

# NNLO QCD predictions for jet observables

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# State of NNLO QCD at the LHC

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NNLO QCD completed for  $2 \rightarrow 1$ ,  $2 \rightarrow 2$  SM processes:

- Colour singlet production:  $pp \rightarrow H$ ,  $pp \rightarrow VV$  (available in MATRIX [Grazzini'17], MCFM [Boughezal'16])
- Massive quark production:  $pp \rightarrow tt\bar{t}$  (+decays) [Czakon'15],  $pp \rightarrow b\bar{b}$  [Kallweit'20], single top [Campbell'17]
- Vector plus jet:  $pp \rightarrow V + \text{jet}$ ,  $pp \rightarrow A + X$ , **flavoured jets**:  $pp \rightarrow Z + b\text{-jets}$ ,  $V + c\text{-jets}$  [NNLOJet '16-'20, Boughezal'15, Czakon'20]
- Di-jets:  $pp \rightarrow j + X$ ,  $pp \rightarrow jj + X$  [NNLOJet '16-'20, Czakon'19]

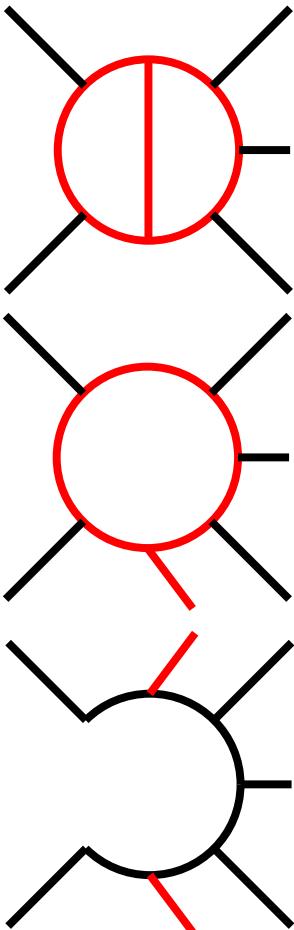
Recently first steps in the realm of  $2 \rightarrow 3$  processes:

- Three photons [Chawdhry '19, Kallweit '20]
- Diphoton plus jet [Chawdhry '21] gg-induced @ N3LO [Badger'21]
- Three jets [Czakon '21]

Beyond fixed order:

- Dedicated resummation calculations for specific observables
- First NNLO + PS appear for colour singlet and  $tt\bar{t}$ : MiNNLOPS with MATRIX [Monni '20]
- Identified hadron production: B-hadrons in  $tt\bar{t}$  production [Czakon '21]
- Photon fragmentation [Gehrmann'21]

# NNLO QCD prediction beyond $2 \rightarrow 2$



$2 \rightarrow 3$  Two-loop amplitudes:

- (Non-) planar 5 point massless 'pheno ready'  
[Chawdry'19'20'21, Abreu'20'21, Agarwal'21, Badger'21]  
fast progress in the last half year  
→ triggered by efficient MI representation [Chicherin'20]
- 5 point with one external mass [Abreu'20, Syrrakos'20, Canko'20, Badger'21]

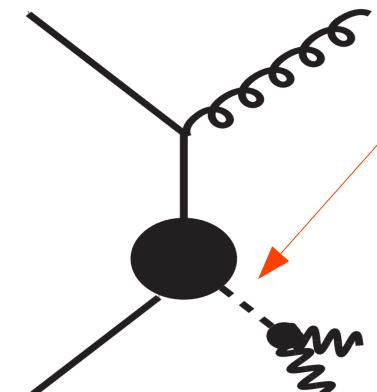
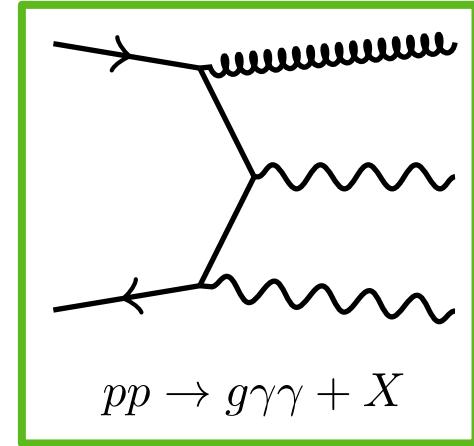
Many leg, IR stable one-loop amplitudes → OpenLoops [Buccioni'19]

Cross sections → Combination with real radiation

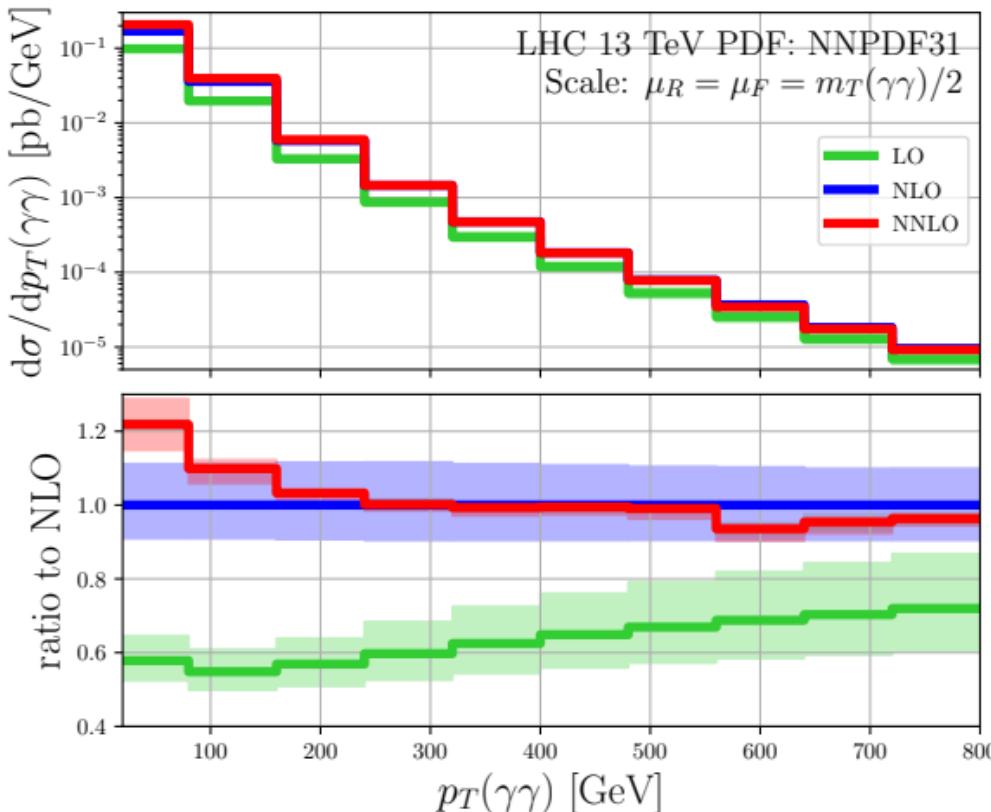
- Various NNLO subtraction schemes are available:  
qT-slicing [Catain'07], N-jettiness slicing [Gaunt'15/Boughezal'15], Antenna  
[Gehrmann'05-'08], Colorful [DelDuca'05-'15], Projection [Cacciari'15], Geometric  
[Herzog'18], Unsubtraction [Aguilera-Verdugo'19], Nested collinear [Caola'17],  
Sector-improved residue subtraction [Czakon'10-'14, '19]

