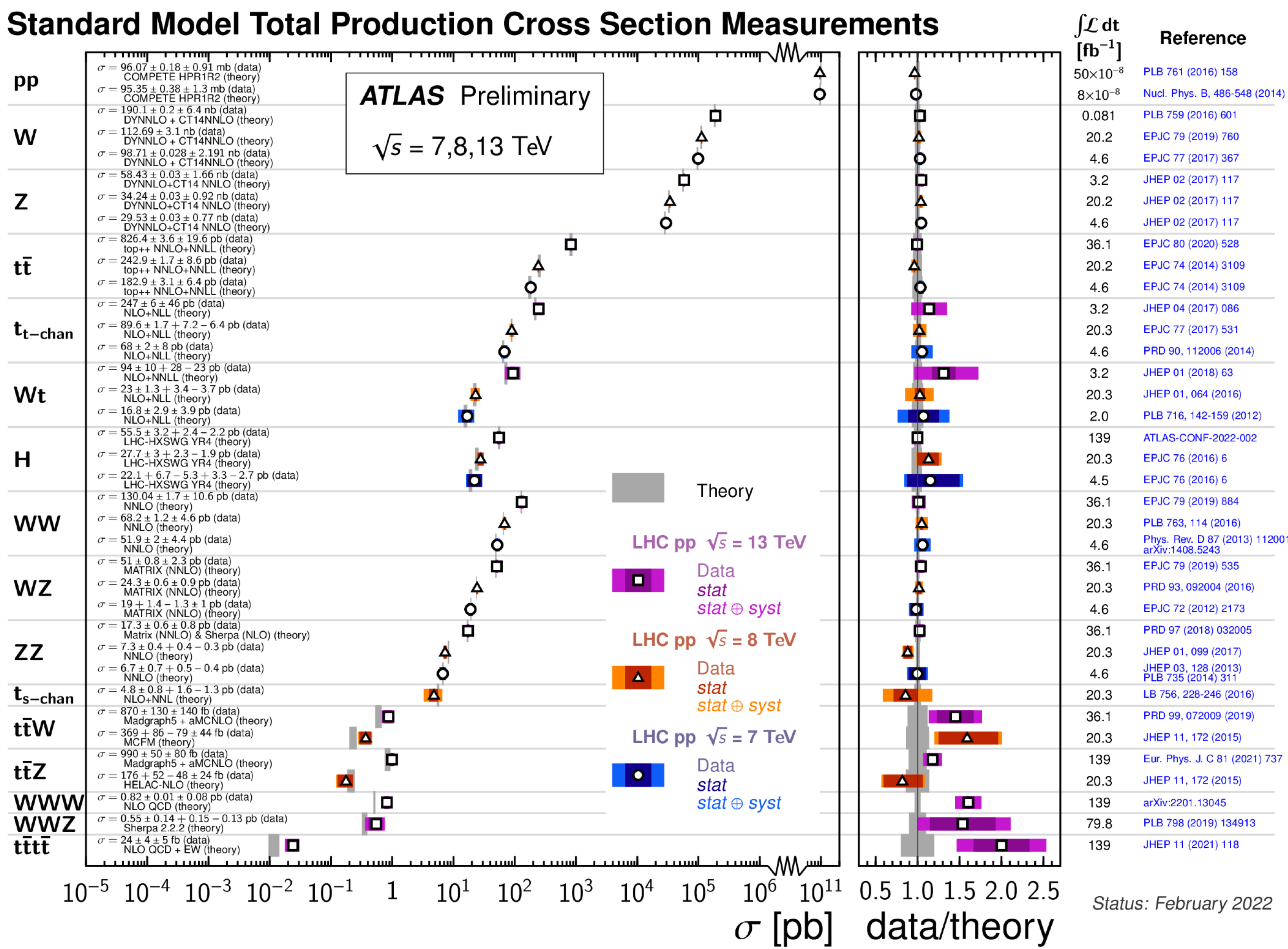
ROBUST ESTIMATES OF THEORETICAL UNCERTAINTIES AT FIXED ORDER IN PERTURBATION THEORY

MATTHEW A. LIM

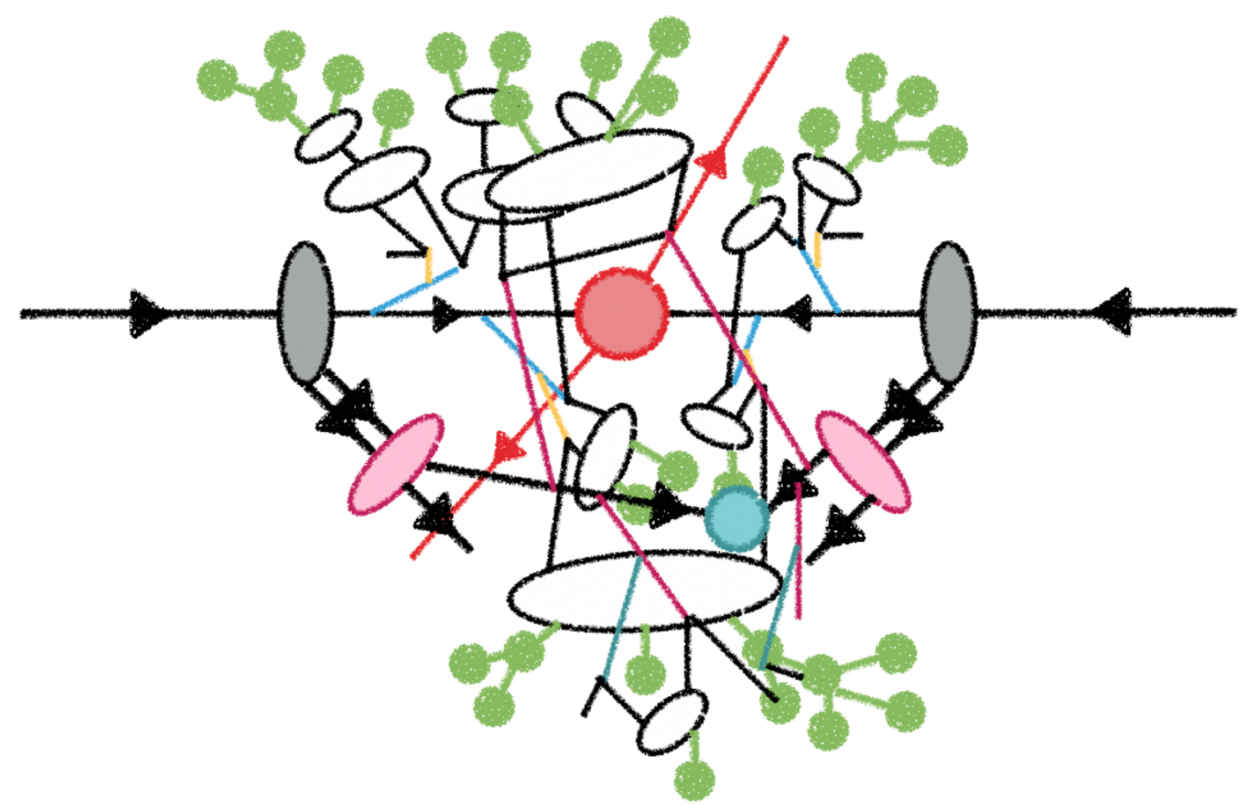
SM@LHC, 09/04/25

BASED ON [LIM, PONCELET, 2412.14910]


