Impact of higher-order theory uncertainties on α_S extractions at the LHC

Rene Poncelet

alphas-2025: Workshop on precision measurements of the strong coupling constant
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THE HENRYK NIEWODNICZAŃSKI
INSTITUTE OF NUCLEAR PHYSICS
POLISH ACADEMY OF SCIENCES

NARODOWE
CENTRUM
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Outline

- **Missing higher order uncertainties**
  - **TEEC → strong-coupling by ATLAS**
    motivation for looking into MHOU
  - **Inclusive jet production at NNLO+NNLL**
    indication that fixed-order MHOU from scale variations are too aggressive
    + two theory-nuisance-parameter approaches
- **Sub-leading colour effects in two-loop amplitudes**
  Full colour results 2 → 3 processes (including three-jet)

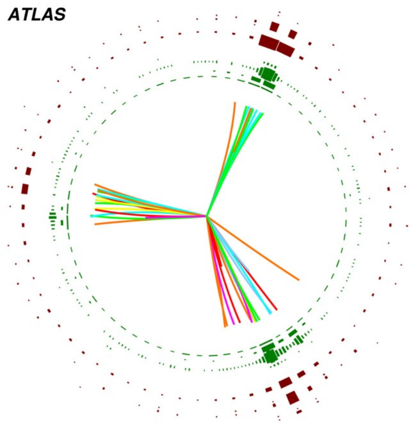
Jet observables at the LHC

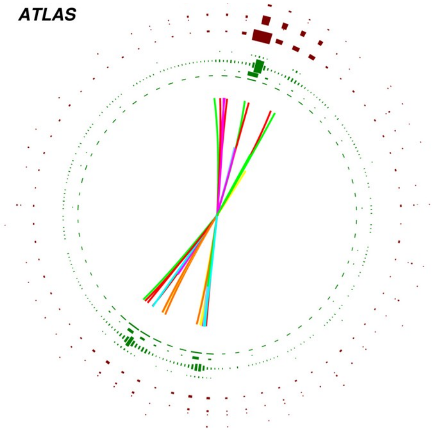
Jet final states:
- Tests of pQCD at high energy
- Tests of MC modelling of LHC events
- Search for new physics

Study of perturbative QCD with **multi-jets**:
- R32 ratios

$$R_{3/2}(X, \mu_R, \mu_F) = \frac{\mathrm{d}\sigma_3(\mu_R, \mu_F)/\mathrm{d}X}{\mathrm{d}\sigma_2(\mu_R, \mu_F)/\mathrm{d}X} \sim \alpha_s$$

→ Extraction of the strong coupling constant
- Transverse Energy-Energy Correlator
- Event shapes





Credits: [ATLAS:2007.12600]

Jet observables at the LHC

Jet final states:
- Tests of pQCD at high energy
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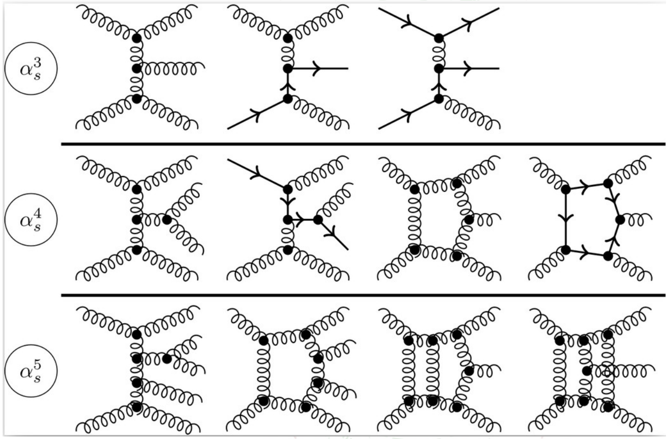
Needs NNLO QCD computation for many parton final states



Study of perturbative QCD with **multi-jets**:
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$$R_{3/2}(X, \mu_R, \mu_F) = \frac{\mathrm{d}\sigma_3(\mu_R, \mu_F)/\mathrm{d}X}{\mathrm{d}\sigma_2(\mu_R, \mu_F)/\mathrm{d}X} \sim \alpha_s$$

→ Extraction of the strong coupling constant

- Transverse Energy-Energy Correlator
- Event shapes

Credits: [ATLAS:2007.12600]

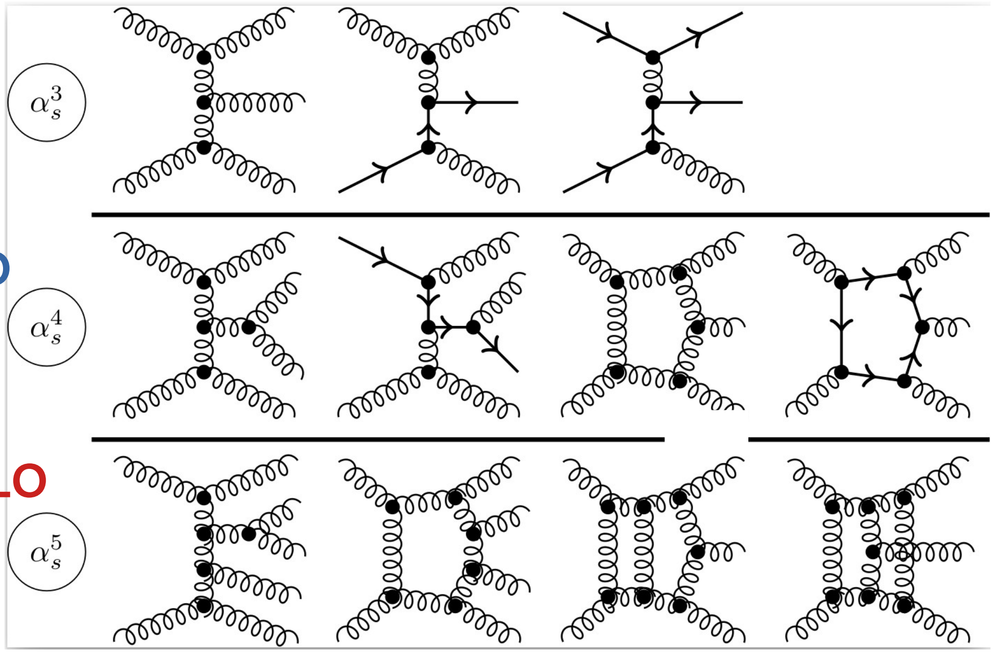
Perturbative QCD through NNLO QCD

$$\sigma_{h_1 h_2 \to X} = \sum_{ij} \int_0^1 \int_0^1 \mathrm{d}x_1 \mathrm{d}x_2 \phi_{i,h_1}(x_1, \mu_F^2) \phi_{j,h_2}(x_2, \mu_F^2) \hat{\sigma}_{ij\to X}(\alpha_s(\mu_R^2), \mu_R^2, \mu_F^2)$$

LO

NLO

NNLO



Partonic cross section:

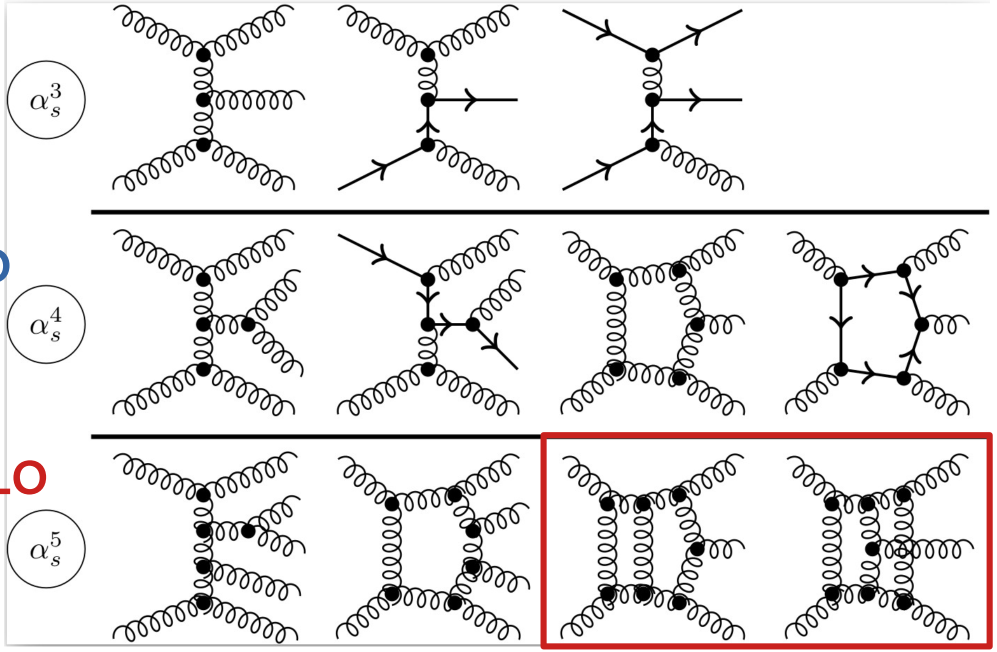
$$\hat{\sigma}_{ab\to X} = \hat{\sigma}^{(0)}_{ab\to X} + \hat{\sigma}^{(1)}_{ab\to X} + \hat{\sigma}^{(2)}_{ab\to X} + \mathcal{O}(\alpha_s^3)$$

Perturbative QCD through NNLO QCD

LO

NLO

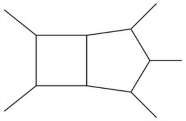
NNLO



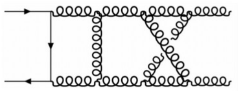
All massless 2→3 are know by now

How to compute
multi-scale two-loop QCD amplitudes?
→ **fast growing complexity:**
rational coef. and **special functions**
→ deeper understanding of the analytical properties
→ refinement of computational tools

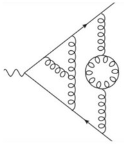
Two-loop 5-point
[Abreu, Agarwal, Badger, Buccioni, Chawdhry, Chicherin,Czakon, de Laurenties, Febres-Cordero, Gambuti, Gehrmann, Henn, Lo Presti, Manteuffel, Ma, Mitov, Page, Peraro, Poncelet, Schabiner Sotnikov, Tancredi, Zhang,...]



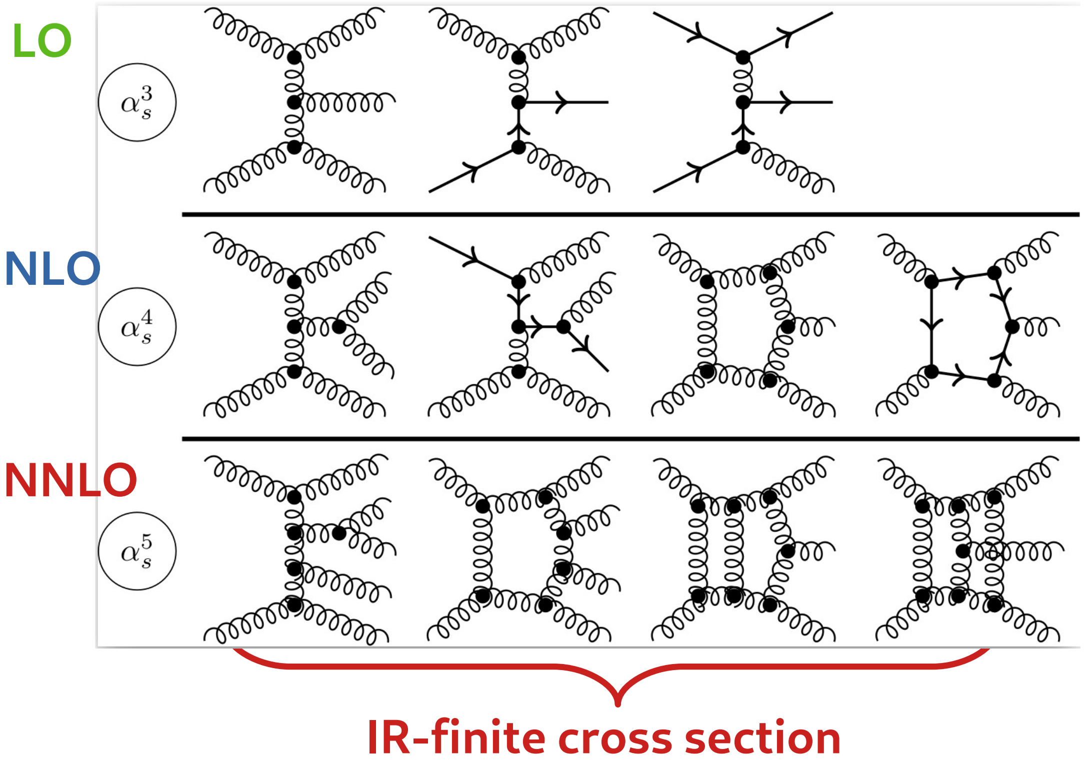
Three-loop 4-point
[Bargiela, Dobadilla, Canko, Caola, Jakubcik, Gambuti, Gehrmann, Henn, Lim, Mella, Mistleberger, Wasser, Manteuffel, Syrrakow, Smirnov, Trancredi, ...]



Four-loop 3-point
[Henn, Lee, Manteuffel, Schabinger, Smirnov, Steinhauser,...]



Perturbative QCD through NNLO QCD



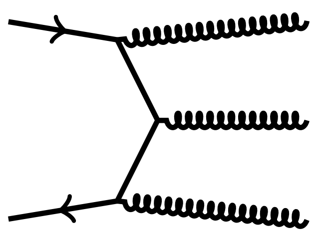
qT-slicing [Catani'07], N-jettiness slicing [Gaunt'15/Boughezal'15], Antenna [Gehrmann'05-'08], Colorful [DelDuca'05-'15], Projetction [Cacciari'15], Geometric [Herzog'18], Unsubtraction [Aguilera-Verdugo'19], Nested collinear [Caola'17], Local Analytic [Magnea'18], **Sector-improved residue subtraction** [Czakon'10-'14,'19]

2) How to achieve **infrared finite differential** cross sections at NNLO QCD?
~20 years to solve this problem
→ highly non-trivial IR structure
→ plethora of subtraction schemes

Three-jet production

- Sector-improved residue subtraction [Czakon'10'14'19]
  - Efficient c++ implementation → STRIPPER
  - Highly automated to deal with enormous amount of channels in three-jet production → O(1k) sectors →O(1M) individual MC integrals
  - Still computationally very challenging! → O(1-100 MCPUh)
- Many-leg, IR stable one-loop amplitudes → OpenLoops [Buccioni'19]
- **Originally**: double virtual amplitudes in **leading-colour approximation** [Abreu'21]
  - Sub-leading colour corrections expected to be small
  - Fast numerical evaluation → very small contribution to computational cost

→ **see update at the end** of the talk lifting this approximation



$pp \to ggg + X$

Only Approximation made:

$$\mathcal{F}^{(2)}(\mu_R^2) = 2\,\mathrm{Re}\left[\mathcal{M}^{\dagger(0)}\mathcal{F}^{(2)}\right](\mu_R^2) + \left|\mathcal{F}^{(1)}\right|^2(\mu_R^2) \equiv \mathcal{F}^{(2)}(s_{12}) + \sum_{i=1}^{4} c_i \ln^i\left(\frac{\mu_R^2}{s_{12}}\right)$$

$$F^{(2)}_{\text{l.c. resc.}}(\mu^2) = \frac{F^{(0)}}{F^{(0)}_{\text{l.c.}}} F^{(2)}_{\text{l.c.}}(Q^2) + \sum_{i=0}^{4} c_i \log^i(\mu^2/Q^2)$$

Multi-jet observables

Test of pQCD and extraction of strong coupling constant

NLO theory unc. > experimental unc.