# Diphoton plus jet production

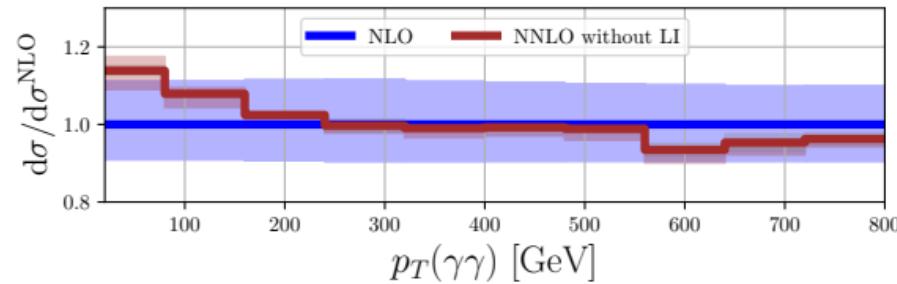
- Photon pair production @ LHC is of particular interest:
  - Main background to cleanest Higgs decay channel
- Inclusive diphoton show large NNLO QCD corrections
  - Perturbative convergence @ N3LO?  
First steps: [Chen's talk at RADCOR+Loopfest2021]
  - Diphoton plus jet @ NNLO QCD ( $p_T(\gamma\gamma) \rightarrow 0$  limit)
- $p_T(\gamma\gamma)$  spectrum itself interesting for Higgs  $\rightarrow \gamma\gamma$ :
  - Higgs –  $p_T$  measurements resolve local Higgs couplings  $\rightarrow$  BSM searches
  - Angular diphoton observables  $\rightarrow$  spin measurements



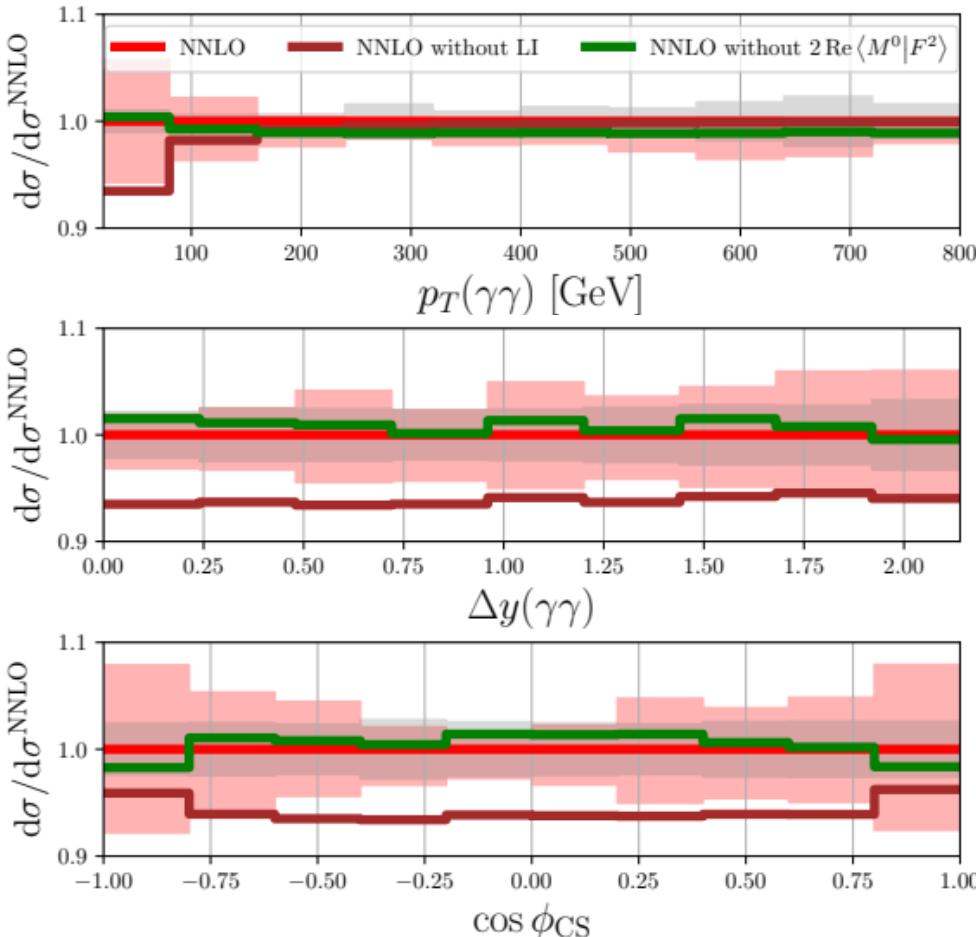
# Diphoton plus jet – pT spectrum



- Beautiful perturbative convergence
- Scale dependence:
  - NLO:  $\sim 10\%$
  - NNLO:  $\sim 1\text{-}2\%$
- Low  $p_T$  region:
  - ? Resummation for  $p_T(\gamma\gamma)/m(\gamma\gamma) \ll 1$
  - Strong effect from the loop induced!



# Diphoton plus jet – two-loop contribution



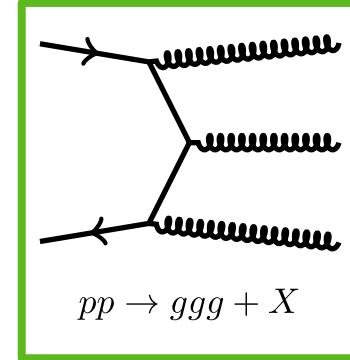
- Two-loop contribution (green line)  $<\sim 1\%$ ,
  - Loop induced contribution:
    - sizeable effects for low  $p_T$  vanishes for high  $p_T$
    - flat effect in 'bulk' observables
    - Dominant source of scale dependence
    - NLO QCD correction (formally N3LO) relevant,
- ~~missing piece~~:  $gg \rightarrow g\gamma\gamma$  two-loop [Badger'21]

# Three jet production

Advances in perturbative QCD allow to tackle the most complicated 2→3 process

## Bottlenecks:

- Handling of real radiation:
  - Sector-improved residue subtraction [Czakon'10'14'19]
  - Computationally very challenging! → O(1M CPUh)
- Double virtual amplitudes in leading colour approximation [Abreu'21]
  - Fast numerical evaluation → very small contribution to computational cost



**Only** Approximation made:

→ taken from [Abreu'21]