Standard Model Total Production Cross Section Measurements
∫ℒ dt [fb⁻¹]
Reference
ATLAS Preliminary
√s = 7,8,13 TeV
pp
σ = 96.07 ± 0.18 ± 0.91 mb (data) COMPETE HPR1R2 (theory)
50×10⁻⁸ PLB 761 (2016) 158
σ = 95.35 ± 0.38 ± 1.3 mb (data) COMPETE HPR1R2 (theory)
8×10⁻⁸ Nucl. Phys. B, 486-548 (2014)
W
σ = 190.1 ± 0.2 ± 6.4 nb (data) DYNNLO + CT14NNLO (theory)
0.081 PLB 759 (2016) 601
σ = 112.69 ± 3.1 nb (data) DYNNLO + CT14NNLO (theory)
20.2 EPJC 79 (2019) 760
σ = 98.71 ± 0.028 ± 2.191 nb (data) DYNNLO + CT14NNLO (theory)
4.6 EPJC 77 (2017) 367
Z
σ = 58.43 ± 0.03 ± 1.66 nb (data) DYNNLO+CT14 NNLO (theory)
3.2 JHEP 02 (2017) 117
σ = 34.24 ± 0.03 ± 0.92 nb (data) DYNNLO+CT14 NNLO (theory)
20.2 JHEP 02 (2017) 117
σ = 29.53 ± 0.03 ± 0.77 nb (data) DYNNLO+CT14 NNLO (theory)
4.6 JHEP 02 (2017) 117
tt̄
σ = 826.4 ± 3.6 ± 19.6 pb (data) top++ NNLO+NNLL (theory)
36.1 EPJC 80 (2020) 528
σ = 242.9 ± 1.7 ± 8.6 pb (data) top++ NNLO+NNLL (theory)
20.2 EPJC 74 (2014) 3109
σ = 182.9 ± 3.1 ± 6.4 pb (data) top++ NNLO+NNLL (theory)
4.6 EPJC 74 (2014) 3109
t t−chan
σ = 247 ± 6 ± 46 pb (data) NLO+NLL (theory)
3.2 JHEP 04 (2017) 086
σ = 89.6 ± 1.7 + 7.2 − 6.4 pb (data) NLO+NLL (theory)
20.3 EPJC 77 (2017) 531
σ = 68 ± 2 ± 8 pb (data) NLO+NLL (theory)
4.6 PRD 90, 112006 (2014)
Wt
σ = 94 ± 10 + 28 − 23 pb (data) NLO+NNLL (theory)
3.2 JHEP 01 (2018) 63
σ = 23 ± 1.3 + 3.4 − 3.7 pb (data) NLO+NLL (theory)
20.3 JHEP 01, 064 (2016)
σ = 16.8 ± 2.9 ± 3.9 pb (data) NLO+NLL (theory)
2.0 PLB 716, 142-159 (2012)
H
σ = 55.5 ± 3.2 + 2.4 − 2.2 pb (data) LHC-HXSWG YR4 (theory)
139 ATLAS-CONF-2022-002
σ = 27.7 ± 3 + 2.3 − 1.9 pb (data) LHC-HXSWG YR4 (theory)
20.3 EPJC 76 (2016) 6
σ = 22.1 + 6.7 − 5.3 + 3.3 − 2.7 pb (data) LHC-HXSWG YR4 (theory)
4.5 EPJC 76 (2016) 6
WW
σ = 130.04 ± 1.7 ± 10.6 pb (data) NNLO (theory)
36.1 EPJC 79 (2019) 884
σ = 68.2 ± 1.2 ± 4.6 pb (data) NNLO (theory)
20.3 PLB 763, 114 (2016)
σ = 51.9 ± 2 ± 4.4 pb (data) NNLO (theory)
4.6 Phys. Rev. D 87 (2013) 112001 arXiv:1408.5243
WZ
σ = 51 ± 0.8 ± 2.3 pb (data) MATRIX (NNLO) (theory)
36.1 EPJC 79 (2019) 535
σ = 24.3 ± 0.6 ± 0.9 pb (data) MATRIX (NNLO) (theory)
20.3 PRD 93, 092004 (2016)
σ = 19 + 1.4 − 1.3 ± 1 pb (data) MATRIX (NNLO) (theory)
4.6 EPJC 72 (2012) 2173
ZZ
σ = 17.3 ± 0.6 ± 0.8 pb (data) Matrix (NNLO) & Sherpa (NLO) (theory)
36.1 PRD 97 (2018) 032005
σ = 7.3 ± 0.4 + 0.4 − 0.3 pb (data) NNLO (theory)
20.3 JHEP 01, 099 (2017)
σ = 6.7 ± 0.7 + 0.5 − 0.4 pb (data) NNLO (theory)
4.6 JHEP 03, 128 (2013) PLB 735 (2014) 311
t s−chan
σ = 4.8 ± 0.8 + 1.6 − 1.3 pb (data) NLO+NNL (theory)
20.3 LB 756, 228-246 (2016)
tt̄W
σ = 870 ± 130 ± 140 fb (data) Madgraph5 + aMCNLO (theory)
36.1 PRD 99, 072009 (2019)
σ = 369 + 86 − 79 ± 44 fb (data) MCFM (theory)
20.3 JHEP 11, 172 (2015)
tt̄Z
σ = 990 ± 50 ± 80 fb (data) Madgraph5 + aMCNLO (theory)
139 Eur. Phys. J. C 81 (2021) 737
σ = 176 + 52 − 48 ± 24 fb (data) HELAC-NLO (theory)
20.3 JHEP 11, 172 (2015)
WWW
σ = 0.82 ± 0.01 ± 0.08 pb (data) NLO QCD (theory)
139 arXiv:2201.13045
WWZ
σ = 0.55 ± 0.14 + 0.15 − 0.13 pb (data) Sherpa 2.2.2 (theory)
79.8 PLB 798 (2019) 134913
tt̄tt̄
σ = 24 ± 4 ± 5 fb (data) NLO QCD + EW (theory)
139 JHEP 11 (2021) 118
Theory
LHC pp √s = 13 TeV
Data
stat
stat ⊕ syst
LHC pp √s = 8 TeV
Data
stat
stat ⊕ syst
LHC pp √s = 7 TeV
Data
stat
stat ⊕ syst
10⁻⁵ 10⁻⁴ 10⁻³ 10⁻² 10⁻¹ 1 10¹ 10² 10³ 10⁴ 10⁵ 10⁶ 10¹¹
σ [pb]
0.5 1.0 1.5 2.0 2.5
data/theory
Status: February 2022

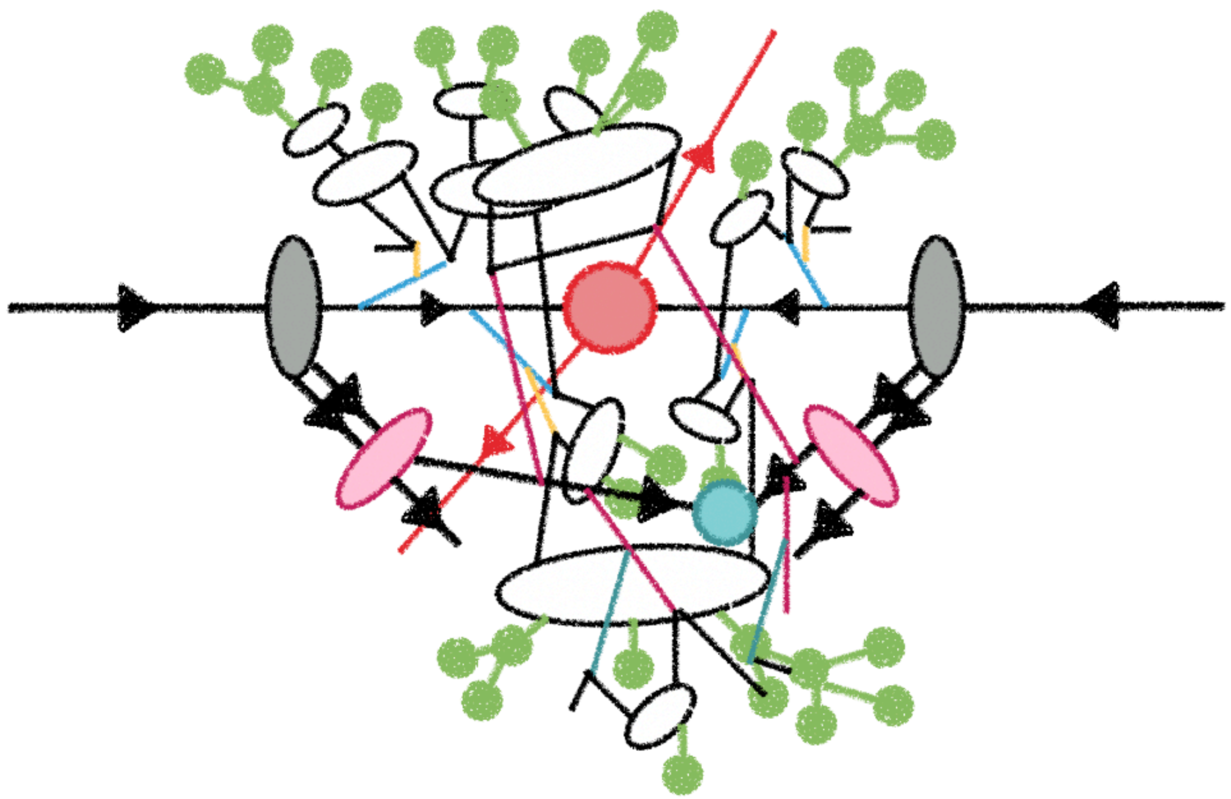
SOURCES OF THEORY UNCERTAINTY

- Parametric uncertainties: SM parameters known to finite precision
- Parton distribution functions: proton structure fit from data
- Non-perturbative/ hadronisation modelling in shower MCs



SOURCES OF THEORY UNCERTAINTY

- Missing Higher Order Uncertainty: arises from truncation of a perturbative series
- Relevant for calculations in resummed and fixed-order perturbation theory



MISSING HIGHER ORDER UNCERTAINTIES

- Let's take a simple example: EoM for a simple pendulum

$$\ddot{\theta} + \omega^2 \sin\theta = 0$$

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$$\ddot{\theta} + \omega^2 \sin\theta = 0$$

