Associated production of a W boson and massive b quarks in NNLO QCD

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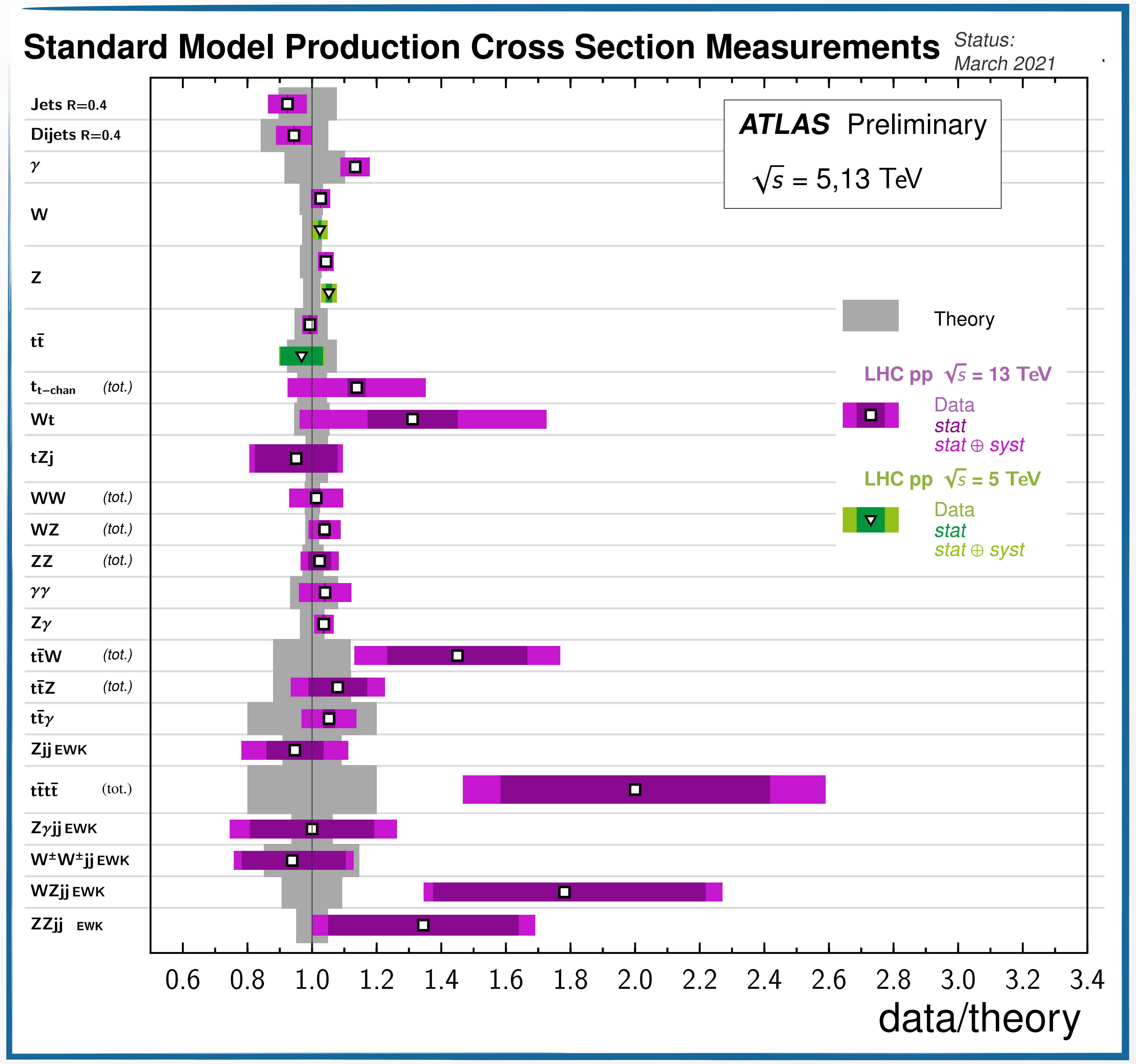
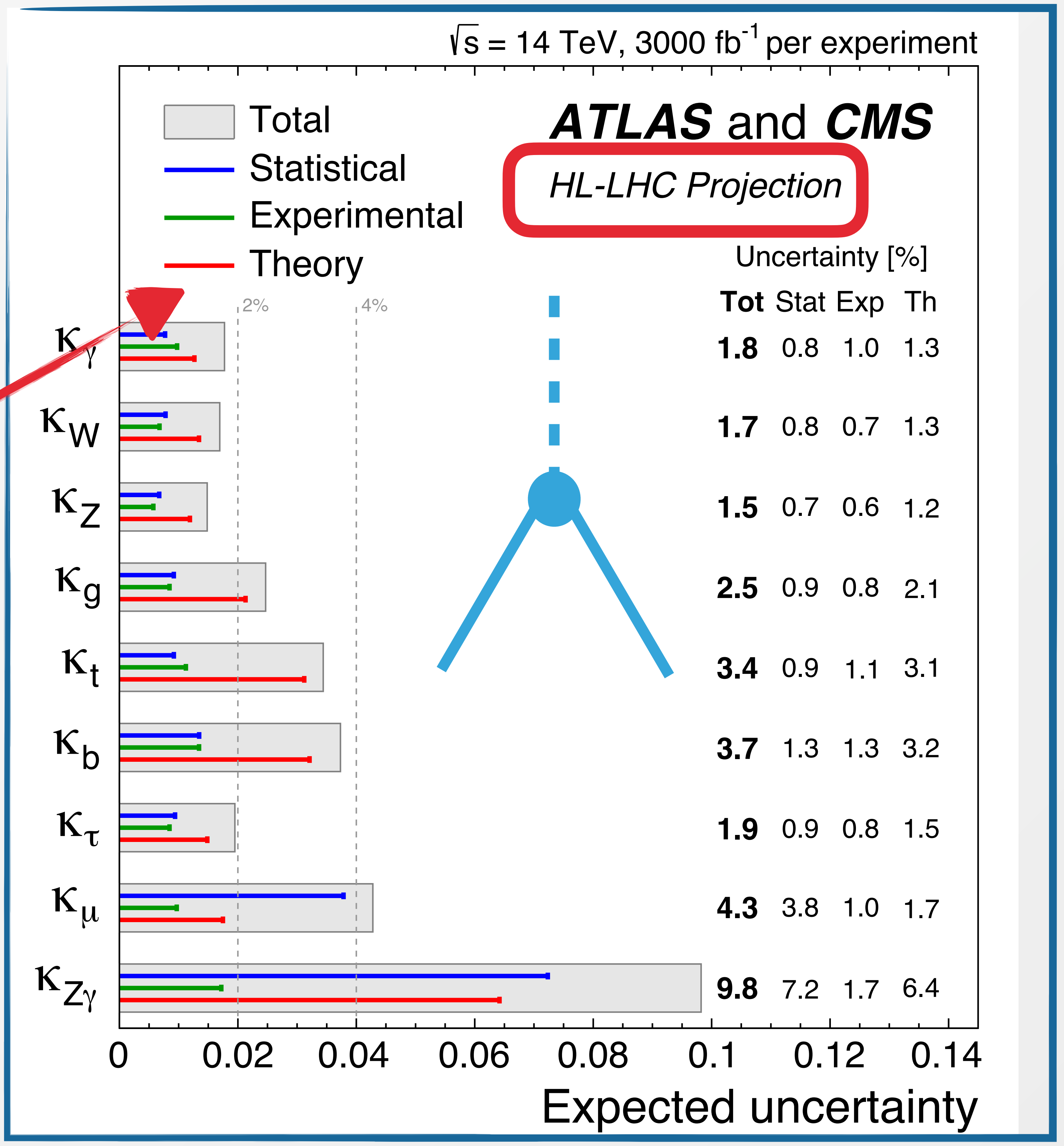
LHC: precision as a path to discovery

- Precision of experimental data across a variety of processes increased after run I and run II at the LHC
- Precision will be increased further at run III and at the **HL-LHC** (luminosity up to ~3000 fb^{-1})



Theoretical uncertainties will be among the **dominant errors** for the extraction of various SM parameters, e.g. Higgs couplings

Sensitivity to deviations of Higgs interactions from SM predictions



[Higgs Physics Report at HE/HL-LHC 2019]

Precise control of signal and backgrounds essential to constrain models for **new physics**

Precision physics at the LHC: the master formula

$$\sigma(s, Q^2) = \sum_{a,b} \int dx_1 dx_2\, f_{a/h_1}(x_1, Q^2) f_{b/h_2}(x_2, Q^2) \hat{\sigma}_{ab\to X}(Q^2, x_1 x_2 s) + \mathcal{O}(\Lambda^p_{\mathrm{QCD}}/Q^p)$$

Input parameters:

strong coupling α_s

PDFs f

few percent uncertainty; improvable

Non-perturbative effects

percent effect; not yet under full control

Precision physics at the LHC: the master formula

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$$\tilde{\sigma} = 1 + \alpha_s\tilde{\sigma}_1 + \alpha_s^2\tilde{\sigma}_2 + \alpha_s^3\tilde{\sigma}_3 + \dots$$

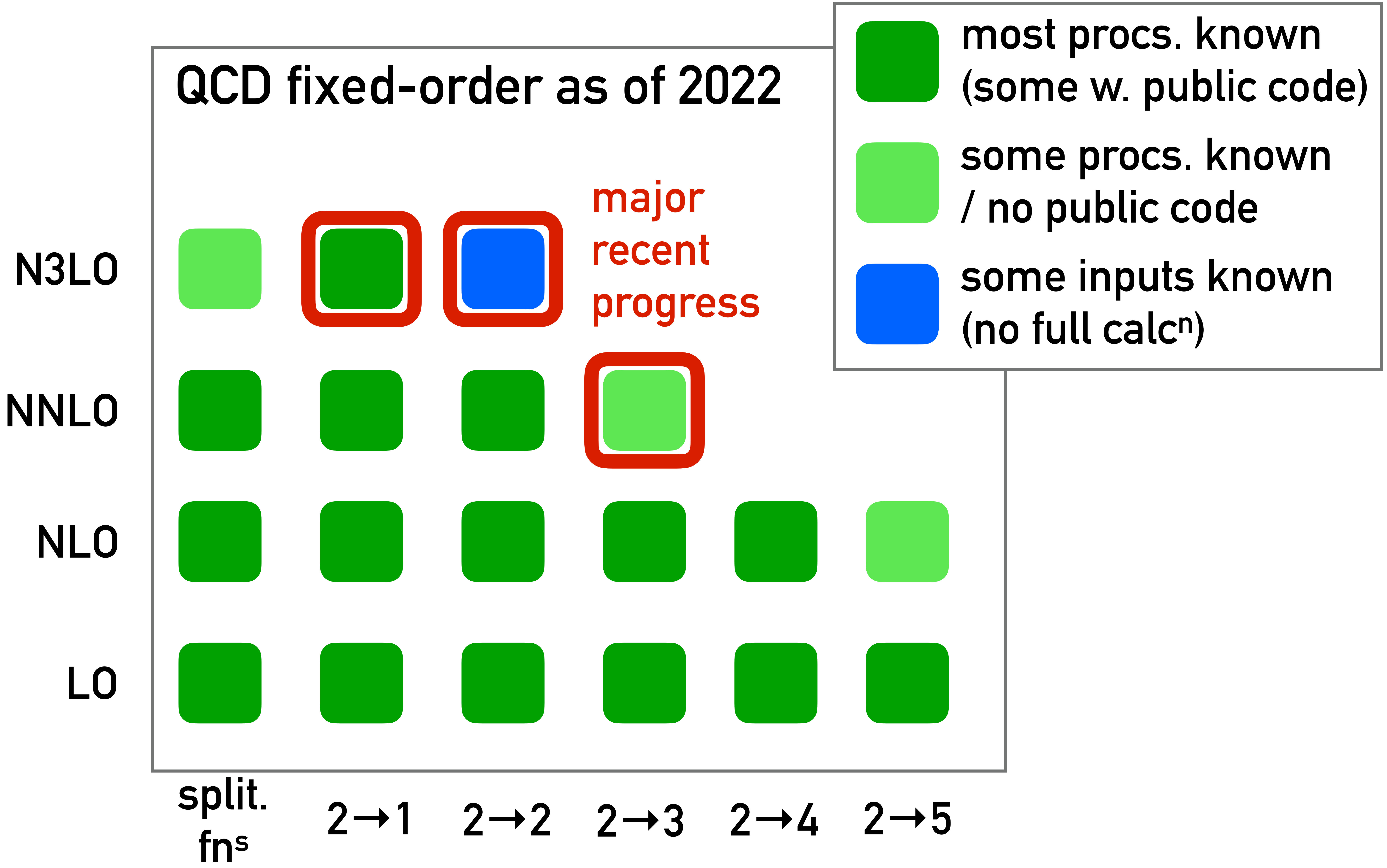
LO_{QCD} **NLO_{QCD}** **NNLO_{QCD}** **$\text{N}^3\text{LO}_{\text{QCD}}$**

$\alpha_s \sim 0.1$

δ~10-20% **NLO_{QCD}**

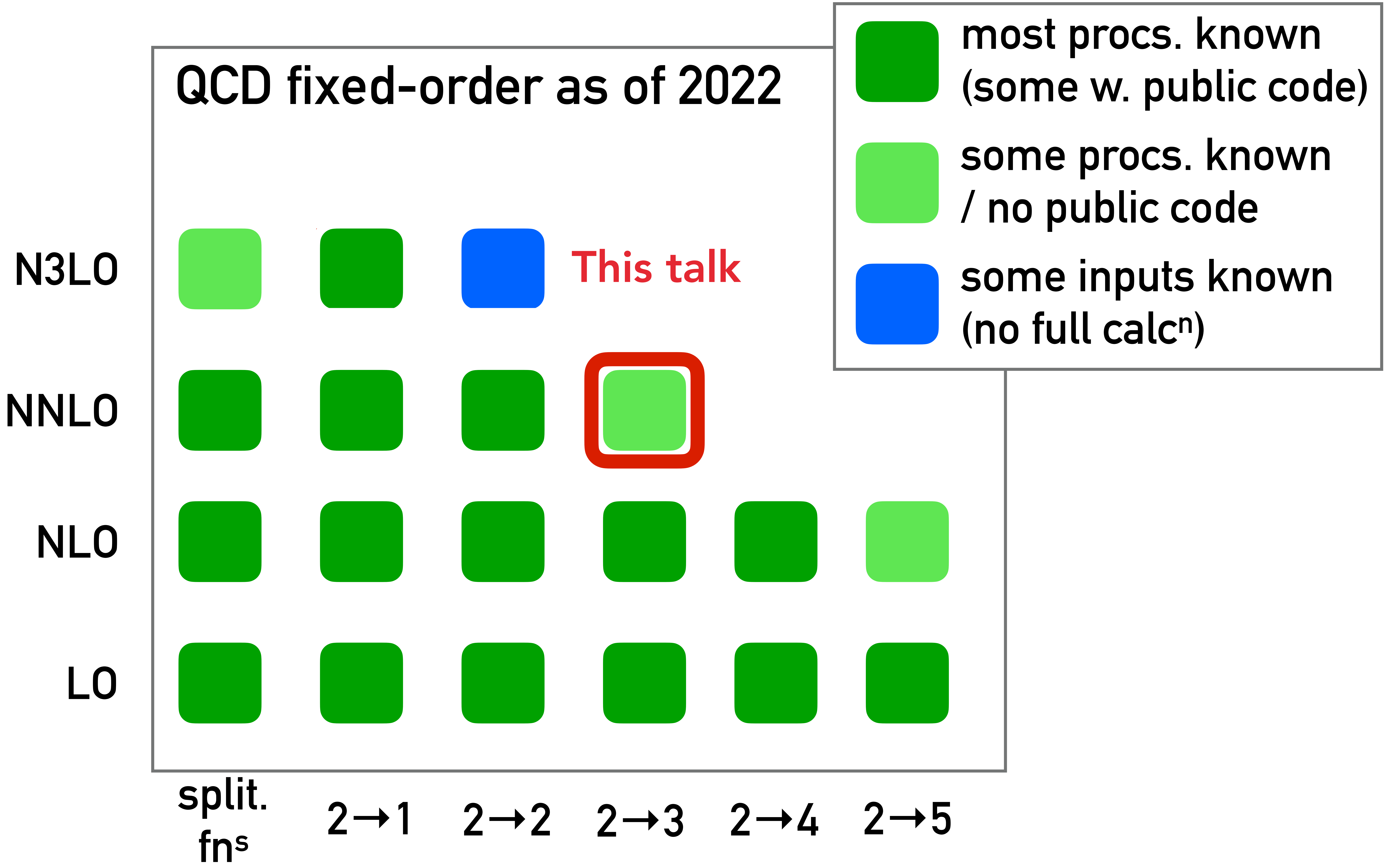
δ~1-5% **NNLO_{QCD}** (or even **$\text{N}^3\text{LO}_{\text{QCD}}$**)

LHC in the precision era



[Gavin Salam @ICHEP 2022]

LHC in the precision era

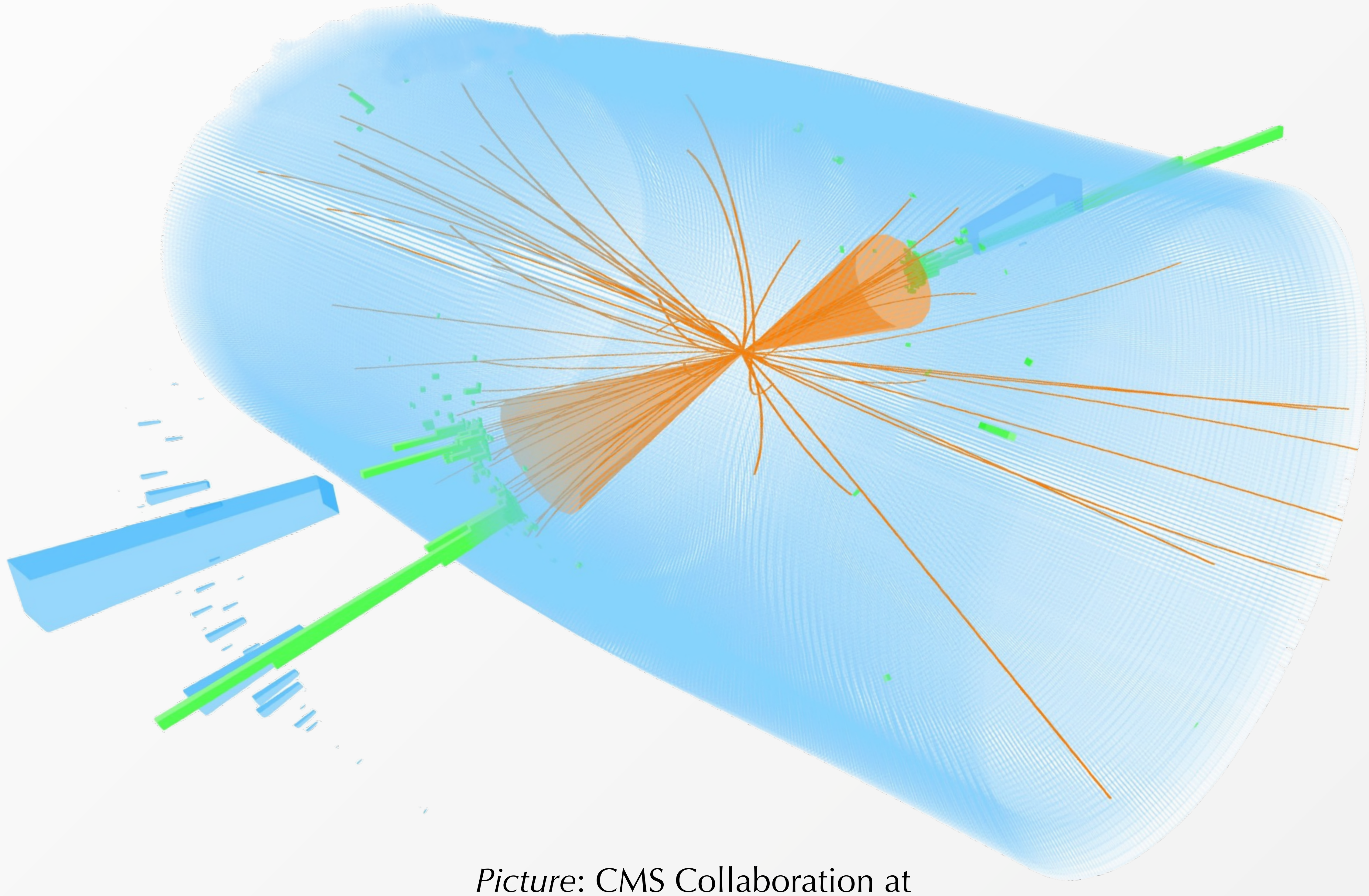


[Gavin Salam @ICHEP 2022]