- NNLO QCD needed for precise theory-data comparisons

  → Restricted to two-jet data [Currie'17+later][Czakon'19]

- NNLO QCD three-jet → access to more observables

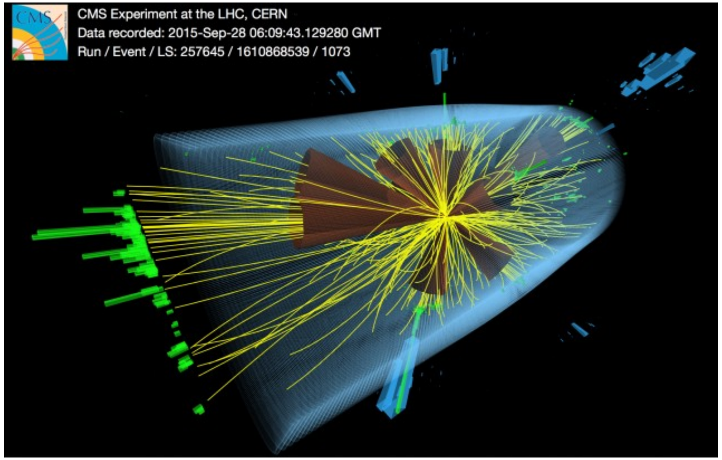
  - Jet ratios

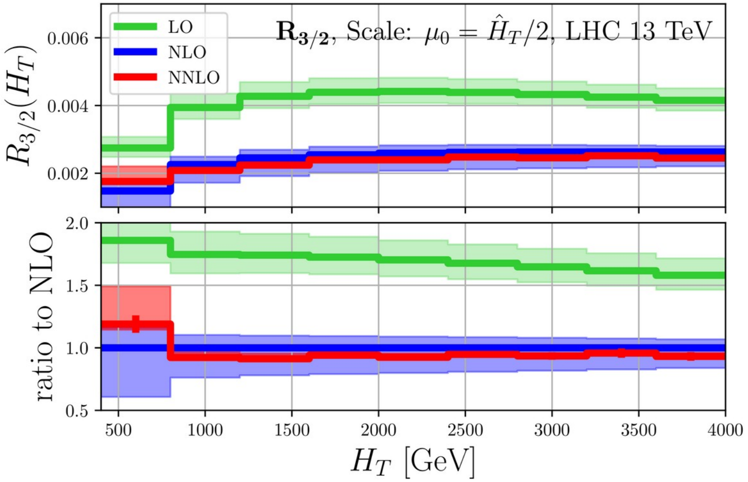
    Next-to-Next-to-Leading Order Study of Three-Jet Production at the LHC
    Czakon, Mitov, **Poncelet** [2106.05331]

$$R^i(\mu_R, \mu_F, \mathrm{PDF}, \alpha_{S,0}) = \frac{\mathrm{d}\sigma_3^i(\mu_R, \mu_F, \mathrm{PDF}, \alpha_{S,0})}{\mathrm{d}\sigma_2^i(\mu_R, \mu_F, \mathrm{PDF}, \alpha_{S,0})}$$

  - Event shapes

    NNLO QCD corrections to event shapes at the LHC
    Alvarez, Cantero, Czakon, Llorente, Mitov, **Poncelet** [2301.01086]



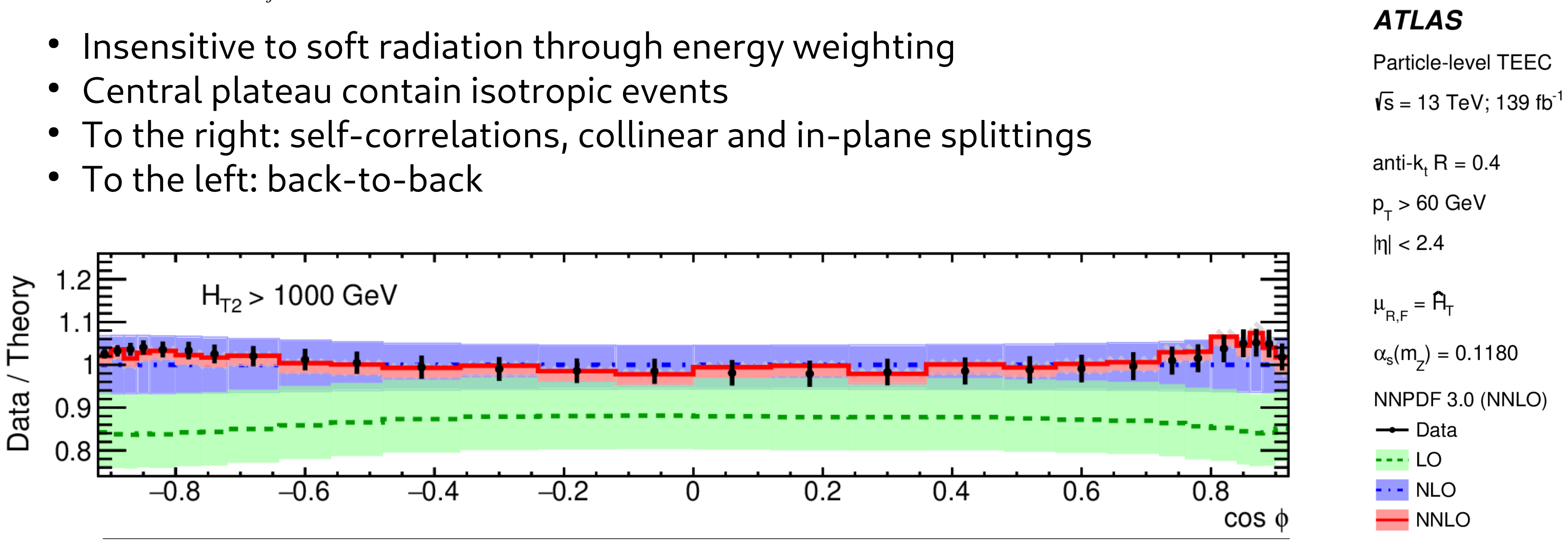


The transverse energy-energy correlator

See also Claudia's talk

$$\frac{1}{\sigma_2}\frac{\mathrm{d}\sigma}{\mathrm{d}\cos\Delta\phi} = \frac{1}{\sigma_2}\sum_{ij}\int \frac{\mathrm{d}\sigma\ x_{\perp,i}x_{\perp,j}}{\mathrm{d}x_{\perp,i}\mathrm{d}x_{\perp,j}\mathrm{d}\cos\Delta\phi_{ij}}\delta(\cos\Delta\phi - \cos\Delta\phi_{ij})\mathrm{d}x_{\perp,i}\mathrm{d}x_{\perp,j}\mathrm{d}\cos\Delta\phi_{ij}\,,$$

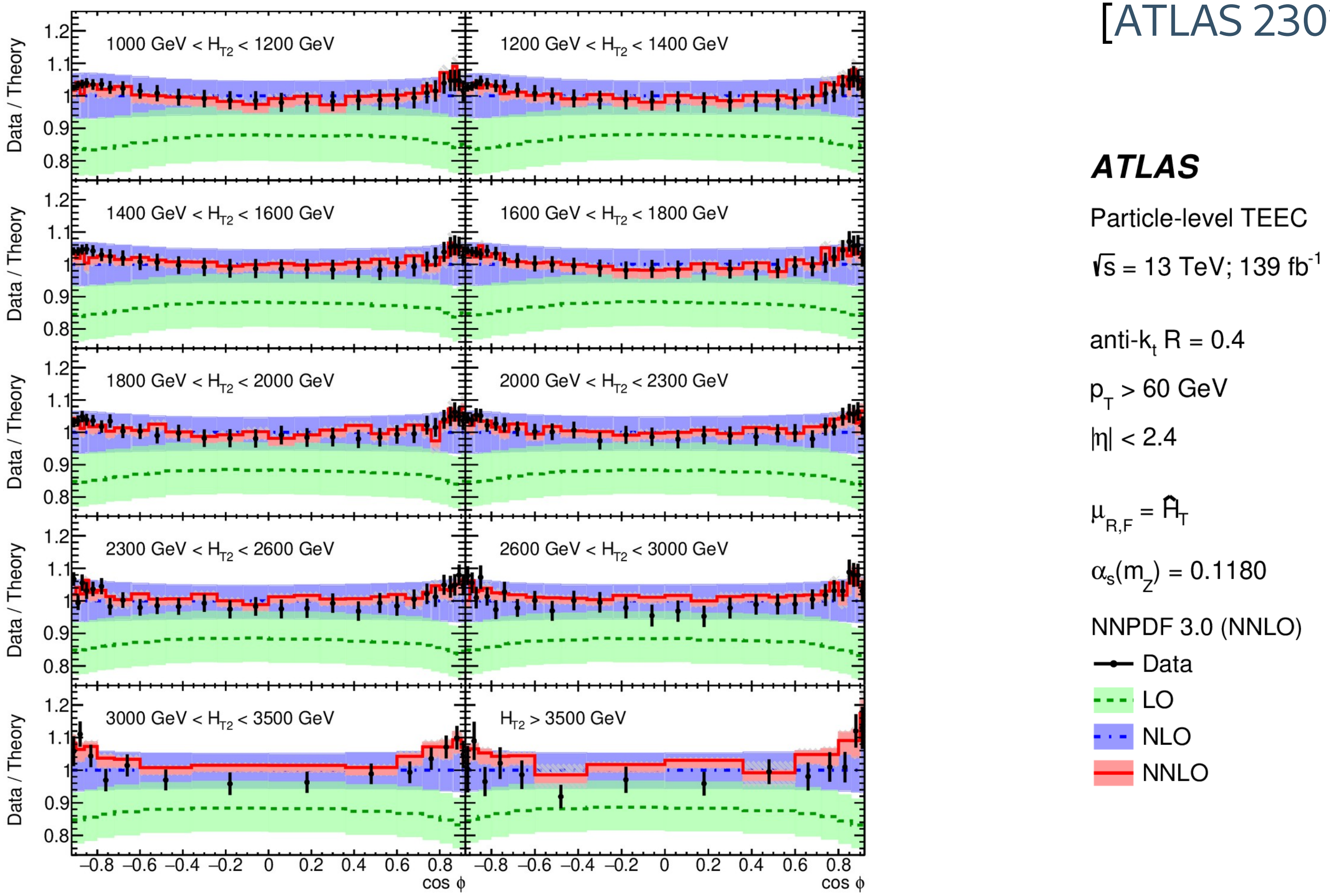
- Insensitive to soft radiation through energy weighting
- Central plateau contain isotropic events
- To the right: self-correlations, collinear and in-plane splittings
- To the left: back-to-back



[ATLAS 2301.09351]

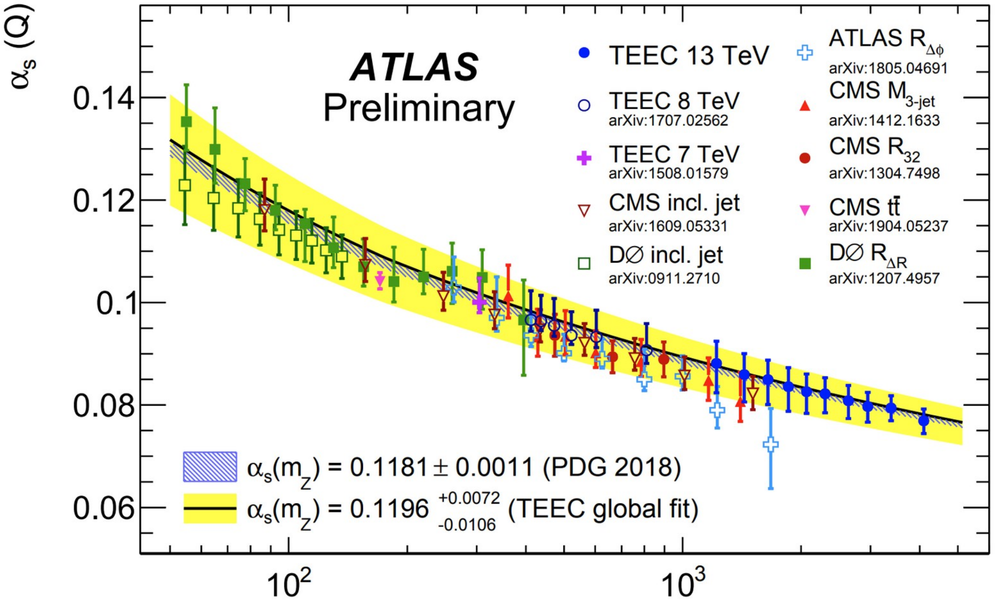
Double differential TEEC

[ATLAS 2301.09351]



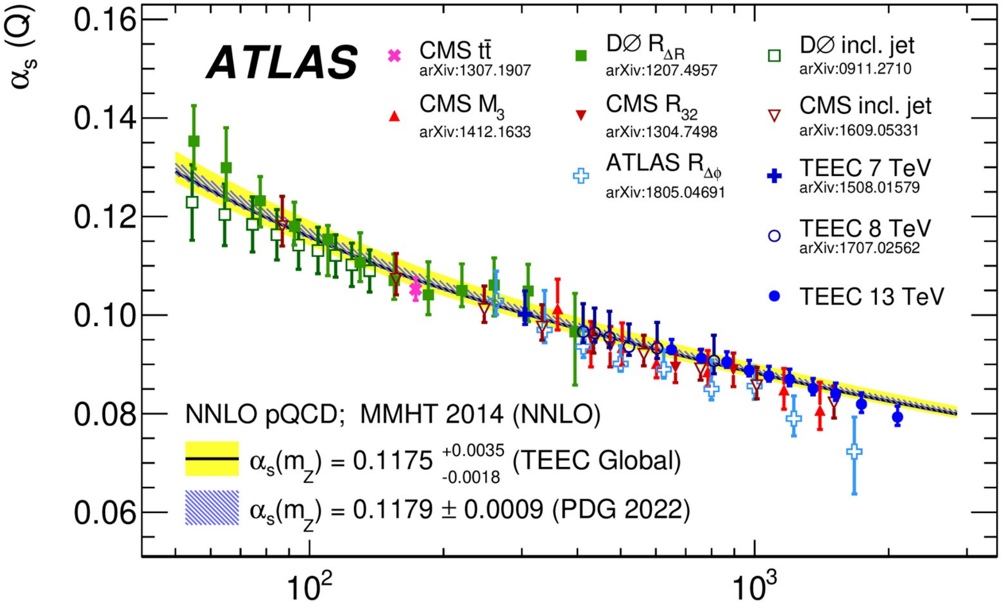
Alphas from TEEC (ATLAS)

NLO QCD



[ATLAS-CONF-2020-025]

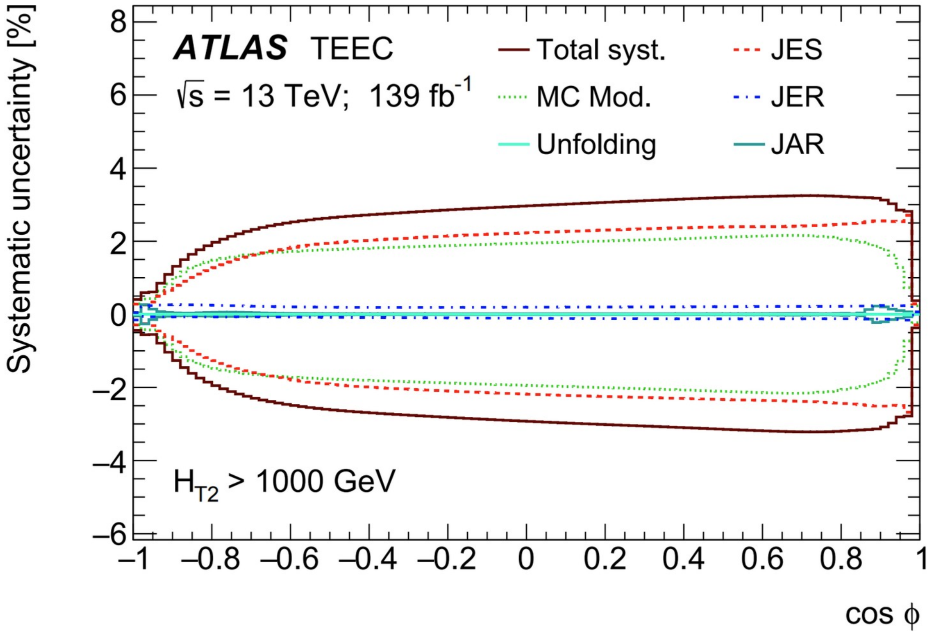
NNLO QCD



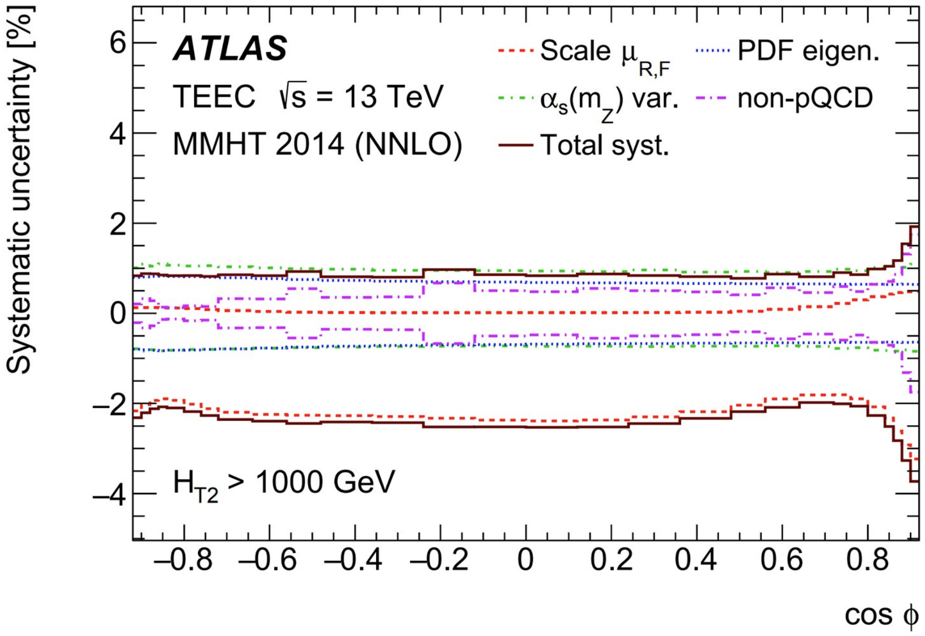
[ATLAS 2301.09351]