- For small displacements, we can expand $\sin\theta \approx \theta + \mathcal{O}(\theta^3)$

$$\ddot{\theta} + \omega^2\theta = 0$$

- Solving, we find for the period of the pendulum

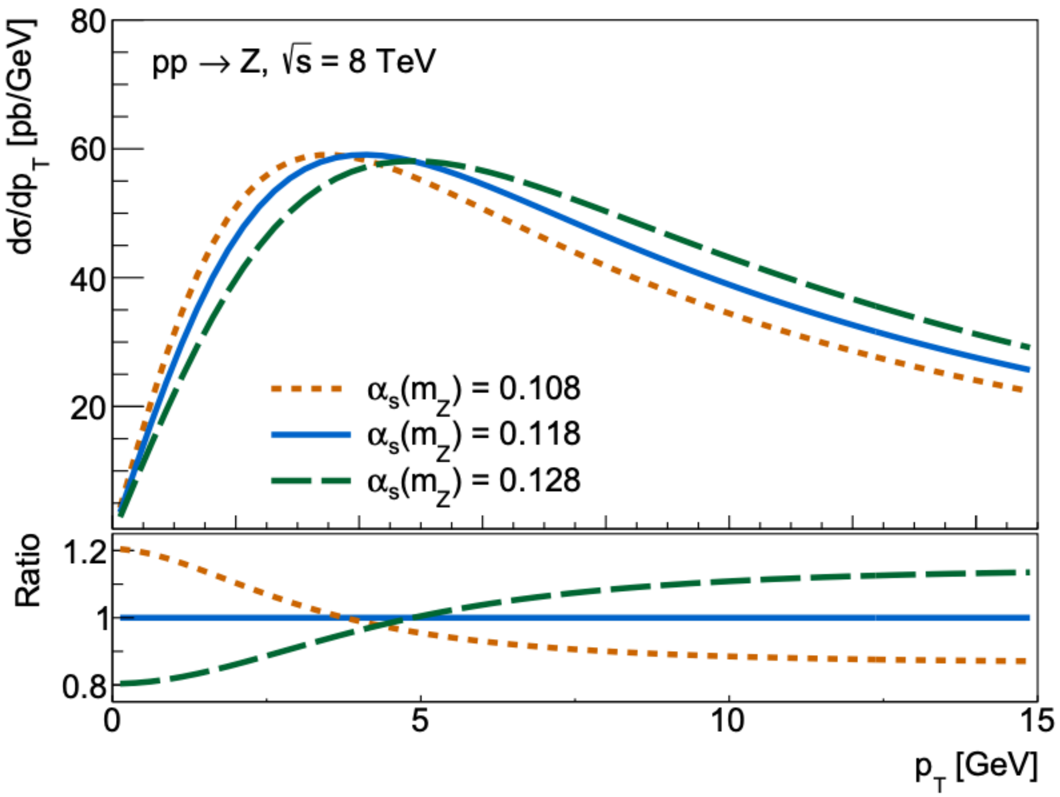
$$T = 2\pi/\omega = 2\pi\sqrt{\frac{\ell}{g}}$$

MISSING HIGHER ORDER UNCERTAINTIES

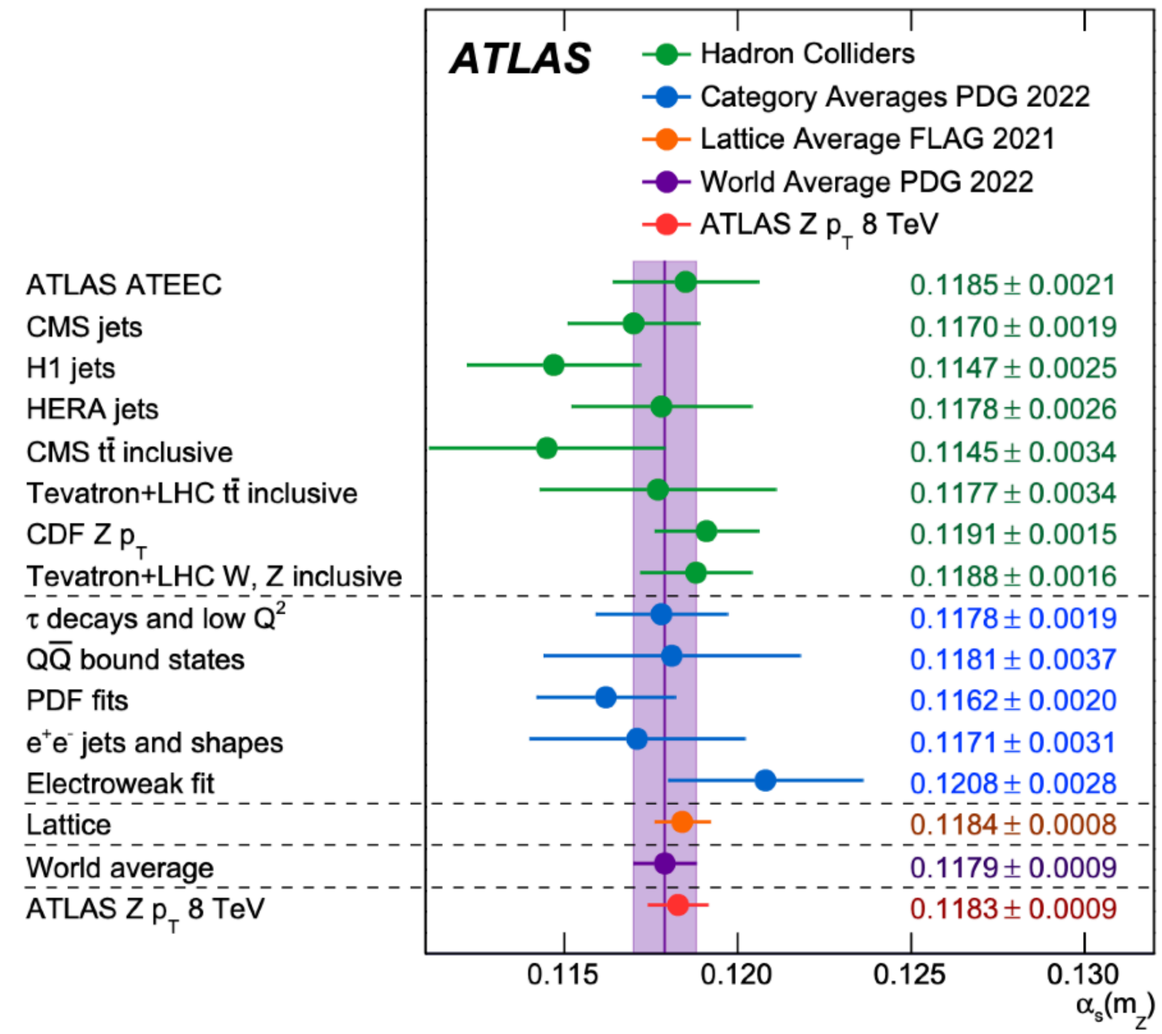
- Question: what is the uncertainty on g due to the inexactness of our expression for T?
- Clearly, we cannot always rely on being able to calculate arbitrary orders.
- Different kind of uncertainty, not related to inexact knowledge of parameters ℓ.
- No auxiliary measurement can improve this systematic.

α_s FROM THE $p_T(Z)$ SPECTRUM

See Giulia's talk!



2309.12986, ATLAS



- Very relevant question given $\sim 0.7\,\%$ extraction of α_s
- Achieved by comparing data with resummed calculation

PERTURBATIVE EXPANSIONS IN QFT

- Calculations beyond leading order depend on a renormalisation scale μ.
- Dependence vanishes at all orders, but at finite order we are required to pick a value μ_0.
- Let's expand at weak coupling $\alpha \equiv \alpha_s(\mu_0)$:

$$f(\alpha) = f_0 + \alpha f_1 + \alpha^2 f_2 + \alpha^3 f_3 + \ldots$$

PERTURBATIVE EXPANSIONS IN QFT

Notation from Tackmann, 2411.18606

- Let's expand at weak coupling $\alpha \equiv \alpha_s(\mu_0)$:

$$f(\alpha) = f_0 + \alpha f_1 + \alpha^2 f_2 + \alpha^3 f_3 + \ldots$$

- What we can actually compute are truncated series:

$$f^{\mathrm{LO}}(\alpha) = \hat{f}_0 \qquad f^{\mathrm{NLO}}(\alpha) = \hat{f}_0 + \alpha \hat{f}_1$$

where the $\hat{f}_i$ are values we actually computed.