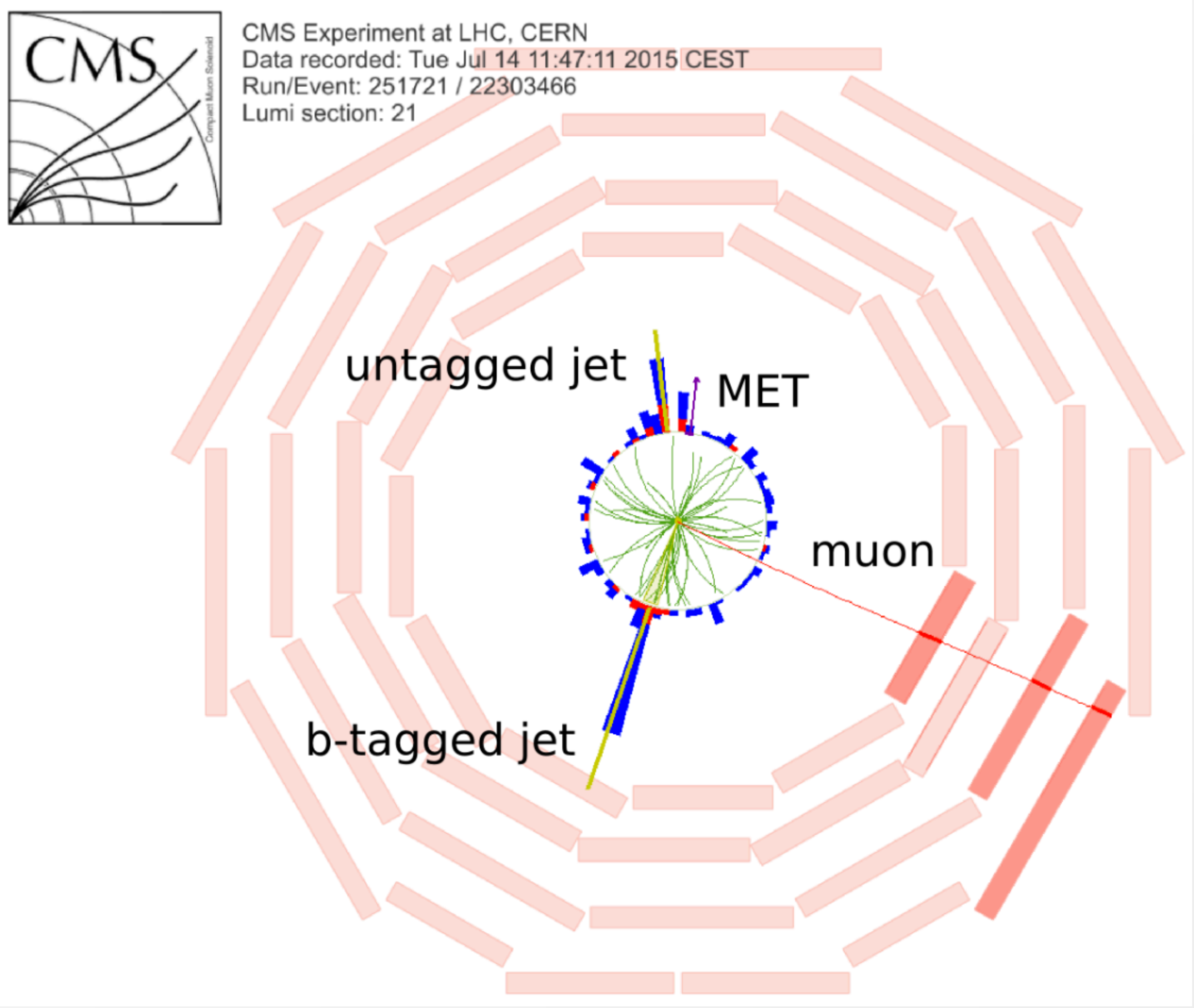
Associated *Wbb* production

***W*+1*bj* and *W*+2*bj* interesting signatures**

- tests of QCD at LHC
- background to $WH(H \to b\bar{b})$ and single top $\bar{b}t(t \to Wb)$
- **bottom quarks modelling:** massive effects, bottom in the PDF, flavour tagging



Picture: CMS Collaboration at the LHC, CERN



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Large normalisation corrections with respect to SM simulation

Process	Z($\nu\nu$)H	W($\ell\nu$)H	Z($\ell\ell$)H low-p_T	Z($\ell\ell$)H high-p_T
W + udscg	1.04 ± 0.07	1.04 ± 0.07	–	–
$\boxed{\text{W + b}}$	2.09 ± 0.16	2.09 ± 0.16	–	–
$\boxed{\text{W + b}\bar{\text{b}}}$	1.74 ± 0.21	1.74 ± 0.21	–	–
Z + udscg	0.95 ± 0.09	–	0.89 ± 0.06	0.81 ± 0.05
Z + b	1.02 ± 0.17	–	0.94 ± 0.12	1.17 ± 0.10
Z + b$\bar{\text{b}}$	1.20 ± 0.11	–	0.81 ± 0.07	0.88 ± 0.08
t$\bar{\text{t}}$	0.99 ± 0.07	0.93 ± 0.07	0.89 ± 0.07	0.91 ± 0.07

from $VH(\to bb)$ analysis [CMS:arXiv:1808.08242]

Associated *Wbb* production: state of the art

NLO corrections for *Wbb* production with massless be quarks known since a long time

[Ellis, Veseli '99]

NLO calculation with massive bottom quarks also long available

[Febres Cordero, Reina, Wackeroth '06, 09]

Combination of 4FS and 5FS computed shortly after

[Campbell, Ellis, Febres Cordero, Maltoni, Reina, Wackeroth, Willenrock '09] [Campbell, Caola, Febres Cordero, Reina, Wackeroth '11]

Matched calculation with parton shower available

[Oleari, Reina '11] [Frederix, Frixione, Hirschi, Maltoni, Pittau, Torrielli '11]
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More recently, calculation with higher jet multiplicities (*Wbb* + 3 jets) computed

[Anger, Febres Cordero, Ita, Sotnikov, 2018]

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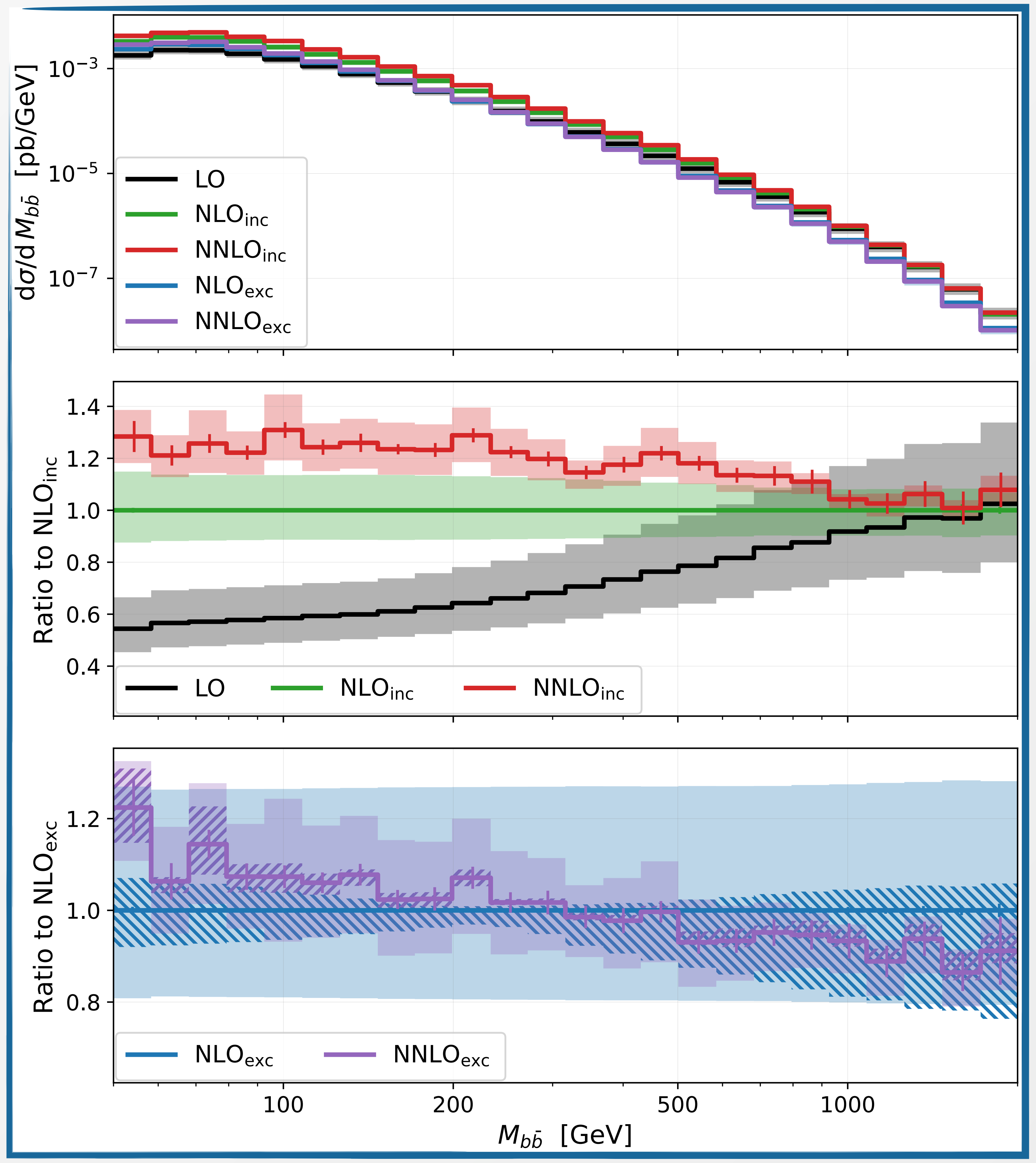
Going beyond NLO requires **computation of 2-loop virtual amplitude** (W + 4 partons)

Analytical results for the 2-loop amplitude computed recently (in the leading colour approximation)

[Badger, Hartanto, Zoia '21] [Abreu, Febres Cordero, Ita, Klinkert, Page, Sotnikov '21]

Wbb @ NNLO with massless *b* quarks

First computation for *Wbb* @ NNLO with massless *b* quarks recently performed [Hartanto, Poncelet, Popescu, Zoia '22]



However, massless calculation is subject to ambiguities related to jet-sensitive jet algorithm

Jet algorithm	σ_{NNLO} [fb]	K_{NNLO}
flavour-k_{T}	$445(5)^{+6.7\%}_{-7.0\%}$	1.23
flavour anti-k_{T} ($a = 0.05$)	$690(7)^{+10.9\%}_{-9.7\%}$	1.38
flavour anti-k_{T} ($a = 0.1$)	$677(7)^{+10.4\%}_{-9.4\%}$	1.36
flavour anti-k_{T} ($a = 0.2$)	$647(7)^{+9.5\%}_{-8.9\%}$	1.33

[Hartanto, Poncelet, Popescu, Zoia '22]

O(50%) difference when using flavour k_T algorithm

Reduced at the K-factor level

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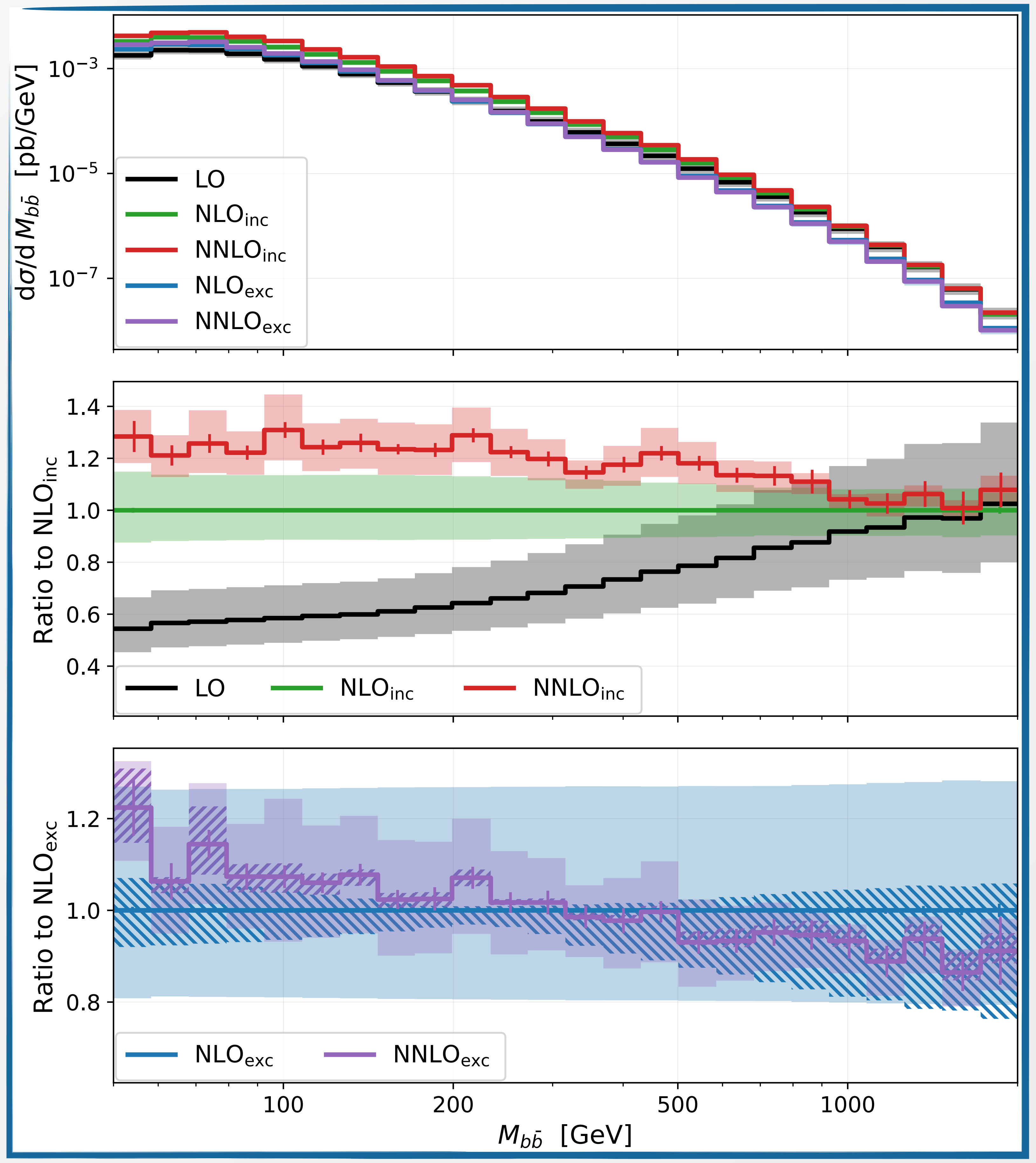
Uncertainties related to the ambiguities reduced when using flavour-aware anti-k_T

[Czakon, Mitov, Poncelet '22]



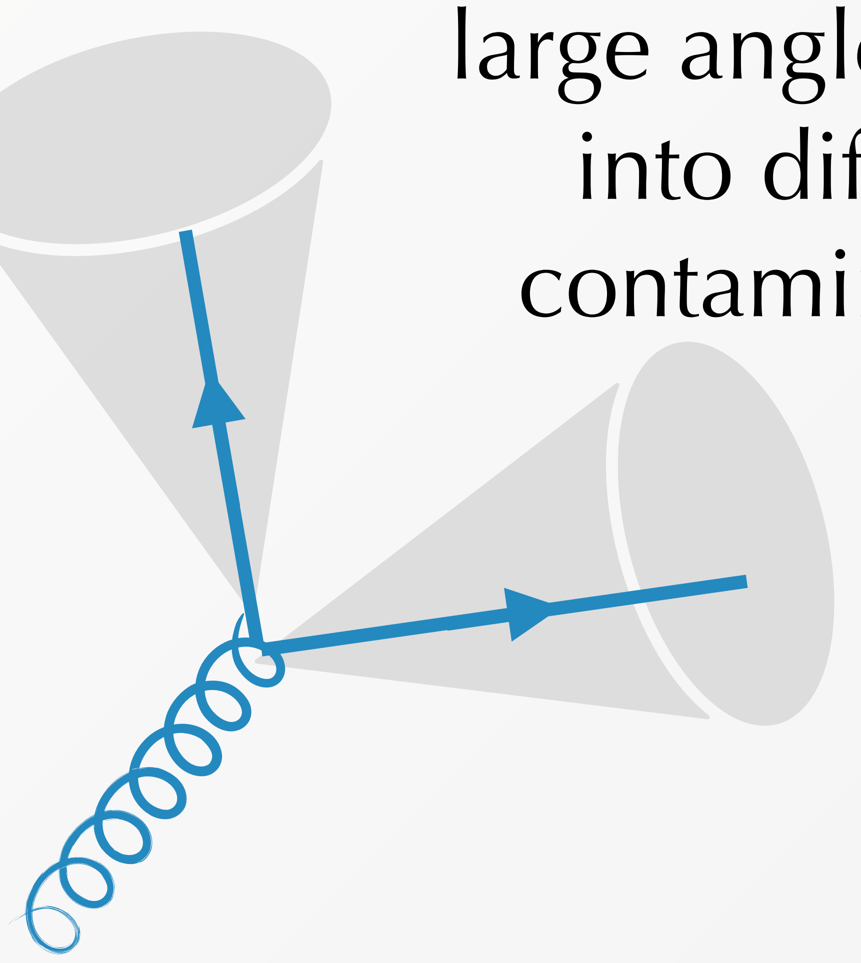
Infrared safety and flavour tagging

Jet algorithms belonging to the k_T family

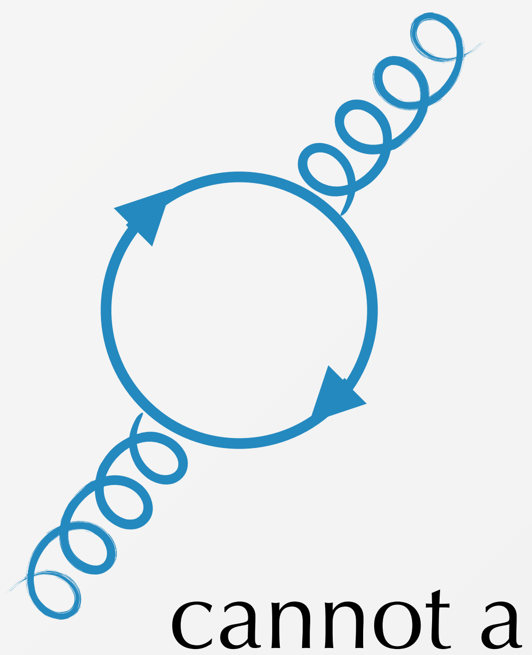
$$d_{ij} = \min\left(k_{T,i}^{2\alpha}, k_{T,j}^{2\alpha}\right) R_{ij}^2, \quad d_{iB} = k_{T,i}^{2\alpha} \qquad\qquad R_{ij}^2 = (y_i - y_j)^2 + (\phi_i - \phi_j)^2$$

For observable sensitive to the flavour assignment, **infrared safety can be an issue**

Problem related **to gluon splitting to quarks in the double soft limit** (starting at NNLO)



large angle $Q\bar{Q}$ is clustered into different jets and contaminates jet flavour



cannot alter tagging

KLN cancellation might be spoiled due to miscancellation between real and virtual configurations due to flavour assignment

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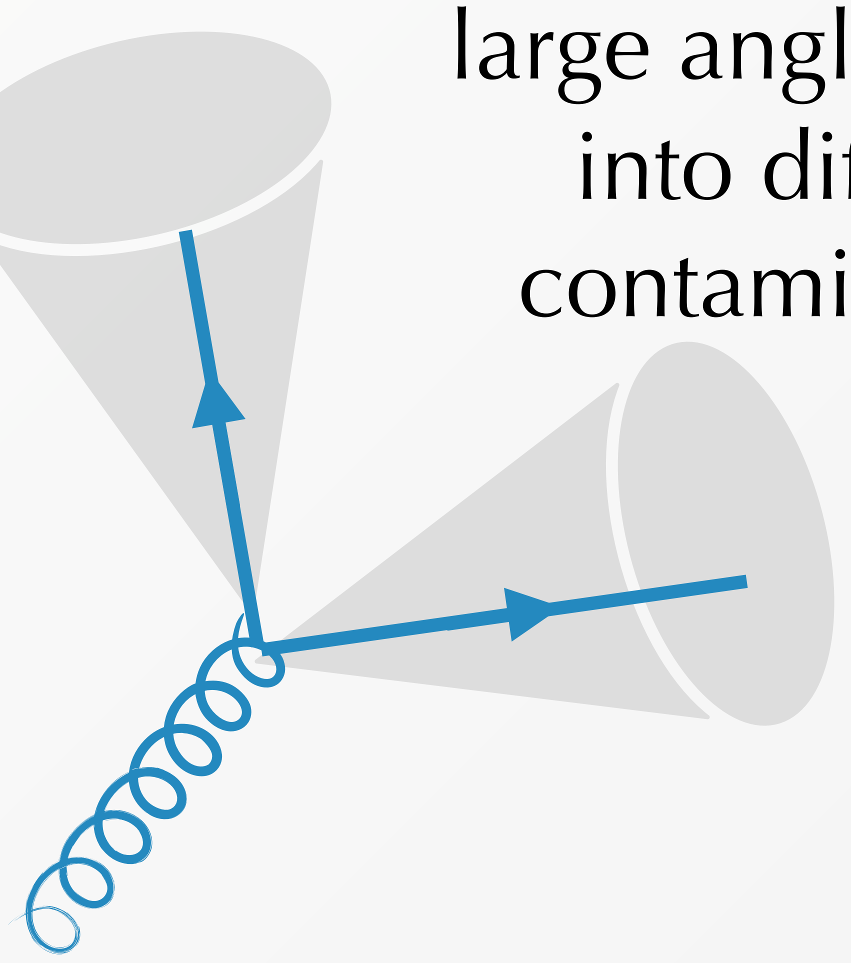

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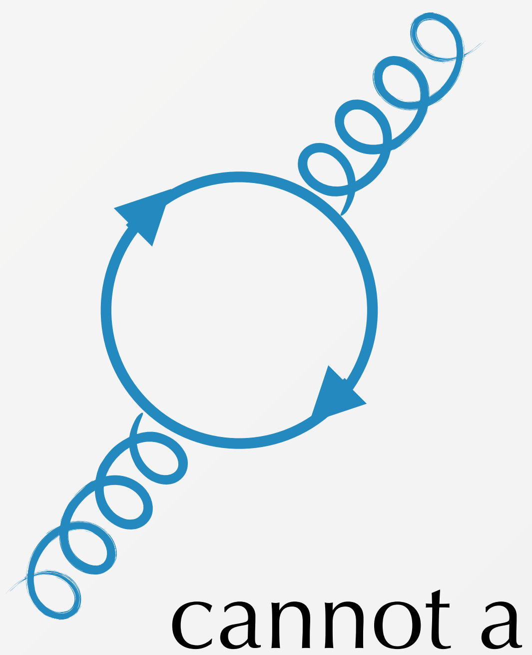

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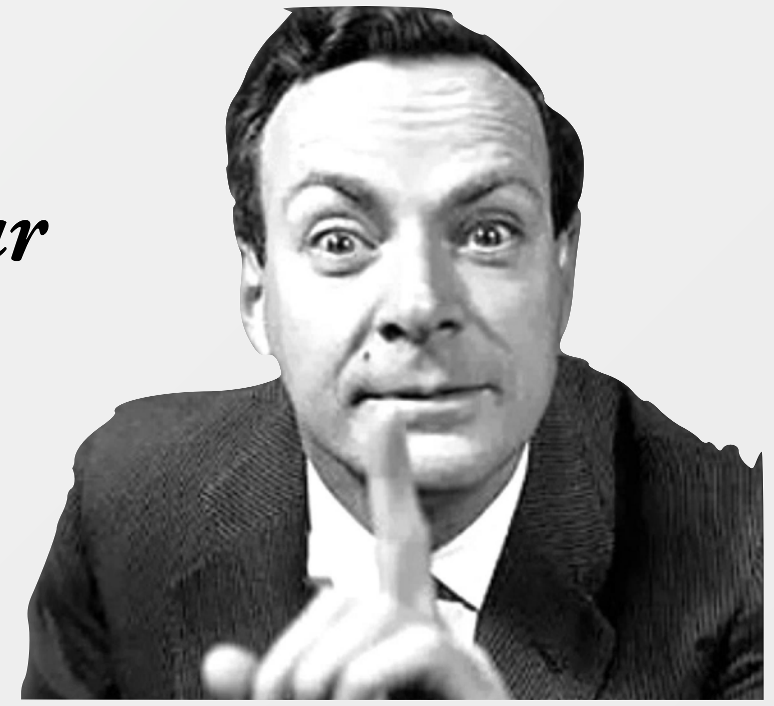
Can jet flavour be made infrared safe?