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

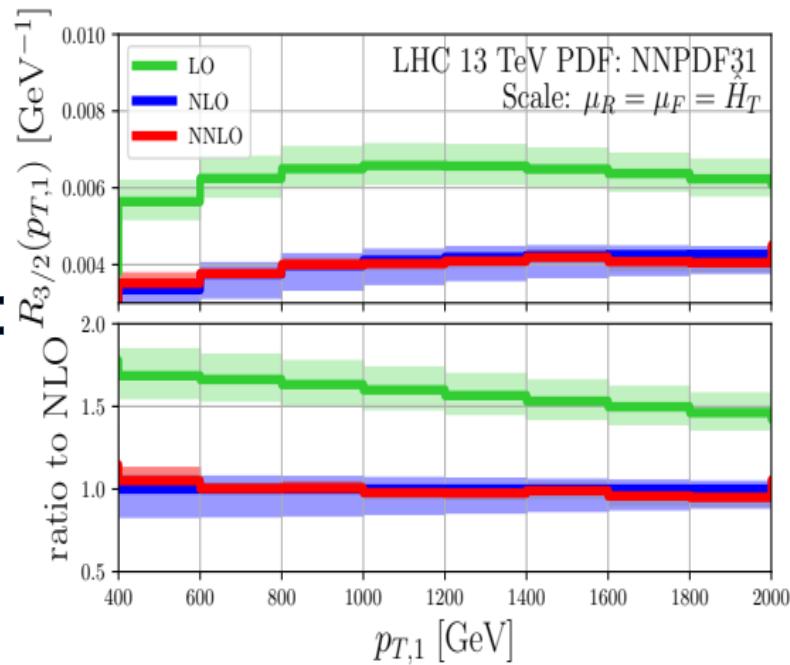
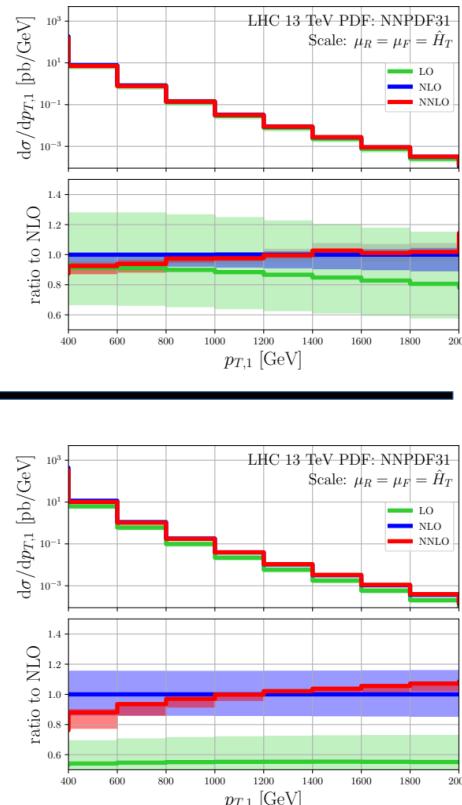
$$\mathcal{R}^{(2)}(s_{12}) \approx \mathcal{R}^{(2)l.c.}(s_{12})$$

# Three jet production - R32(pT1)

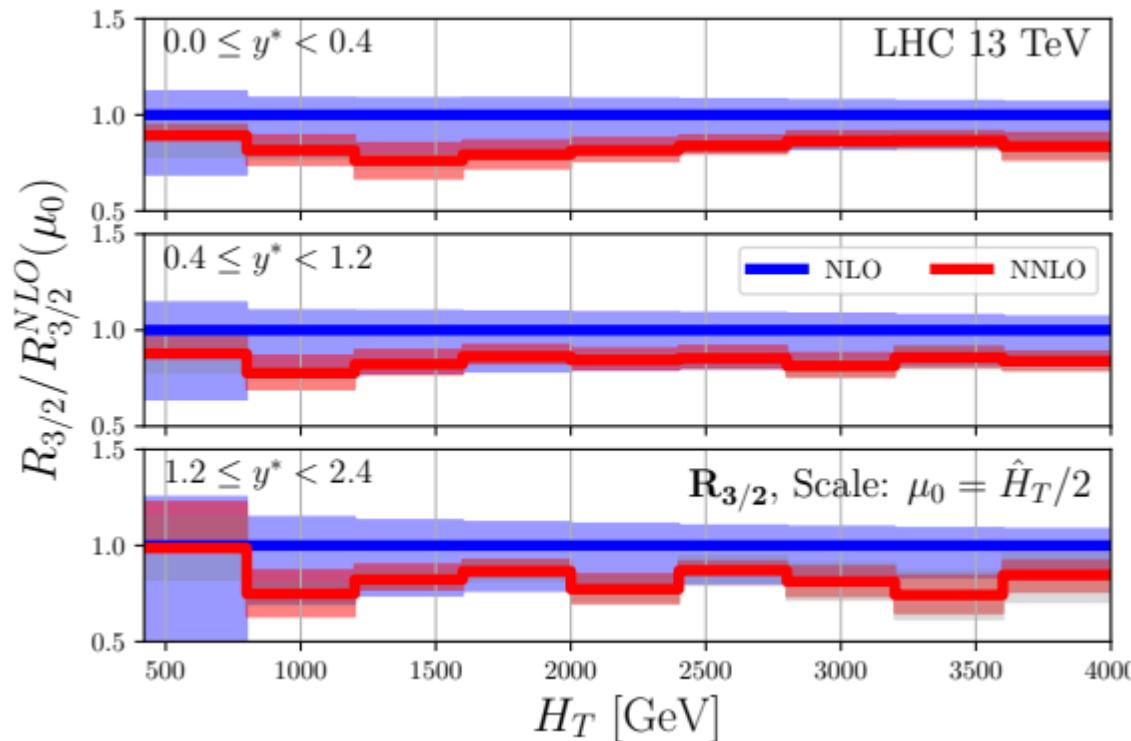
- LHC @ 13 TeV, NNPDF31
- Require at least three (two) jets:
  - $p_T(j) > 60$  GeV and  $|y(j)| < 4.4$
  - $H_{T,2} = p_T(j_1) + p_T(j_2) > 250$  GeV
- Scales:

$$\mu_R = \mu_F = \hat{H}_T = \sum_{\text{partons}} p_T$$

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



# Three jet production – R<sub>3/2</sub>(HT,y\*)



Double differential w.r.t.  $H_T = \sum_{\text{jets}} p_T$  and  $y^* = |y(j_1) - y(j_2)|/2$

Central scale choice:  $\hat{H}_T/2$

# Three jet production – azimuthal decorrelation

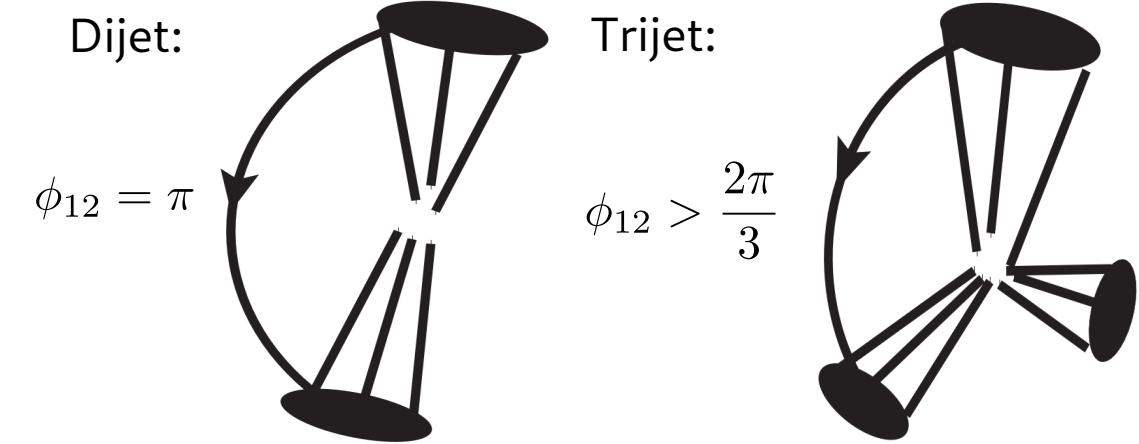
Kinematic constraints on the azimuthal separation between the two leading jets ( $\phi_{12}$ )

$\phi_{12}$  sensitive to the jet multiplicity:

$$2j: \phi_{12} = \pi$$

$$3j: \phi_{12} > \frac{2\pi}{3}$$

4j: unconstrained

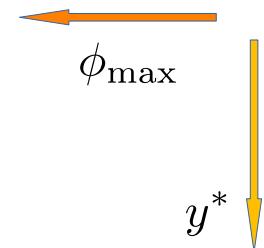


Study of the ratio:

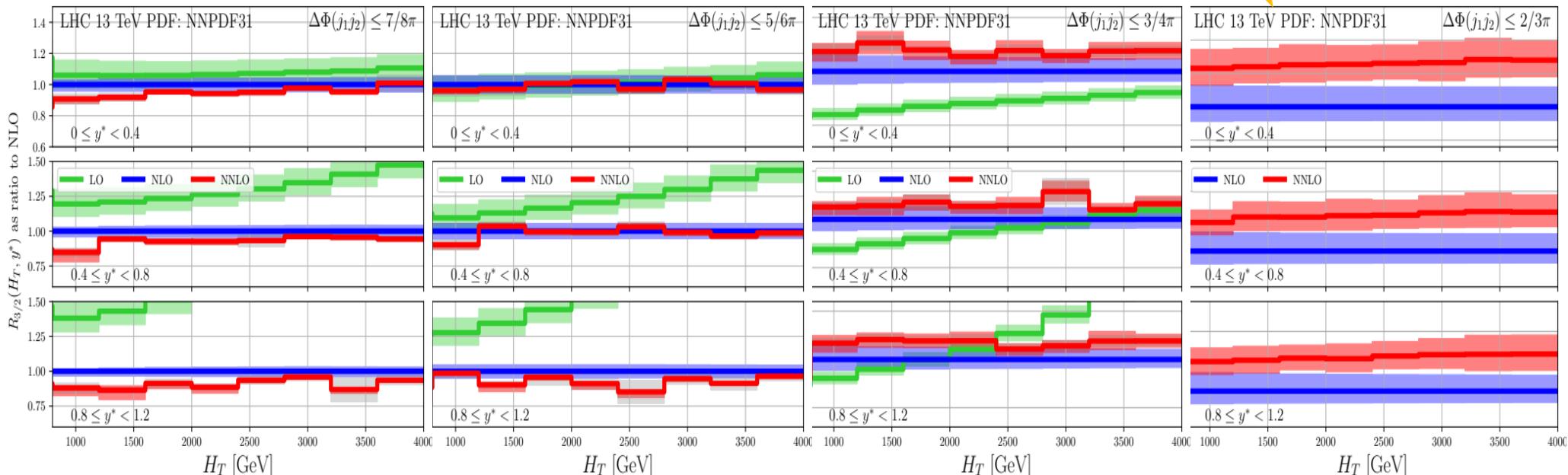
$$R_{32}(H_T, y^*, \phi_{\max}) = \frac{d\sigma_3(H_T, y^*, \phi_{12} < \phi_{\max})}{d\sigma_2(H_T, y^*)}$$

# Three jet production - azimuthal decorrelation

NNLO/NLO K-factor smaller than NLO/LO  
Scale dependence is reduced



Work in progress: phasespace in [1805.04691]

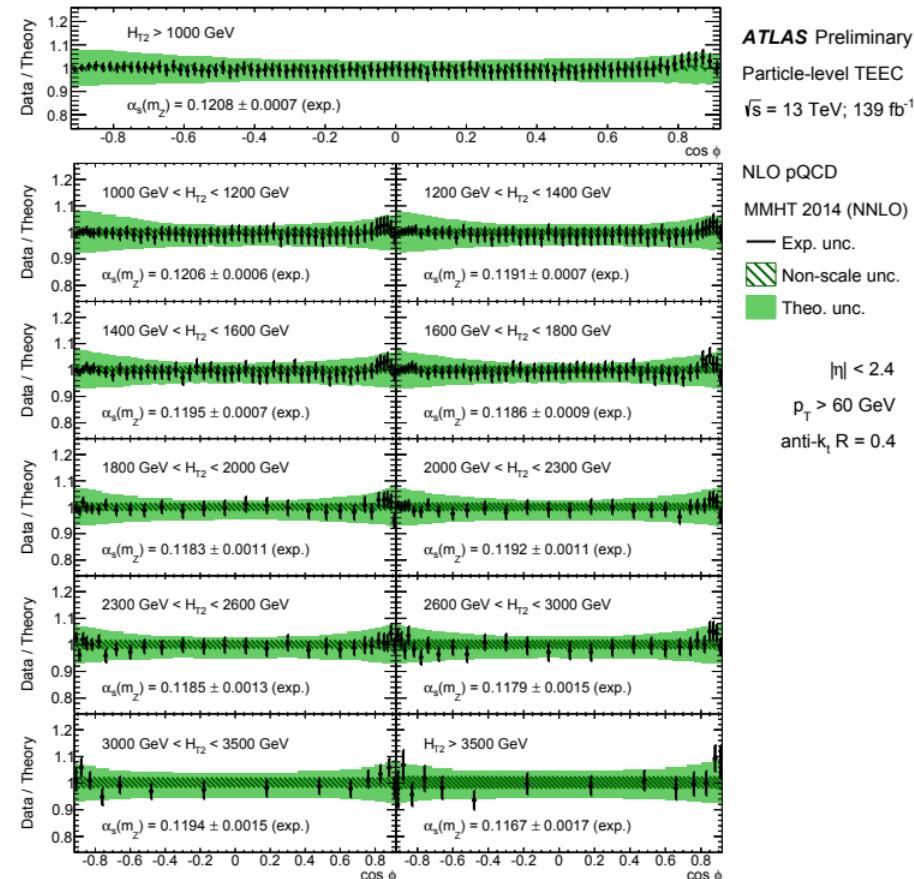
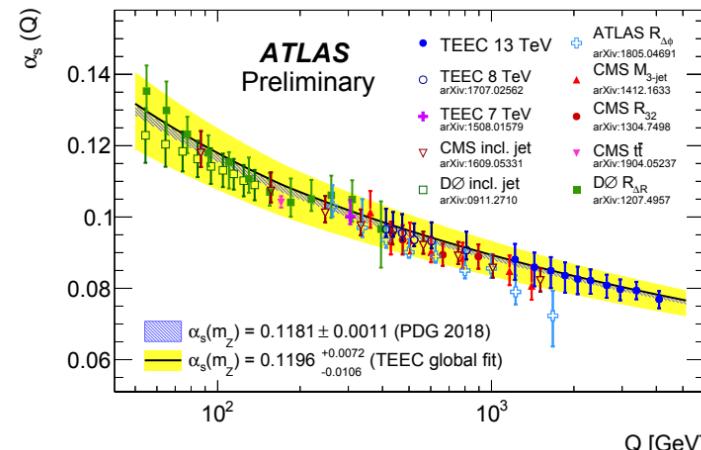


# Energy correlators at the LHC

In collaboration with ATLAS group:  
 Strong coupling measurement in TEEC  
 → three jet is leading contribution  
 → normalization through dijet rates

## TEEC: Transverse Energy-Energy Correlation

$$\frac{1}{\sigma} \frac{d\Sigma}{d \cos \phi} = \frac{1}{N} \sum_{A=1}^N \sum_{ij} \frac{E_{\perp,i}^A E_{\perp,j}^A}{\left( \sum_k E_{T,k}^A \right)^2} \delta(\cos \phi - \cos \phi_{ij})$$



[ATLAS-CONF-2020-025]