- Missing terms are the source of uncertainty (convergence implies leading missing term is dominant)

$$f^{\mathrm{N^{0+1}LO}}(\alpha) = \hat{f}_0 + \alpha f_1 \qquad f^{\mathrm{N^{1+1}LO}}(\alpha) = \hat{f}_0 + \alpha \hat{f}_1 + \alpha^2 f_2$$

SCALE VARIATION APPROACH

- Changing the renormalisation scale, we define a new coupling $\tilde{\alpha} \equiv \alpha_s(\mu_1)$ related to α via

$$\alpha = \alpha(\tilde{\alpha}) = \tilde{\alpha} + \tilde{\alpha}^2 b_0 + \mathcal{O}(\tilde{\alpha}^3) \qquad b_0 = \frac{\beta_0}{2\pi} \log \frac{\mu_0}{\mu_1}$$

- Expanding in the new coupling,

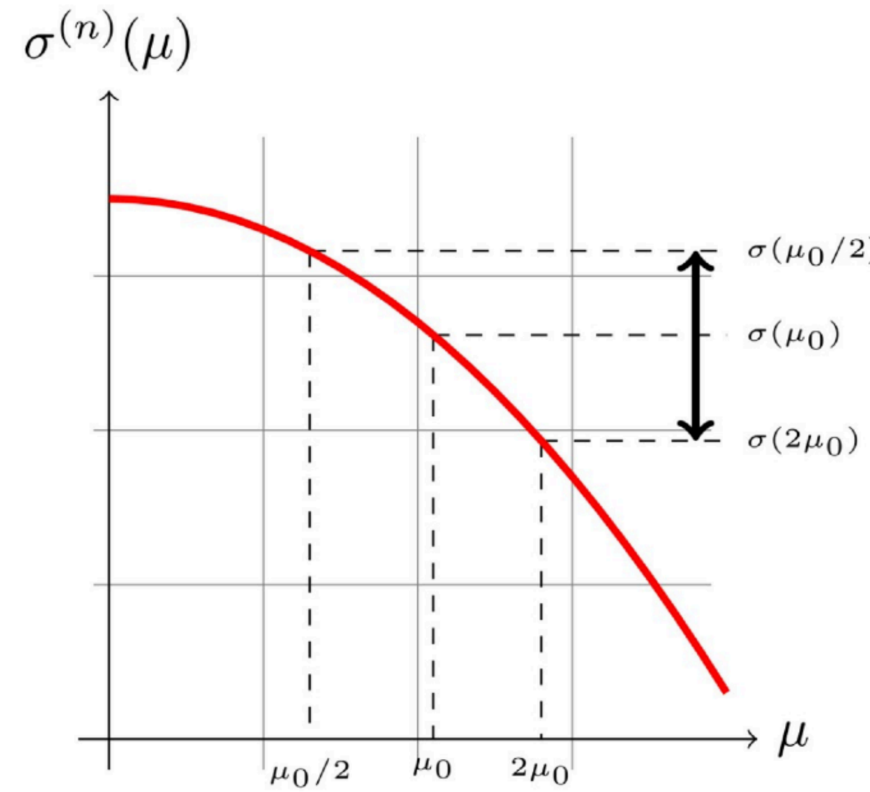
$$\tilde{f}^{\mathrm{LO}}(\tilde{\alpha}) = \hat{\tilde{f}}_0 \qquad \tilde{f}^{\mathrm{NLO}}(\tilde{\alpha}) = \hat{\tilde{f}}_0 + \tilde{\alpha}\,\hat{\tilde{f}}_1 = \hat{f}_0 + \alpha\,\hat{f}_1 + \alpha^2 b_0\,\hat{f}_1 + \mathcal{O}(\alpha^3)$$

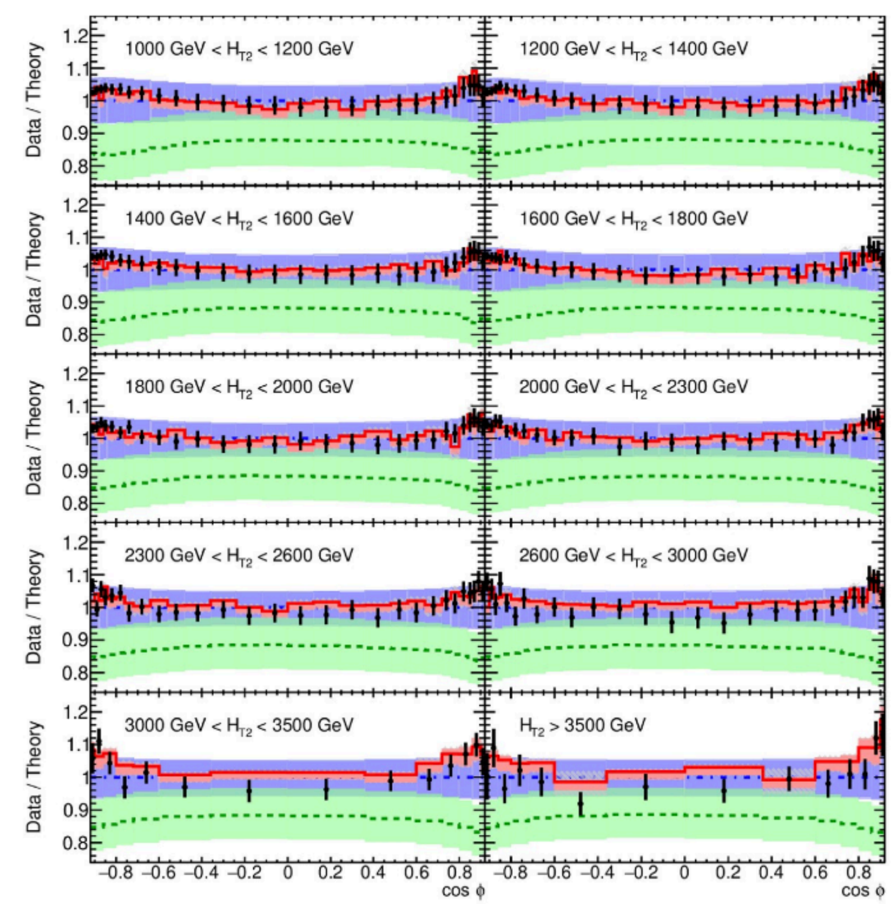
- We then take as uncertainty estimate

$$\boxed{\Delta f^{\mathrm{NLO}} = f^{\mathrm{NLO}}(\alpha) - \tilde{f}^{\mathrm{NLO}}(\tilde{\alpha}) = -\,\alpha^2 b_0\, f_1}$$

SCALE VARIATION APPROACH

- This is genuinely of higher order.
- Normal (arbitrary) prescription is to pick a central scale related to the process, and vary up and down by a factor 2, envelope variations.
- Prescriptions exist to choose the central scale value, normally aiming to increase convergence rate.





2301.09351, ATLAS

SHORTCOMINGS OF SCALE VARIATION

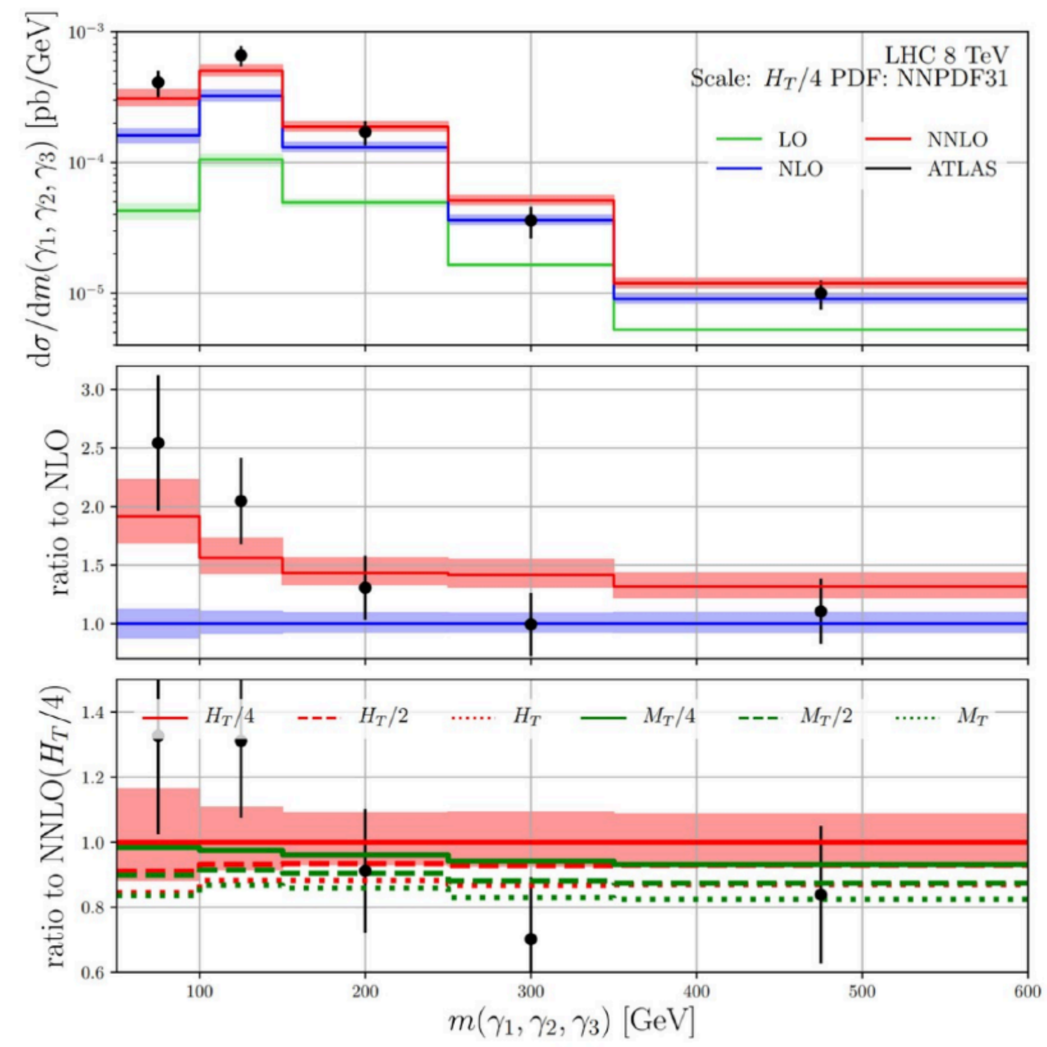
- Our NLO uncertainty estimate was given by

$$\Delta f^{\mathrm{NLO}} = -\,\alpha^2 b_0\, f_1$$

- Nothing guarantees this is any good!
- The true f_2 is generally more complex than f_1
- b_0 is an arbitrary constant and normally the same for any f
- Correlations between bins of a distribution are not captured correctly, and enveloping means propagation of uncertainties is unclear