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For observable sensitive to the flavour assignment, **infrared safety can be an issue**

Problem related **to gluon splitting to quarks in the double soft limit** (starting at NNLO)

To ensure infrared safety, two necessary conditions must hold for a wide-angle double-soft limit of two opposite flavoured parton i and j **[Czakon, Mitov, Poncelet, 2022]**

1. d_{ij} vanishes for every R_{ij}
2. d_{ij} vanishes faster than the distance of either i or j to the remaining (hard) pseudojets

Flavour aware jet algorithms: flavour k_T

[Banfi, Salam, Zanderighi '06]

Standard k_T algorithm

$$d_{ij} = \min\left(k_{T,i}^2, k_{T,j}^2\right) R_{ij}^2, \quad d_{iB} = k_{T,i}^2$$

condition 1 automatically satisfied

Flavour aware k_T algorithm (usually $\alpha = 2$):
flavour information available at each step of the clustering procedure

$$d_{ij}^{(F)} = R_{ij}^2 \times \begin{cases} \left[\max\left(k_{T,i}^2, k_{T,j}^2\right)\right]^{\alpha} \left[\min\left(k_{T,i}^2, k_{T,j}^2\right)\right]^{2-\alpha}, & \text{if softer of } i,j \text{ is flavoured} \\ \min\left(k_{T,i}^2, k_{T,j}^2\right), & \text{if softer of } i,j \text{ is flavourless} \end{cases}$$

this ensures condition 2 among final state protojets, as soft flavoured quark-anti-quark pair clusters first

Flavour aware jet algorithms: flavour k_T

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$$d_{ij} = \min\left(k_{T,i}^2, k_{T,j}^2\right) R_{ij}^2, \quad d_{iB} = k_{T,i}^2$$

condition 1 automatically satisfied

Flavour aware k_T algorithm (usually $\alpha = 2$):
flavour information available at each step of the clustering procedure

Also beam distance problematic:
a soft flavoured parton can be identified as a protojet and removed from the list)

$$d_{iB(\bar{B})}^{(F)} = R_{ij}^2 \times \begin{cases} \left[\max\left(k_{T,i}^2, k_{T,B(\bar{B})}^2\right)\right]^{\alpha} \left[\min\left(k_{T,i}^2, k_{T,B(\bar{B})}^2\right)\right]^{2-\alpha}, & \text{if } i \text{ is flavoured} \\ \min\left(k_{T,i}^2, k_{T,B(\bar{B})}^2\right), & \text{if } i \text{ is flavourless} \end{cases}$$

$$k_{T,B}(y) = \sum_i k_{T,i}\left(\Theta(y_i - y) + \Theta(y - y_i)e^{y_i - y}\right) \qquad k_{T,\bar{B}}(y) = \sum_i k_{T,i}\left(\Theta(y - y_i) + \Theta(y_i - y)e^{y - y_i}\right)$$

Flavour aware jet algorithms: flavour k_T

[Banfi, Salam, Zanderighi '06]

Theoretically sound, but problematic for data-theory comparison

1. Flavour assignment and jet reconstruction performed at the particle level experimentally
2. Analyses typically employ anti-k_T ad default jet algorithm

k_T algorithm

$$d_{ij} = \min\left(k_{T,i}^2, k_{T,j}^2\right) R_{ij}^2, \quad d_{iB} = k_{T,i}^2$$

anti-k_T algorithm

$$d_{ij} = \min\left(k_{T,i}^{-2}, k_{T,j}^{-2}\right) R_{ij}^2, \quad d_{iB} = k_{T,i}^{-2}$$

anti-k_T favours clustering of hard particles, thus providing a IRC safe algorithm that gives circular hard jets

Flavour aware jet algorithms: flavour k_T

[Banfi, Salam, Zanderighi '06]

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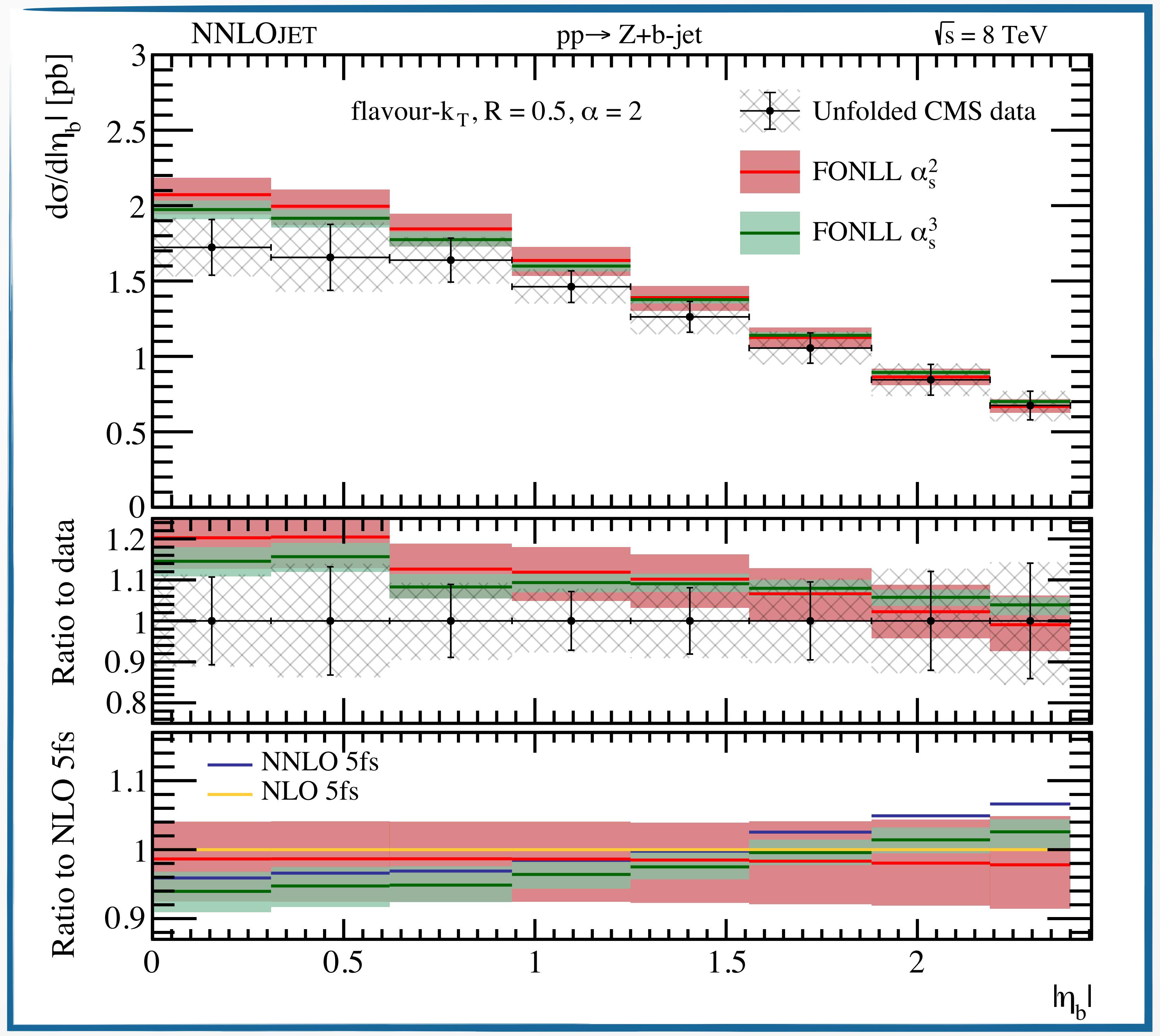


[Gauld, Gehrmann–De Ridder, Glover, Huss, Majer '20]

Theory/data comparison requires the unfolding of the experimental data to the theory calculation performed with the flavour k_T algorithm

The unfolding correction can be sizeable, e.g. larger than 10% in *Z+b* jet production (estimate using NLO+PS)

For *Wbb,* which involves two jets at the lowest order, large differences between the two algorithms appear already at LO

Flavour aware jet algorithms: flavour anti-k_T

$$d_{ij} = \min\left(k_{T,i}^{-2}, k_{T,j}^{-2}\right) R_{ij}^2, \quad d_{iB} = k_{T,i}^{-2}$$

Algorithm must be modified in the wide-angle double-soft limit of two opposite flavoured parton i and j to ensure infrared safety [Czakon, Mitov, Poncelet '22]

$$d_{ij}^{(F)} = d_{ij} \times \begin{cases} \mathcal{S}_{ij}, & \text{if both } i \text{ and } j \text{ have non-zero flavour of opposite sign} \\ 1, & \text{otherwise} \end{cases}$$

$$\mathcal{S}_{ij} = 1 - \theta(1-\kappa)\cos\left(\frac{\pi}{2}\kappa\right)$$

$$\kappa = \frac{1}{a}\frac{k_{T,i}^2 + k_{T,j}^2}{2k_{T,max}^2}$$

$$\mathcal{S}_{ij} \sim E^4 \implies d_{ij}^{(F)} \sim E^2$$

the suppression factor overcompensates the divergent behaviour in the double soft limit

Infrared safety **checked at NNLO**

Suppression factor depends on (unphysical) parameter a: in the limit $a \to 0$, the standard anti-k_T algorithm is recovered. Best choice of the parameter a from comparison at NLO+PS (aiming at minimising unfolding)

Flavour-dependent metric, still needs some (possibly small) unfolding

Flavour aware jet algorithms: new proposals

In the past year several proposal have been brought forward to address the flavour problem

Use **Soft Drop** to remove soft quarks

No unfolding needed

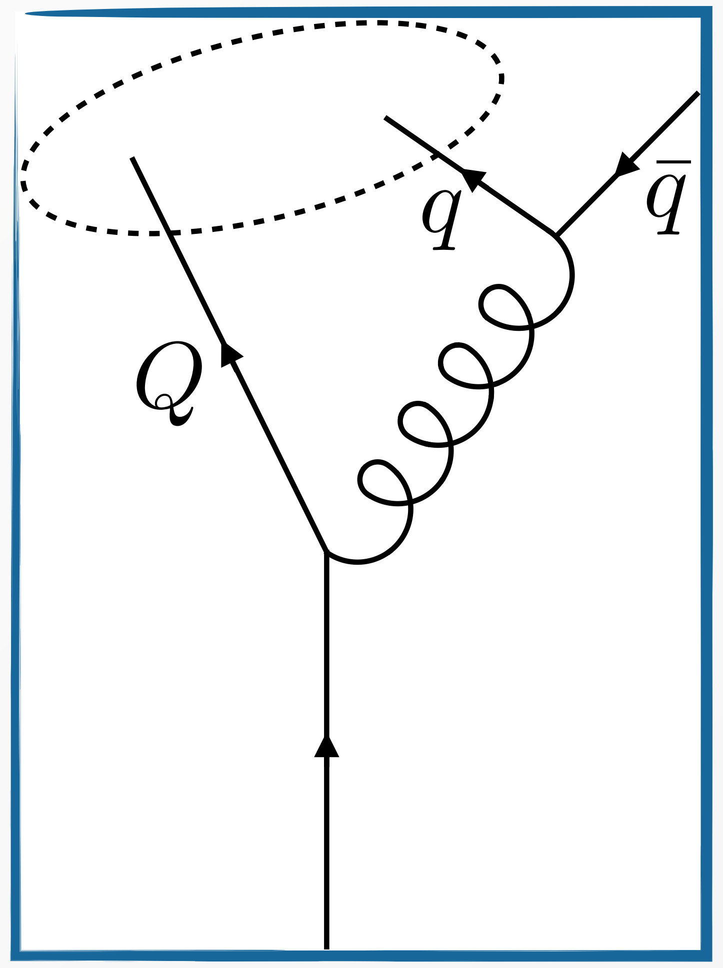
Requires reclustering with JADE (issue with IRC safety beyond NNLO)

Assign a **flavour dressing** to jets reconstructed with any IRC flavour-blind jet algorithms

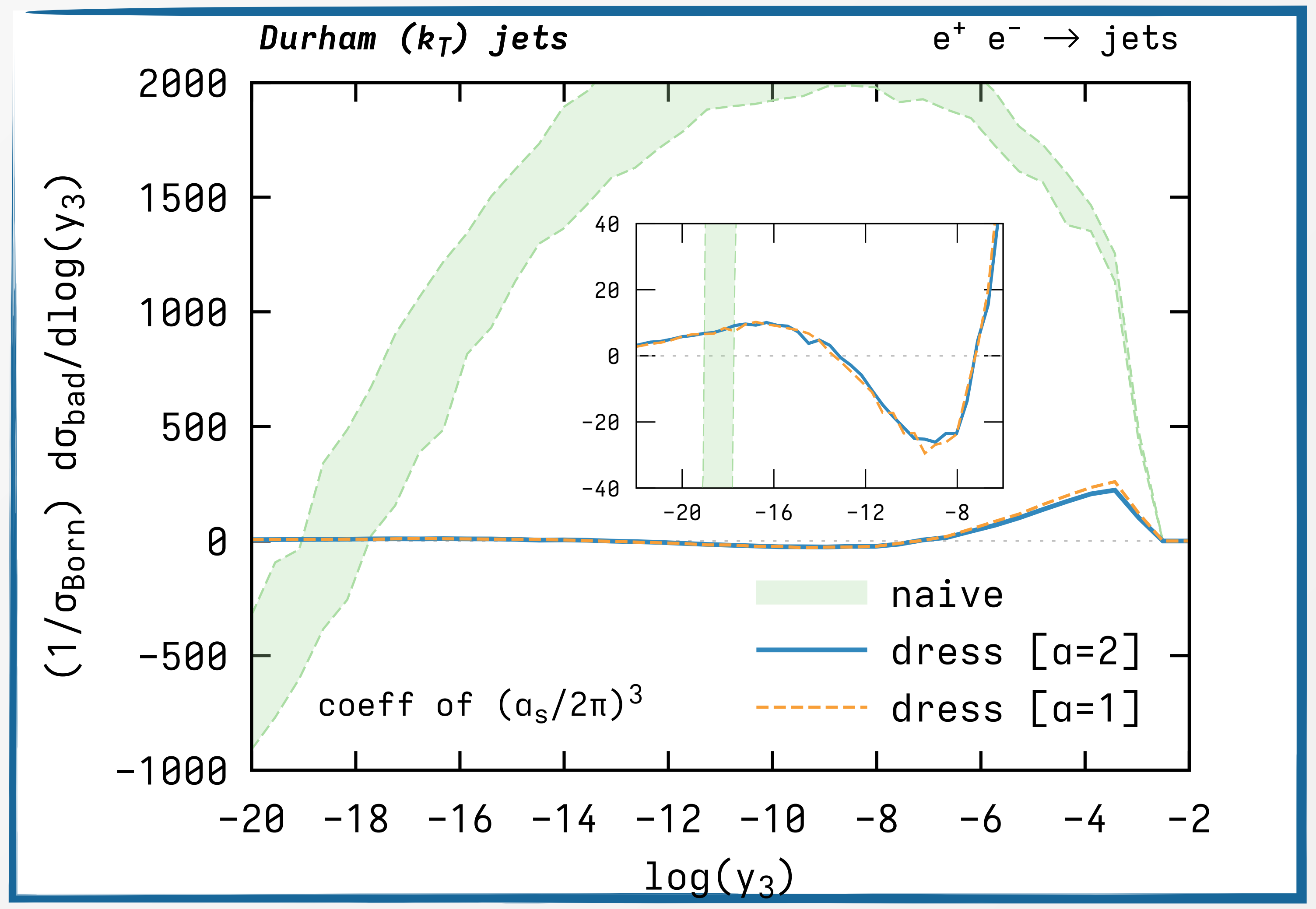
Requires flavour information of many particles in the event

Recluster using the flavour aware **Winner-Take-All** (WTA) recombination scheme (**soft-safe**)

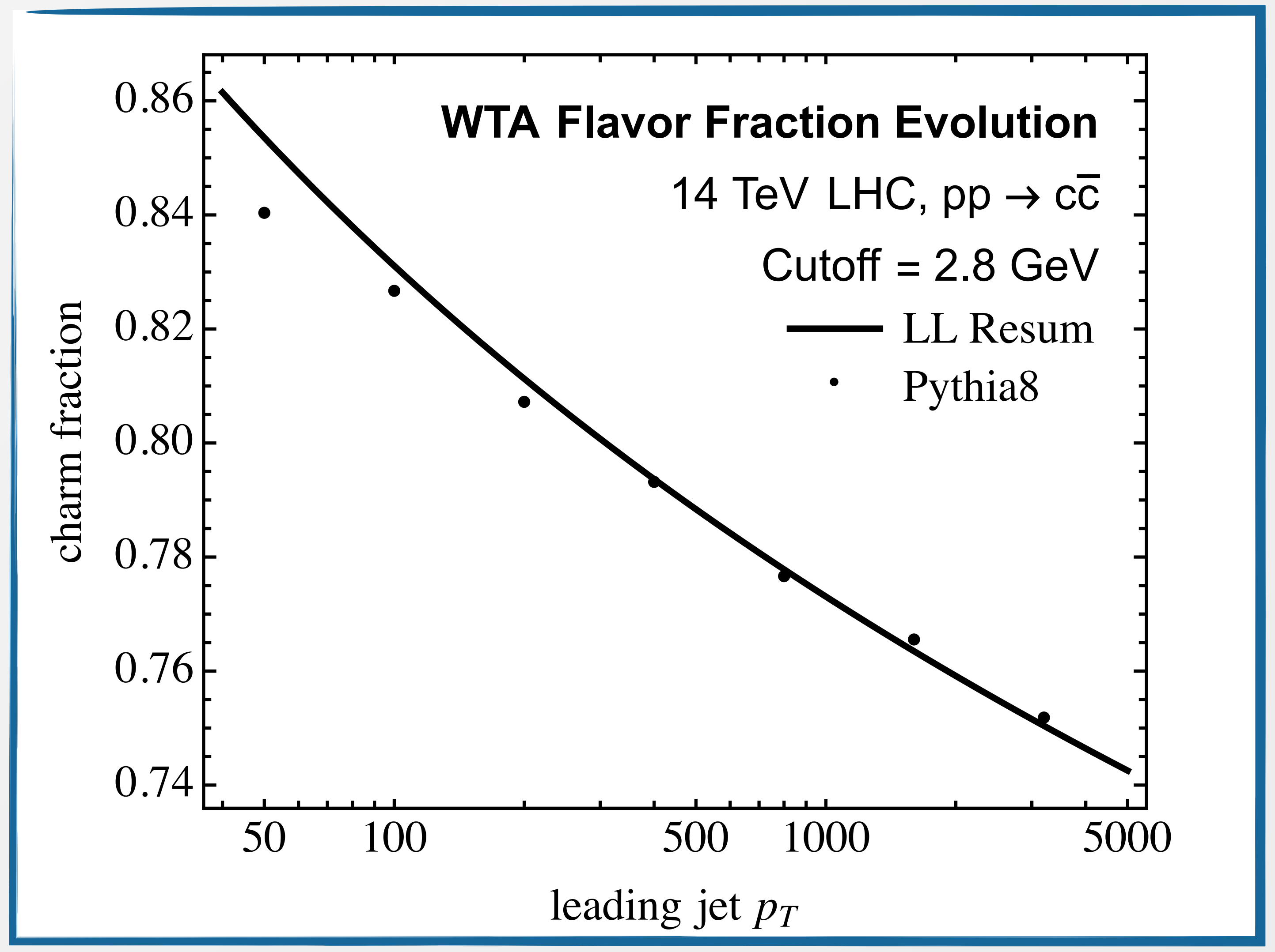
Requires fully perturbative WTA flavour fragmentation function (for **collinear safety**)



[Caletti, Larkoski, Marzani, Reichelt '22]



[Gauld, Huss, Stagnitto '22]



[Caletti, Larkoski, Marzani, Reichelt '22]

Massive calculation

In a massive calculation, the quark mass acts as a **physical IR regulator** suppressing naturally the double soft limit

Ambiguities of the massless calculation avoided

No requirement for flavour-aware jet algorithms: any **flavour-blind algorithm** can be used, in particular **anti-k_T**

Direct comparison with experimental data possible (unfolding corrections limited to non-perturbative modelling and hadronisation)