Systematic Uncertainties TEEC

Experimental uncertainties

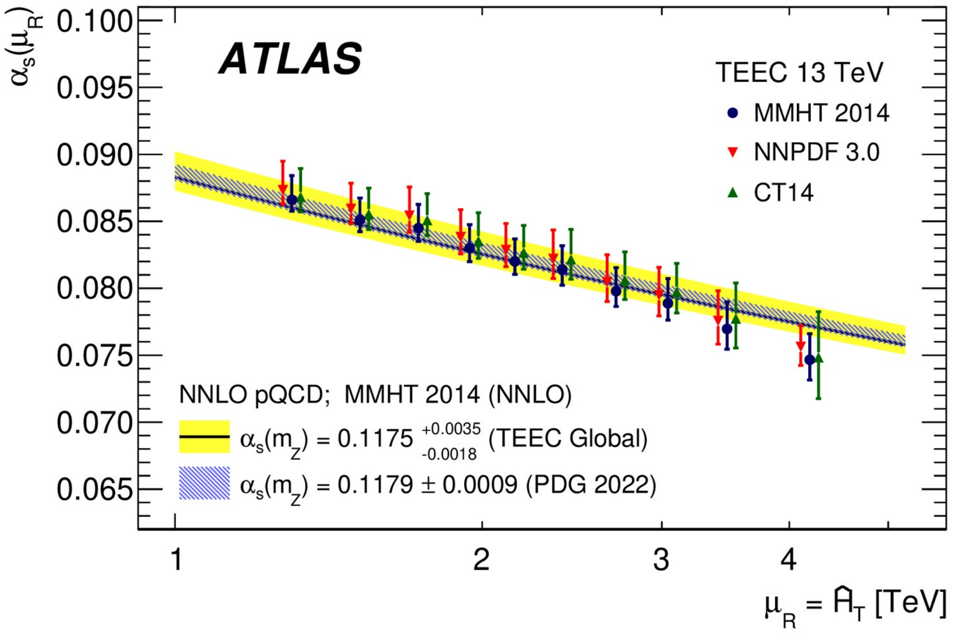


Theory uncertainties



Scale dependence is the dominating theory uncertainty

Where does the slope come from?



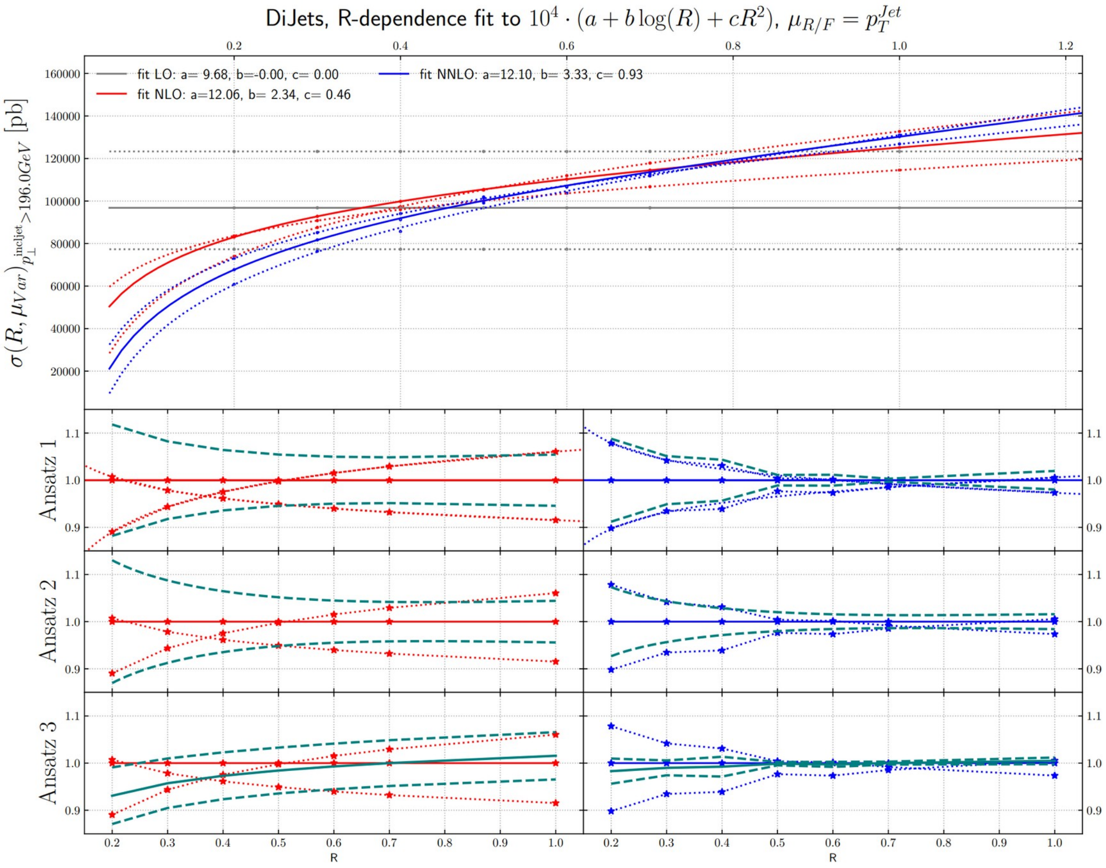
- Residual PDF effects → very high Q^2 ?
  → **need re-run with modern PDFs (a bit expensive, needs improved performance)**
- EW corrections? → **cancelling in ratio**
  Full NLO corrections to 3-jet production and R32 at the LHC Reyer, Schönherr, Schumann, 1902.01763
- Maybe effect from LC approximation in two-loop ME? → **see end of the talk**
- Resummation/PS effect? → **wip**
- **MHOU?**
  wip → start with inclusive jets are simpler!

Theory uncertainties in inclusive jet production

→ NNLO QCD corrections imply very small theory uncertainty for R = 0.4 to 1.0

→ Significant jet radius dependence of uncertainties from scale variations

→ small radius needs resummation



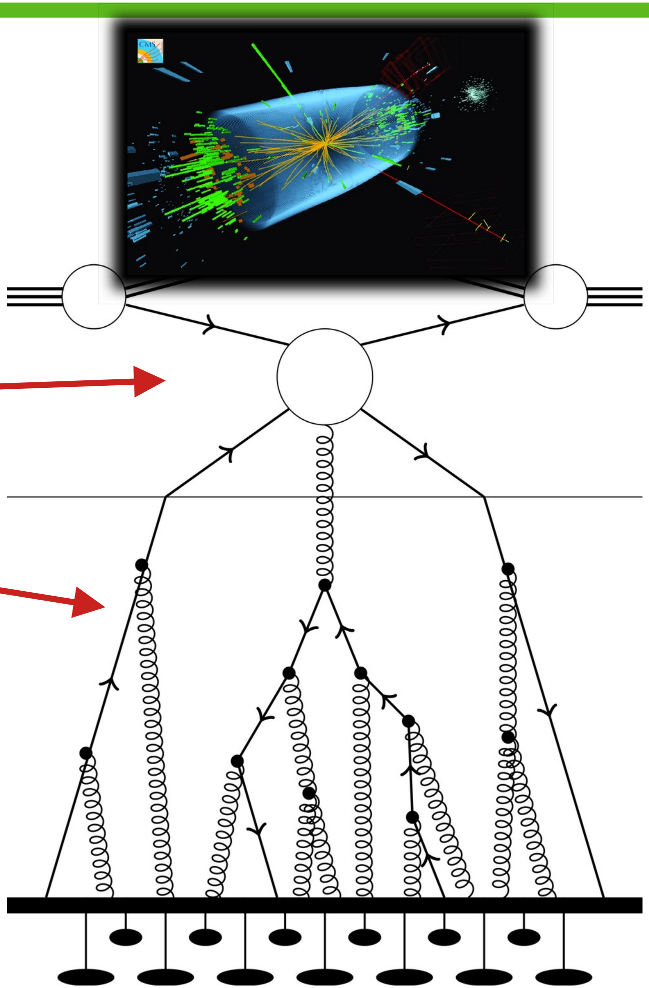
[1903.12563 Bellm et al]

Theory picture of hadron collision events

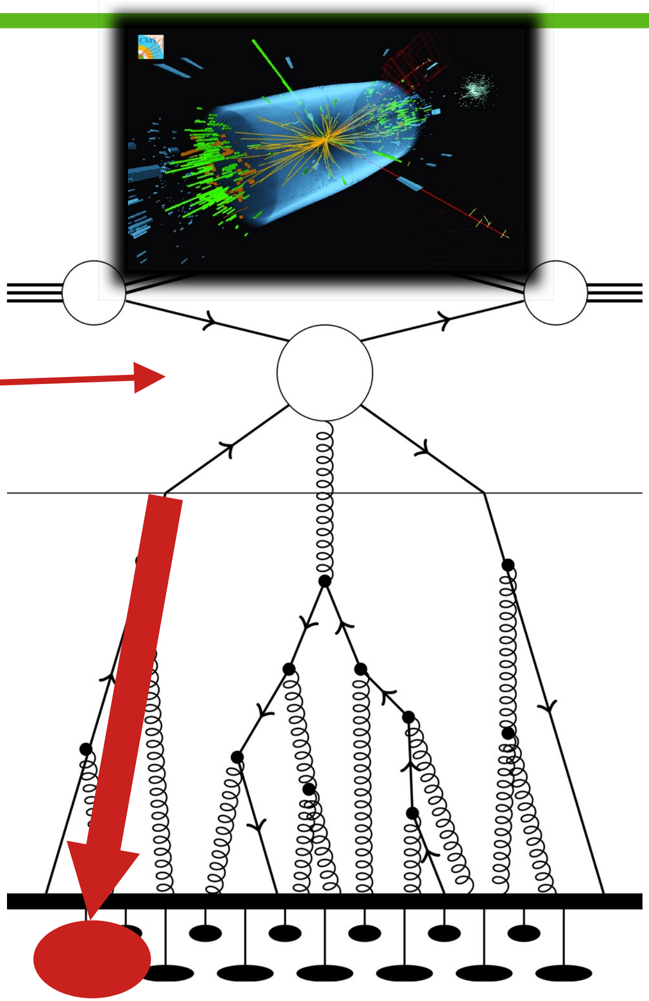
$Q \gg \Lambda_{\mathrm{QCD}}$ **Fixed-order perturbation theory**
scattering of individual partons

$Q \gtrsim \Lambda_{\mathrm{QCD}}$ **Parton-shower/Resummation**
all-order bridge between perturbative and non-perturbative physics

$Q \sim \Lambda_{\mathrm{QCD}}$ **"Hadronization"/MPI/…**
non-perturbative physics



Beyond fixed-order perturbation theory



$Q \gg \Lambda_{\mathrm{QCD}}$ **Fixed-order perturbation theory**
scattering of individual partons

Parton to identified object transition "**Fragmentation**"
→ Resummation of collinear logs through 'DGLAP'
→ Non perturbative fragmentation functions
Example: B-hadrons in e+e-

$$\frac{d\sigma_B(m_b, z)}{dz} = \sum_i \left\{ \frac{d\sigma_i(\mu_{Fr}, z)}{dz} \otimes D_{i\to B}(\mu_{Fr}, m_b, z) \right\}(z) + \mathcal{O}(m_b^2)$$

Jet substructure

Semi-inclusive jet function [1606.06732, 2410.01902]

$$\frac{d\sigma_{\mathrm{LP}}}{dp_T d\eta} = \sum_{i,j,k} \boxed{\int_{x_{i,\min}}^{1} \frac{dx_i}{x_i} f_{i/P}(x_i,\mu) \int_{x_{j,\min}}^{1} \frac{dx_j}{x_j} f_{j/P}(x_j,\mu) \int_{z_{\min}}^{1} \frac{dz}{z} \mathcal{H}_{ij}^{k}(x_i, x_j, p_T/z, \eta, \mu)} \times \boxed{J_k\left(z, \ln\frac{p_T^2 R^2}{z^2\mu^2}, \mu\right)},$$

The same hard function as for identified hadrons!

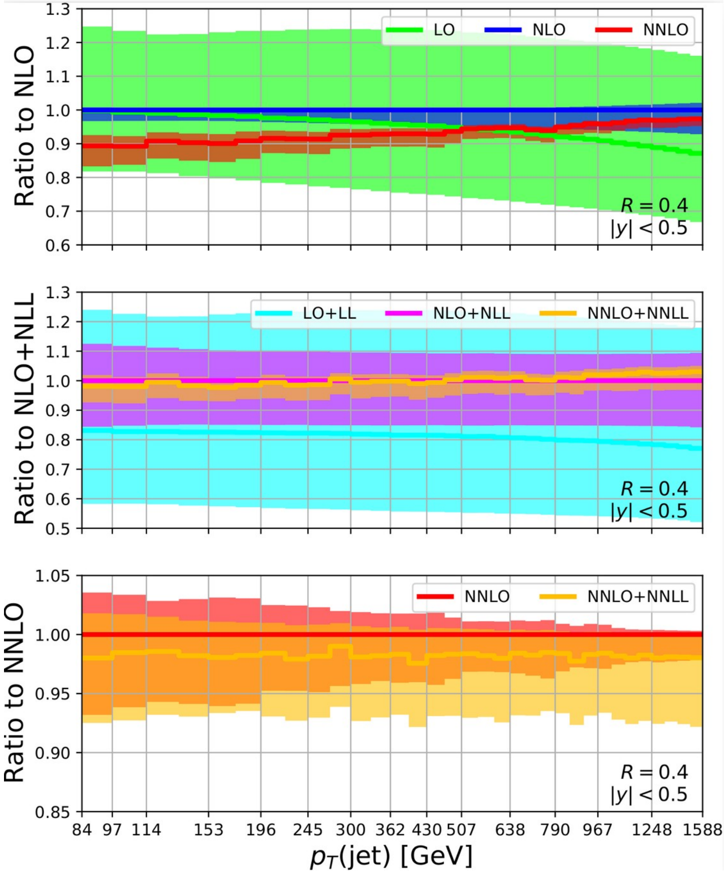
Inclusion of fragmentation@NNLO QCD:
[Czakon, Generet, Mitov, Poncelet]
- B-hadrons in top-decays [2210.06078,2102.08267]
- Open-bottom [2411.09684]
- Identified hadrons [2503.11489]

Modified RGE wrt DGLAP: [2402.05170,2410.01902]

$$\frac{d\vec{J}\left(z, \ln\frac{p_T^2 R^2}{z^2\mu^2}, \mu\right)}{d\ln\mu^2} = \int_z^1 \frac{dy}{y} \vec{J}\left(\frac{z}{y}, \ln\boxed{\frac{y^2 p_T^2 R^2}{z^2\mu^2}}, \mu\right) \cdot \widehat{P}_T(y)$$

Inclusive jet production: small-R resummation NNLO+NNLL

[Generet, Lee, Moult, Poncelet, Zhang’25]



FO scale variations

R=0.4

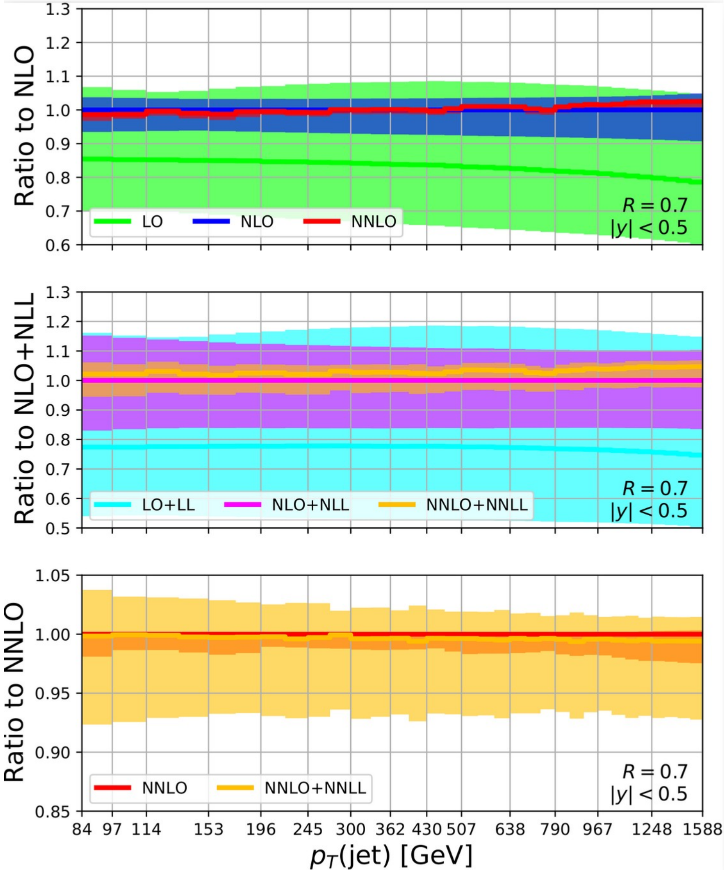
→ underestimation of NNLO correction

R=0.7

→ very small NNLO uncertainty

Resummation

→ stabilization of pert. series and uncertainties.