SHORTCOMINGS OF SCALE VARIATION

- Complex processes and phase spaces may mean that this fails completely.
- Ultimately μ is not a physical parameter - it has no true value and does not become better known at higher orders!
- Uncertainty reduces only because μ-dependence decreases.



1911.00479, Chawdhry, Czakon, Mitov, Poncelet

THEORY NUISANCE PARAMETERS

Notation from Tackmann, 2411.18606

- Parameterise unknown higher terms

$$f^{\mathrm{N}^{0+1}\mathrm{LO}}(\alpha) = \hat{f}_0 + \alpha f_1(\theta) \qquad f^{\mathrm{N}^{1+1}\mathrm{LO}}(\alpha) = \hat{f}_0 + \alpha \hat{f}_1 + \alpha^2 f_2(\theta)$$

- The θ_i are now Theory Nuisance Parameters.
- They have a true value, viz.

$$f_i(\hat{\theta}) = \hat{f}_i$$

- Distributions for the θ_i can be inferred e.g. from existing higher order computations

THEORY NUISANCE PARAMETERS

- In the simplest case $f(\alpha)$ is only a function of α - then the parameterised higher order terms are simply numbers,

$$f_n(\theta) = \theta$$

- In general, extra functional dependence may be present.
- Particularly nice for transverse momentum resummation: many ingredients can be directly parameterised in this way

$$F(\alpha_s) = F_0 + \alpha_s F_1 + \ldots + \alpha_s^n F_n(\theta)$$
$$\Gamma(\alpha_s) = \alpha_s[\Gamma_0 + \alpha_s \Gamma_1 + \ldots + \alpha_s^n \Gamma_n(\theta)]$$
$$\gamma(\alpha_s) = \alpha_s[\gamma_0 + \alpha_s \gamma_1 + \ldots + \alpha_s^n \gamma_n(\theta)]$$

See Giulia's talk!

ADVANTAGES OF THE TNP APPROACH

- TNPs have a true value - they can even be constrained from data
- Typical size can be estimated from existing calculations
- Can be included in fits and treated as other systematics
- Capture correlations correctly
- Can be used to include partial higher order information without needing full computation

TNPS FOR FIXED ORDER COMPUTATIONS

- In the resummed case, a lot about the higher order structure of the computation is known a priori
- Anomalous dimensions are often simply numbers and can easily be parameterised
- For simple processes (e.g. Drell-Yan), hard and soft functions are also numbers
- Beam functions more tricky, as they depend on partonic x
- None of this applies for fixed order computations!

TNPS FOR DIFFERENTIAL FIXED ORDER COMPUTATIONS

2412.14910, MAL, Poncelet

$$\mathrm{d}\sigma = \alpha_s^n N_c^m \mathrm{d}\bar{\sigma}^{(0)} \left[1 + \alpha_s N_c \left(\frac{\mathrm{d}\bar{\sigma}^{(1)}}{\mathrm{d}\bar{\sigma}^{(0)}} \right) + \alpha_s^2 N_c^2 \left(\frac{\mathrm{d}\bar{\sigma}^{(2)}}{\mathrm{d}\bar{\sigma}^{(0)}} \right) + \ldots \right]$$

- Experience suggests that $\mathrm{d}\bar{\sigma}^{(i)}/\mathrm{d}\bar{\sigma}^{(0)} \sim \mathcal{O}(1)$
- Try a parameterisation using lower order information:

$$\frac{\mathrm{d}\bar{\sigma}_{\mathrm{TNP}}^{(N+1)}}{\mathrm{d}\bar{\sigma}^{(0)}} = \sum_{j=1}^{N} f_k^{(j)} \left(\vec{\theta}, x \right) \left(\frac{\mathrm{d}\bar{\sigma}^{(j)}}{\mathrm{d}\bar{\sigma}^{(0)}} \right)$$

- x is a mapped kinematic variable

TNPS FOR DIFFERENTIAL FIXED ORDER COMPUTATIONS

- Try a parameterisation using lower order information:

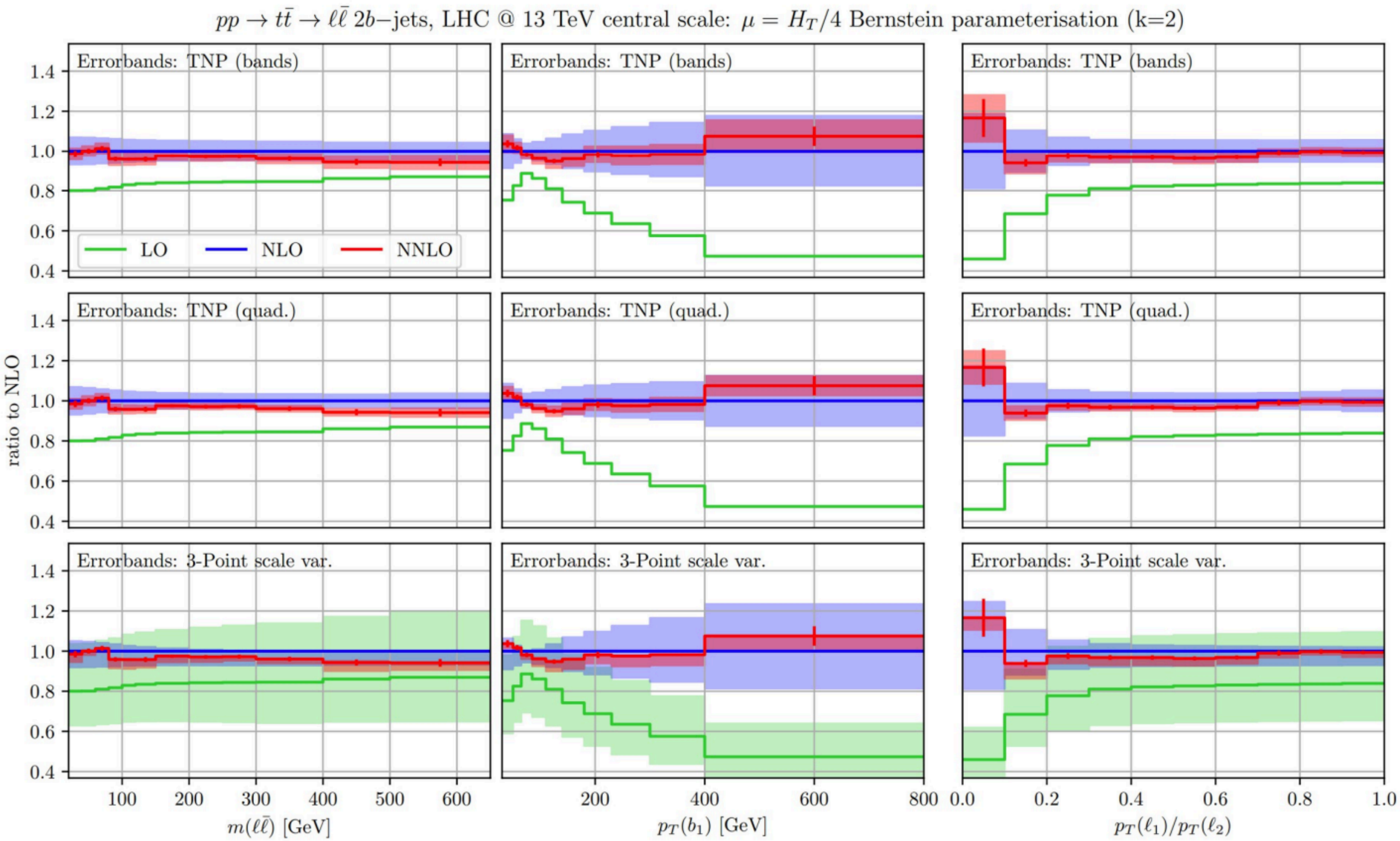
$$\frac{\mathrm{d}\bar{\sigma}^{(N+1)}_{\mathrm{TNP}}}{\mathrm{d}\bar{\sigma}^{(0)}} = \sum_{j=1}^{N} f_k^{(j)}\left(\overrightarrow{\theta}, x\right)\left(\frac{\mathrm{d}\bar{\sigma}^{(j)}}{\mathrm{d}\bar{\sigma}^{(0)}}\right)$$