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# Event-shapes at the LHC

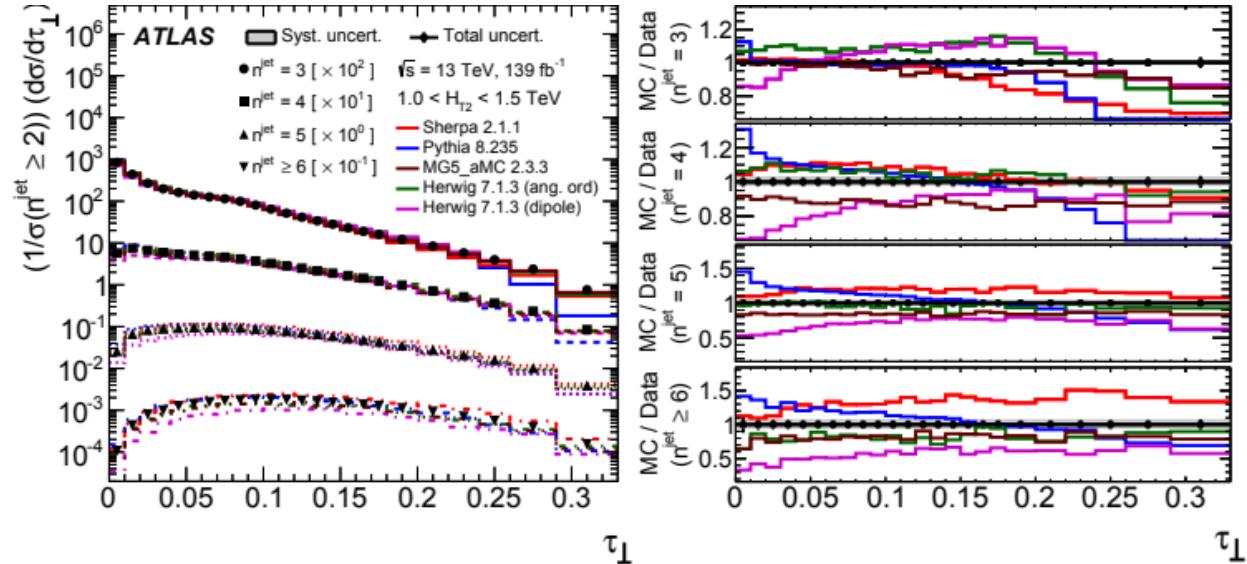
ATLAS measurement of event shapes [2007.12600]

Transverse Thrust:

$$\tau_T = 1 - \frac{\sum_i |\vec{p}_{T,i} \cdot \hat{n}|}{\sum |\vec{p}_{T,i}|}$$

Linearised sphericity tensor:

$$\mathcal{M}_{xyz} = \frac{1}{\sum_i |\vec{p}_i|} \sum_i \frac{1}{|\vec{p}_i|} \begin{pmatrix} p_{x,i}^2 & p_{x,i}p_{y,i} & p_{x,i}p_{z,i} \\ p_{y,i}p_{x,i} & p_{y,i}^2 & p_{y,i}p_{z,i} \\ p_{z,i}p_{x,i} & p_{z,i}p_{y,i} & p_{z,i}^2 \end{pmatrix}$$

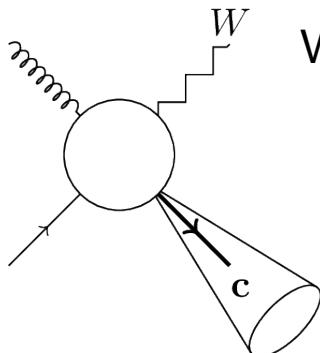


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# Flavoured jets and fragmentation

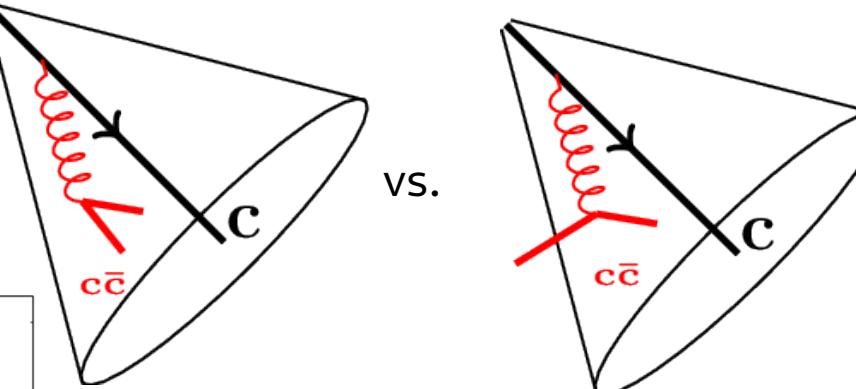
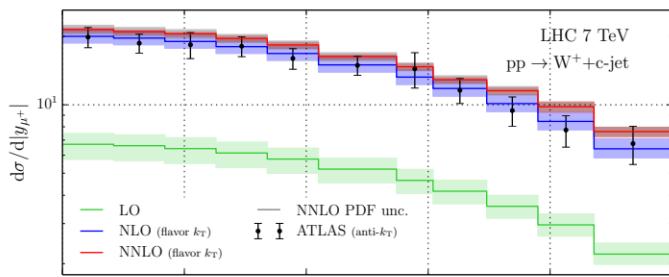
# IR safe jet flavour

Example:



Well known problem in massless NNLO QCD [Banfi'06]:

[Czakon'20]



A possible solution:  
change the clustering  
→ Flavour –  $k_T$  algorithm

NNLO QCD with flavour  $k_T$

ATLAS data with standard anti- $k_T$

A proper comparison would require to  
unfold experimental data

# What about flavour anti-kT?

Anti-kT:  $d_{ij} = \min(k_{T,i}^{-2}, k_{T,j}^{-2})R_{ij}^2$      $d_i = k_{T,i}^{-2}$

The energy ordering in anti-kT prevents correct recombination of flavoured pairs in the double soft limit.

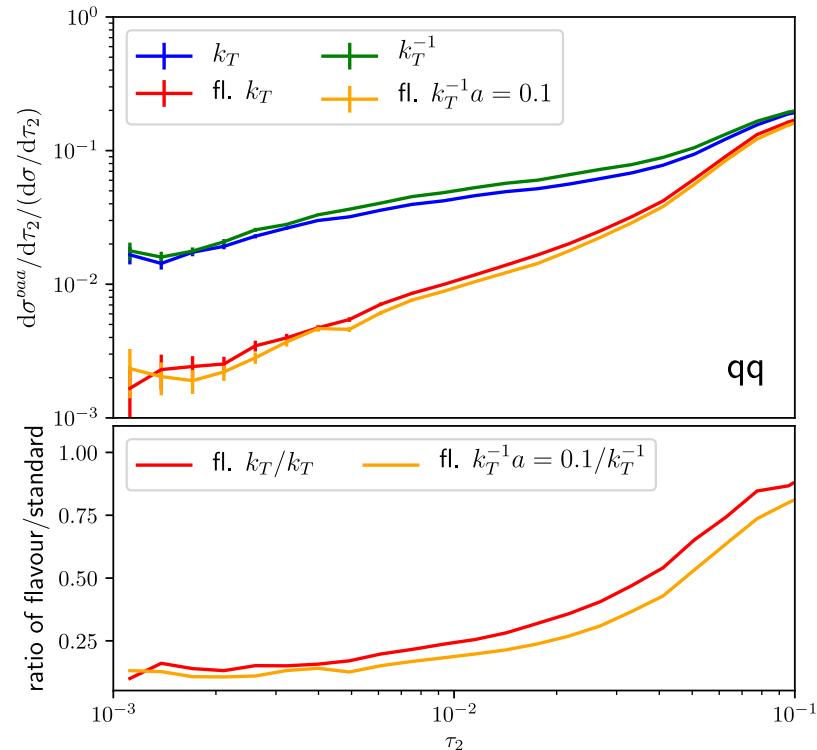
Proposed modification [to be published soon]:

A soft term designed to modify the distance of flavoured pairs.

$$d_{i,j}^{(F)} = d_{i,j} \begin{cases} \mathcal{S}_{ij} & i,j \text{ is flavoured pair} \\ 1 & \text{else} \end{cases}$$

$$\mathcal{S}_{ij} = 1 - \theta(1-x) \cos\left(\frac{\pi}{2}x\right) \quad \text{with} \quad x = \frac{k_{T,i}^2 + k_{T,j}^2}{2ak_{T,\max}^2}$$

IR safety check:



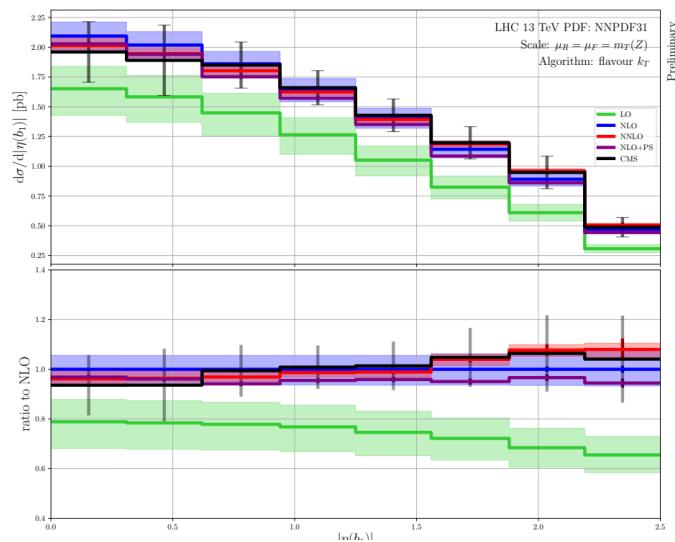
# Phenomenology: Tunable parameter

Benchmark process:  $pp \rightarrow Z(l\bar{l}) + b\text{-jet}$

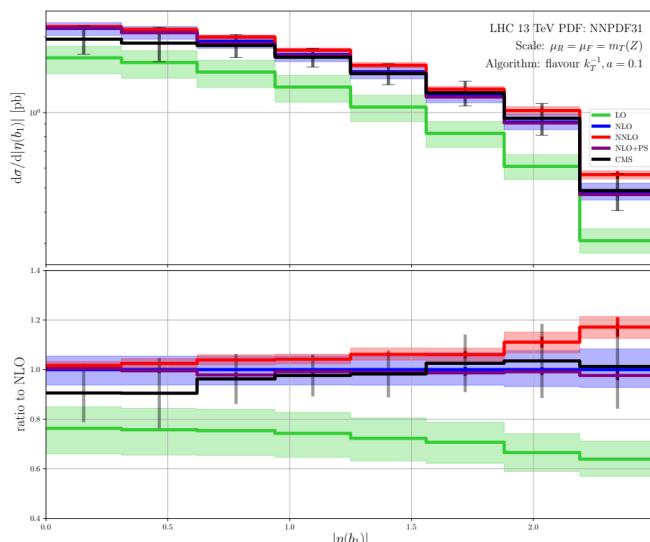
Tunable parameter  $a$ :

- Limit  $a \rightarrow 0 \Leftrightarrow$  original anti- $k_T$  (IR unsafe)
- Large  $a \Leftrightarrow$  large modification of cluster sequence

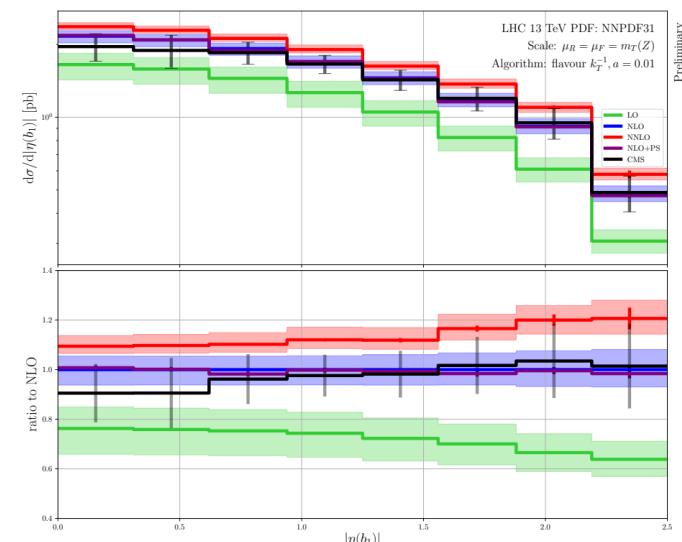
Flavour  $k_T$ :



Flavour anti- $k_T$ :  $a = 0.1$

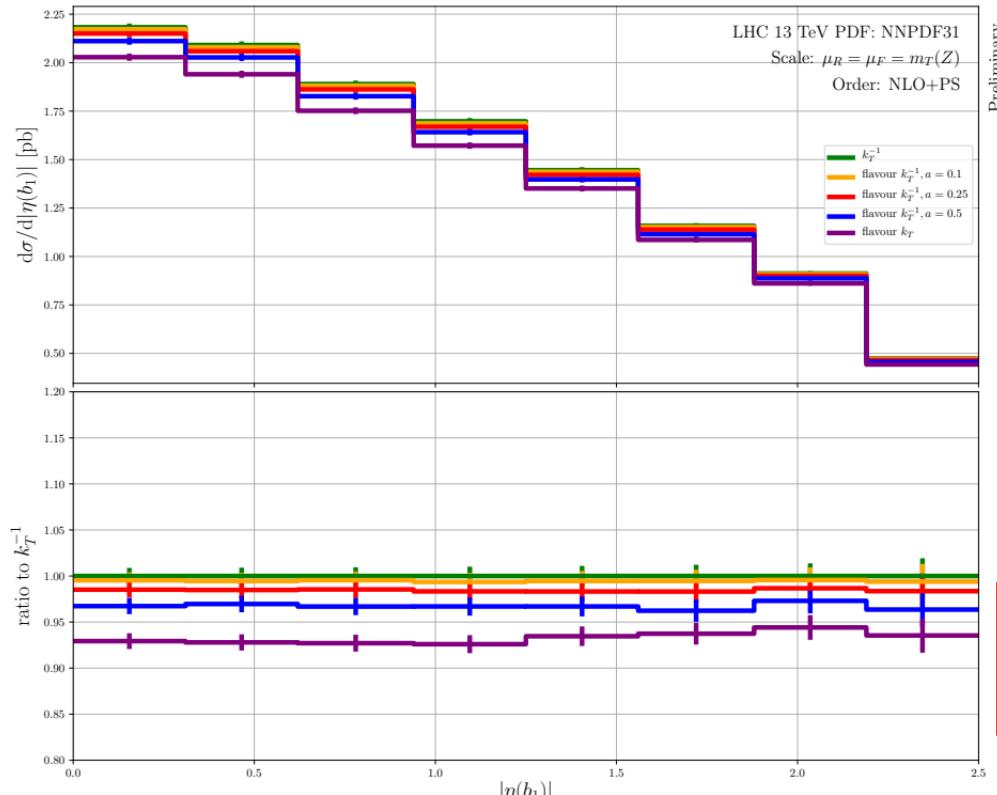


Flavour anti- $k_T$ :  $a = 0.01$



# Phenomenology: Tunable parameter II

What happens in the presence of many flavoured partons? → NLO PS



Tunable parameter a:

- Flavour anti-kT results are similar to standard anti-kT  
→ small unfolding factors
- Flavour-kT has larger difference

Combine with perturbative convergence:  
→  $a \sim 0.1$  is a good candidate

# Fixed-order Fragmentation

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Fixed order QCD predictions with a final state hadron

Considering partonic computation  
+ transition of parton to hadron (collinear fragmentation of massless partons)

Advantage is that the hadrons momentum is measurable while the quark's is not

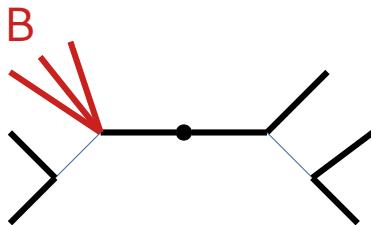
Fragmentation function (similar to PDFs)  
Probability to find a hadron with a fraction  $x$  of the quarks momentum:  $D_{i \rightarrow h}(x)$

No Parton-shower needed

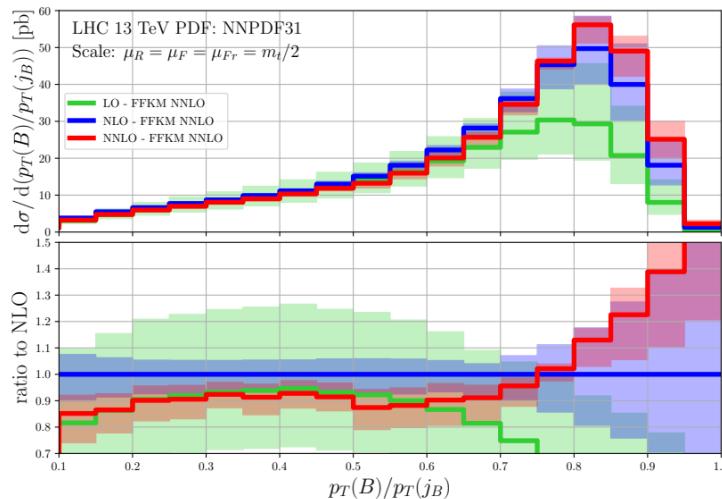
Implementation in the STRIPPER framework

# B-hadrons in ttbar production

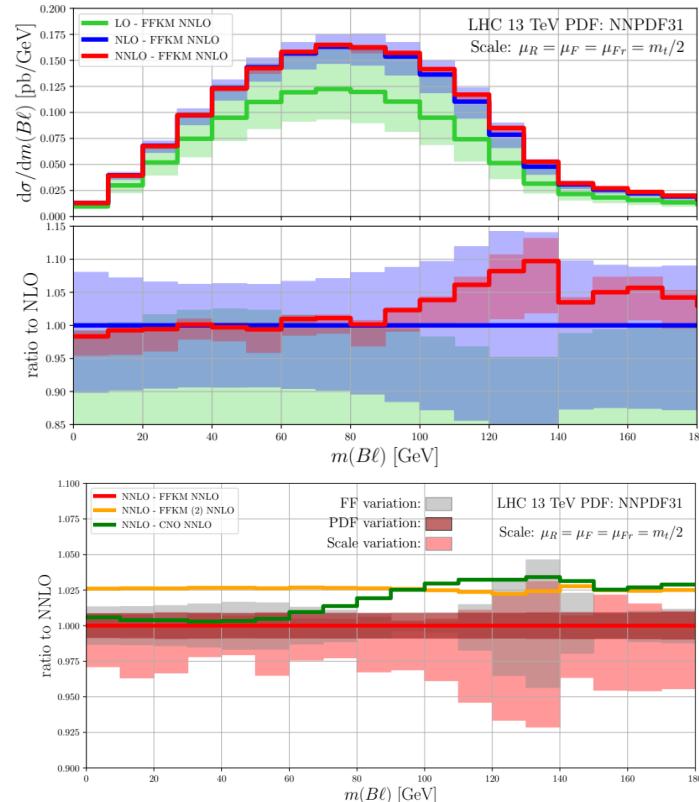
$$pp \rightarrow t\bar{t} \rightarrow B\ell\bar{\ell}\nu\bar{\nu}b + X$$



$pT(B)/pT(j_B)$ : sensitive to B-hadron fraction x



$m(lB)$ : sensitive to top-quark mass



# Applications

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Exploration of applications:

- Measurement of fragmentation functions at the LHC (so far mostly data from LEP)?
  - What observables?  $pT(B)/pT(jB)$  and similar look promising.
- Using the B-hadron to tag jets in partonic computation? → flavoured jets

Fragmentation implementation not limited to ttbar:

- Open b
- V + hadron

**Work in progress:** fragmentation function fits with the right conventions

# Summary and Outlook

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NNLO predictions with the sector-improved residue subtraction framework

- First computations of  $2 \rightarrow 3$  processes: 3 photon, 2 photon+jet and three jet production
- Three jets @ the LHC:
  - R32 ratios → reduction of scale uncertainties, stabilization of K-factors
  - Planned applications: alphaS extractions from R32 ratios, event-shapes & TEEC
- Flavoured jet observables: new ideas for flavoured jet definitions with anti-kT
- Identified hadron production in fixed-order fragmentation:
  - Applications: measurement of fragmentation functions, top-quark mass measurements,...

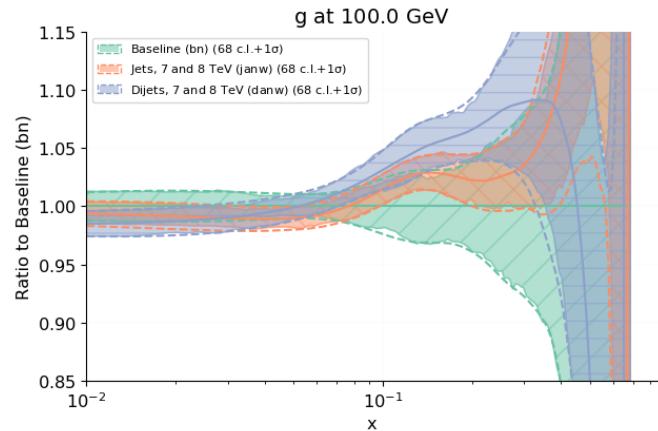
Many interesting applications ahead!  
Stay tuned!

Thank you for your attention!



# Backup

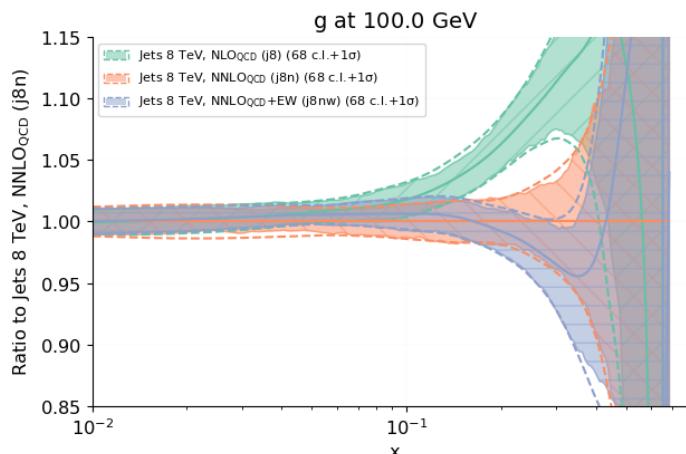
# Higher order pQCD: PDF fits with jets



Idea (quite old actually [[Giele'94](#)]):