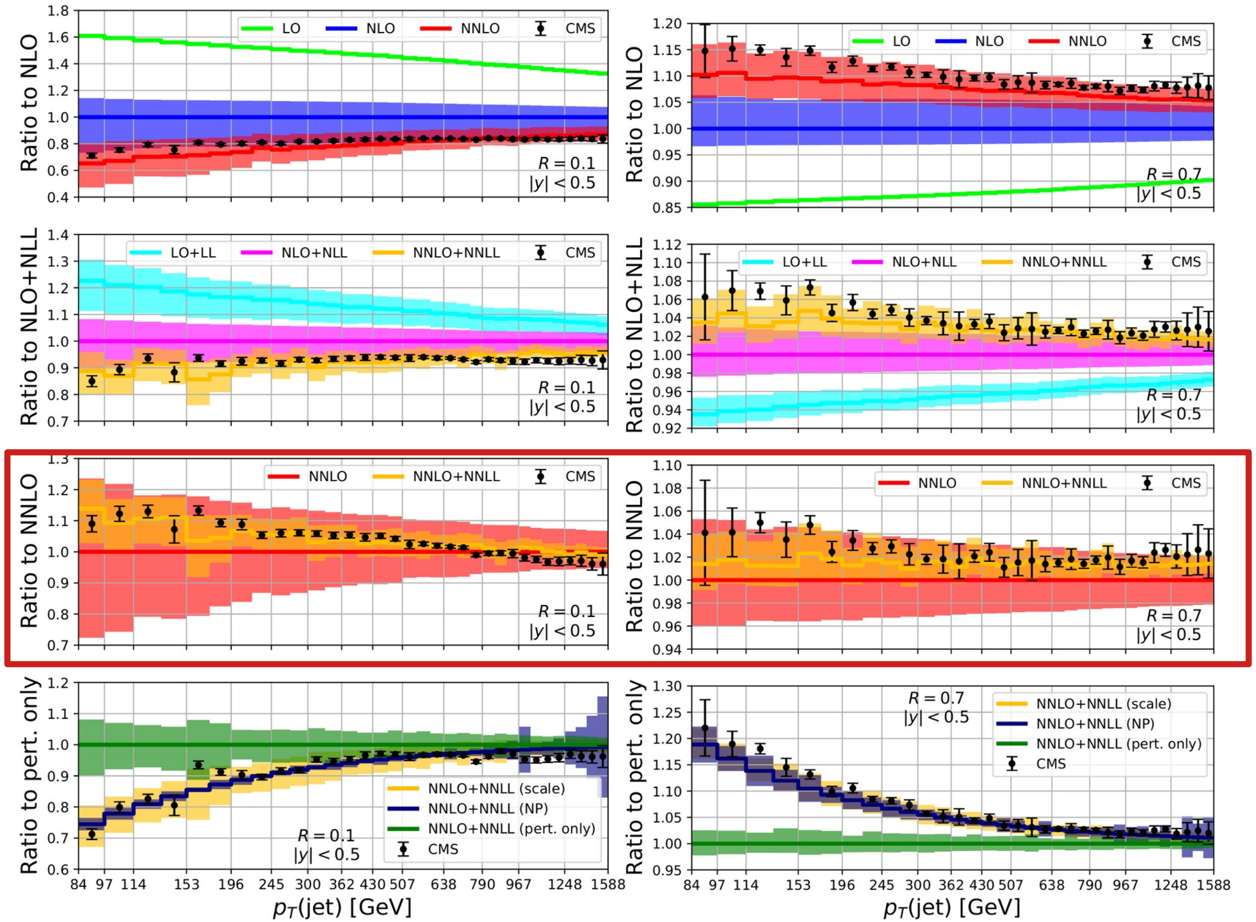


Small-R jets

Application to small-R jets
[Generet, Lee, Moult, Poncelet, Zhang]
[2503.21866]

'Triple' differential measurement by CMS:
Y, pT, R [2005.05159]

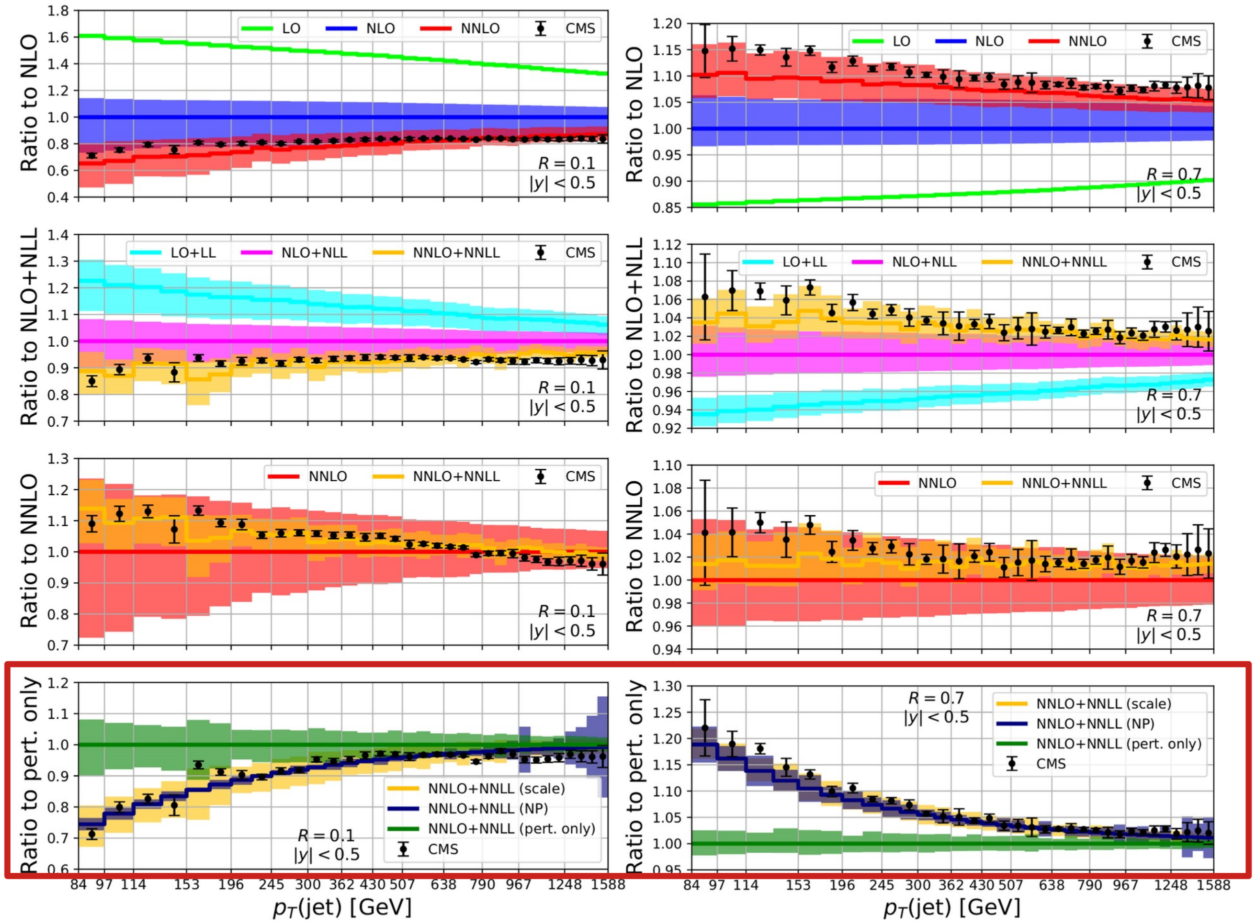
→ provided as ratios over R=0.4
[→ having the absolute spectra would be super useful...]



Small-R jets

Non-perturbative effects huge
→ analytic knowledge of R dep.
helps in this case [0712.3014]

→ unc. ~ MHOU for R = 0.7



Theory uncertainties from scale variations

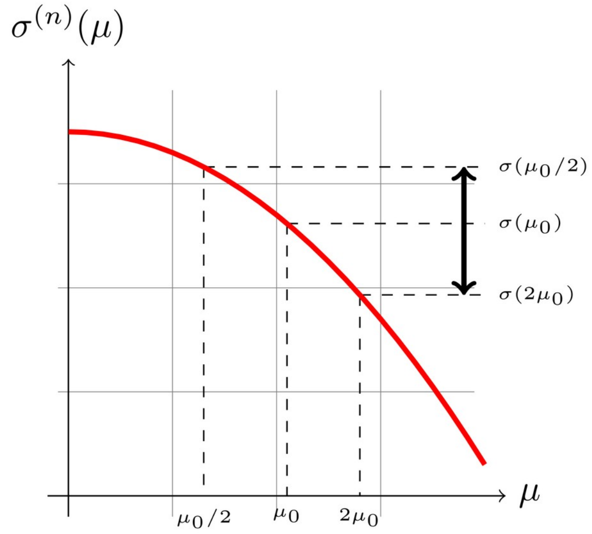
Lets focus on QCD as an example: $\alpha = \alpha_s(\mu_0)$

$$\mathrm{d}\sigma = \mathrm{d}\sigma^{(0)} + \alpha_s \mathrm{d}\sigma^{(1)} + \alpha_s^2 \mathrm{d}\sigma^{(2)} + \ldots \xrightarrow{\text{RGE}} \mu \frac{\mathrm{d}\sigma^{(n)}}{\mathrm{d}\mu} = \mathcal{O}\left(\alpha_s^{(n_0+n+1)}\right)$$

Of same order as the next dominant term → exploiting this to estimate size of $\mathrm{d}\sigma^{(n+1)}$

Scale variation prescription (ad-hoc and heuristic choice)

- choose 'sensible' μ_0
  - → principle of fasted apparent convergence: $\sigma^{(n)}(\mu_{\mathrm{FAC}}) = 0$
  - → principle of minimal sensitivity: $\mu \frac{\mathrm{d}\sigma(\mu)}{\mathrm{d}\mu}\Big|_{\mu=\mu_{\mathrm{PMC}}} = 0$
  - → ...
- vary with a factor (typically 2)
- take envelope as uncertainty



Short comings of scale variations

- not always reliable … however in most cases issues are understood/expected:
  new channels, phase space constraints, etc. → often we can design workarounds
- however, some issues are more fundamental:
  - → how to choose the central scale? → not a physical parameter, no 'true' value
    (Principle of fasted apparent convergence, principle of minimal sensitivity,...)
  - → how to propagate the estimated uncertainty, no statistical interpretation!
  - → what about correlations? Based on 'fixed form' of the lower orders and RGE.

(At the moment) two alternative approaches under investigation:

"Bayesian"

[Cacciari,Houdeau 1105.5152]
[Bonvini 2006.16293]
[Duhr, Huss, Mazeliauskas, Szafron 2106.04585]

"Theory Nuisance Parameter"

[Tackmann 2411.18606]
→ W mass extraction: [CMS 2412.13872]
[Cal,Lim, Scott,Tackmann Waalewijn 2408.13301]
[Lim, Poncelet, 2412.14910]
[Cridge,Marinelli,Tackmann,2506.13874]

1. TNP approach for fixed-order computations

[Lim, Poncelet, 2412.14910]

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

Observation, i.e. “expert knowledge”: $\frac{\mathrm{d}\bar{\sigma}^{(i)}}{\mathrm{d}\bar{\sigma}^{(0)}} \sim \mathcal{O}(1)$

Use some knowledge about lower orders but introduce parametric dependence:

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

x → mapped kinematic variable

Approximation of original TNP philosophy
→ there is only $f_i(\hat{\theta}) \approx \hat{f}_i$

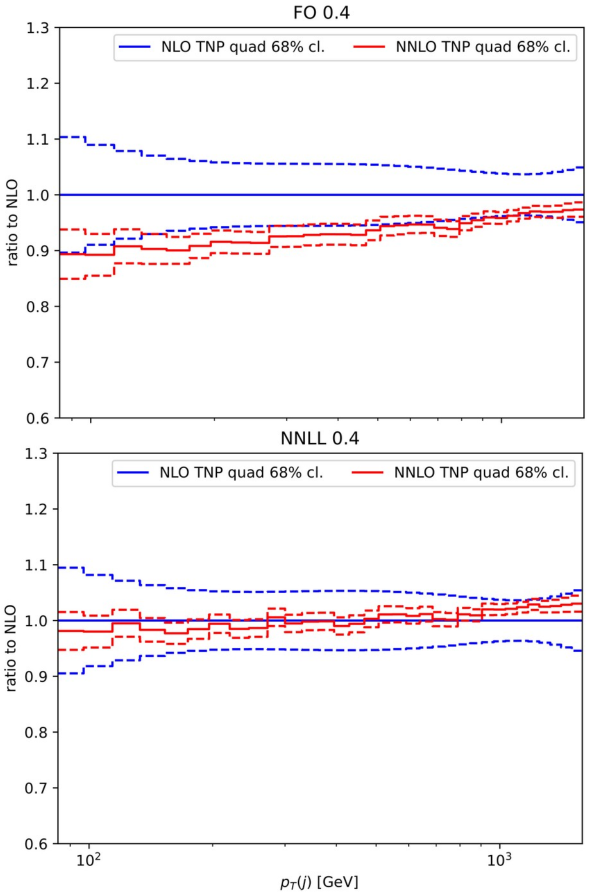
Chebyshev: $f_k^C\left(\vec{\theta}, x\right) = \frac{1}{2} \sum_{i=0}^{k} \theta_i T_i(x)$ $\quad x \in [-1, 1]$