- x is a mapped kinematic variable

- Different choices for polynomial f possible:

$$f_k^B\left(\overrightarrow{\theta}, x\right) = \sum_{i=0}^{k} \theta_i \binom{k}{i} x^{k-i}(1-x)^i,\ x \in [0,1] \qquad f_k^C\left(\overrightarrow{\theta}, x\right) = \frac{1}{2}\sum_{i=0}^{k} \theta_i T_i(x),\ x \in [-1,1]$$

TNP UNCERTAINTIES - $t\bar{t}$ + DECAYS

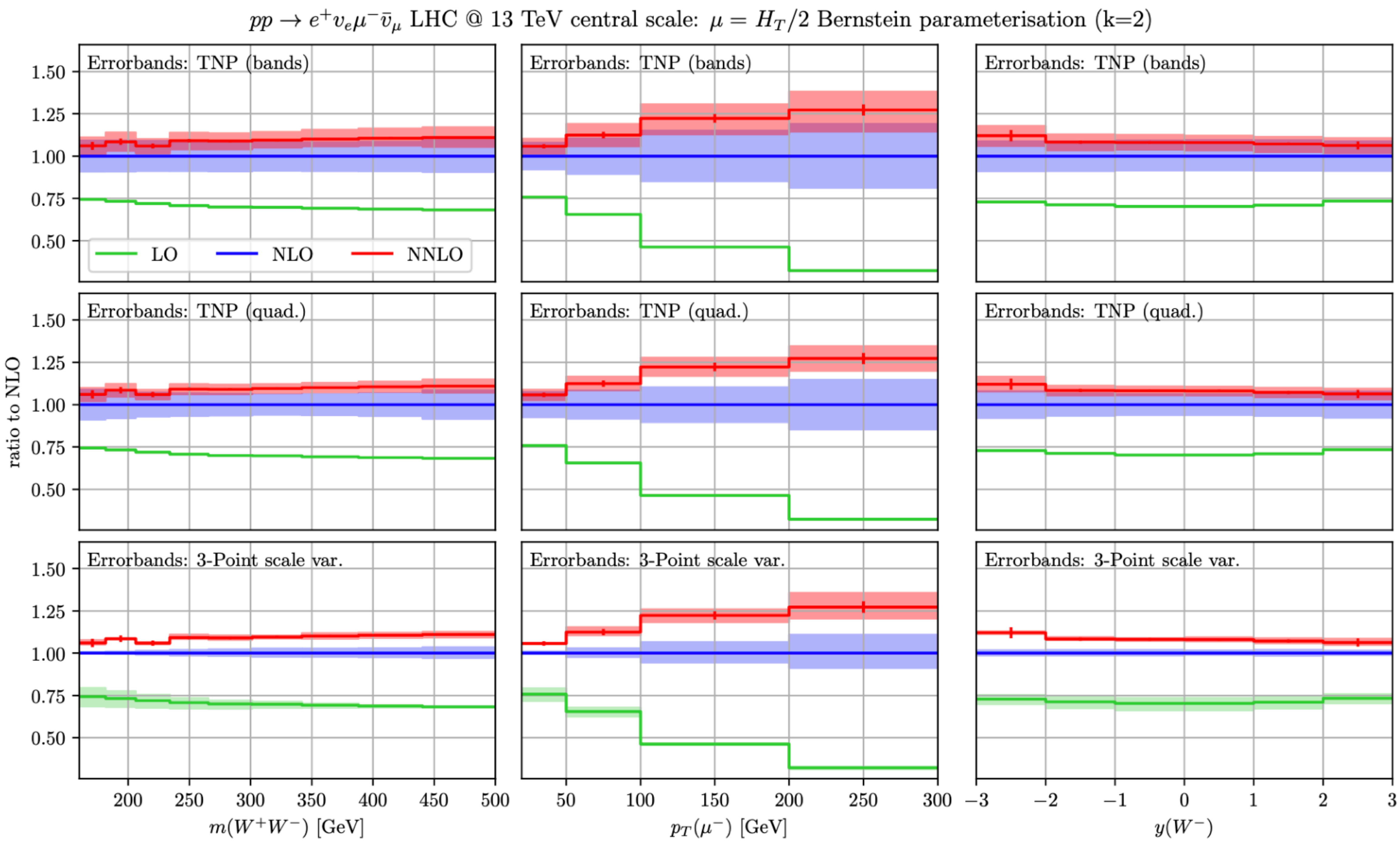


Band : sample $\theta \in [-1,1]$

Quad: add individual $\theta = \pm 1$ in quadrature

2412.14910, MAL, Poncelet

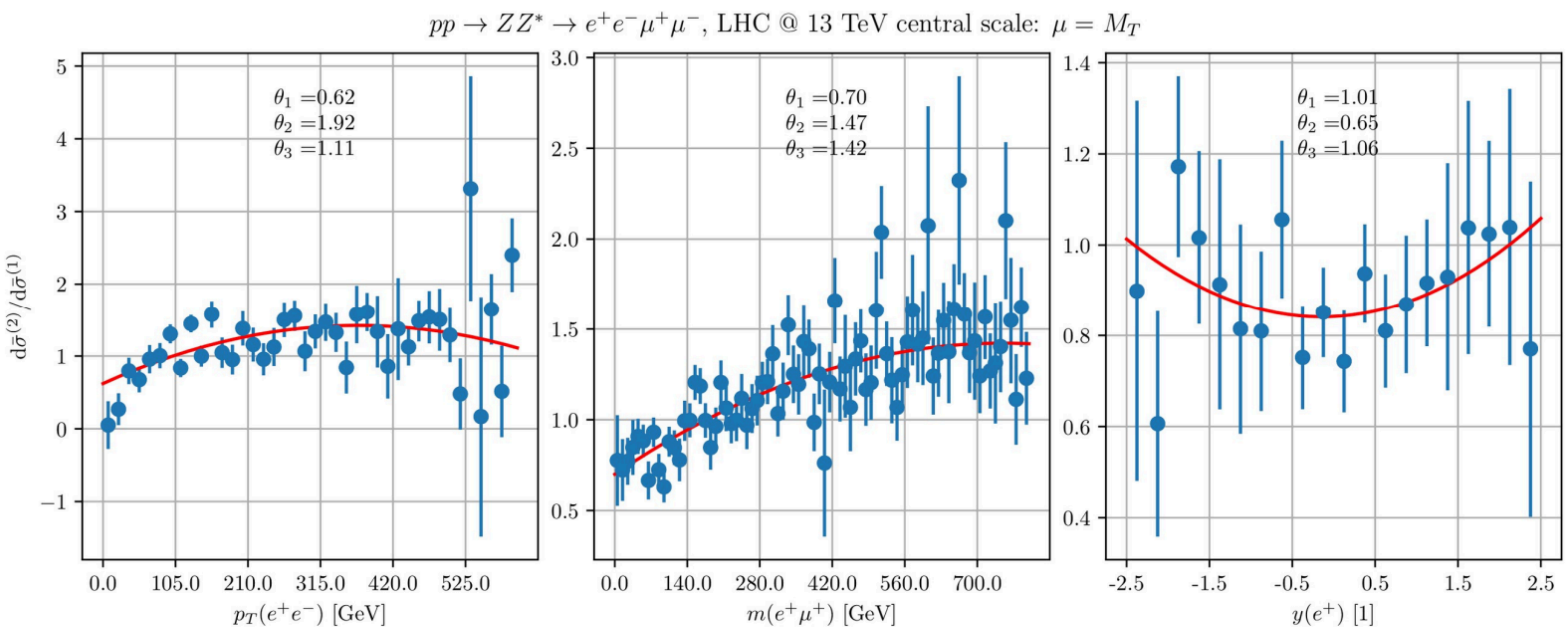
TNP UNCERTAINTIES - WW + DECAYS



2412.14910, MAL, Poncelet

EXAMPLE OF TNP FIT: ZZ

$$\frac{\mathrm{d}\bar{\sigma}^{(N+1)}_{\mathrm{TNP}}}{\mathrm{d}\bar{\sigma}^{(0)}} = \sum_{j=1}^{N} f_k^{(j)}\left(\vec{\theta}, x\right)\left(\frac{\mathrm{d}\bar{\sigma}^{(j)}}{\mathrm{d}\bar{\sigma}^{(0)}}\right) \qquad f_k^B\left(\vec{\theta}, x\right) = \sum_{i=0}^{k} \theta_i \begin{pmatrix} k \\ i \end{pmatrix} x^{k-i}(1-x)^i$$