Caveat and challenges

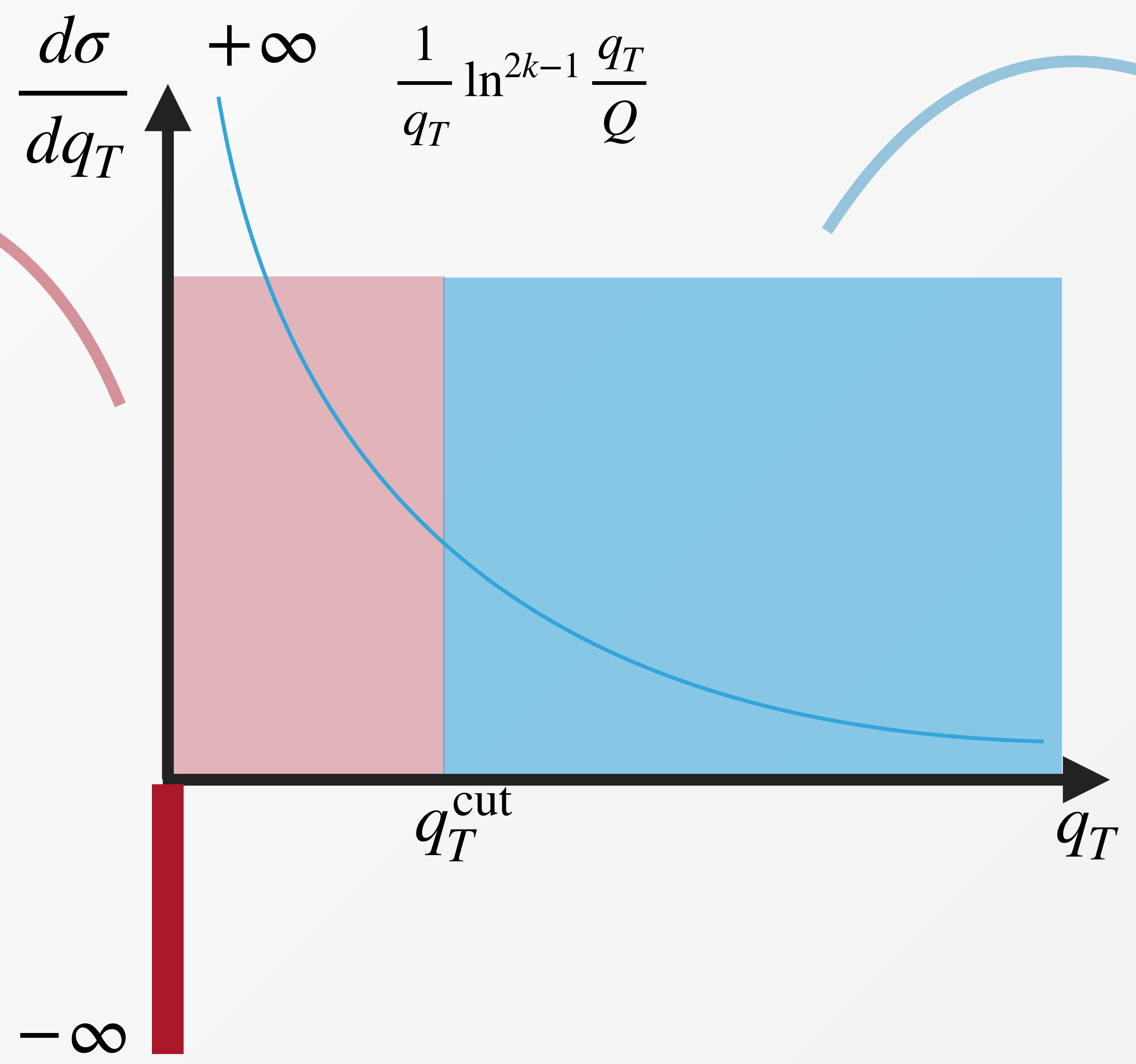
Left over IR sensitivity in the form of logarithms of the heavy quark mass at each order in perturbative theory

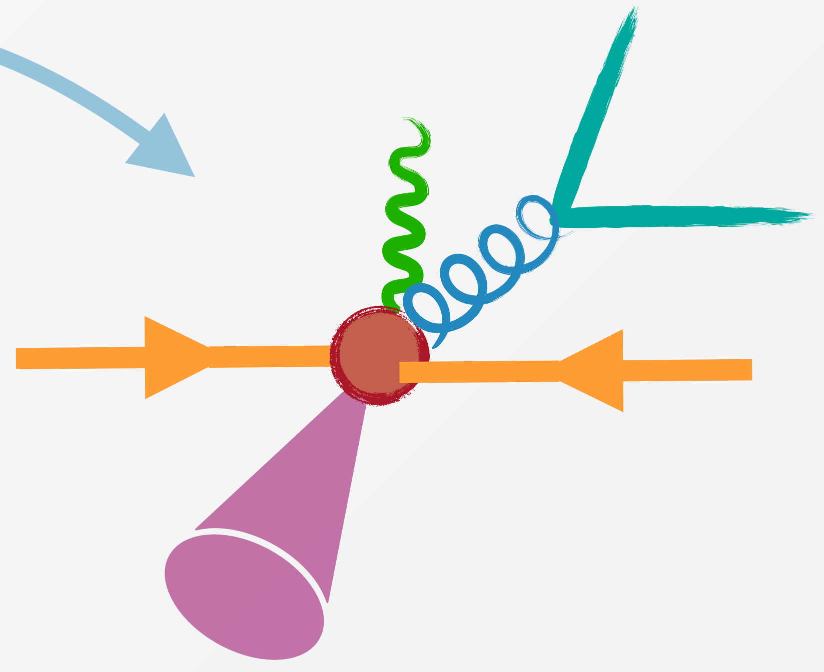
Calculation with massive quarks is challenging

Methodology: q_T-subtraction formalism

q_T resummation

- Expand to fixed order
- $\mathcal{O}(\alpha_s^2)$ ingredients





X+j @ N^{k-1}LO

$$d\sigma_V^{\mathrm{N^kLO}} \equiv d\sigma_V^{\mathrm{N^kLO}}\Big|_{q_T<q_T^{\mathrm{cut}}} + d\sigma_V^{\mathrm{N^kLO}}\Big|_{q_T>q_T^{\mathrm{cut}}}$$

q_T-subtraction formalism
[Catani, Grazzini ’08]

$$d\sigma_X^{\mathrm{N^kLO}} \equiv \mathscr{H}_{\mathrm{X}}^{\mathrm{N^kLO}} \otimes d\sigma_{\mathrm{X}}^{\mathrm{LO}} + \left[d\sigma_{\mathrm{X+jet}}^{\mathrm{N^{k-1}LO}} - \left[d\sigma_X^{\mathrm{N^kLL}}\right]_{\mathcal{O}(\alpha_s^k)}\right]_{q_T>q_t^{\mathrm{cut}}} + \mathcal{O}((q_T^{\mathrm{cut}}/M)^n)$$

q_T-subtraction formalism: extension to massive final states

$$d\sigma_X^{\mathrm{N^kLO}} \equiv \mathscr{H}_{\mathrm{X}}^{\mathrm{N^kLO}} \otimes d\sigma_{\mathrm{X}}^{\mathrm{LO}} + \left[d\sigma_{\mathrm{X+jet}}^{\mathrm{N^{k-1}LO}} - \left[d\sigma_X^{\mathrm{N^kLL}} \right]_{\mathscr{O}(\alpha_s^k)} \right]_{q_T > q_t^{\mathrm{cut}}} + \mathscr{O}((q_T^{\mathrm{cut}}/M)^n)$$

All ingredients for *Wbb+j* @ NLO available and implemented in public libraries such as OpenLoops2 ✓

[Buccioni, Lang, Lindert, Maierhöfer, Pozzorini, Zhang, Zoller '19]

q_T-subtraction formalism: extension to massive final states

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$\mathcal{H}$ contains virtual correction after subtraction of IR singularities and contribution of soft/collinear origin

- Beam functions ✓
- Soft function
- Two-loop virtual

[Catani, Cieri, de Florian, Ferrera, Grazzini '12]
[Gehrmann, Luebbert, Yang '14]
[Echevarria, Scimemi, Vladimirov '16]
[Luo, Wang, Xu, Yang, Yang, Zhu '19]

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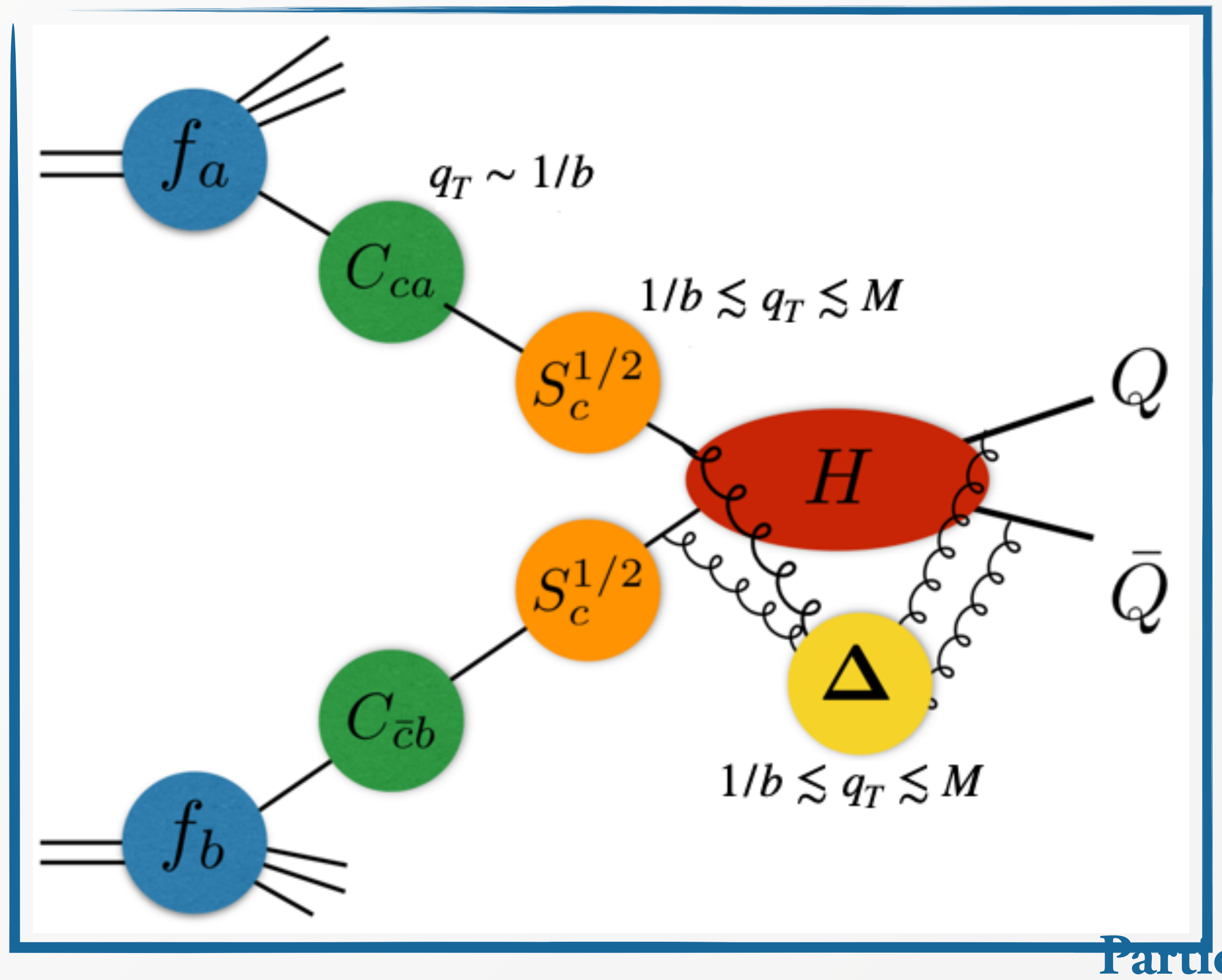


The resummation formula for heavy quark production shows a **richer structure** because of additional soft singularities (four coloured partons at LO)

- Soft logarithms controlled by the **transverse momentum anomalous dimension $\boldsymbol{\Gamma}_t$** known up to NNLO [Mitov, Sterman, Sung '09] [Neubert, et al '09]
- Hard coefficient gets a **non-trivial** colour structure (matrix in colour-space)
- Non trivial azimuthal correlations

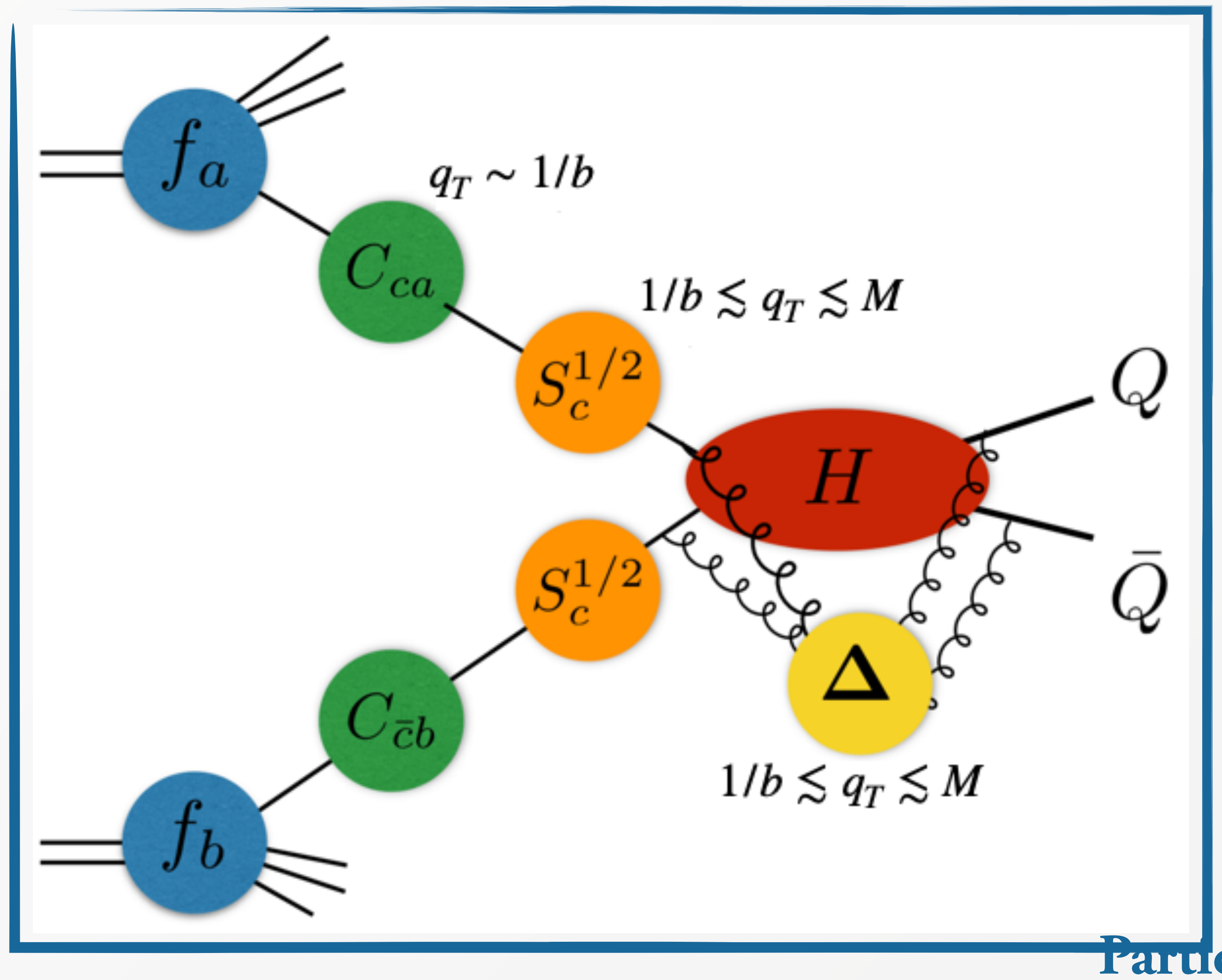
q_T-subtraction formalism: extension to massive final states

$$d\sigma_X^{\mathrm{N^kLO}} \equiv \boxed{\mathcal{H}_X^{\mathrm{N^kLO}} \otimes d\sigma_X^{\mathrm{LO}}} + \left[d\sigma_{X+\mathrm{jet}}^{\mathrm{N^{k-1}LO}} - \boxed{\left[d\sigma_X^{\mathrm{N^kLL}} \right]_{\mathcal{O}(\alpha_s^k)}} \right]_{q_T > q_T^{\mathrm{cut}}} + \mathcal{O}((q_T^{\mathrm{cut}}/M)^n)$$

$\mathcal{H}$ contains virtual correction after subtraction of IR singularities and contribution of soft/collinear origin

- Beam functions ✓
- Soft function
- Two-loop virtual

The resummation formula for heavy quark production shows a **richer structure** because of additional soft singularities (four coloured partons at LO)



q_T subtraction formalism extended to the case of **heavy quarks** production and applied to $t\bar{t}$ and $b\bar{b}$ production

[Catani, Grazzini, Torre '14]

[Catani, Devoto, Grazzini, Kallweit, Mazzitelli, Sargsyan '19]
[Catani, Devoto, Grazzini, Kallweit, Mazzitelli '21]

q_T-subtraction formalism: extension to massive final states

$$d\sigma_X^{\mathrm{N^kLO}} \equiv \mathscr{H}_X^{\mathrm{N^kLO}} \otimes d\sigma_X^{\mathrm{LO}} + \left[d\sigma_{X+\mathrm{jet}}^{\mathrm{N^{k-1}LO}} - \left[d\sigma_X^{\mathrm{N^kLL}} \right]_{\mathcal{O}(\alpha_s^k)} \right]_{q_T > q_t^{\mathrm{cut}}} + \mathcal{O}((q_T^{\mathrm{cut}}/M)^n)$$

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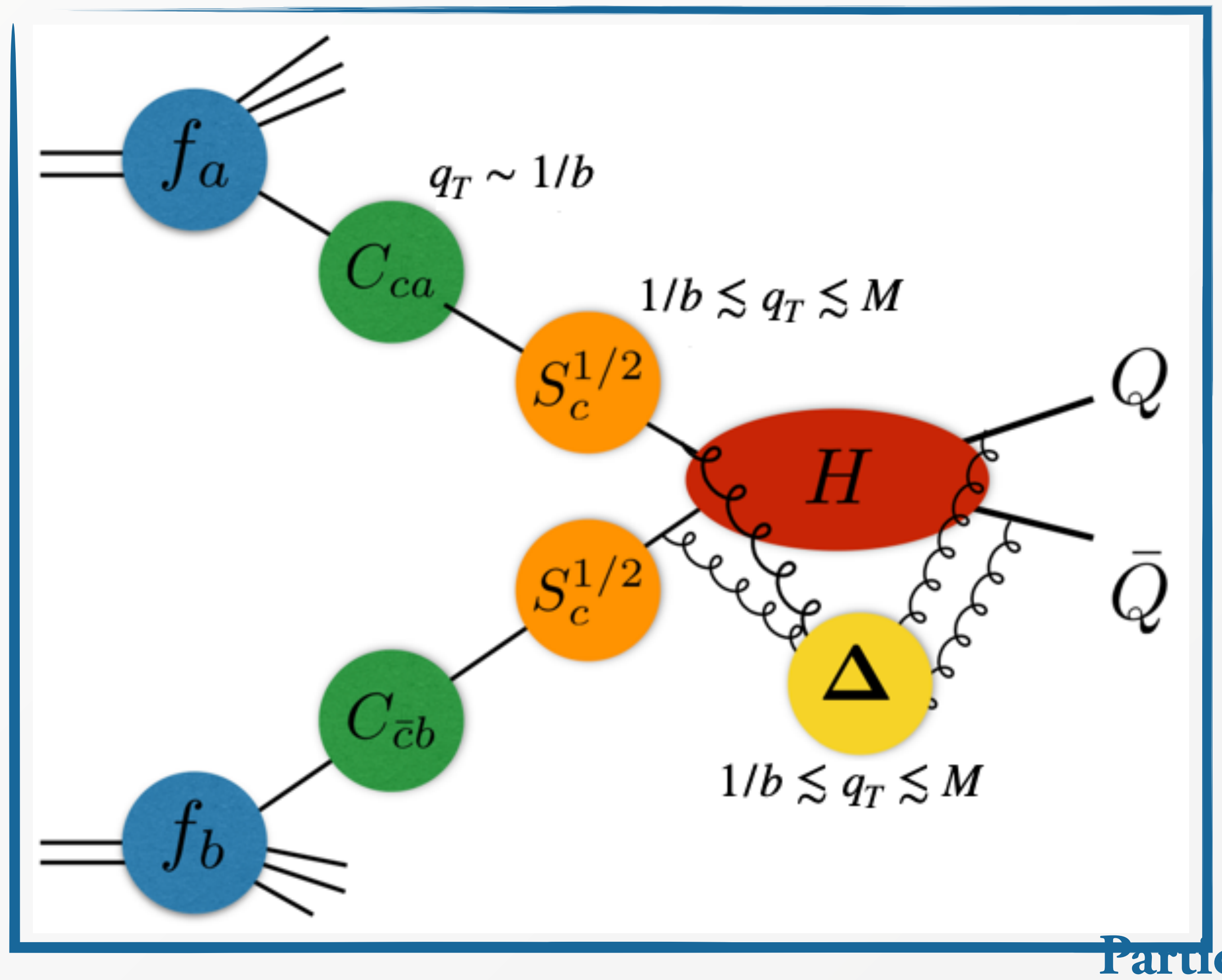


To reach NNLO accuracy, the **two-loop soft function for heavy quark production** is needed

Two-loop soft function in back-to-back Born kinematics
[Catani, Devoto, Grazzini, Mazzitelli '23]

Recently generalized to **arbitrary kinematics**
[Devoto, Mazzitelli in preparation]