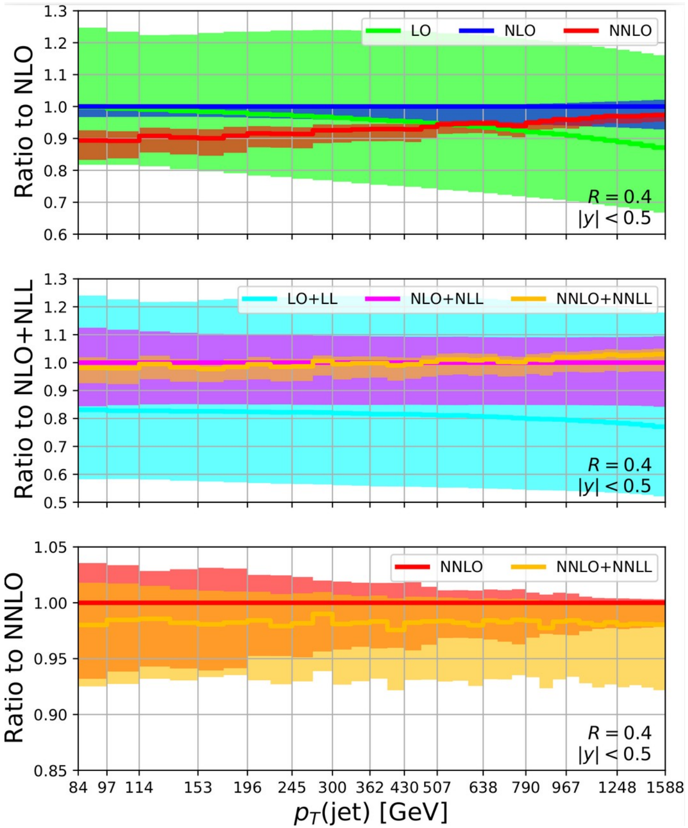
1. TNP uncertainties for inclusive jet production

R = 0.4

TNP uncertainties

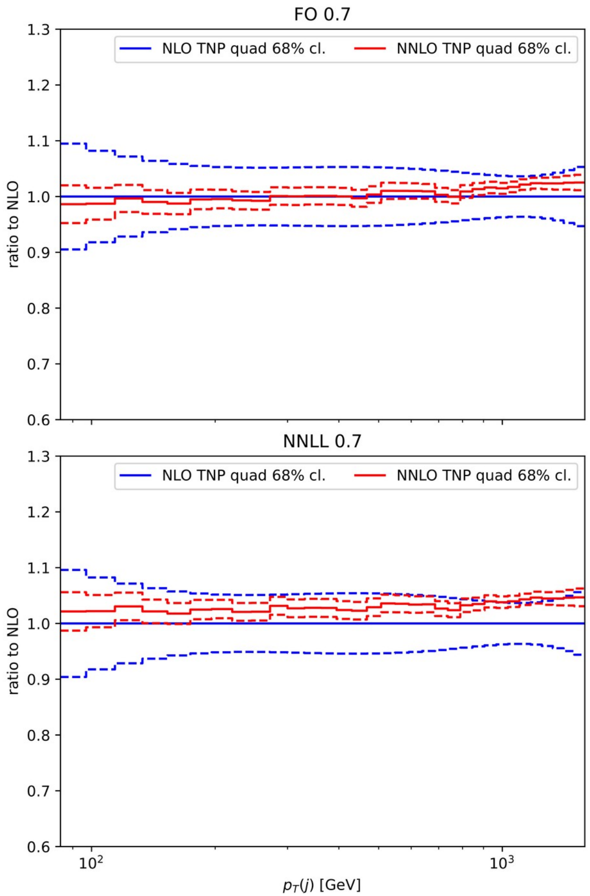
- More sensible NLO uncertainties
- Similar to resummed scale variation

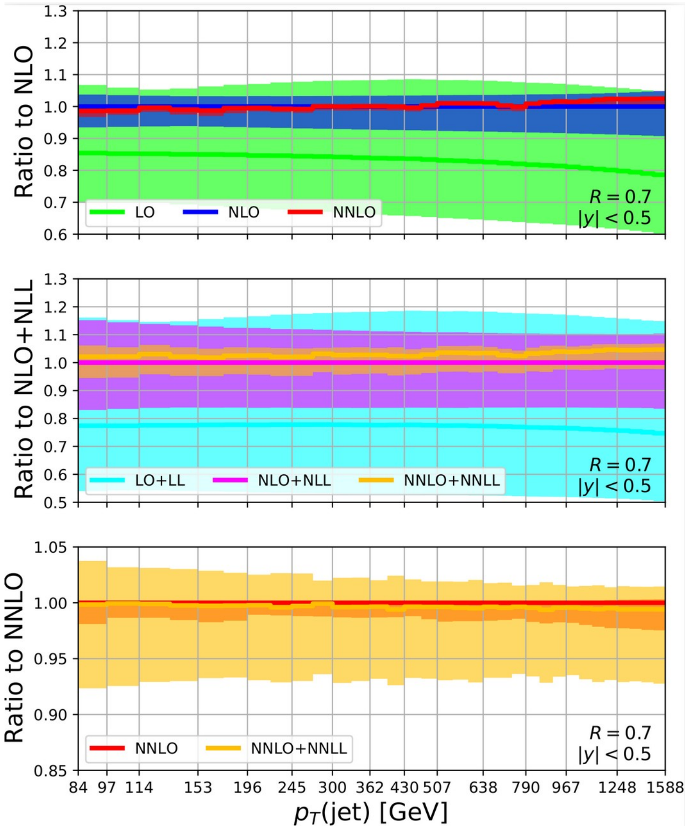




1. TNP uncertainties for inclusive jet production

R = 0.7





TNP uncertainties

- More sensible NNLO QCD uncertainties
- Similar to resummed scale variation

2. TNP: A more realistic approach

Thanks to Terry Generet to put this together!

The pT spectrum is a steeply falling function → effectively only few Mellin moments contribute

$$\frac{d\sigma}{dp_T} \approx \sum_{a,b} L_{ab}(\hat{E}/E = 2p_T/E)\frac{d\hat{\sigma}_{ab}}{dp_T}(N = \tilde{n}(2p_T/E))$$

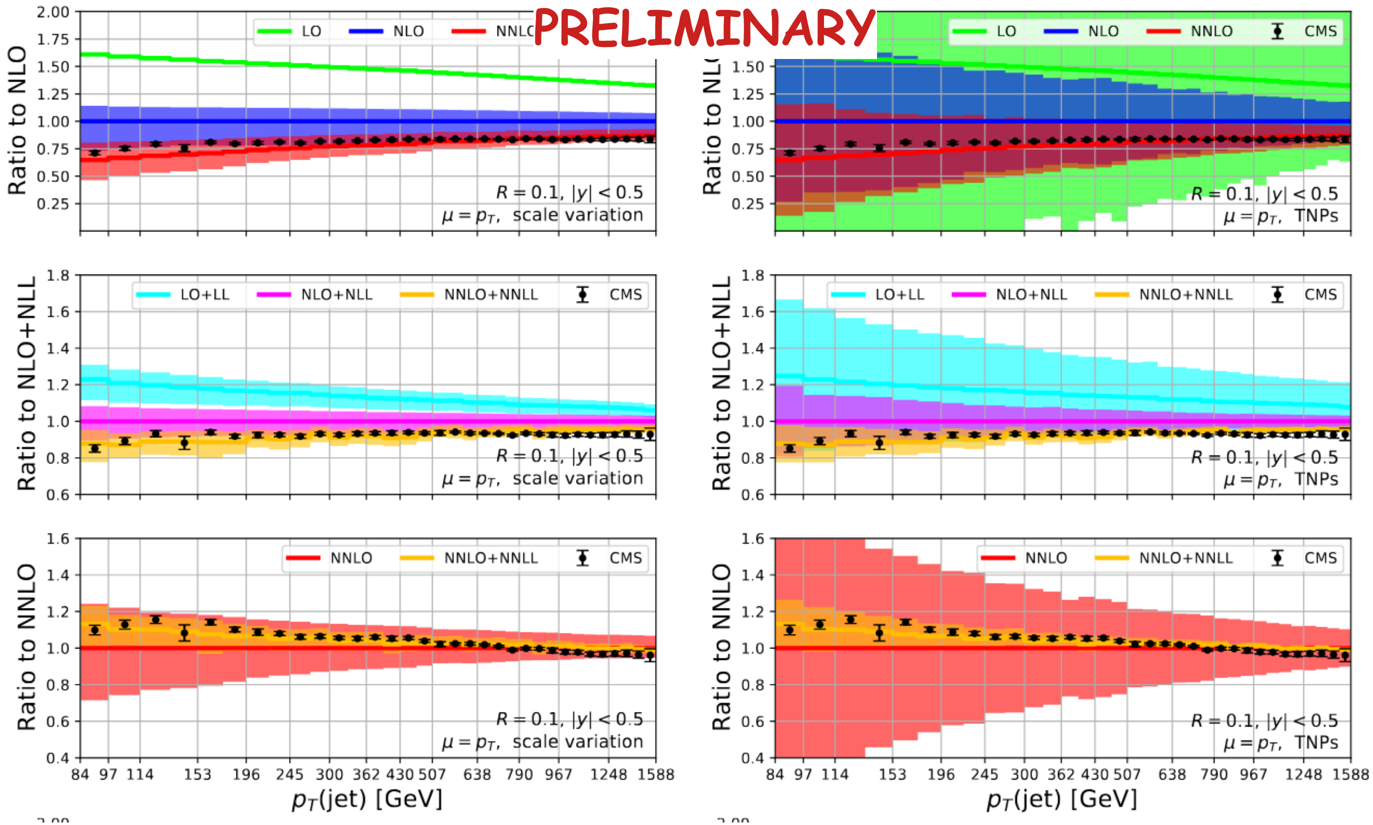
$$\begin{aligned} d\hat{\sigma}_{ab\to cd}(N) = {} & J_{\rm in}^{(a)}\left(\frac{\hat{s}}{N_{0a}^2\mu^2}, \alpha_s(\mu)\right) J_{\rm in}^{(b)}\left(\frac{\hat{s}}{N_{0b}^2\mu^2}, \alpha_s(\mu)\right) \\ & \times J_{\rm fr}^{(c)}\left(\frac{\hat{s}}{N_0^2\mu^2}, \alpha_s(\mu)\right) J_{\rm rec}^{(d)}\left(\frac{\hat{s}}{N_0\mu^2}, \frac{\hat{s}}{N_0^2\mu^2}, \alpha_s(\mu)\right) \\ & \times {\rm Tr}\left[\mathbf{H}_{ab\to cd}\left(\frac{\hat{s}}{\mu^2}, \alpha_s(\mu)\right)\mathbf{S}_{ab\to cd}\left(\frac{\hat{s}}{N_0^2\mu^2}, \alpha_s(\mu)\right)\right] + \mathcal{O}\left(\frac{1}{N}\right) \end{aligned}$$

These then can be broken down into scalar series:
(soft+hard functions require approx. of
colour matrix → error on the error)

$$\begin{aligned} J_{\rm in}^{(i)}\left(\frac{\hat{s}}{N_{0i}^2\mu^2}, \alpha_s(\mu)\right) = J_{\rm fr}^{(i)}\left(\frac{\hat{s}}{N_{0i}^2\mu^2}, \alpha_s(\mu)\right) = R_i(\alpha_s(\mu)) \\ \times \exp\left[\int_{\sqrt{\hat{s}}/N_{0i}}^{\mu} \frac{d\mu'}{\mu'}\left(A_i(\alpha_s(\mu'))\ln\left(\frac{\mu'^2 N_{0i}^2}{\hat{s}}\right) - \frac{1}{2}D_i(\alpha_s(\mu'))\right)\right] \end{aligned}$$

2. TNP: A more realistic approach

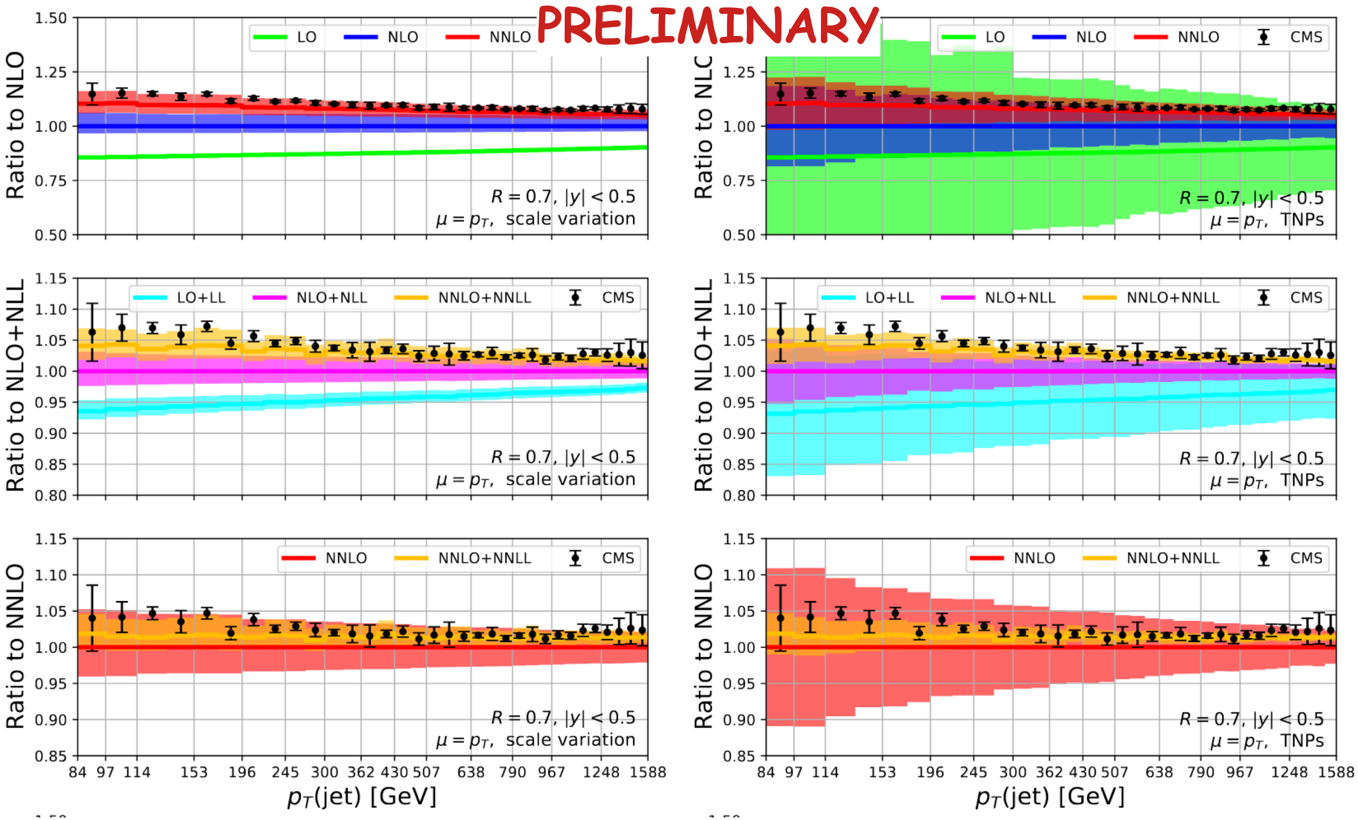
Small R: expect fixed-order to fail and resummation to be stable



side note
these are ratios (R/R=0.4),
TNPs allow
correct correlation!