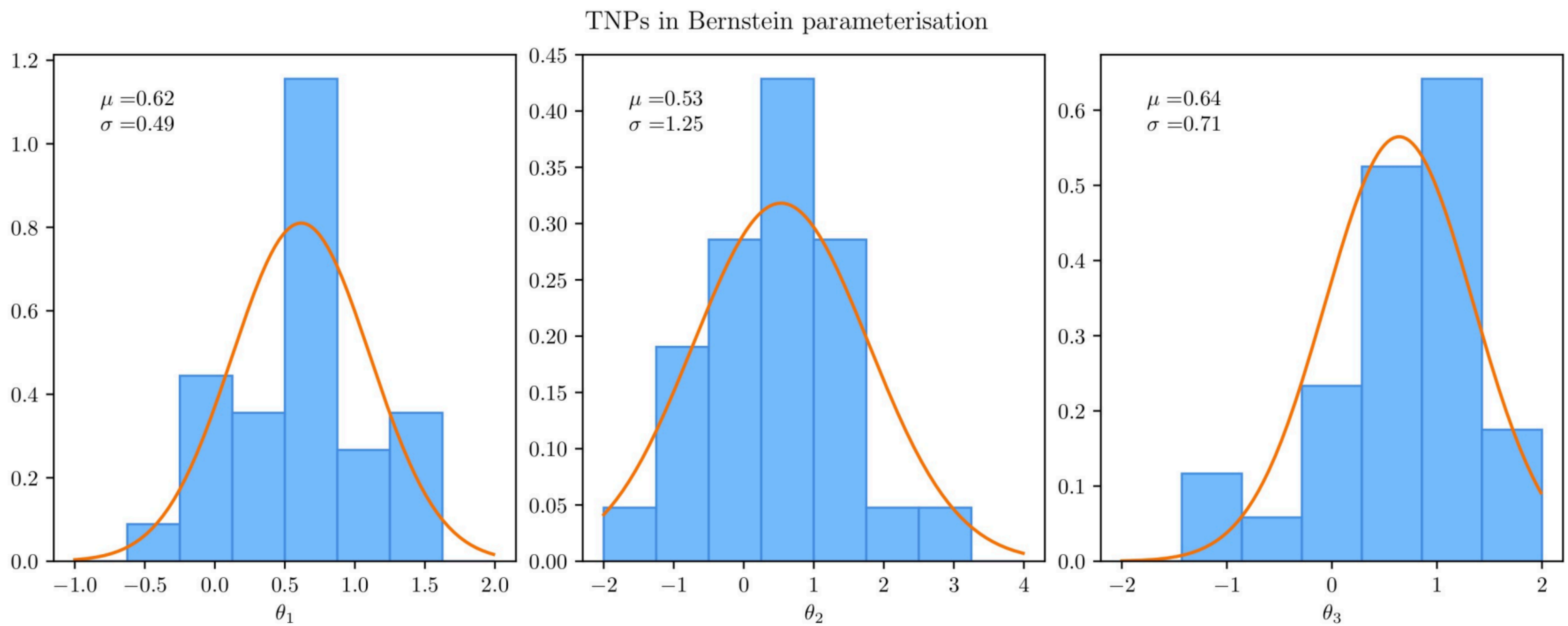
2412.14910, MAL, Poncelet

PROCESS META-STUDY

Process	$\sqrt{s}$/TeV	Scale	PDF	Distributions
$pp \to H$ (full theory)	13	$m_H/2$	`NNPDF3.1`	y_H
$pp \to ZZ^* \to e^+e^-\mu^+\mu^-$	13	M_T	`NNPDF3.1`	$M_{e^+\mu^+}$, $p_T^{e^+e^-}$, y_{e^+}
$pp \to WW^* \to e\nu_e\mu\nu_\mu$	13	m_W	`NNPDF3.1`	M_{WW}, $p_T^{\mu^-}$, y_{W^-}
$pp \to (W \to \ell\nu) + c$	13	$E_T + p_T^c$	`NNPDF3.1`	p_T^ℓ ,$\lvert y_\ell \rvert$,
$pp \to t\bar{t}$	13	$H_T/4$	`NNPDF3.1`	$M_{t\bar{t}}$, p_T^t, y_t
$pp \to t\bar{t} \to b\bar{b}\ell\bar{\ell}$	13	$H_T/4$	`NNPDF3.1`	$M_{\ell\bar{\ell}}$, $p_T^{b_1}$, $p_{T,\ell_1}/p_{T,\ell_2}$
$pp \to \gamma\gamma$	8	$M_{\gamma\gamma}$	`NNPDF3.1`	$M_{\gamma\gamma}$, $p_T^{\gamma_1}$, $y_{\gamma\gamma}$
$pp \to \gamma\gamma j$	13	$H_T/2$	`NNPDF3.1`	$M_{\gamma\gamma}$, $p_T^{\gamma\gamma}$, $\cos\phi_{\mathrm{CS}}$, $\lvert y_{\gamma_1} \rvert$, $\Delta\phi_{\gamma\gamma}$
$pp \to jjj$	13	$\hat{H}_T$	`MMHT2014`	TEEC with $H_{T,2} \in [1000, 1500), [1500, 2000), [3500, \infty)$ GeV
$pp \to \gamma jj$	13	H_T	`NNPDF3.1`	$M_{\gamma jj}$, p_T^j, $\lvert y_{\gamma-\mathrm{jet}} \rvert$, $E_{T,\gamma}$

2412.14910, MAL, Poncelet

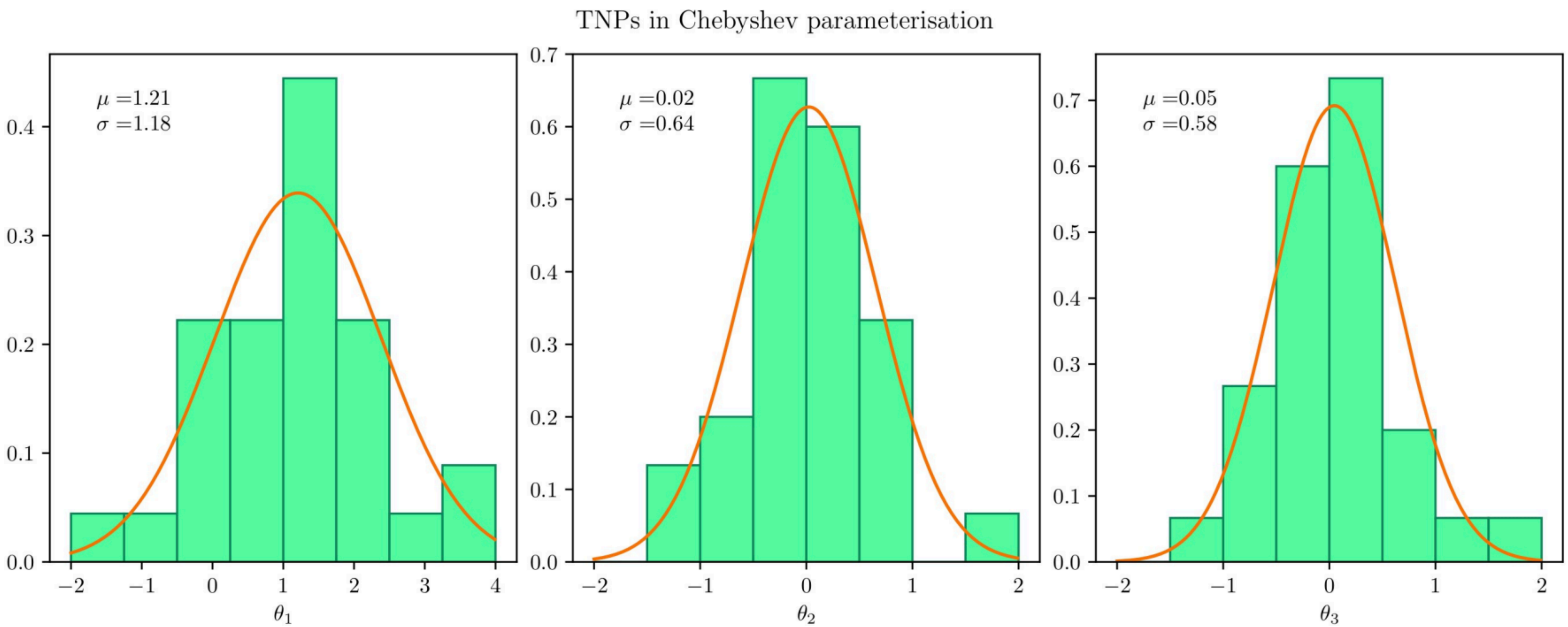
FITS: BERNSTEIN PARAMETERISATION



$$f_k^B\left(\vec{\theta}, x\right) = \sum_{i=0}^{k} \theta_i \begin{pmatrix} k \\ i \end{pmatrix} x^{k-i}(1-x)^i$$

2412.14910, MAL, Poncelet

FITS: CHEBYSHEV PARAMETERISATION



$$f_k^C\left(\vec{\theta}, x\right) = \frac{1}{2}\sum_{i=0}^{k} \theta_i T_i(x)$$

2412.14910, MAL, Poncelet

CAVEATS AND OPEN QUESTIONS

- How does uncertainty estimate depend on central scale choice?
- How sensitive is this to the exact parameterisation?
- How do you deal with multi-differential distributions?
- What about EW corrections?
- How do you correctly correlate processes?