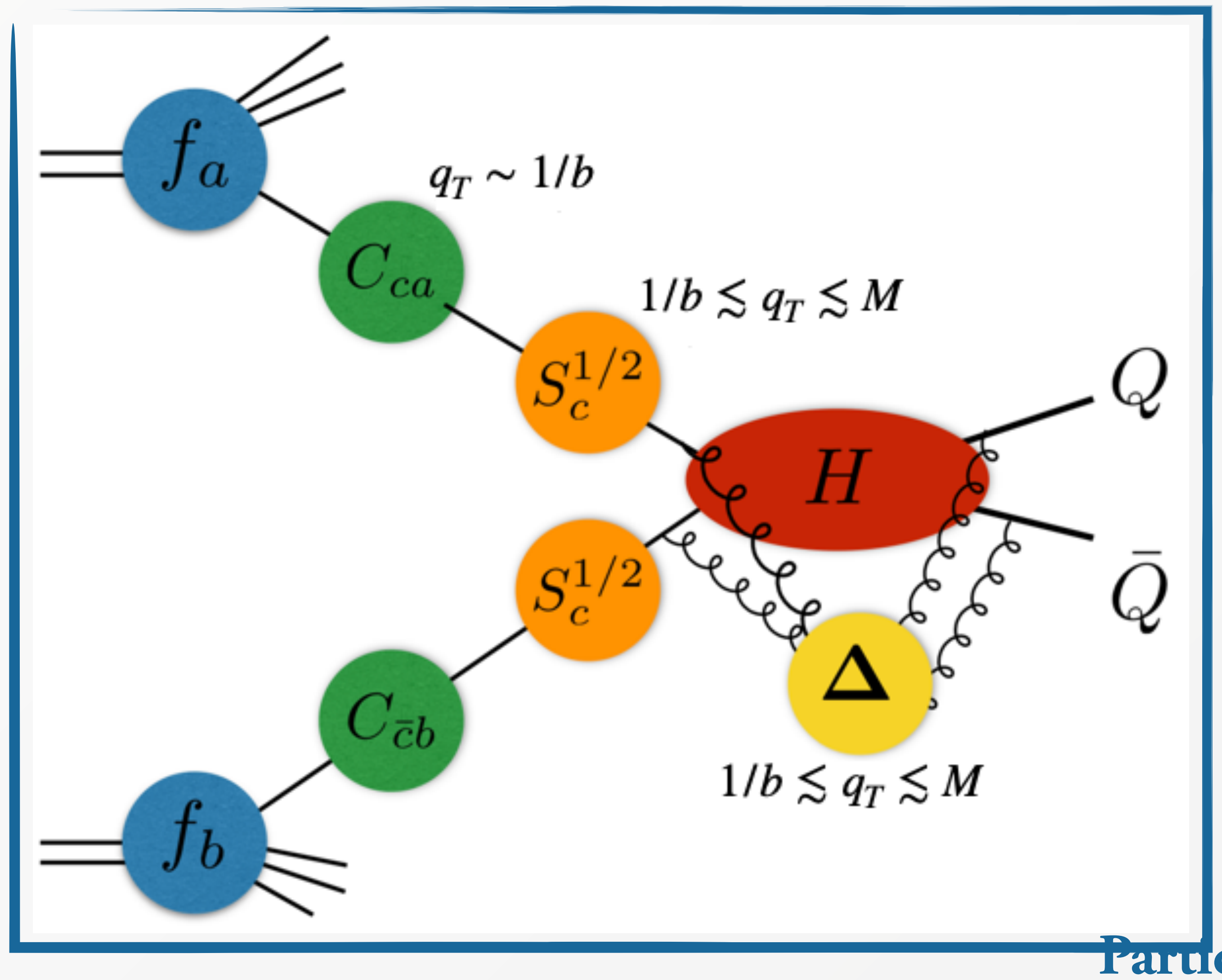
q_T-subtraction formalism: extension to massive final states

$$d\sigma_X^{\mathrm{N^kLO}} \equiv \boxed{\mathscr{H}_X^{\mathrm{N^kLO}} \otimes d\sigma_X^{\mathrm{LO}}} + \left[d\sigma_{X+\mathrm{jet}}^{\mathrm{N^{k-1}LO}} - \boxed{\left[d\sigma_X^{\mathrm{N^kLL}} \right]_{\mathcal{O}(\alpha_s^k)}} \right]_{q_T > q_t^{\mathrm{cut}}} + \mathcal{O}((q_T^{\mathrm{cut}}/M)^n)$$

$\mathscr{H}$ contains virtual correction after subtraction of IR singularities and contribution of soft/collinear origin

- Beam functions ✓
- Soft function ✓
- Two-loop virtual

Once an expression for the two-loop virtual is provided, the formula yields the fully-differential NNLO correction for the associated production of a heavy quark pair and a colour singlet



First application $t\bar{t}H$ @ NNLO

[Catani, Devoto, Grazzini, Kallweit, Mazzitelli, Savoini '23]

Two-loop virtual amplitude

Compute the born amplitude for two massless quarks into W and a pair of bottom quarks with Feyncalc, treating the bottom quarks as massive

To compute the Born amplitude for two massless quarks into a W and a pair of bottom quarks, we can use FeynCalc, a Mathematica package for high-energy physics calculations. We will treat the bottom quarks as massive, which means that we need to use the full propagator for the bottom quarks instead of the massless approximation.

Here is the FeynCalc code to compute the Born amplitude:

mathematica   Copy code

```mathematica
<< FeynCalc`

SetOptions[FC, ScreenDumps -> False];

$Dimension = D;
```

Two-loop virtual amplitude

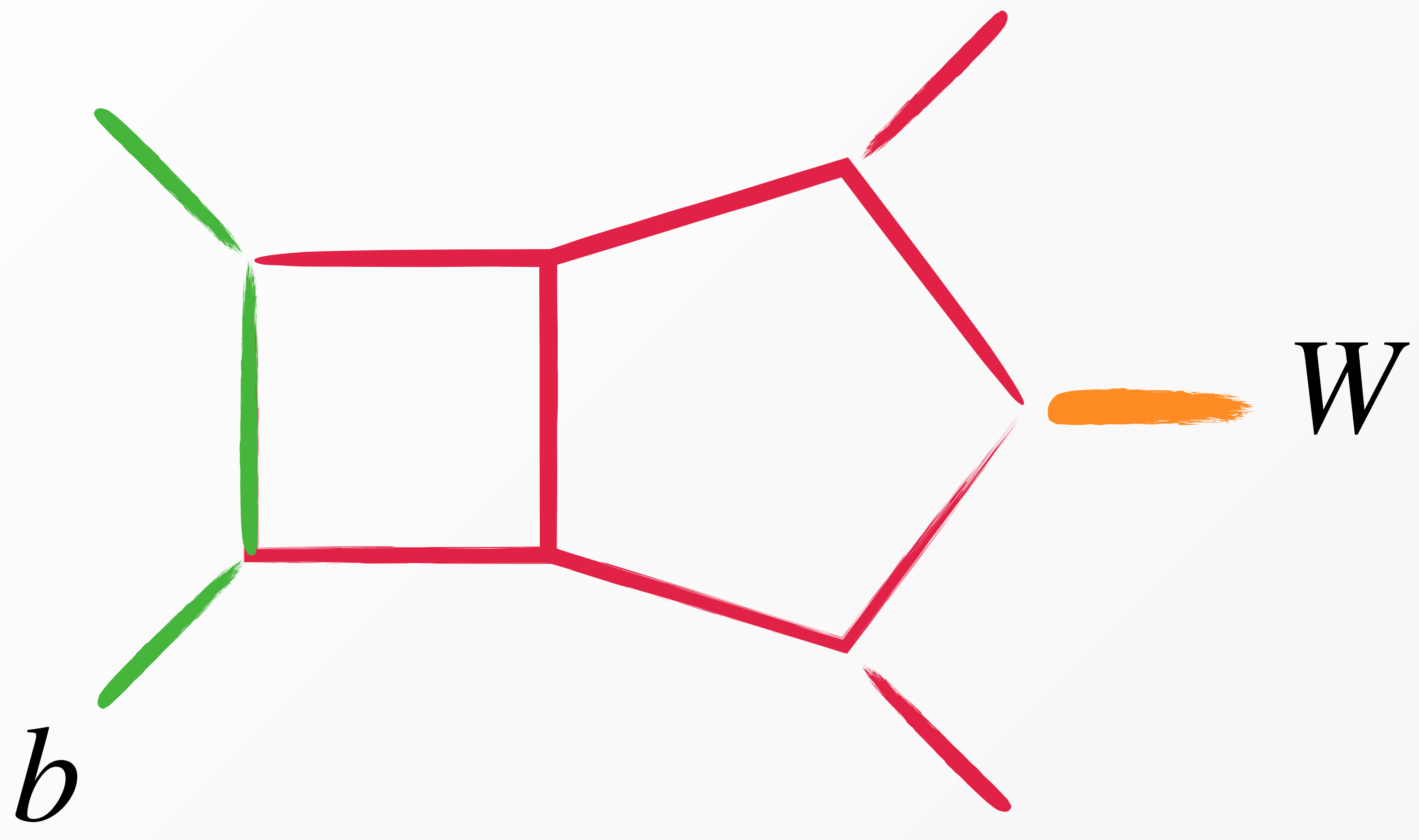
Calculate the amplitude at two loops

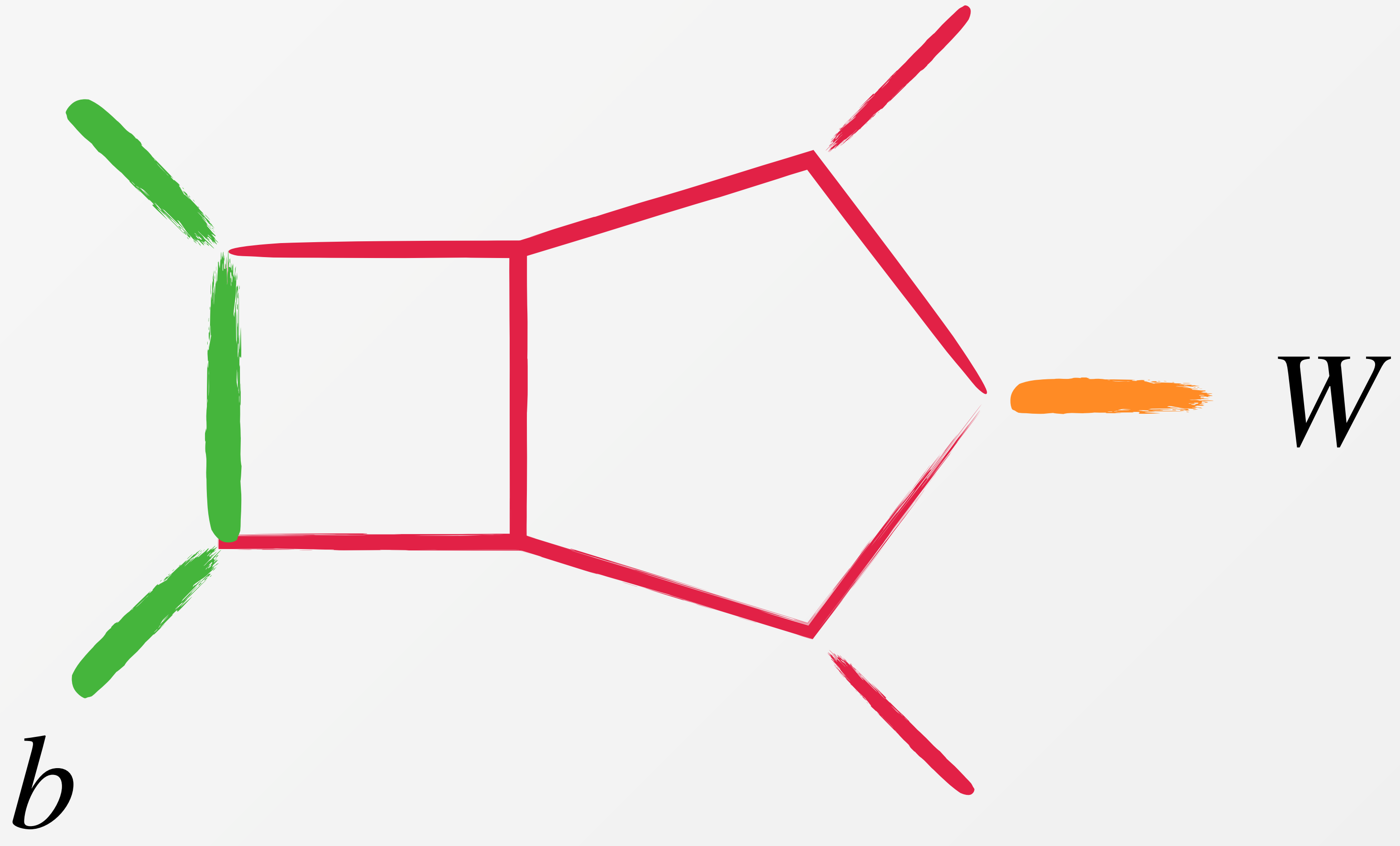
Calculating the amplitude at two loops is a very challenging task as it requires evaluating a large number of Feynman diagrams with many loops, which can quickly become computationally intractable.

In general, the calculation of multi-loop amplitudes requires the use of advanced techniques such as dimensional regularization, renormalization, and sophisticated algebraic manipulation tools like the integration-by-parts method or the differential equations method.

Therefore, it is beyond the scope of a simple answer in this Q&A format to provide a complete calculation of the two-loop amplitude for the given process. However, FeynCalc can be used to generate the Feynman diagrams for the two-loop amplitude, which can provide some insight into the complexity of the calculation.

Two-loop virtual amplitude: massification procedure





5-point two loop amplitude with massless b quarks and one external massive leg is the current state of the art

[Badger, Hartanto, Zoia '21] [Abreu, Febres Cordero, Ita, Klinkert, Page, Sotnikov '21]

Current technology does not allow for the analytical computation of the amplitude with additional massive legs

However, the large hierarchy between the bottom mass and the W mass can be exploited

Massification of the massless amplitude up to power corrections $m_b/Q \ll 1$

Massification procedure

[Mitov, Moch, 2007]

Massification procedure is based on the **factorisation properties** of QCD amplitudes

Basic idea: in the small mass limit, the massive amplitude $\mathscr{M}^{[p],(m)}$ and the massless one $\mathscr{M}^{[p],(m=0)}$ are connected as the mass screens some collinear divergences "trading" poles in the dimensional regulator ϵ for logarithms of the mass

This can be viewed as a **change in the renormalisation scheme** which leads to a universal **"multiplicative renormalization"** relation between (*ultraviolet renormalised*) massive and massless amplitudes

$$\mathscr{M}^{[p],(m)} = \prod_{i\in\{\text{all legs}\}} \left(Z_{[i]}^{(m|0)}\right)^{\frac{1}{2}} \mathscr{M}^{[p],(m=0)} + \mathcal{O}(m^k)$$

universal factors which depend only on the external parton and admit a perturbative expansion in α_s

$$Z_{[i]} = 1 + \sum_k \left(\frac{\alpha_s}{2\pi}\right)^k Z_{[i]}^k$$

$$\mathscr{M}^{[p],(m)} = \sum_{k=0} \left(\frac{\alpha_s}{2\pi}\right)^k \mathscr{M}_{(k)}^{[p],(m)}$$

$$\mathscr{M}_0^{Wbb,(m)} = \mathscr{M}_0^{Wbb,(m=0)}$$

$$\mathscr{M}_{(1)}^{Wbb,(m)} = \mathscr{M}_{(1)}^{Wbb,(m=0)} + Z_{[q]}^{(1)} \mathscr{M}_{(0)}^{Wbb,(m=0)}$$

$$\mathscr{M}_{(2)}^{Wbb,(m)} = \mathscr{M}_{(2)}^{Wbb,(m=0)} + Z_{[q]}^{(1)} \mathscr{M}_{(1)}^{Wbb,(m=0)} + Z_{[q]}^{(2)} \mathscr{M}_{(0)}^{Wbb,(m=0)}$$

Two-loop virtual amplitude: massification

[Mitov, Moch '07]

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universal factors which depend only on the external parton and admit a perturbative expansion in α_s

The massification procedure predicts **poles, logarithms of mass and mass independent terms (constants)** of $\mathcal{M}^{[p],(m)}$ while **power corrections** in the mass and the contribution of **heavy loops** cannot be retrieved using this approach

WQQAmp: a massive C++ implementation

[Buonocore, LR, Savoini, https://gitlab.com/lrottoli/WQQAmp]

We have implemented the one-loop and two-loop amplitudes (in the leading colour approximation) of in a **C++ library** for the efficient numerical evaluation of the **massive amplitudes** (< 5s for phase-space point)

PentagonFunctions-cpp

[Chicherin, Sotnikov, Zoia '21]

Pentagon functions entering in the one and two-loop expressions

Massless amplitudes

[Abreu et al' 22]

$$PS = \{p_1, p_2, \ldots, p_6\}$$

massive phase space point **mapped** into a massless one

WbbAmp

$$\frac{2\Re < M_0 | M_2^{\text{fin}} >}{|M_0|^2}$$

Finite remainder defined subtracting the IR poles as defined in [Ferroglia, Neubert, Pecjac, Yang '09]

OpenLoops 2

evaluation of exact one-loop amplitudes [Buccioni et al '19]

Massification

[Mitov, Moch '07]

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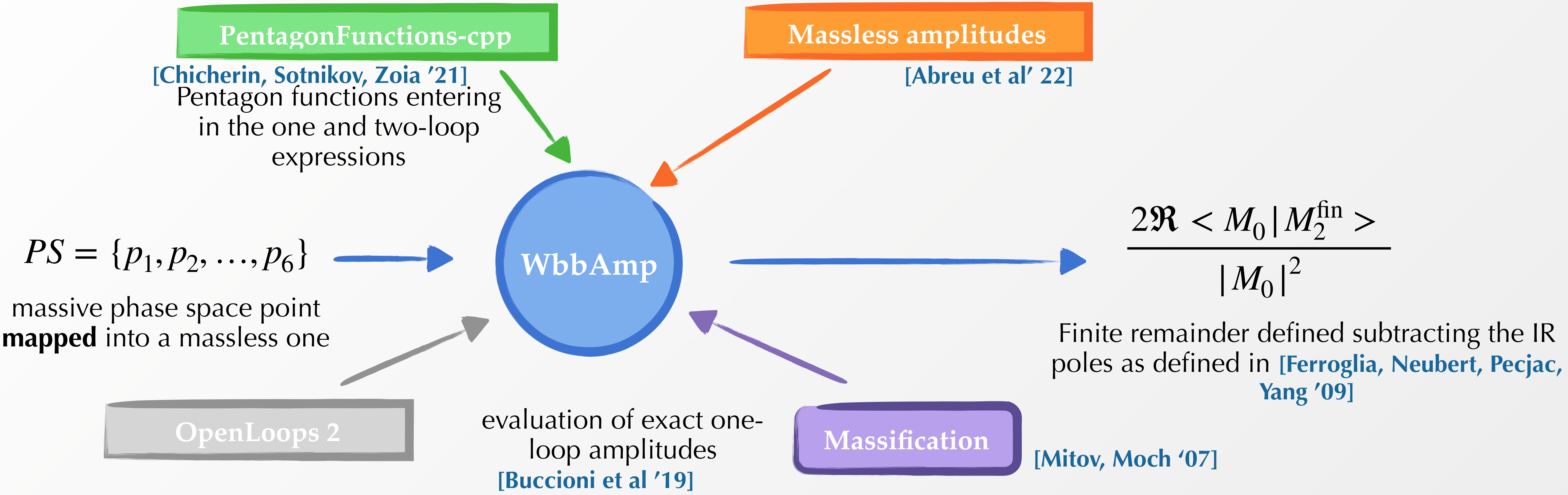


- Two-loop virtual ✓

Library interfaced to the **MATRIX code** which provides the underlying framework for the evaluation of *Wbb* production
[Grazzini, Kallweit, Wiesemann 2018]

WQQAmp: a massive C++ implementation

[Buonocore, LR, Savoini, https://gitlab.com/lrottoli/WQQAmp]

One-Loop amplitudes: $\mathcal{O}(1000)$ source files of small-moderate size (<100 Kb)

- algebraic expressions (rational function of the invariants) simplified using MultiVariate Apart **[Heller, von Manteuffel, 2021]** at the level of Mathematica before exporting them
- automatised generation of C++ source files from the Mathematica expressions; very simple optimisation introducing abbreviations (https://github.com/lecopivo/OptimizeExpressionToC)

Two-Loop amplitudes: $\mathcal{O}(3000)$ source files of moderate size (<250 Kb)

- algebraic expressions **too long and complex**; no pre-simplification step
- breakdown of each expression in small blocks (**crucial** for numerical stability)
- automatised generation of C++ source files for each block
- handling of **numerical instabilities a posteriori with a simple rescue system** (at integration time)

Numerous validations checks performed to test the numerical implementation:

- Phase-space check against Mathematica for crossed amplitudes, most point agree within single float precision. Occasionally it fails spectacularly (simple mechanism to remove problematic points)
- One-loop amplitudes in the LCA tested against MCFM
- Cancellation of the poles in the LCA for the massive amplitude against **[Ferroglia, Neubert, Pecjac, Yang, 2009]**

Phenomenology: setup

$$W + 2\, b_{\text{(jet)}} + X \text{ @ } \sqrt{s} = 13.6\,\text{TeV}$$

α_s and PDF scheme	4-flavour scheme (4FS), m_b=4.92 GeV
EW	G_μ-scheme, CKM diagonal
Jet clustering algortihm	anti-k_T (and k_T) algorithm with $R = 0.4$
pdf sets	NNPDF30_as_0118_nf_4 (LO) NNPDF31_as_0118_nf_4 (NLO, NNLO)

We consider two setups:

- **(fully) inclusive** (with a technical cut $m_{\ell\nu} > 5\,\text{GeV}$): study the convergence of the perturbative series
- **fiducial**: inspired by ATLAS $VH(\to b\bar{b})$ **boosted** analysis **[ATLAS:arXiv:2007.02873]**

$$p_{T,\ell} > 25\text{ GeV} \qquad |\eta_\ell| < 2.5 \qquad p_T^W > 150\,\text{GeV}$$

Jet selection

$$p_{T,j} > 20\text{ GeV} \quad \text{and} \quad |\eta_\ell| < 2.5 \quad \text{or}$$
$$p_{T,j} > 30\text{ GeV} \quad \text{and} \quad 2.5 < |\eta_\ell| < 4.5$$