2. TNP: A more realistic approach

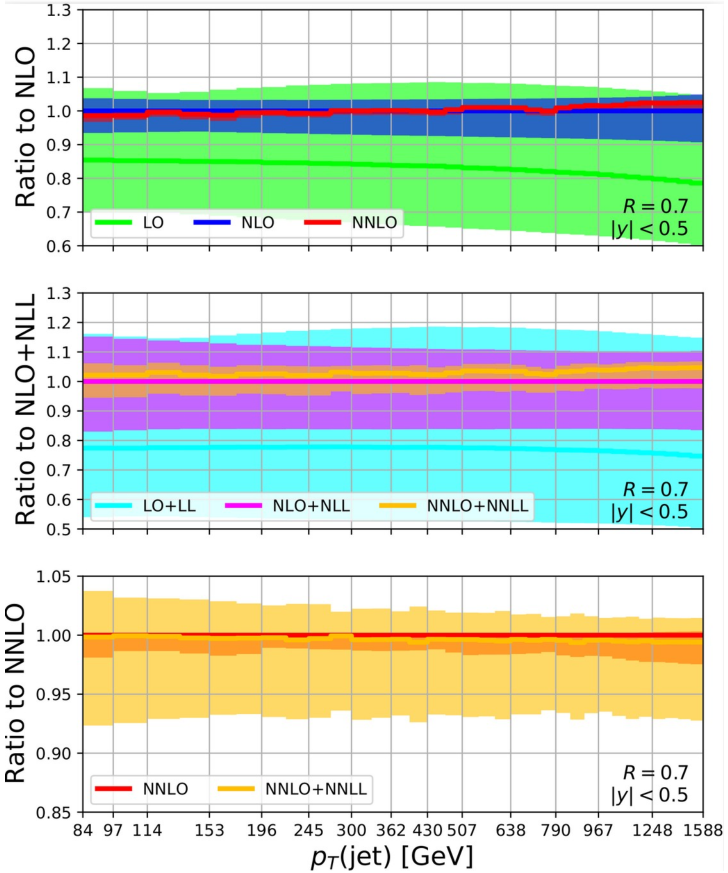
Intermediate R: observed small scale dependence → TNPs more realistic



Quick summary on MHOU in inclusive jets

- Resummation and TNP analysis suggests that MHOU are massively underestimated (even for larger R)
- R32 ratio of cross sections should be less sensitive
  → some hope for TEEC
- but eventually we need to compute it…
  → **next step di-jet** with resummation
  → same as the production of two hadrons [2503.11489]!

$$d\sigma_{pp\to h_1 h_2}(p_1,p_2) \;=\; \sum_{i,j}\int dz_1 \int dz_2\; d\hat{\sigma}_{pp\to ij}\left(\frac{p_1}{z_1},\frac{p_2}{z_2}\right) \times D_{i\to h_1}(z_1) D_{j\to h_2}(z_2)\,, \qquad (2)$$



Sub-leading colour effects

2 → 3 processes

	Leading colour amplitudes	Full colour amplitudes
$pp \to \gamma\gamma\gamma$	[1911.00479][2010.15834] [2012.13553]	[2305.17056]
$pp \to \gamma\gamma j$	[2102.01820][2103.04319]	[2105.04585]
$pp \to \gamma j j$		[2304.06682]
$pp \to j j j$	[1904.00945] [2102.13609]	[2311.09870] [2311.10086] [2311.18752]

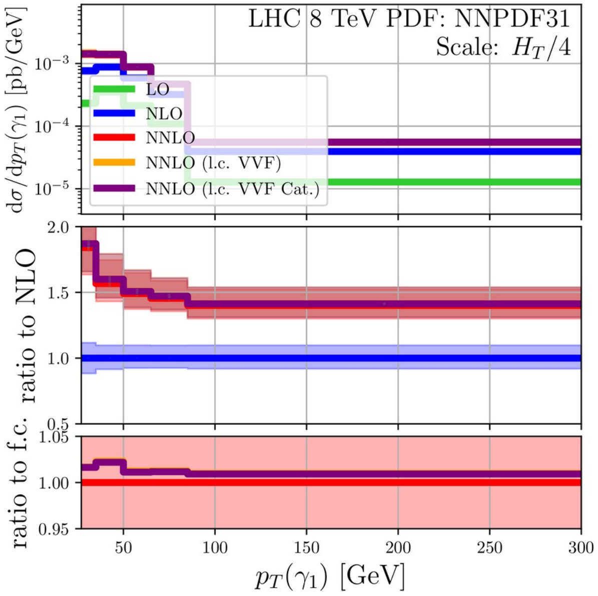
Approximation made in 2 → 3 calculations:

$$\mathcal{F}^{(2)}(\mu_R^2) = 2\,\mathrm{Re}\left[\mathcal{M}^{\dagger(0)}\mathcal{F}^{(2)}\right](\mu_R^2) + \left|\mathcal{F}^{(1)}\right|^2(\mu_R^2) \equiv \mathcal{F}^{(2)}(s_{12}) + \sum_{i=1}^{4} c_i \ln^i\left(\frac{\mu_R^2}{s_{12}}\right)$$

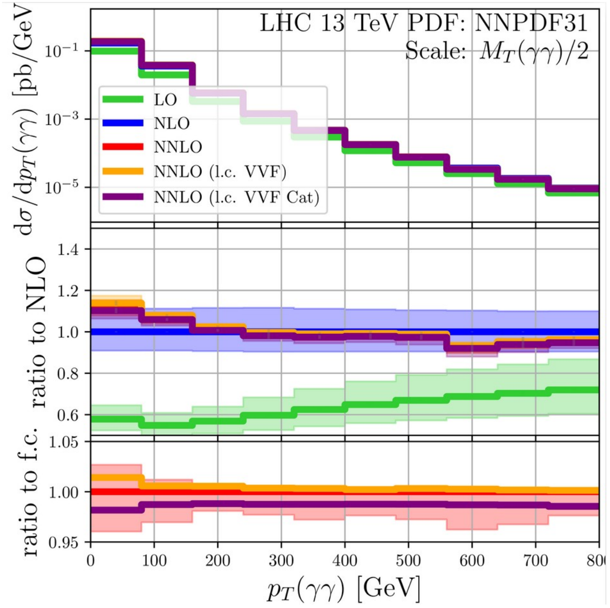
$$F^{(2)}_{\text{l.c. resc.}}(\mu^2) = \frac{F^{(0)}}{F^{(0)}_{\text{l.c.}}} F^{(2)}_{\text{l.c.}}(Q^2) + \sum_{i=0}^{4} c_i \log^i(\mu^2/Q^2)$$

Photon processes

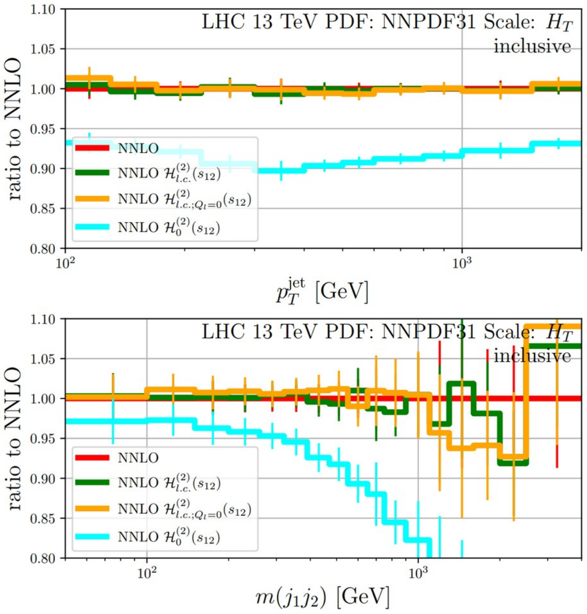
$pp \to \gamma\gamma\gamma$



$pp \to \gamma\gamma j$



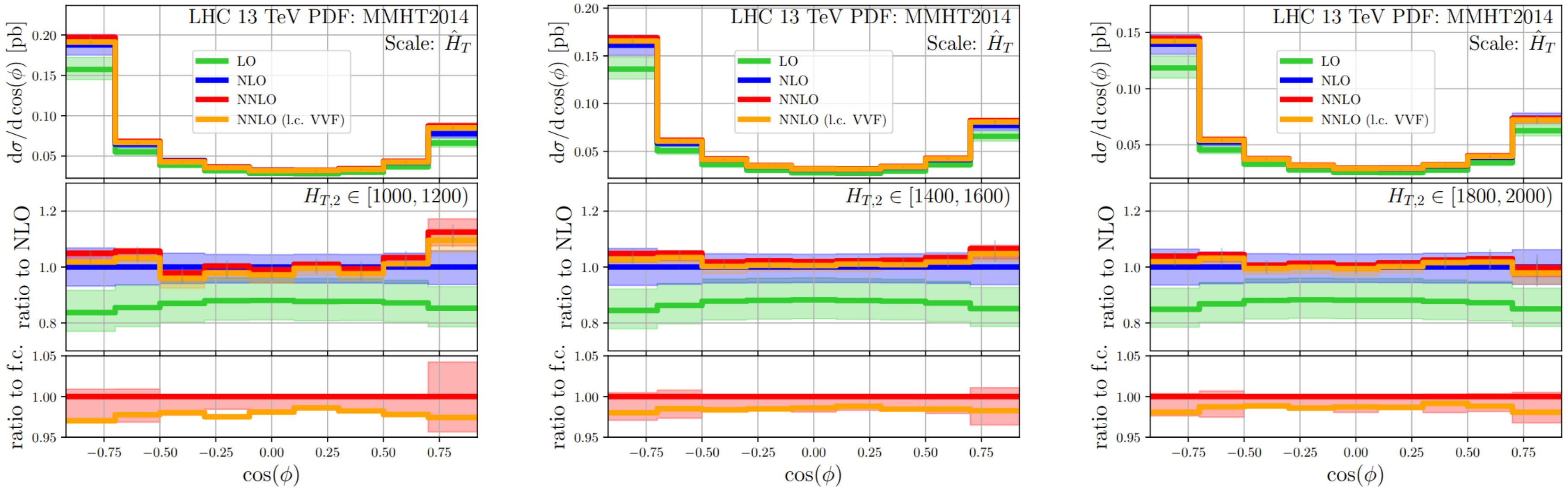
$pp \to \gamma jj$



Long story short → effect is small as expected.

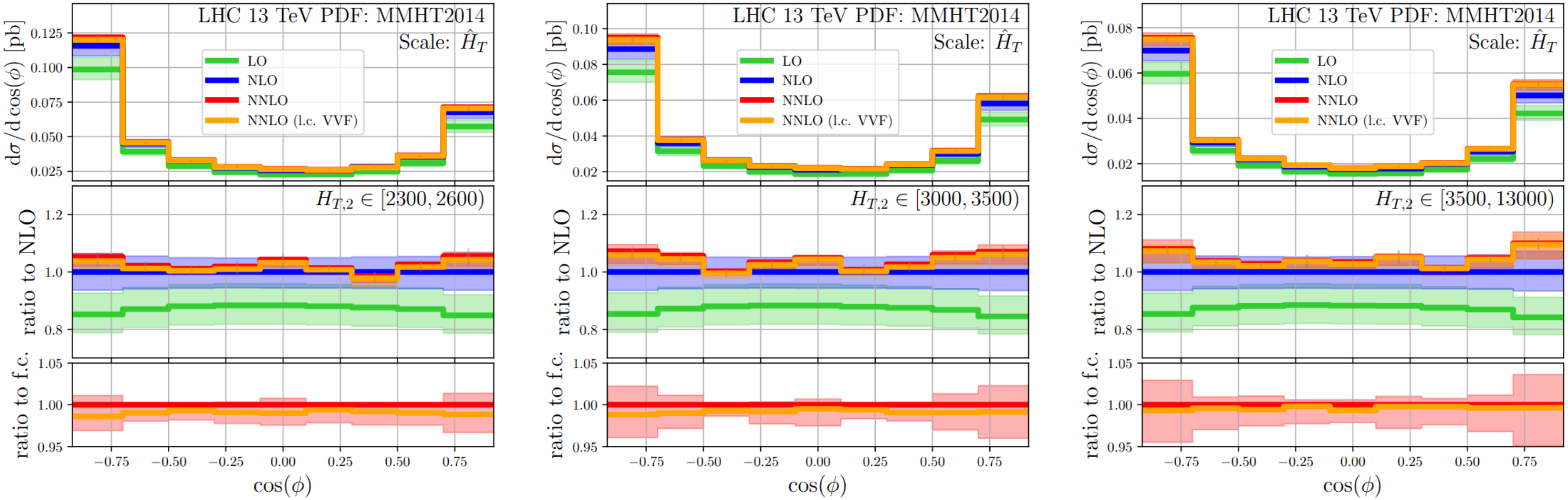
Sub-leading colour effects on TEEC I

$pp \to jjj$



Sub-leading colour effects on TEEC II

$pp \to jjj$

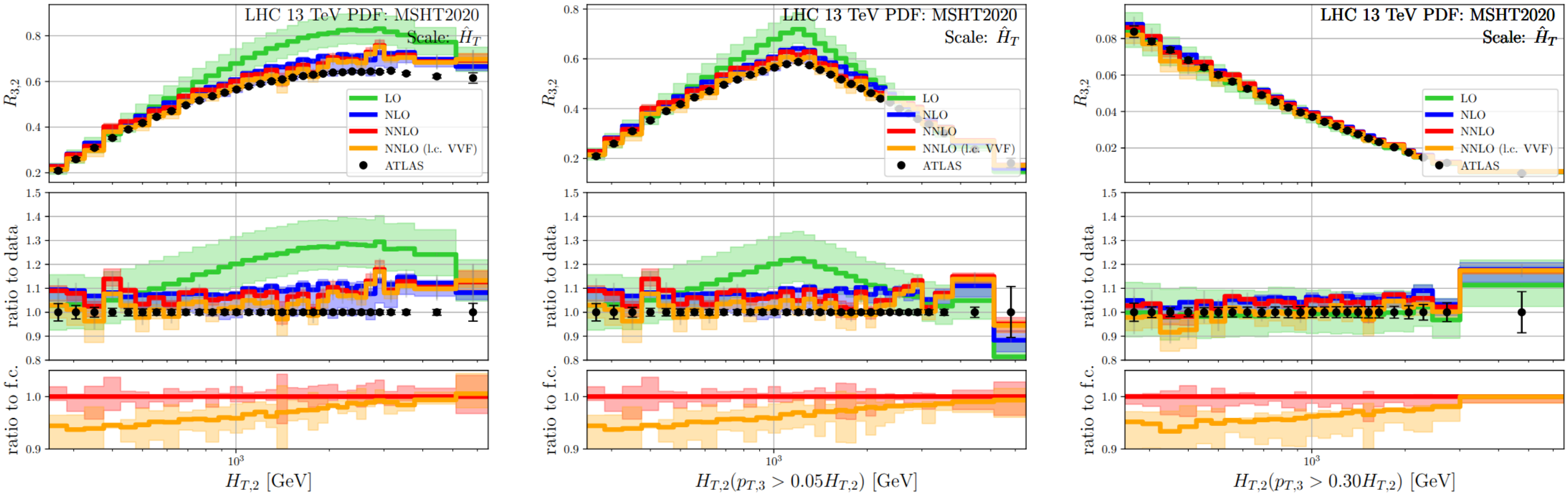


Effect covered by scale variations and decreasing with energy scale

Sub-leading colour effects in R32

ATLAS R32 [2405.20206]
→ data public

Dynamical pT3 cut



At low pT → 5% effect

Example: how to assign an 'sub-leading colour' uncertainty

Higher-order QCD corrections to top-quark pair production in association with a jet,
Badger, Becchetti, Brancaccio, Czakon, Hartanto, **Poncelet**, Zoia [arxiv:2511.11431]

Full NNLO QCD except for two-loop virtuals:

$$F^{(2)}_{\mathrm{l.c.\ resc.}}(\mu^2) = \frac{F^{(0)}}{F^{(0)}_{\mathrm{l.c.}}} F^{(2)}_{\mathrm{l.c.}}(Q^2) + \sum_{i=0}^{4} c_i \log^i(\mu^2/Q^2)$$

Leading colour amplitudes from:

Double virtual QCD corrections to tt̄+jet production at the LHC,
Badger, Becchetti, Brancaccio, Czakon, Hartanto, **Poncelet**, Zoia
[arxiv:2511.11424]

Naive 'TNP'-parameterization of sub-leading colour:

$$\frac{F^{(2)}_{l.c.}}{F^{(0)}_{l.c.}} \to \frac{F^{(2)}_{l.c.}}{F^{(0)}_{l.c.}} + \frac{\theta}{N_c^2} \frac{F^{(2)}_{l.c.}}{F^{(0)}_{l.c.}}$$

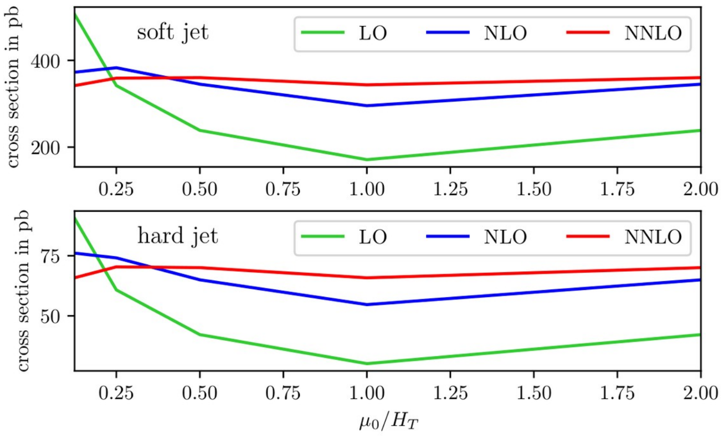
LHC phase spaces at 13 TeV

Soft-jet:

$$p_T(j) > 30\,\mathrm{GeV},\ |y(j)| < 2.5$$

Hard-jet:

$$p_T(j) \geq 120\,\mathrm{GeV},\ p_T(j) \geq 0.4(p_T(t) + p_T(\bar{t})),\ |y(j)| < 2.4$$