SUMMARY AND OUTLOOK

- Accurate theory uncertainties a must for the LHC
- Scale variation has well-known shortcomings, in particular inability to correctly describe correlations
- TNPs provide an appealing alternative
- For single differential fixed order, can reproduce scale variation where it works well and provide significant improvements where it fails

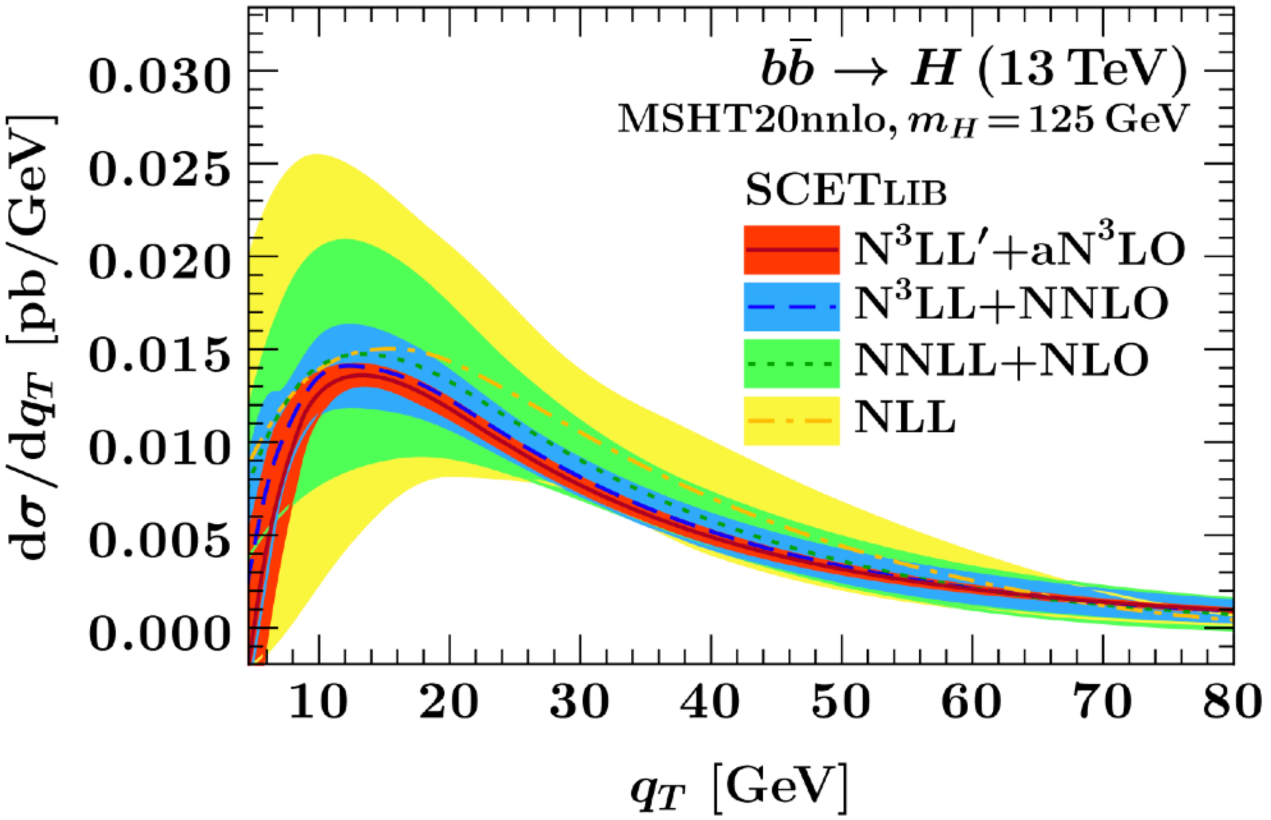
BACKUP SLIDES

SCALE VARIATION APPROACH

- Resummed calculations depend on many scales due to factorisation of cross section:

$$\frac{\mathrm{d}\hat{\sigma}}{\mathrm{d}p_T} \approx H(m_H, \mu_H)\, B_i(p_T, \mu_B) \otimes B_j(p_T, \mu_B) \otimes S(p_T, \mu_S)$$

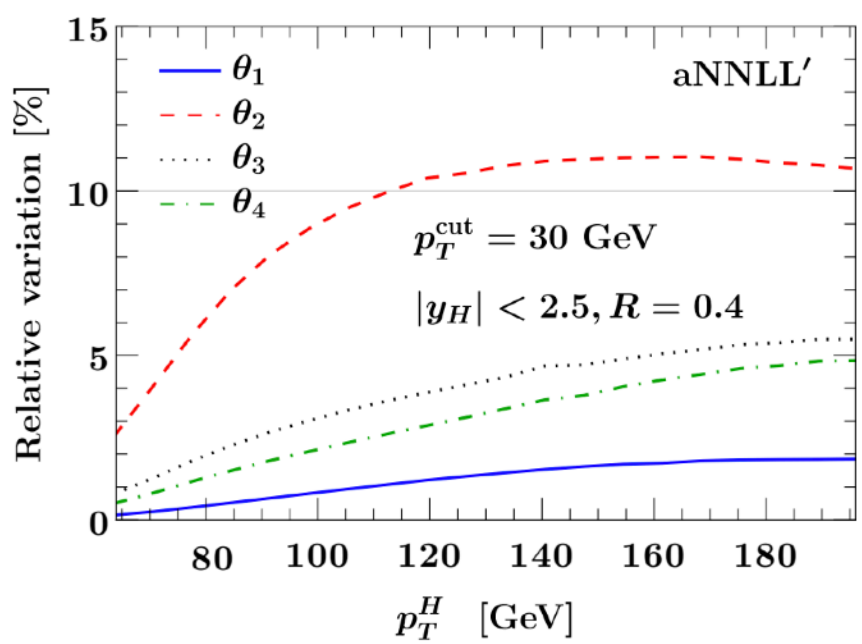
- Most reliable uncertainty estimation prescription involves simultaneous variation of all scales and enveloping.

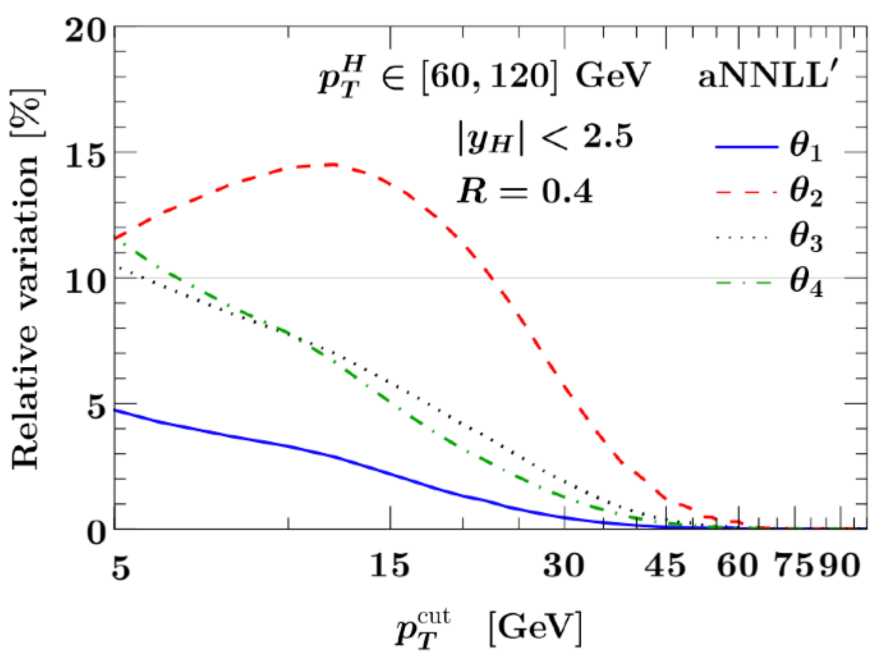


2306.16458, Cal, von Kuk, MAL, Tackmann

PARTIAL HIGHER ORDERS: JET VETO RESUMMATION

- Jet veto resummation for $H+j$ known to NLL′ - many NNLL ingredients known, but a few two-loop ingredients missing
- Approximate NNLL′ order can be achieved by treating unknown terms as nuisance parameters
- Correlation between distributions captured correctly





2408.13301, Cal, MAL, Scott, Tackmann, Waalewijn