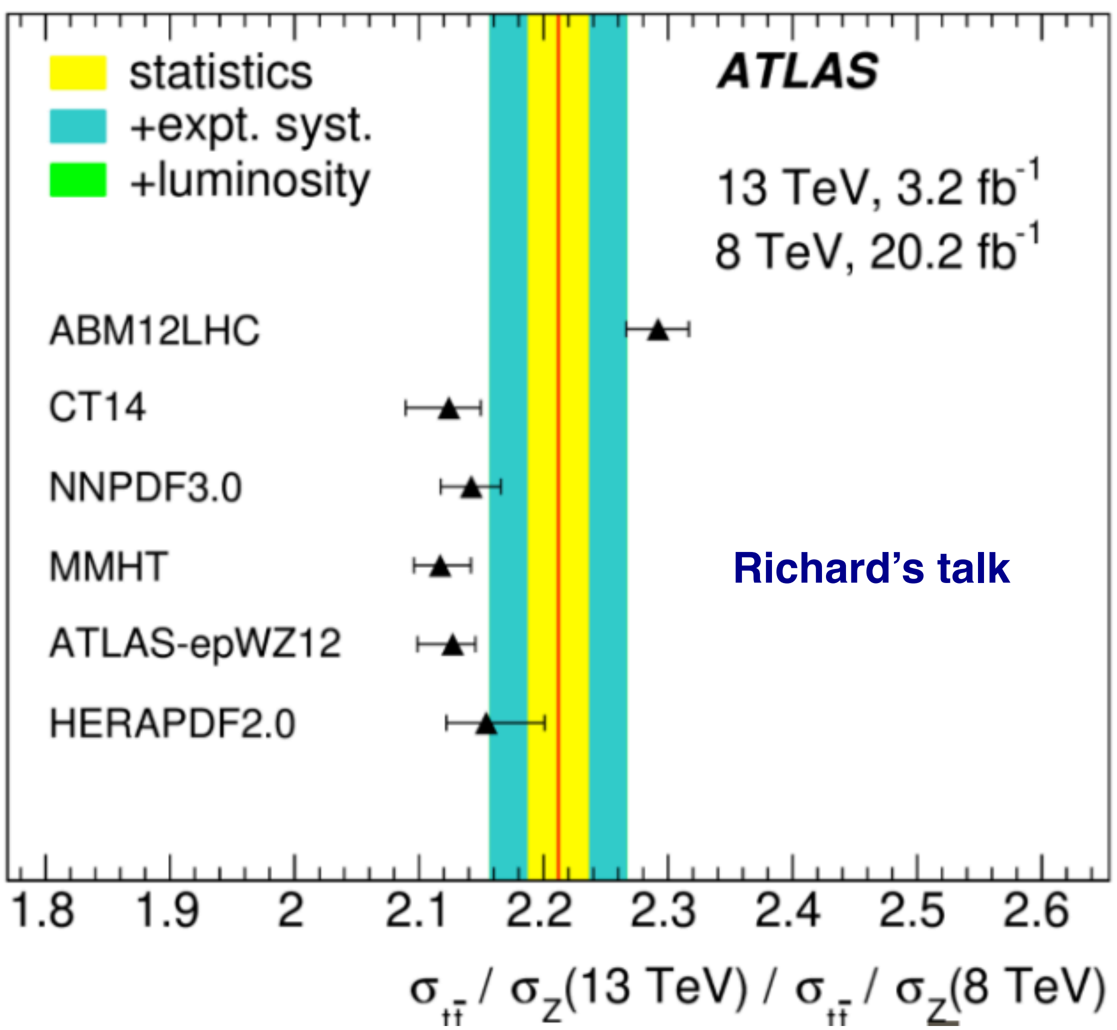
Tailored observables

By cleverly **designing new observables**, we can reduce the sensitivity of theory predictions wrt to some source of uncertainty (i.e. MHOU) and **emphasise another** (i.e. PDFs)

- Ratios between the same observable at **different CoM energies**
- Ratios between different observables sharing **common systematics**
- Ratios between the same observable evaluated in **complementary kinematic regions**



Gauld and JR 16



Lots of room for new ideas, looking forward to discussions about this!

Summary and outlook

- The ultimate potential of the **LHC precision program** can only be achieved with a thorough understanding of our theoretical predictions, pushing forward their limitations
- Amazing new results in SM predictions, but improved accuracy does not (necessarily) equal improved precision
- Moving to theory predictions with 1% precision requires non-trivial, coordinated progress in **PDFs, higher orders, shower Monte Carlos, and non-perturbative QCD phenomena**
- We should be wary of pushing for the **most precise measurement and/or interpretation** while neglecting (known and unknown) some theory uncertainties

Summary and outlook

- The ultimate potential of the **LHC precision program** can only be achieved with a thorough understanding of our theoretical predictions, pushing forward their limitations
- Amazing new results in SM predictions, but improved accuracy does not (necessarily) equal improved precision
- Moving to theory predictions with 1% precision requires non-trivial, coordinated progress in **PDFs, higher orders, shower Monte Carlos, and non-perturbative QCD phenomena**
- We should be wary of pushing for the **most precise measurement and/or interpretation** while neglecting (known and unknown) some theory uncertainties