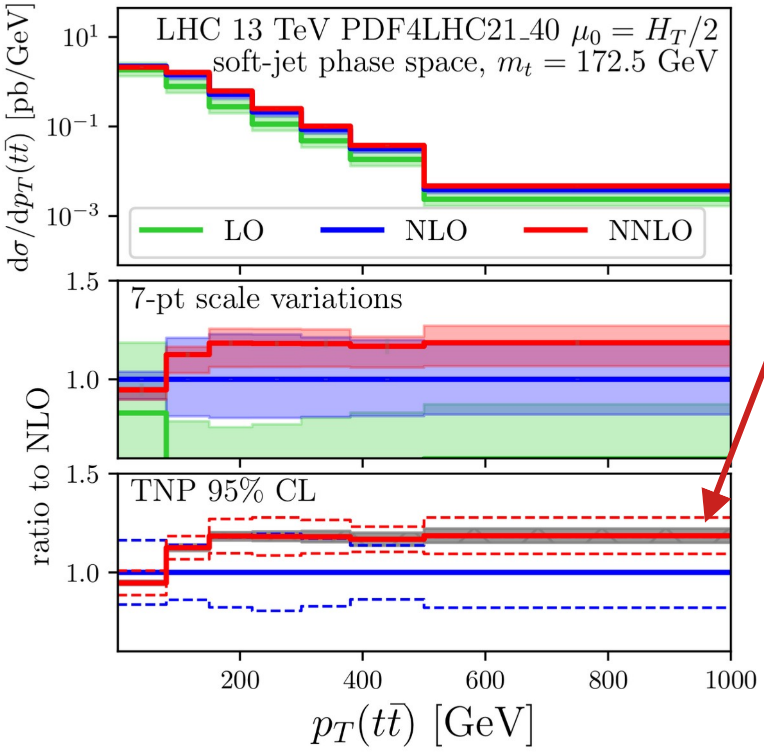


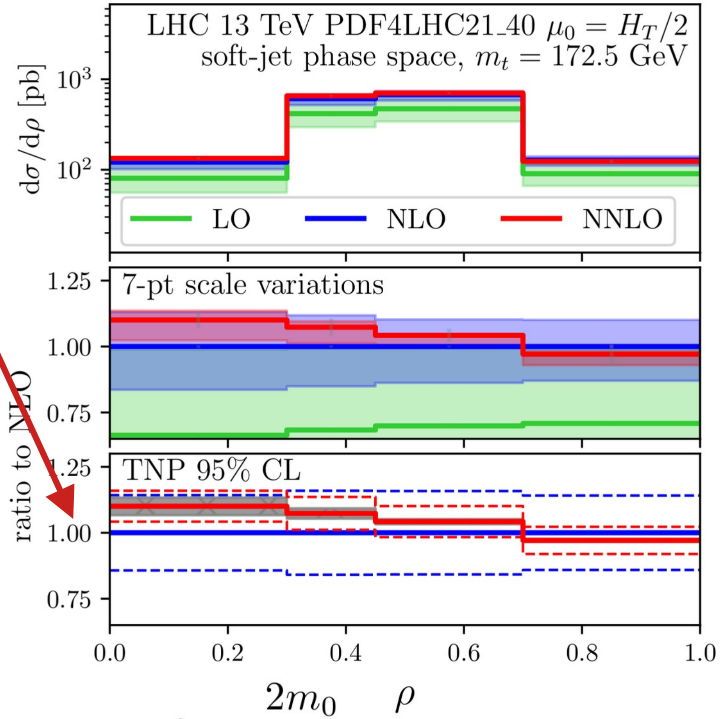
$$H_T = M_T(t) + M_T(\bar{t}) + p_T(j_1)$$

$$\mu_R = \mu_F = \mu_0 = H_T/n$$

Top-quark pair+jet production: differential observables

Sub-leading colour unc. → grey band





$$\rho = \frac{2m_0}{m(t\bar{t}j)}$$

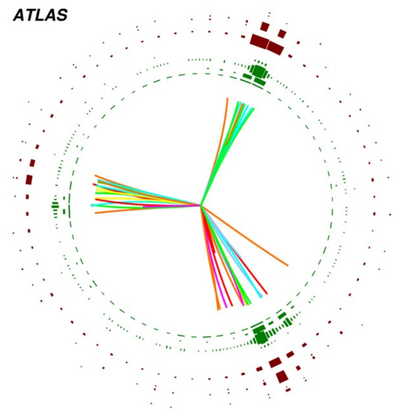
Caveat: will fail close to threshold due to octet contribution!

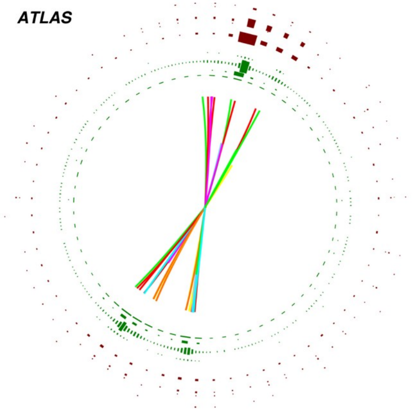
Summary

- Discussion of theory uncertainties entering into TEEC and inclusive jets
- MHOU estimates are crucial
  → scale variation does not lead to a consistent picture
  → NNLO+NNLL hints at larger MHOU than 7-point scale variations at fixed-order
  → WIP: TNP approaches indicate similar conclusions
- Sub-leading colour effects in two-loop amplitudes
  → in general small because two-loop contributions are small
  → however specific phase space regions show larger sensitivity
  (low pT jets, threshold for example...)

Backup

Encoding QCD dynamics in event shapes





Using (global) event information to separate different regimes of QCD event evolution:

- **Thrust & Thrust-Minor** $$T_\perp = \frac{\sum_i |\vec{p}_{T,i} \cdot \hat{n}_\perp|}{\sum_i |\vec{p}_{T,i}|}\,, \quad \text{and} \quad T_m = \frac{\sum_i |\vec{p}_{T,i} \times \hat{n}_\perp|}{\sum_i |\vec{p}_{T,i}|}\,.$$
- **Energy-energy correlators** $$\frac{1}{\sigma_2}\frac{\mathrm{d}\sigma}{\mathrm{d}\cos\Delta\phi} = \frac{1}{\sigma_2}\sum_{ij}\int \frac{\mathrm{d}\sigma\; x_{\perp,i}x_{\perp,j}}{\mathrm{d}x_{\perp,i}\mathrm{d}x_{\perp,j}\mathrm{d}\cos\Delta\phi_{ij}}\delta(\cos\Delta\phi - \cos\Delta\phi_{ij})\mathrm{d}x_{\perp,i}\mathrm{d}x_{\perp,j}\mathrm{d}\cos\Delta\phi_{ij}\,,$$

Separation of energy scales: $H_{T,2} = p_{T,1} + p_{T,2}$

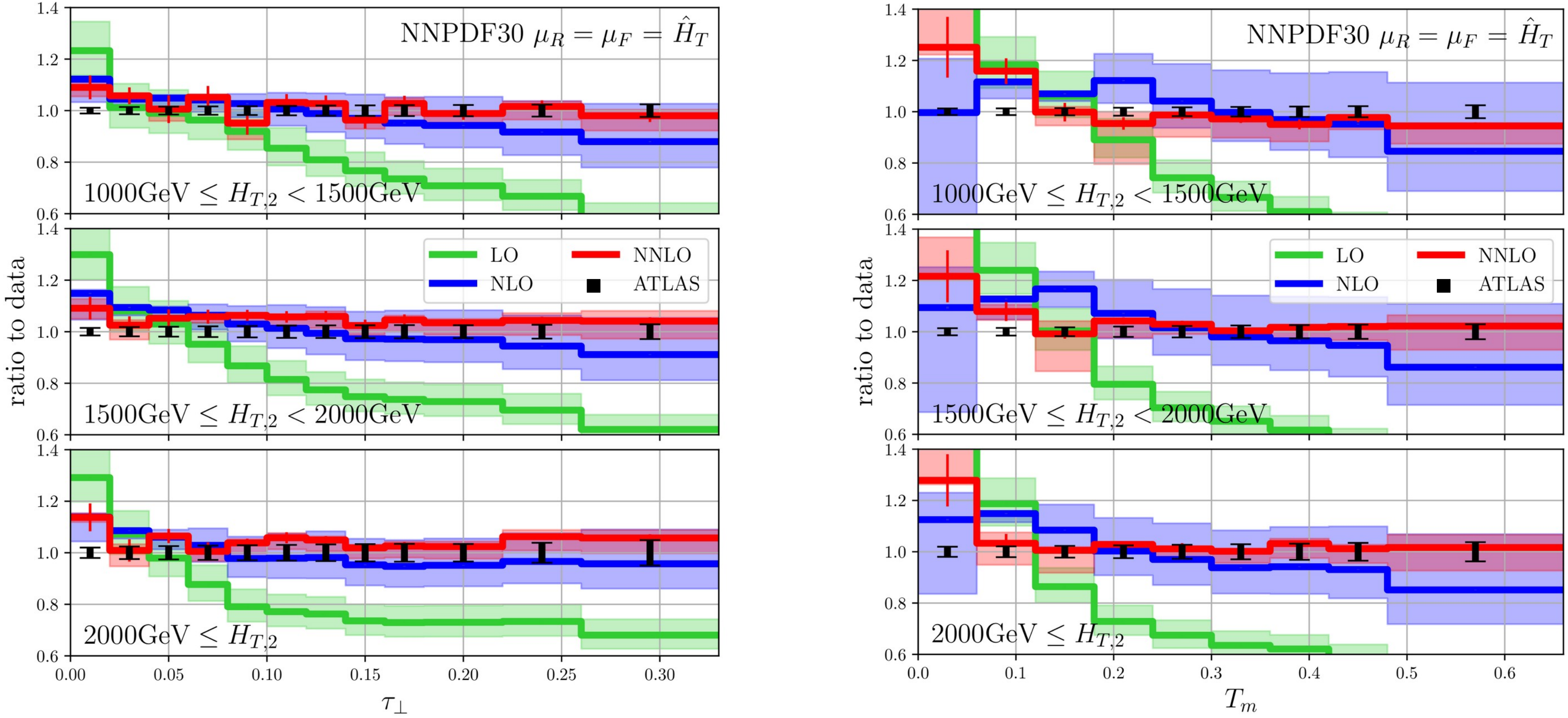
Ratio to 2-jet: $$R^i(\mu_R, \mu_F, \mathrm{PDF}, \alpha_{S,0}) = \frac{\mathrm{d}\sigma_3^i(\mu_R, \mu_F, \mathrm{PDF}, \alpha_{S,0})}{\mathrm{d}\sigma_2^i(\mu_R, \mu_F, \mathrm{PDF}, \alpha_{S,0})}$$

Here: use jets as input → experimentally advantageous
(better calibrated, smaller non-pert.)

Transverse Thrust @ NNLO QCD

NNLO QCD corrections to event shapes at the LHC
Alvarez, Cantero, Czakon, Llorente, Mitov, Poncelet [2301.01086]

ATLAS [2007.12600]



Uncertainties in precision phenomenology

Experiments are getting more precise → theory uncertainties matter!

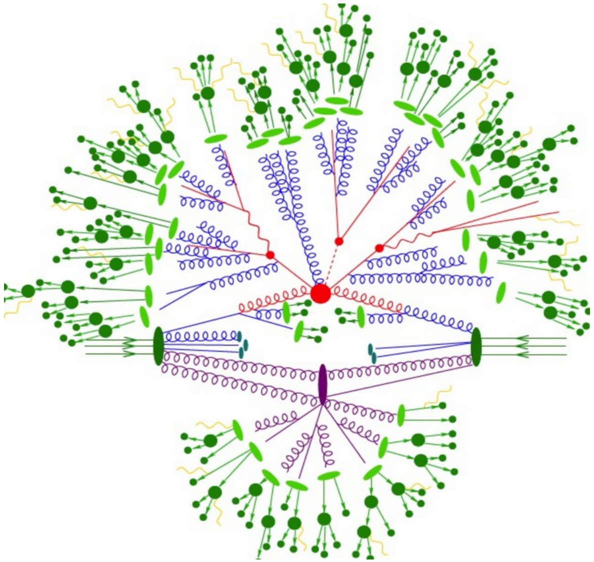
Sources of theory uncertainties:

- parametric (values of coupling parameters etc.)
→ variation of parameters within their uncertainties

- parton distribution functions (PDFs)
→ different error propagation methods (fit parameter, replicas,...)

- non-perturbative parameters in Monte Carlo simulations.
→ needs data constraints by definition. Problematic if dominant effect...

- missing higher orders in fixed-order and resummed predictions (MHOU)
→ tricky because we are trying to estimate the unknown....



[Credit: SHERPA]

Missing higher orders

Notation from: [Tackmann 2411.18606]
Beyond Scale Variations: Perturbative Theory Uncertainties from Nuisance Parameters

Generic perturbative expansion:

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

f_i : the coefficient of the series, potentially unknown

We can compute the truncated series: $\hat{f}_i$: the true value, i.e. a value we actually computed

$$f^{\mathrm{LO}}(\alpha) = \hat{f}_0 \qquad f^{\mathrm{NLO}}(\alpha) = \hat{f}_0 + \hat{f}_1\alpha \qquad f^{\mathrm{NNLO}}(\alpha) = \hat{f}_0 + \hat{f}_1\alpha + \hat{f}_2\alpha^2$$

The missing terms are the source of uncertainty.
(assume convergence → the first missing is the dominant one)

$$f^{\mathrm{LO+1}}(\alpha) = \hat{f}_0 + f_1\alpha \qquad f^{\mathrm{NLO+1}}(\alpha) = \hat{f}_0 + \hat{f}_1\alpha + f_2\alpha^2 \qquad f^{\mathrm{NNLO+1}}(\alpha) = \hat{f}_0 + \hat{f}_1\alpha + \hat{f}_2\alpha^2 + f_3\alpha^3$$

Challenge: how to estimate f_1, f_2, f_3, … without computing them?

Short comings of scale variations

- not always reliable … however in most cases issues are understood/expected:
  new channels, phase space constraints, etc. → often we can design workarounds
- however, some issues are more fundamental:
  → how to choose the central scale? → not a physical parameter, no ‘true’ value
  (Principle of fasted apparent convergence, principle of minimal sensitivity,...)
  → how to propagate the estimated uncertainty, no statistical interpretation!
  → what about correlations? Based on ‘fixed form’ of the lower orders and RGE.

(At the moment) two alternative approaches under investigation:

“Bayesian”

[Cacciari,Houdeau 1105.5152]
[Bonvini 2006.16293]
[Duhr, Huss, Mazeliauskas, Szafron 2106.04585]

“Theory Nuisance Parameter”

[Tackmann 2411.18606]
→ W mass extraction: [CMS 2412.13872]
[Cal,Lim, Scott,Tackmann Waalewijn 2408.13301]
[Lim, Poncelet, 2412.14910]

Some remarks on TNPs in resummation

Picture: simple ingredients that enter different computations/processes etc.

→ ideal situation

But actually not that simple:

- Scheme dependence of ingredients? E.g. scales, IR subtraction, …
  → might need modified parametrisations
- Some TNPs represent directly numbers: $\Gamma,\ \gamma,\ H$ for simple processes
  but others are functions → Beam functions, hard functions for more complicated processes
- Parametrisation works for the resummed spectrum. What about other observables?
- "Easy to implement" for use-cases so far
  → might be really expensive if each variation needs a full computation (Monte Carlos,...)

Is there a simpler, say "effective", way to do this for a general computation?