Requirements on b-tagged jets

$$n_b = 2, \quad p_{T,b_1} > 45\text{ GeV}, \quad 0.5 < \Delta R_{bb} < 2$$

$$bin\ I : 150 < p_T^W < 250\,\text{GeV}$$
$$bin\ II : p_T^W > 250\,\text{GeV}$$

Inclusive cross section and perturbative convergence

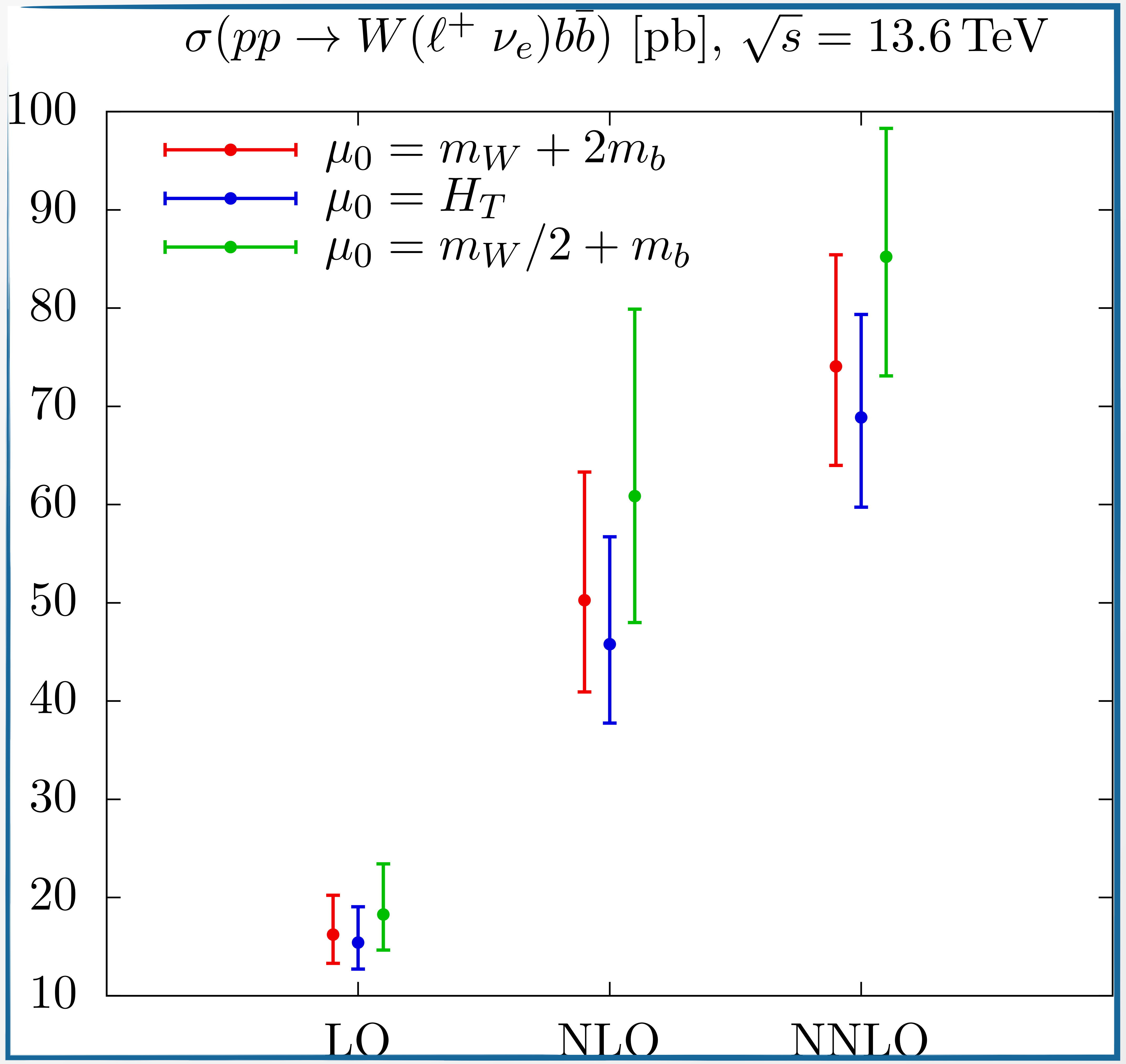
Fixed scale

$$\mu_0 = m_W + 2m_b$$

$$\mu_0 = m_W/2 + m_b$$

Dynamical scales

$$H_T = E_T(\ell\nu) + p_T(b_1) + p_T(b_2) \quad E_T(\ell\nu) = \sqrt{M^2(\ell\nu) + p_T^2(\ell\nu)}$$



Inclusive cross section and perturbative convergence

Qualitatively similar results when using either scale choice

Very large NLO corrections, as already noted in the literature, due to the opening of the gluon channel

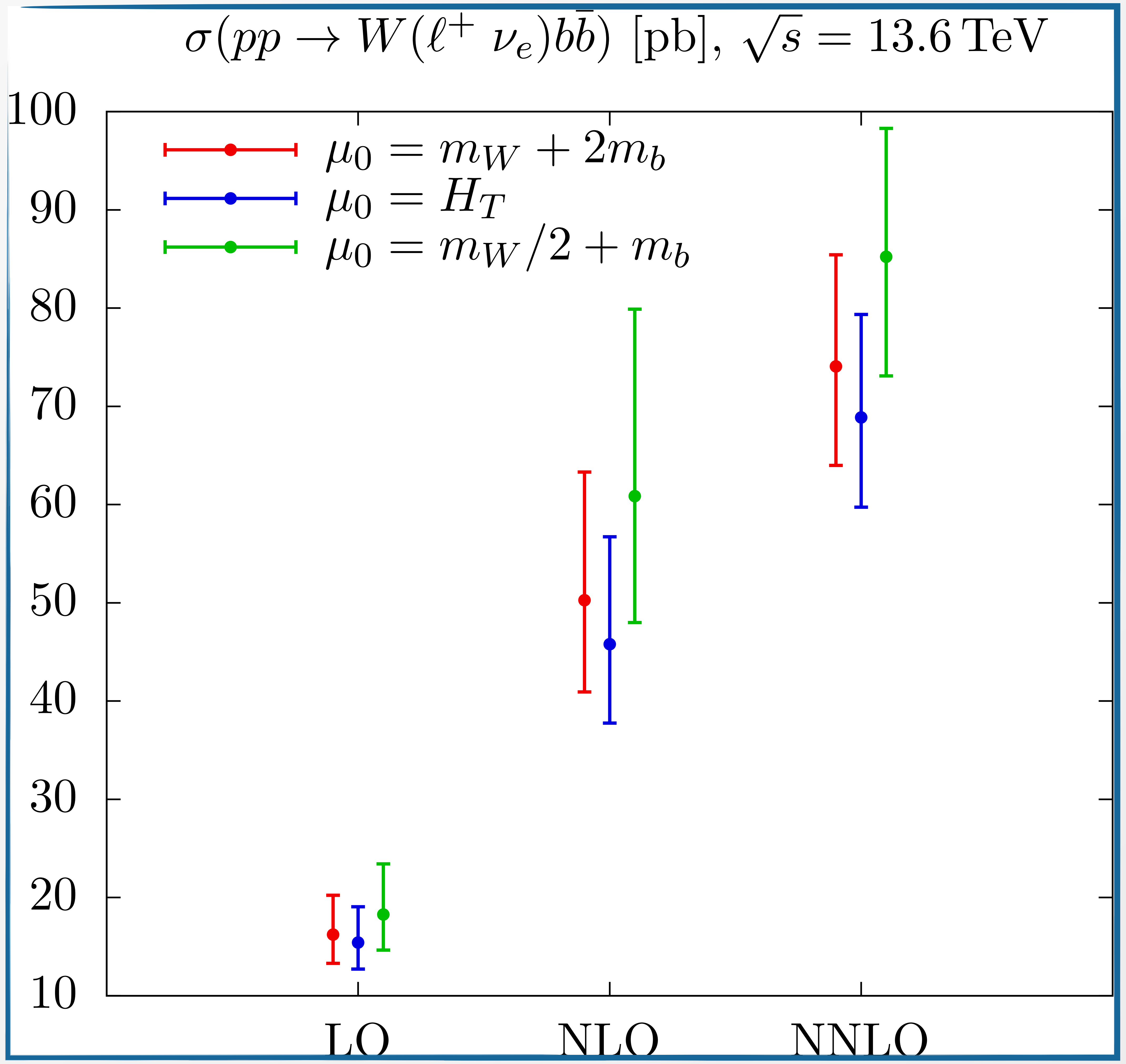
NLO cross section almost three times larger than the LO cross section. Uncertainty band at LO completely unreliable

Signals of convergence of the perturbative series at NNLO, where the *K*-factor gets smaller (~1.5) and more reliable scale uncertainties

Convergence slightly improved when using half of the fixed scale (as noted in similar processes)

$\mu_0 = m_W/2 + m_b$

order	σ_{incl} [pb]
LO	$18.270(2)^{+28\%}_{-20\%}$
NLO	$60.851(7)^{+31\%}_{-21\%}$
NNLO	$85.23(9)^{+15\%}_{-14\%}$

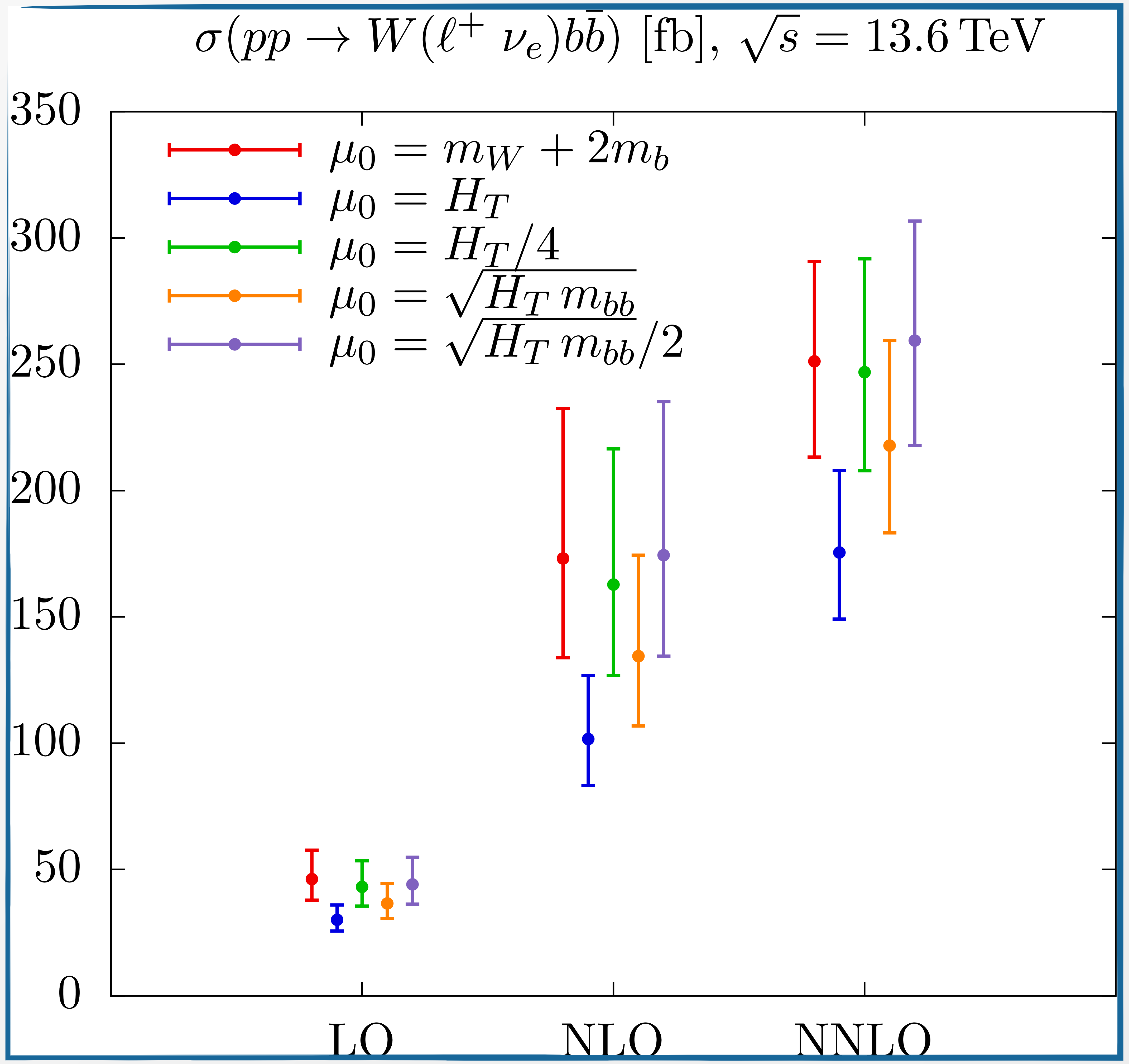


Partial reduction of scale uncertainties at NNLO

Fiducial cross section: scale choice

In the fiducial case, the choice of the scale is more delicate

ALL SCALES ARE EQUAL BUT
SOME SCALES ARE MORE
EQUAL THAN OTHERS



Fiducial cross section: scale choice

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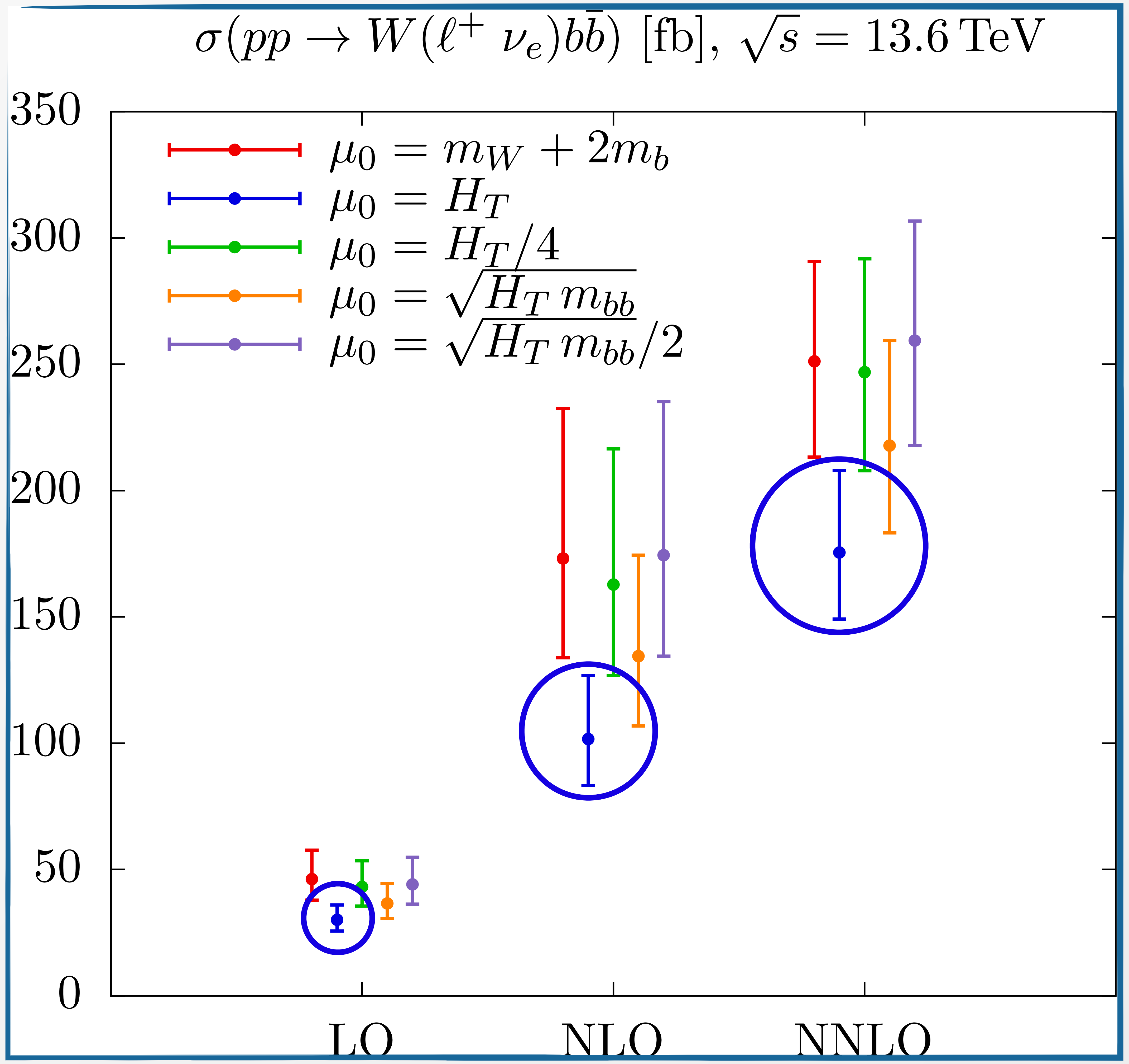
Fixed scale choice **not well physically motivated**

The choice of a dynamical scale such as H_T would be naively a better choice; nevertheless, it displays a **poor perturbative convergence** (NNLO and NLO bands not overlapping), alleviated when lowering the central value



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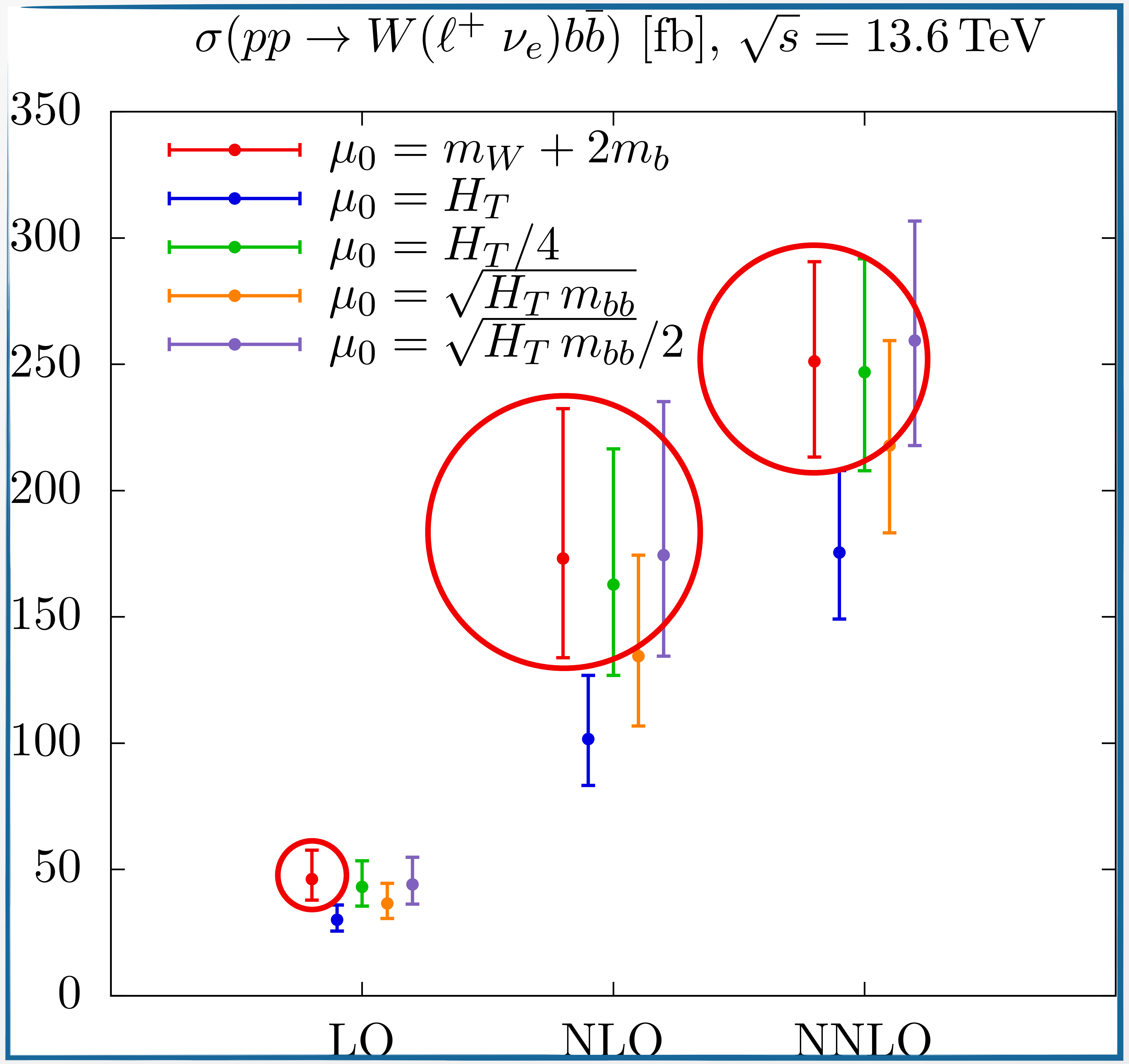

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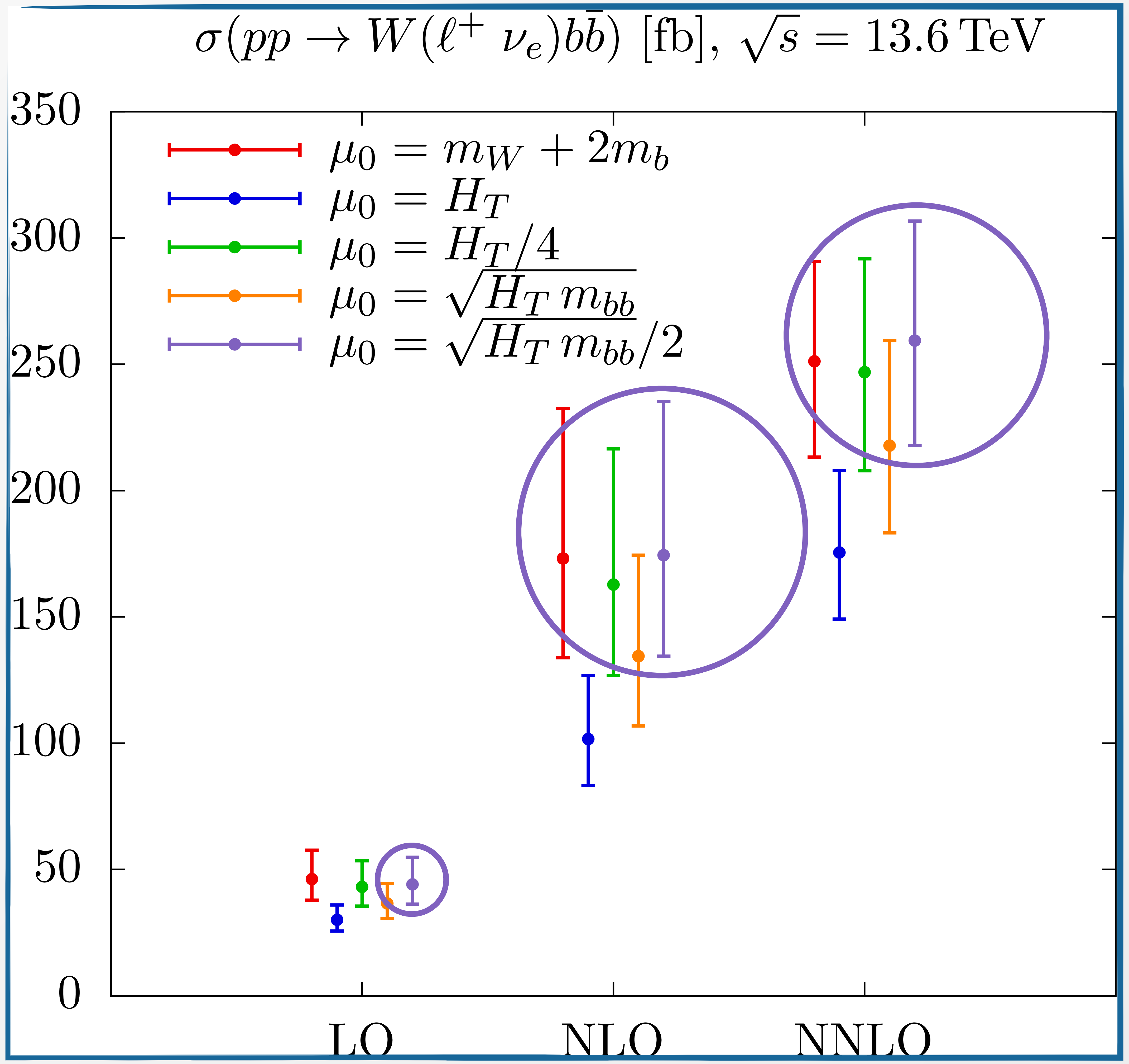
Multi-scale nature of the process in the fiducial setup is best captured averaging the scales