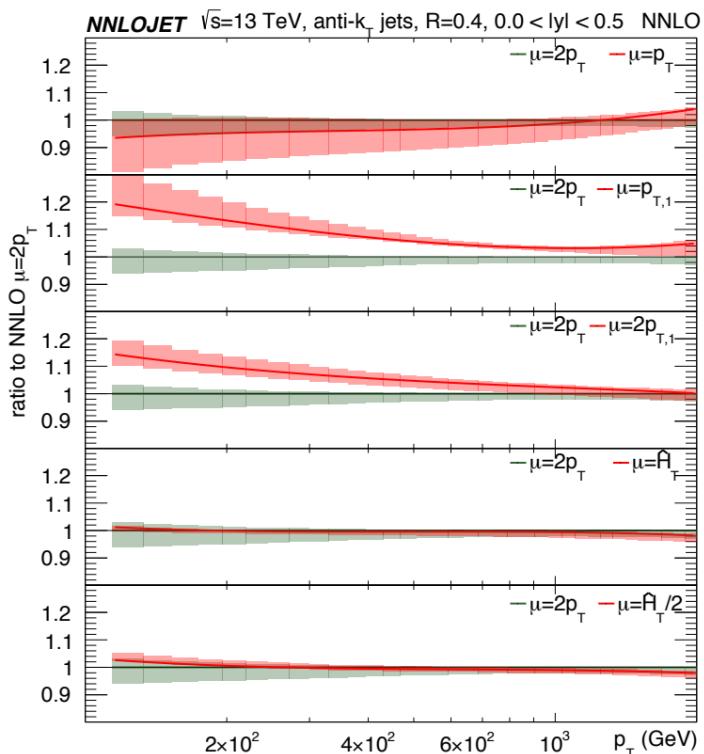
Here by a collaboration of NNLOJet and NNPDF [[Khalek'20](#)]:

Combine single inclusive and dijet triple differential measurements by ATLAS and CMS to constrain the large gluon-x



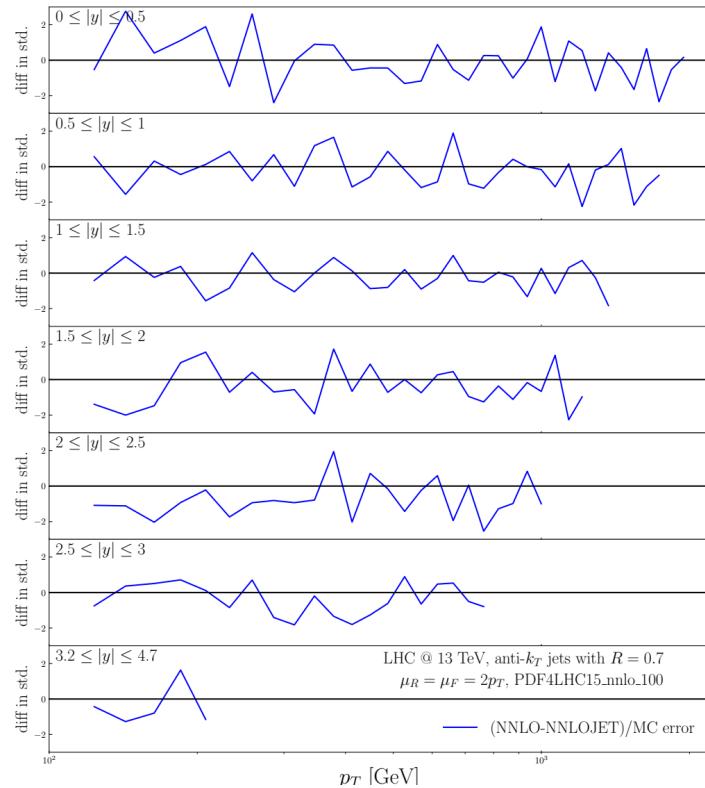
- Reduced uncertainty in large-x gluon PDF
- **NNLO QCD corrections crucial** to obtain consistent results between data sets
- NLO EW [[Dittmaier'12](#)] or full NLO corrections [[Frederix'17, Reyer'19](#)]

# Higher order pQCD: lessons from dijet



Detailed studies of  
scale dependence:  
Event-based choices vs.  
single jet choices  
[Currie'18]

Study of  
sub-leading colour  
effects  
in quark channels:  
smaller than  $O(1\%)$   
[Czakon'19]



# Diphoton plus jet - setup

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[Chawdry'21]: Inspired by Higgs  $\rightarrow \gamma\gamma$  measurement phase spaces

- Smooth photon isolation criteria:  $E_T = 10$  GeV,  $R_\gamma = 0.4$ ,  $\Delta R(\gamma, \gamma) > 0.4$
- $p_T(\gamma_1) > 30$  GeV,  $p_T(\gamma_2) > 18$  GeV and  $|y(\gamma)| < 2.4$
- $m(\gamma\gamma) > 90$  GeV and  $p_T(\gamma\gamma) > 20$  GeV, below resummation important
- No further restrictions on jets (IR safety from  $p_T(\gamma\gamma)$  cut)

Technicalities:

- LHC 13 TeV, PDF: NNPDF31, Scale:  $\mu_R^2 = \mu_F^2 = \frac{1}{4}m_T^2(\gamma\gamma) = \frac{1}{4}(m(\gamma\gamma)^2 + p_T(\gamma\gamma)^2)$
- 5 massless flavours and top-quarks (in all one-loop amps)
- Approximation of two-loop amps:  
 $2 \operatorname{Re}(\mathcal{M}^{(0)\dagger} \mathcal{F}^{(2)}) + \mathcal{F}^{(1)\dagger} \mathcal{F}^{(1)}$  without top-quark loops  
and  $2 \operatorname{Re}(\mathcal{M}^{(0)\dagger} \mathcal{F}^{(2)})$  in leading colour limit [Chawdhry'21]  
→ Update to full colour planned [Agarwal'21]

# Solution: Modified jet algorithms

Standard kT algorithm [Ellis'93]:

Pair distance:  $d_{ij} = \min(k_{T,i}^2, k_{T,j}^2) R_{ij}^2$

$$R_{ij}^2 = (\Delta\phi_{ij}^2 + \Delta\eta_{ij}^2)/R^2$$

Beam distance:  $d_i = k_{T,i}^2$

Flavour kT algorithm [Banfi'06]:

Pair distance:

$$d_{ij} = R_{ij}^2 \begin{cases} \max(k_{T,i}, k_{T,j})^\alpha \min(k_{T,i}, k_{T,j})^{2-\alpha} & \text{softer of } i,j \text{ is flavoured} \\ \min(k_{T,i}, k_{T,j})^\alpha & \text{else} \end{cases}$$

Beam distance:

$$d_{i,B} = \begin{cases} \max(k_{T,i}, k_{T,B}(y_i))^\alpha \min(k_{T,i}, k_{T,B}(y_i))^{2-\alpha} & i \text{ is flavoured} \\ \min(k_{T,i}, k_{T,B}(y_i))^\alpha & \text{else} \end{cases}$$

$$d_B(\eta) = \sum_i k_{T,i} (\theta(\eta_i - \eta) + \theta(\eta - \eta_i) e^{\eta_i - \eta}$$

$$d_{\bar{B}}(\eta) = \sum_i k_{T,i} (\theta(\eta - \eta_i) + \theta(\eta_i - \eta) e^{\eta - \eta_i}$$

Numerical check in 2jet events:  
Misidentification rate as  
a function of  $y_{3kt}$