Introducing theory nuisance parameters (TNPs)

Generic perturbative expansion:

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

Beyond Scale Variations: Perturbative Theory Uncertainties from Nuisance Parameters, Frank Tackmann [2411.18606]

$$f^{\mathrm{LO+1}}(\alpha) = \hat{f}_0 + f_1(\theta)\alpha$$

$$f^{\mathrm{NLO+1}}(\alpha) = \hat{f}_0 + \hat{f}_1\alpha + f_2(\theta)\alpha^2$$

$$f^{\mathrm{NNLO+1}}(\alpha) = \hat{f}_0 + \hat{f}_1\alpha + \hat{f}_2\alpha^2 + f_3(\theta)\alpha^3$$

Introduce a parametrisation of unknown coefficients in terms of

"Theory nuisance parameters" θ

- The parametrization such that there is a true value: $f_i(\hat{\theta}) = \hat{f}_i$
- Distributions of θ "known" (for example from already existing computations)

→ Expert knowledge to construct such a parametrisation

Example: TNPs in resummed cross sections

[Tackman 2411.18606]

Transverse momentum resummation:

$$\frac{\mathrm{d}\sigma}{\mathrm{d}p_T} = [\underbrace{H \times B_a \times B_b \times S}](\alpha_s, \ln\left(\frac{p_T}{Q}\right)) + \mathcal{O}\left(\frac{p_T}{Q}\right)$$

$$X(\alpha_s, L) = X(\alpha_s) \exp \int_0^L \mathrm{d}L' \{\Gamma(\alpha_s(L'))L' + \gamma_X(\alpha_s(L'))\}$$

Perturbative expansion of resummation ingredients:

$$X(\alpha_s) = X_0 + \alpha_s X_1 + \alpha_s^2 X_2 + \cdots \boxed{+ \alpha_s^n X_n(\theta)}$$

$$\Gamma(\alpha_s) = \alpha_s[\Gamma_0 + \alpha_s \Gamma_1 + \alpha_s^2 \Gamma_2 + \cdots \boxed{+ \alpha_s^n \Gamma_n(\theta)]}$$

$$\gamma(\alpha_s) = \alpha_s[\gamma_0 + \alpha_s \gamma_1 + \alpha_s^2 \gamma_2 + \cdots \boxed{+ \alpha_s^n \gamma_n(\theta)]}$$

Task: find suitable parametrization and variation range

These are numbers for simple processes → only need normalisation

TNP parametrisations for resummation

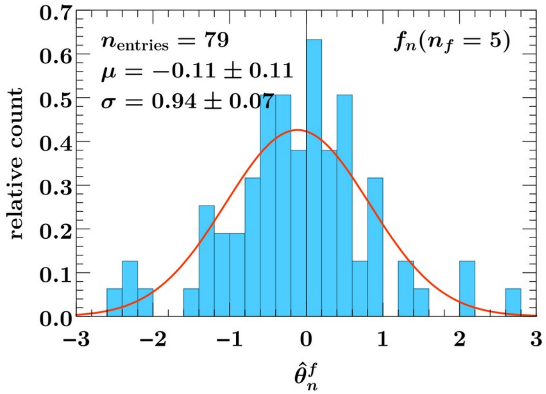
[Tackman 2411.18606]

$\gamma(\alpha_s)$	N_n	$\hat{\gamma}_0/N_0$	$\hat{\gamma}_1/N_1$	$\hat{\gamma}_2/N_2$	$\hat{\gamma}_3/N_3$	$\hat{\gamma}_4/N_4$
β	1	−15.3	−77.3	−362	−9652	−30941
	4^{n+1}	−3.83	−4.83	−5.65	−37.7	−30.2
	$4^{n+1}C_F C_A^n$	**−1.28**	**−0.54**	**−0.21**	**−0.47**	**−0.12**
γ_m	1	−8.00	−112	−950	−5650	−85648
	4^{n+1}	−2.00	−7.028	−14.8	−22.1	−83.6
	$4^{n+1}C_F C_A^n$	**−1.50**	**−1.76**	**−1.24**	**−0.61**	**−0.77**
$2\Gamma^q_{\mathrm{cusp}}$	1	+10.7	+73.7	+478	+282	(+140000)
	4^{n+1}	+2.67	+4.61	+7.48	+1.10	(+137)
	$4^{n+1}C_F C_A^n$	**+2.00**	**+1.15**	**+0.62**	**+0.03**	**(+1.27)**

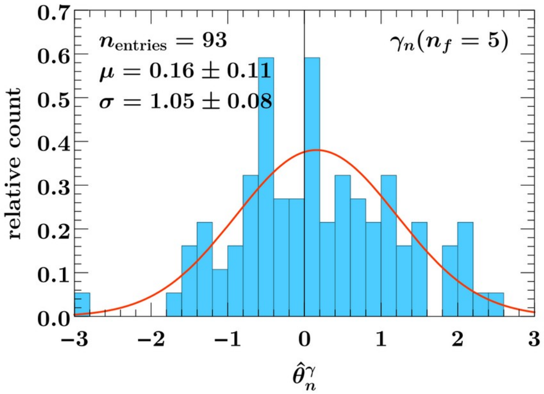
⋮

"Statistics over many computations"

Matrix elements



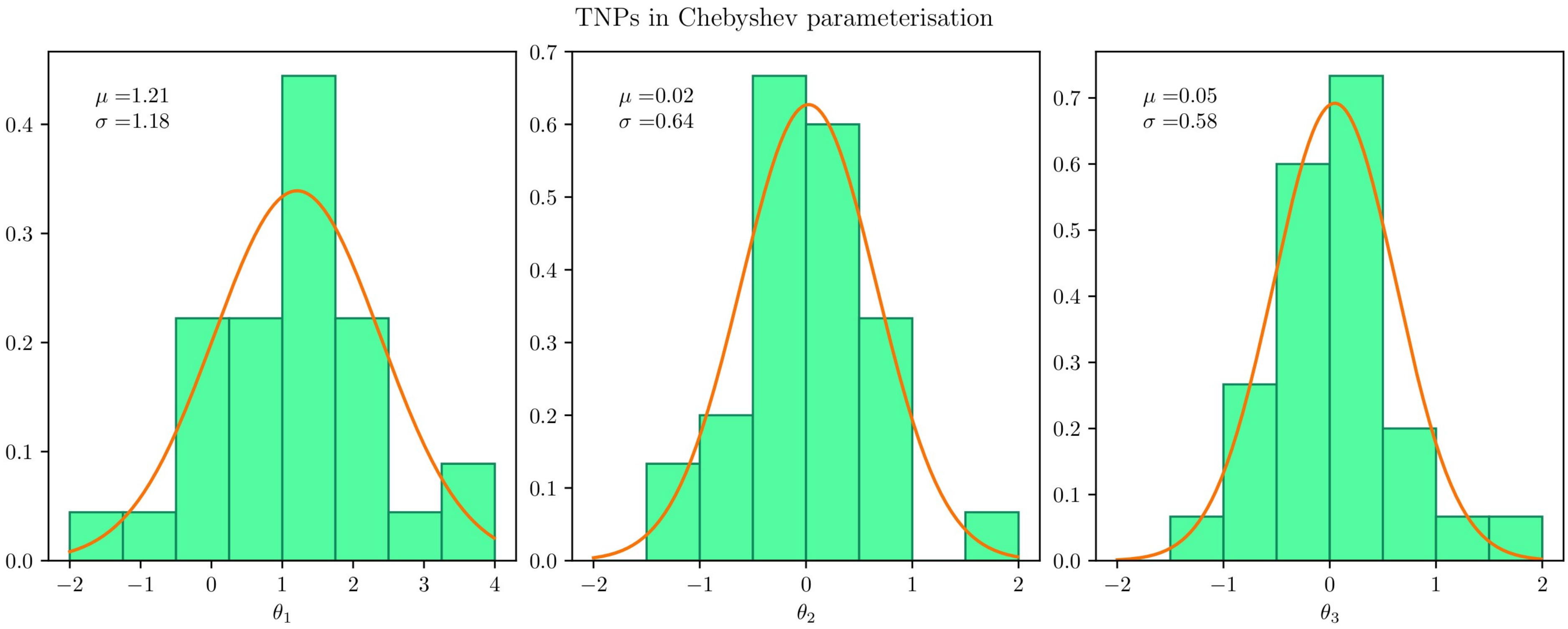
Anomalous dimensions



Process meta study

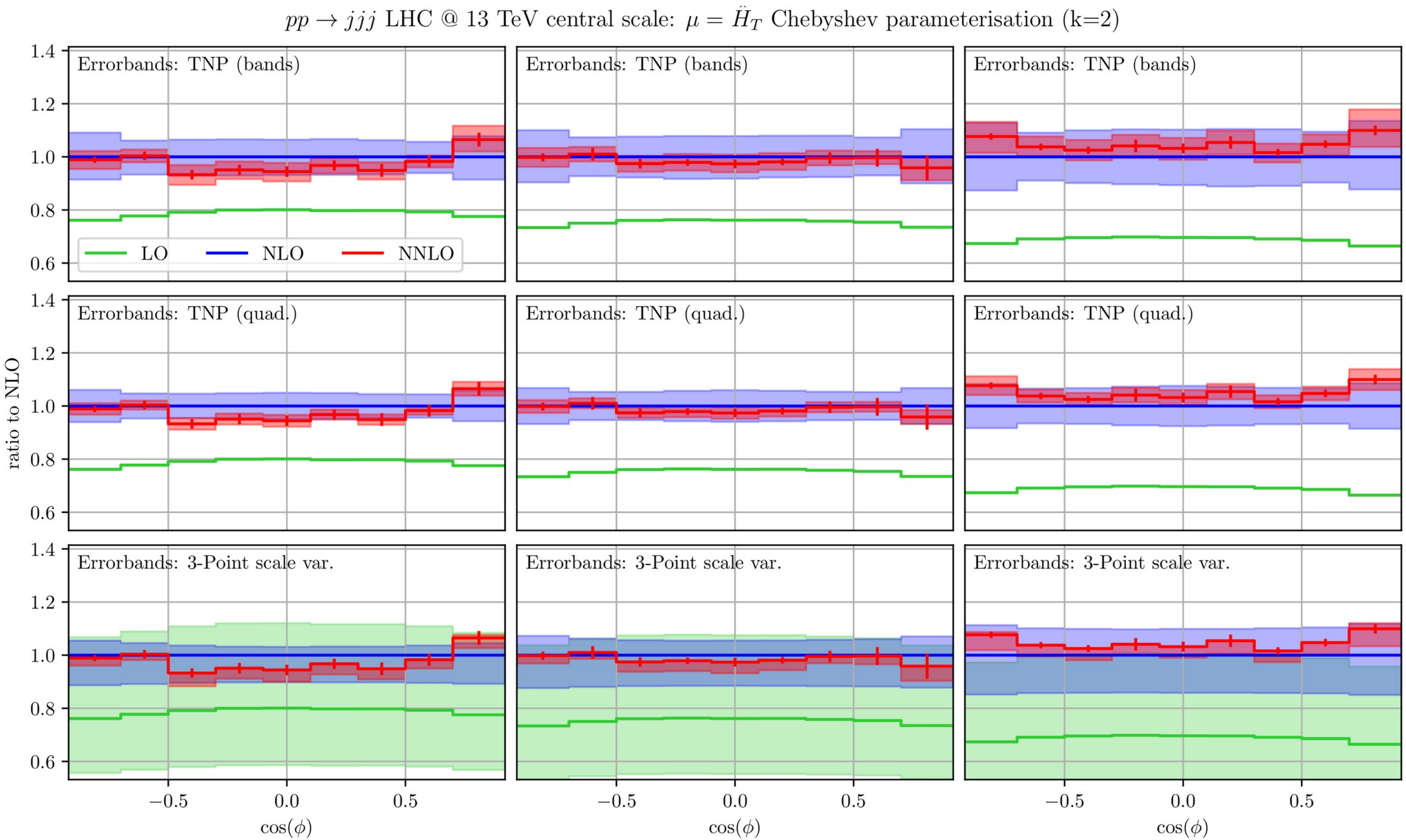
Process	$\sqrt{s}$/TeV	Scale	PDF	Distributions
$pp \to H$ (full theory)	13	$m_H/2$	`NNPDF3.1`	y_H
$pp \to ZZ^* \to e^+e^-\mu^+\mu^-$	13	M_T	`NNPDF3.1`	$M_{e^+\mu^+}$, $p_T^{e^+e^-}$, y_{e^+}
$pp \to WW^* \to e\nu_e\mu\nu_\mu$	13	m_W	`NNPDF3.1`	M_{WW}, $p_T^{\mu^-}$, y_{W^-}
$pp \to (W \to \ell\nu) + c$	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, $\lvert y_{\gamma-\mathrm{jet}} \rvert$, $E_{T,\gamma}$

Fits - Chebyshev parametrisation



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

Example: TEEC



Sensitivity to the strong coupling constant

- R32 ratio: $R^i(\mu_R, \mu_F, \mathrm{PDF}, \alpha_{S,0}) = \dfrac{\mathrm{d}\sigma_3^i(\mu_R, \mu_F, \mathrm{PDF}, \alpha_{S,0})}{\mathrm{d}\sigma_2^i(\mu_R, \mu_F, \mathrm{PDF}, \alpha_{S,0})}$
- Using the strong coupling's running: $\alpha_S(\mu_R, \alpha_{S,0}) = \alpha_{S,0}\left(1 - \alpha_{S,0} b_0 \ln\left(\dfrac{\mu_R^2}{m_Z^2}\right) + \mathcal{O}({\alpha_{S,0}}^2)\right)$
- Absorb running in the perturbative expansion → linear dependence

$$
\begin{aligned}
R^{\mathrm{NNLO}}(\mu, \alpha_{S,0}) &= \frac{\mathrm{d}\sigma_3^{\mathrm{NNLO}}(\mu, \alpha_{S,0})}{\mathrm{d}\sigma_2^{\mathrm{NNLO}}(\mu, \alpha_{S,0})} \\
&= \frac{{\alpha_{S,0}}^3\left(\mathrm{d}\tilde{\sigma}_3^{(0)}(\mu) + \alpha_{S,0}\mathrm{d}\tilde{\sigma}_3^{(1)}(\mu) + {\alpha_{S,0}}^2\mathrm{d}\tilde{\sigma}_3^{(2)}(\mu) + \mathcal{O}({\alpha_{S,0}}^3)\right)}{{\alpha_{S,0}}^2\left(\mathrm{d}\tilde{\sigma}_2^{(0)}(\mu) + \alpha_{S,0}\mathrm{d}\tilde{\sigma}_2^{(1)}(\mu) + {\alpha_{S,0}}^2\mathrm{d}\tilde{\sigma}_2^{(2)}(\mu) + \mathcal{O}({\alpha_{S,0}}^3)\right)}\,.
\end{aligned}
$$

- In practise using LHAPDF running and perform fit to Taylor expansion around $\alpha_s = 0.118$:

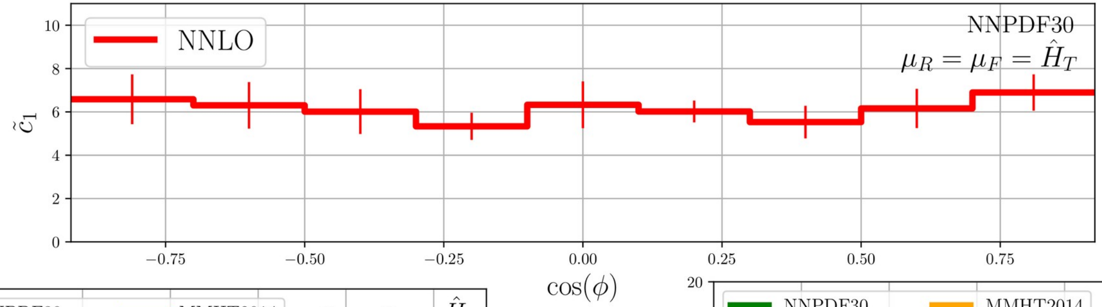
$$R^{\mathrm{NNLO,fit}}(\mu, \alpha_{S,0}) = c_0 + c_1(\alpha_{S,0} - 0.118) + c_2(\alpha_{S,0} - 0.118)^2 + c_3(\alpha_{S,0} - 0.118)^3$$

dependence mostly linear

Strong coupling dependence (differential)

For visualisation:

$$\tilde{c}_1 = \frac{c_1}{R^{\mathrm{NNLO}}(\alpha_{S,0} = 0.118)}$$



TEEC
scale unc. ~2%

Thrust &
Thrust-Minor
scale unc. ~3-5%