H_T

high-p_T kinematics $\longrightarrow$ $\sqrt{H_T \cdot m_{bb}}$

m_{bb} (possibly divided by a factor of 2)

gluon splitting kinematics



Fiducial cross section: results

Results

- Reference scale: $\sqrt{H_T \cdot m_{bb}}/2$
- Large NLO K-factors as in inclusive case: $K_{\mathrm{NLO}} \gtrsim 3$
- **Relative large positive NNLO corrections**, $K_{\mathrm{NNLO}} \sim 1.5$ (comparable in size to the normalisation factors applied by experimentalists)
- **More reliable** theory uncertainties estimated by scale variations with a reduction to the $15-20\,\%$ level

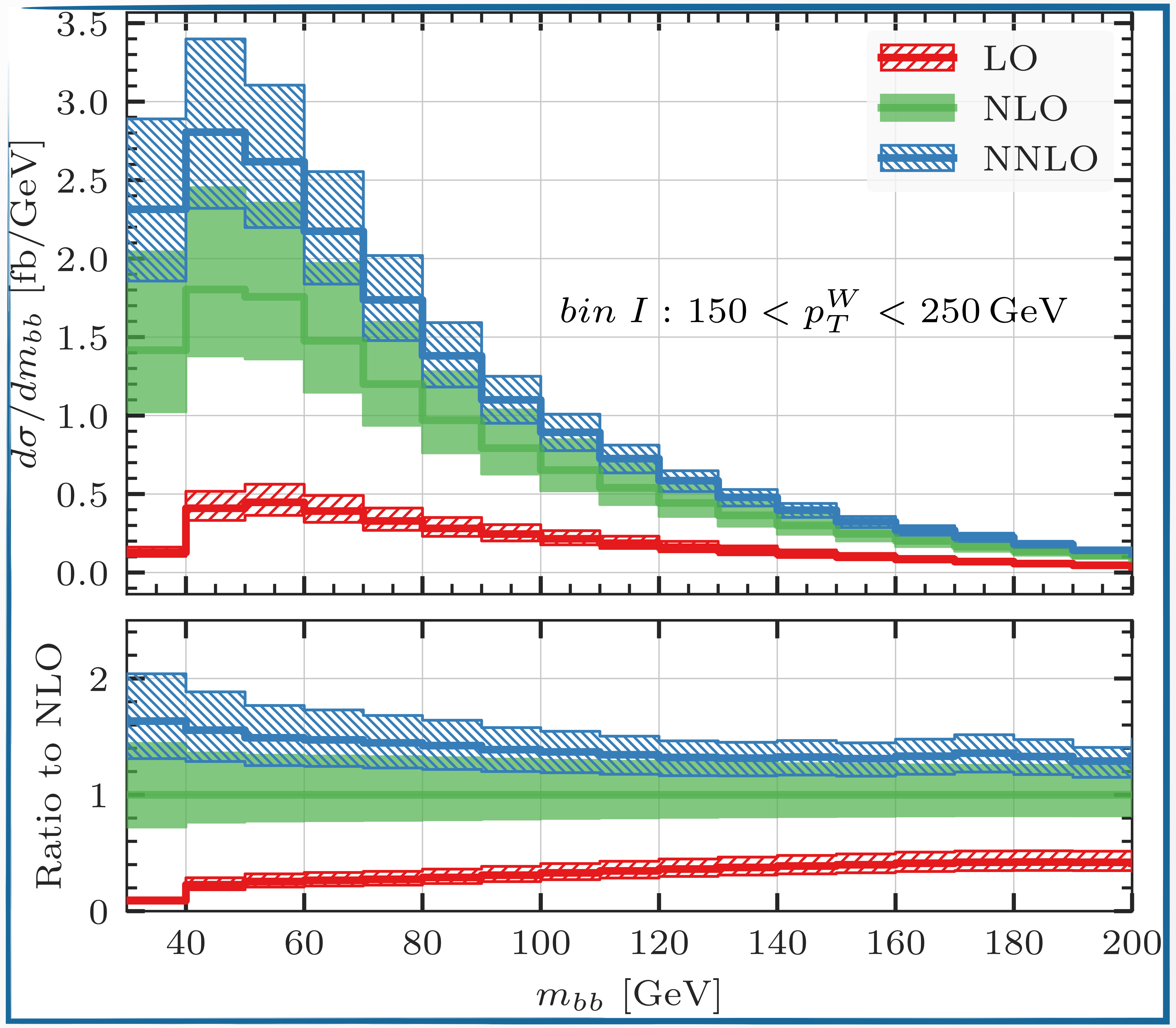
order	$\sigma_{\mathrm{fid}}^{bin\ I}$ [fb]	$\sigma_{\mathrm{fid}}^{bin\ II}$ [fb]
LO	$35.49(1)^{+25\%}_{-18\%}$	$8.627(1)^{+25\%}_{-18\%}$
NLO	$137.20(5)^{+34\%}_{-23\%}$	$37.24(1)^{+38\%}_{-24\%}$
NNLO	$201.0(8)^{+17\%}_{-16\%}$	$58.5(1)^{+21\%}_{-18\%}$

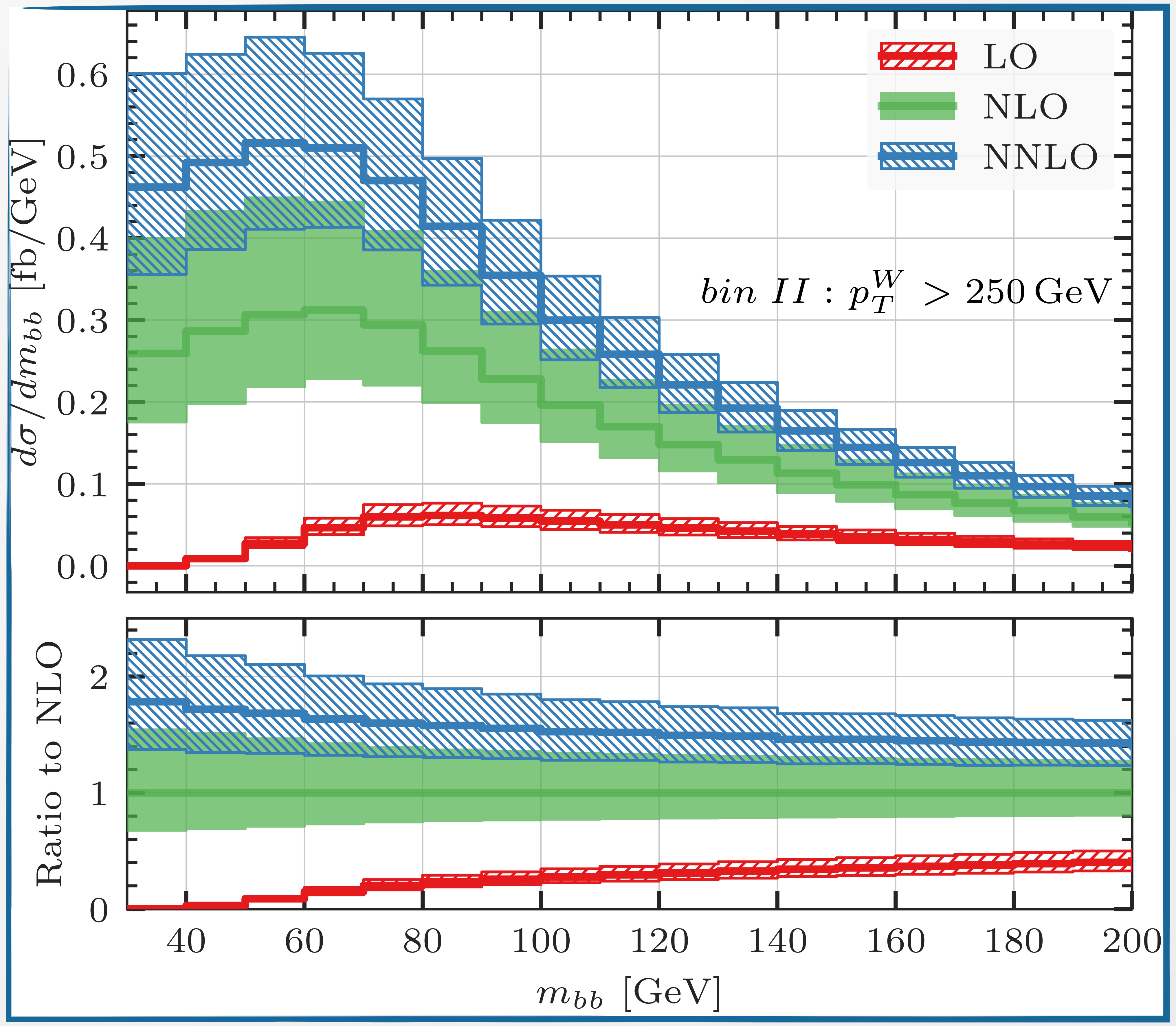
Other theoretical uncertainties are subdominant:

- Variation of bottom mass: $m_b = 4.91 \to 4.2\,\mathrm{GeV} \implies \delta\sigma_{\mathrm{NNLO}}/\sigma_{\mathrm{NNLO}} = +\,2\,\%$
- Impact of massification estimated at NLO: $|\,\delta(\Delta\sigma_{\mathrm{NLO}})/\Delta\sigma_{\mathrm{NLO}}^{exact}\,| = 3\,\%$
- Leading-colour approximation responsible for an additional 1-2% uncertainty of the full NNLO correction

Phenomenology: invariant mass of the bottom dijet system

- Pattern of the NNLO corrections similar in the two considered p_T^W bins
- NNLO corrections **not uniform**, larger for smaller invariant-mass values
- **Reduction** of scale uncertainties, **partial overlap** of NLO and NNLO bands





Phenomenology: massless and massive calculations

$$W + 2\ b_{jet} + X \textbf{ (inclusive) } @ \sqrt{s} = 8\,\text{TeV}$$

[CMS:arXiv:1608.07561]

Selection cuts

$$p_{T,\ell} > 30\ \text{GeV} \qquad |\eta_\ell| < 2.1$$

$$n_b = 2 : p_{T,b} > 25\ \text{GeV} \qquad |\eta_\ell| < 2.4$$

$$p_{T,j} > 25\ \text{GeV} \qquad |\eta_\ell| < 2.4$$

Reference scale

$$H_T = E_T(\ell\nu) + p_T(b_1) + p_T(b_2)$$

$$E_T(\ell\nu) = \sqrt{M^2(\ell\nu) + p_T^2(\ell\nu)}$$

	HPPZ	**This work**
α_s and PDF scheme	5FS	4FS
Jet clustering algortihm	flavour k_T and flavour anti-k_T algorithm (R=0.5)	k_T and anti-k_T algorithm (R=0.5)
pdf sets	NNPDF31_as_0118 (LO, NLO, NNLO) [Hartanto, Poncelet, Popescu, Zoia '22]	NNPDF30_as_0118_nf_4 (LO) NNPDF31_as_0118_nf_4 (NLO, NNLO NNLO)

Phenomenology: massless and massive calculations

order	$\sigma^{4\text{FS}}$ [fb]	$\sigma^{5\text{FS}}_{a=0.05}$ [fb]	$\sigma^{5\text{FS}}_{a=0.1}$ [fb]	$\sigma^{5\text{FS}}_{a=0.2}$ [fb]
LO	$210.42(2)^{+21.4\%}_{-16.2\%}$	$262.52(10)^{+21.4\%}_{-16.1\%}$	$262.47(10)^{+21.4\%}_{-16.1\%}$	$261.71(10)^{+21.4\%}_{-16.1\%}$
NLO	$468.01(5)^{+17.8\%}_{-13.8\%}$	$500.9(8)^{+16.1\%}_{-12.8\%}$	$497.8(8)^{+16.0\%}_{-12.7\%}$	$486.3(8)^{+15.5\%}_{-12.5\%}$
NNLO	$636.4(1.6)^{+11.9\%}_{-10.5\%}$	$690(7)^{+10.9\%}_{-9.7\%}$	$677(7)^{+10.4\%}_{-9.4\%}$	$647(7)^{+9.5\%}_{-9.4\%}$

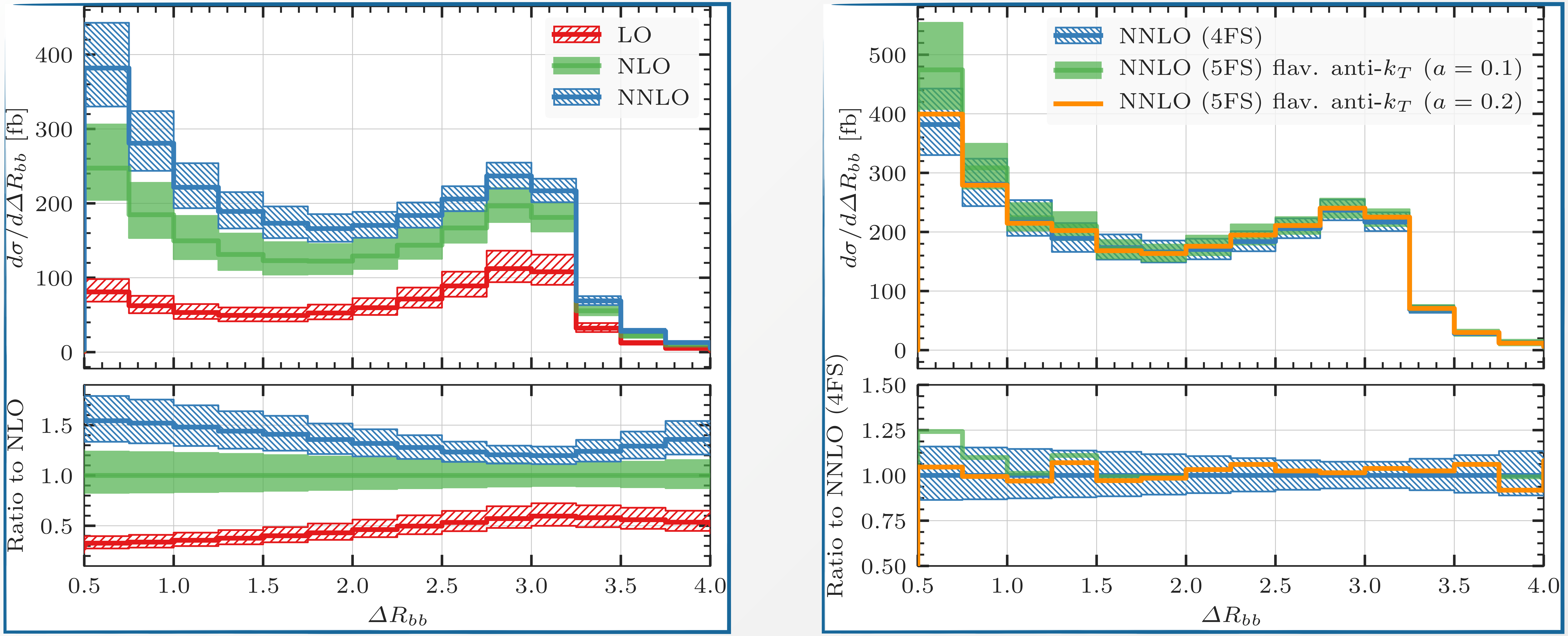
Remarks

- The **parameter** a of the flavour anti k_T algorithm plays a role similar to m_b in our massive calculation
- Uncertainty estimated by varying $a \in [0.05, 0.2]$ amounts to $7\,\%$; considerably **smaller** uncertainty (2%) estimated by generously varying $m_b \in [4.2, 4.92]$
- General **agreement within scale variations**, with the massive calculation performed in the 4FS **systematically below**

Phenomenology: massless and massive calculations

Sizeable NNLO corrections which lead to a steeper slope at small ΔR_{bb} (where scale uncertainties are larger)

Good agreement between flavour and standard anti-k_T for the largest value $a = 0.2$



Conclusion and outlook

- Description of *Wbb* production process plays an important role in the physics precision programme at the LHC
- Calculation in the massive case possible using the q_T-subtraction methods thanks to recent availability of two-loop ingredients: soft function and two-loop virtual amplitude
- **First calculation of *Wbb*** production in NNLO QCD in the **4FS (massive b-quarks)**
- We rely on the **massification procedure** starting from the corresponding massless amplitude to obtain the missing two-loop virtual amplitude
- NNLO QCD corrections **crucial for precision phenomenology**
- Our calculation **minimises problems related to flavour tagging allowing a more direct comparison to data**

Future steps

- Matching to parton shower in a full NNLO+PS implementation
- Study of W production in association to a single *b* (comparison with the combined 4FS+5FS @NLO)

Backup

Massification procedure

[Mitov, Moch, 2007]

Amplitude factorisation in massless QCD [Catani, 1998][Sterman, Tejeda-Yeomans, 2003]

$$|\mathscr{M}^{[p]} > \, = \mathscr{J}^{[p]}\left(\frac{Q^2}{\mu^2}, \alpha_S(\mu^2), \epsilon\right) \times \mathscr{S}^{[p]}\left(\{k_i\}\frac{Q^2}{\mu^2}, \alpha_S(\mu^2), \epsilon\right) \times |\mathscr{H}^{[p]} >$$

Amplitude factorisation in QCD with a **massive** parton of mass $m^2 \ll Q^2$

$$|\mathscr{M}^{[p],(m)} > \, = \mathscr{J}^{[p]}\left(\frac{Q^2}{\mu^2}, \frac{m_i^2}{\mu^2}\alpha_S(\mu^2), \epsilon\right) \times \mathscr{S}^{[p]}\left(\{k_i\}\frac{Q^2}{\mu^2}, \alpha_S(\mu^2), \epsilon\right) \times |\mathscr{H}^{[p]} > + \, \mathscr{O}\left(\frac{m^2}{Q^2}\right)$$

$$\mathscr{J}^{[p]}\left(\frac{Q^2}{\mu^2}, \frac{m_i^2}{\mu^2}\alpha_S(\mu^2), \epsilon\right) = \prod_i \mathscr{J}^i\left(\frac{Q^2}{\mu^2}, \frac{m_i^2}{\mu^2}\alpha_S(\mu^2), \epsilon\right) = \prod_i \left(\mathscr{F}^i\left(\frac{Q^2}{\mu^2}, \frac{m_i^2}{\mu^2}\alpha_S(\mu^2), \epsilon\right)\right)^{1/2}$$

space-like massive form factor

Massification procedure

[Mitov, Moch, 2007]

Master formula of "massification"

$$|\mathscr{M}^{[p],(m)}> = \prod_i \left[Z_{[i]}\left(\frac{m^2}{\mu^2}, \alpha_s(\mu^2), \epsilon\right)\right]^{1/2} \times |\mathscr{M}^{[p]}> + \mathcal{O}\left(\frac{m^2}{Q^2}\right)$$

$$Z_{[i]}\left(\frac{m^2}{\mu^2}, \alpha_S(\mu^2), \epsilon\right) = \mathscr{F}^i\left(\frac{Q^2}{\mu^2}, \frac{m_i^2}{\mu^2}, \alpha_S(\mu^2), \epsilon\right)\left[\mathscr{F}^i\left(\frac{Q^2}{\mu^2}, 0, \alpha_S(\mu^2), \epsilon\right)\right]^{-1}$$

History & Remarks

- The formula retrieves mass logarithms and constant terms [Glover, TauskandJ, VanderBij, 2001] [Penin 2005-2006]
- Consistent with previous results for NNLO QED correction to Bhabha scattering
- Successfully employed to derive and cross check results for $q\bar{q} \to Q\bar{Q}$ and $gg \to Q\bar{Q}$ amplitudes [Czakon, Mitov, Moch, 2007]
- Recently extended to the case of two different external masses $(M \gg m)$
- [Engel, Gnendiger, Signera, Ulrich 2019]

Massification procedure

[Mitov, Moch, 2007]

The massification procedure is based on the **factorisation properties** of QCD amplitudes

Basic idea: in the small mass limit, the massive amplitude $\mathcal{M}^{[p],(m)}$ and the massless one $\mathcal{M}^{[p],(m=0)}$ are connected as the mass screens some collinear divergences "trading" poles in the dimensional regulator ϵ for logarithms of the mass

This can be viewed as a **change in the renormalisation scheme** which leads to a universal **"multiplicative renormalization"** relation between (*ultraviolet renormalised*) massive and massless amplitudes

$$\mathcal{M}^{[p],(m)} = \prod_{i\in\{\text{all legs}\}} \left(Z_{[i]}^{(m|0)}\right)^{\frac{1}{2}} \mathcal{M}^{[p],(m=0)} + \mathcal{O}(m^k)$$

- The function $Z_{[i]}^{(m|0)}$ are universal, depend only on the external parton (quark or gluon) and admit a perturbative expansion in α_s:

$$Z_{[i]} = 1 + \sum_k \left(\frac{\alpha_s}{2\pi}\right)^k Z_{[i]}^k$$

$$\mathcal{M}^{[p],(m)} = \sum_{k=0} \left(\frac{\alpha_s}{2\pi}\right)^k \mathcal{M}_{(k)}^{[p],(m)}$$

$\rightarrow$

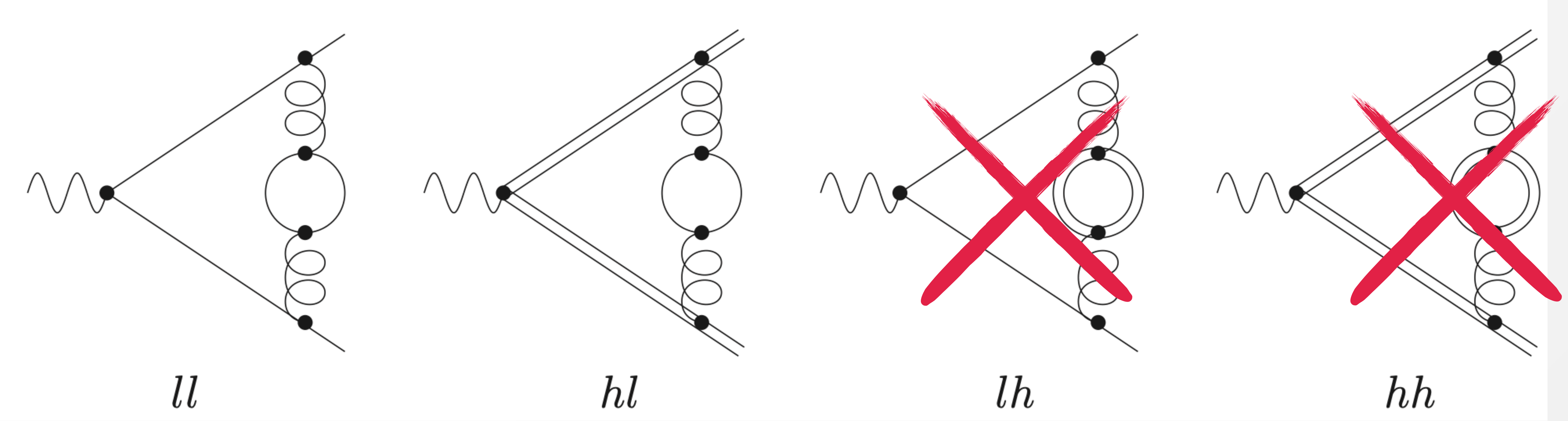
$$\boxed{\begin{aligned}
\mathcal{M}_0^{Wbb,(m)} &= \mathcal{M}_0^{Wbb,(m=0)} \\
\mathcal{M}_{(1)}^{Wbb,(m)} &= \mathcal{M}_{(1)}^{Wbb,(m=0)} + Z_{[q]}^{(1)} \mathcal{M}_{(0)}^{Wbb,(m=0)} \\
\mathcal{M}_{(2)}^{Wbb,(m)} &= \mathcal{M}_{(2)}^{Wbb,(m=0)} + Z_{[q]}^{(1)} \mathcal{M}_{(1)}^{Wbb,(m=0)} + Z_{[q]}^{(2)} \mathcal{M}_{(0)}^{Wbb,(m=0)}
\end{aligned}}$$

Massification procedure

[Mitov, Moch, 2007]

$$\mathscr{M}^{[p],(m)} = \prod_{i\in\{\text{all legs}\}} \left(Z_{[i]}^{(m|0)}\right)^{\frac{1}{2}} \mathscr{M}^{[p],(m=0)} + \mathcal{O}(m^k)$$

- The $Z_{[i]}^{(m|0)}$ are given by the **ratio of massive and massless form factors** ($\gamma^* qq$ for the quark case)



- Starting from two loops, contributions from **heavy quarks loops** (*lh* and *hh*) arise. Their description requires additional process dependent terms and **have been excluded** from the definition of the $Z_{[i]}^{(m|0)}$

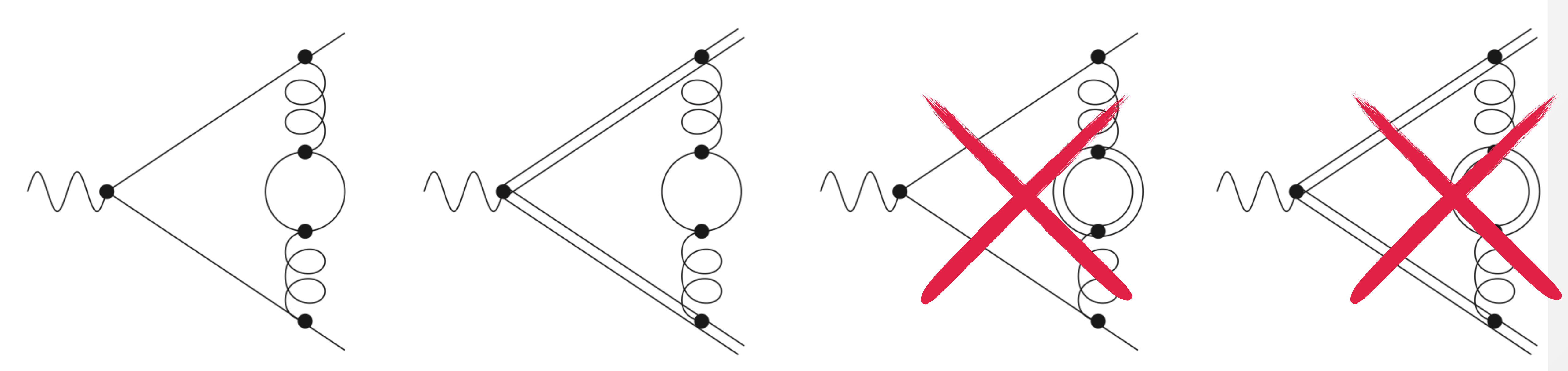
The massification procedure predicts **poles, logarithms of mass and mass independent terms (constants)** of $\mathscr{M}^{[p],(m)}$ while **power corrections** in the mass and the contribution of **heavy loops** cannot be retrieved using this approach

Massification procedure

[Mitov, Moch, 2007]

$$\mathcal{M}^{[p],(m)} = \prod_{i \in \{\text{all legs}\}} \left(Z_{[i]}^{(m|0)} \right)^{\frac{1}{2}} \mathcal{M}^{[p],(m=0)} + \mathcal{O}(m^k)$$

- The $Z_{[i]}^{(m|0)}$ are given by the **ratio of massive and massless form factors** ($\gamma^* qq$ for the quark case)



Remarks

- The functions $Z_{[i]}^{(m|0)}$ are **trivial objects in colour space** and are expressed in terms of colour Casimir
- At each perturbative order, $Z_{[i]}^{(k)}$ is given by a Laurent series in ϵ

$$Z_{[q]}^{(1)} = C_F \left[\frac{1}{\epsilon^2} + \frac{1}{\epsilon} \left(\ln \frac{\mu^2}{m^2} + \frac{1}{2} \right) + \ldots \right] \longrightarrow$$

requires knowledge of the massless one-loop amplitude $\mathcal{M}_{(1)}^{Wbb,(m=0)}$ up to $\mathcal{O}(\epsilon^2)$

Two-loop massless amplitudes

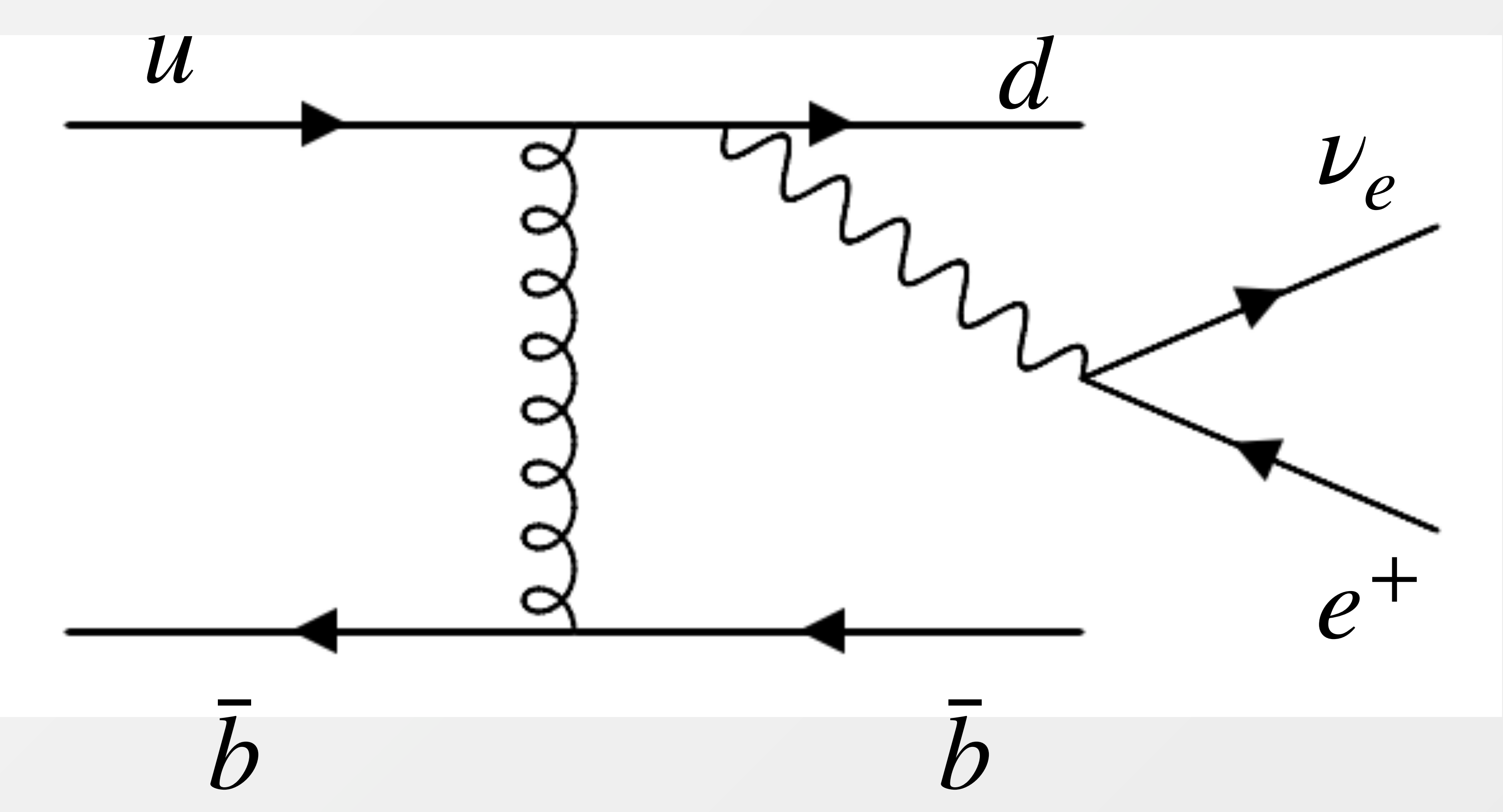
[Abreu, Febres-Cordero, Ita, Klinkert, Page, Sotnikov, 2022]

Two-loop helicity virtual amplitudes for W boson and four partons only available in **leading colour app**. (LCA)

- Analytical expressions obtained within the framework of numerical unitary (using numerical samples)
- Final results are expressed as a function of **one-mass pentagon functions** [Chicherin, Sotnikov, Zoia 2021]
- **W boson treated off-shell** (exact treatment of leptonic decays)
- publicly available http://www.hep.fsu.edu/~ffebres/W4partons
- **analytical expressions of the one-loop amplitudes up to** $\mathcal{O}(\epsilon^2)$ available in LCA

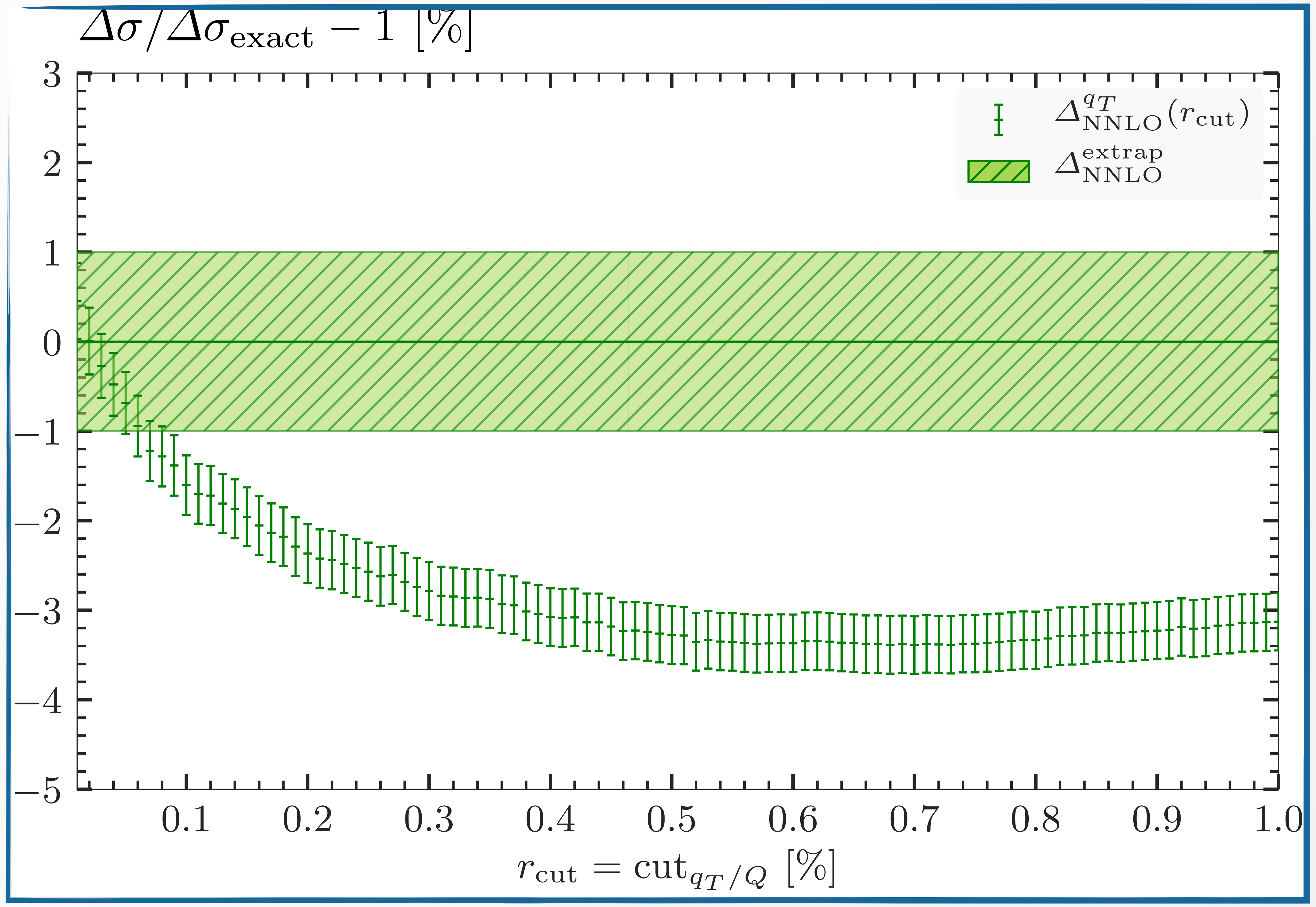
Remarks

- Amplitudes only available as (lengthy) mathematical expressions, not usable directly for computations (~1-2 minute per phase space point)
- Rather long algebraic expressions prone to numerical round-off errors
- Reference process is $u\bar{b} \to \bar{b}de^+\nu_e$. Initial-final state crossing require suitable permutation the action of the permutation transforms the **pentagon functions** into each others, no need for analytic continuation. All permutations available in a Mathematica script [Chicherin, Sotnikov, Zoia 2021]



r_{cut} dependence

$$d\sigma_X^{\mathrm{N^kLO}} \equiv \mathcal{H}_X^{\mathrm{N^kLO}} \otimes d\sigma_X^{\mathrm{LO}} + \left[d\sigma_{\mathrm{X+jet}}^{\mathrm{N^{k-1}LO}} - \left[d\sigma_X^{\mathrm{N^kLL}} \right]_{\mathcal{O}(\alpha_s^k)} \right]_{q_T > q_t^{\text{cut}}} + \mathcal{O}((q_T^{\text{cut}}/M)^n)$$



Behaviour of the power corrections compatible with a **linear scaling** as expected from processes with massive final state

Overall mild power corrections

Control of the NNLO correction at $\mathcal{O}(1\%)$
$\to \mathcal{O}(0.2\%)$ at the level of the total cross section

Comparison with HPPZ: fiducial cross sections

order	$\sigma^{4\mathrm{FS}}$ [fb]	$\sigma^{5\mathrm{FS}}_{a=0.05}$ [fb]	$\sigma^{5\mathrm{FS}}_{a=0.1}$ [fb]	$\sigma^{5\mathrm{FS}}_{a=0.2}$ [fb]
LO	$210.42(2)^{+21.4\%}_{-16.2\%}$	$262.52(10)^{+21.4\%}_{-16.1\%}$	$262.47(10)^{+21.4\%}_{-16.1\%}$	$261.71(10)^{+21.4\%}_{-16.1\%}$
NLO	$468.01(5)^{+17.8\%}_{-13.8\%}$	$500.9(8)^{+16.1\%}_{-12.8\%}$	$497.8(8)^{+16.0\%}_{-12.7\%}$	$486.3(8)^{+15.5\%}_{-12.5\%}$
NNLO	$636.4(1.6)^{+11.9\%}_{-10.5\%}$	$690(7)^{+10.9\%}_{-9.7\%}$	$677(7)^{+10.4\%}_{-9.4\%}$	$647(7)^{+9.5\%}_{-9.4\%}$

Remarks

Change of scheme @NLO **[Cacciari, Nason, Greco, 1998]**

1. Use same running coupling and PDF set of the 5FS calculation
2. Add the extra factor (due to the conversion between $\overline{MS}$ and decoupling schemes) : $-\alpha_s \frac{2T_R}{3\pi} \ln \frac{\mu_R^2}{m^2} \sigma^{\mathrm{LO}}_{q\bar{q}}$

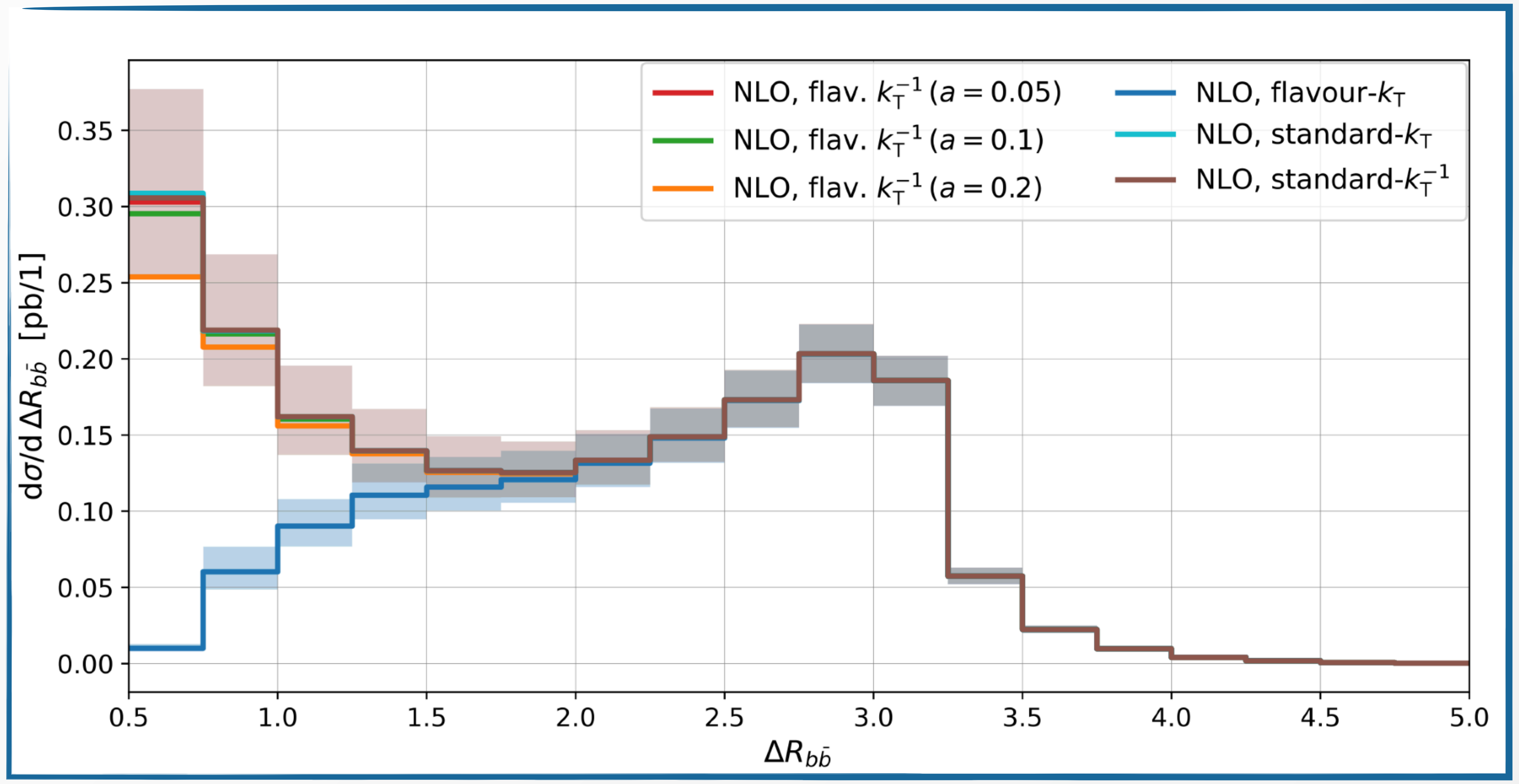
   No corrective term for pdfs at this order
3. Take the massless limit $m_b \to 0$

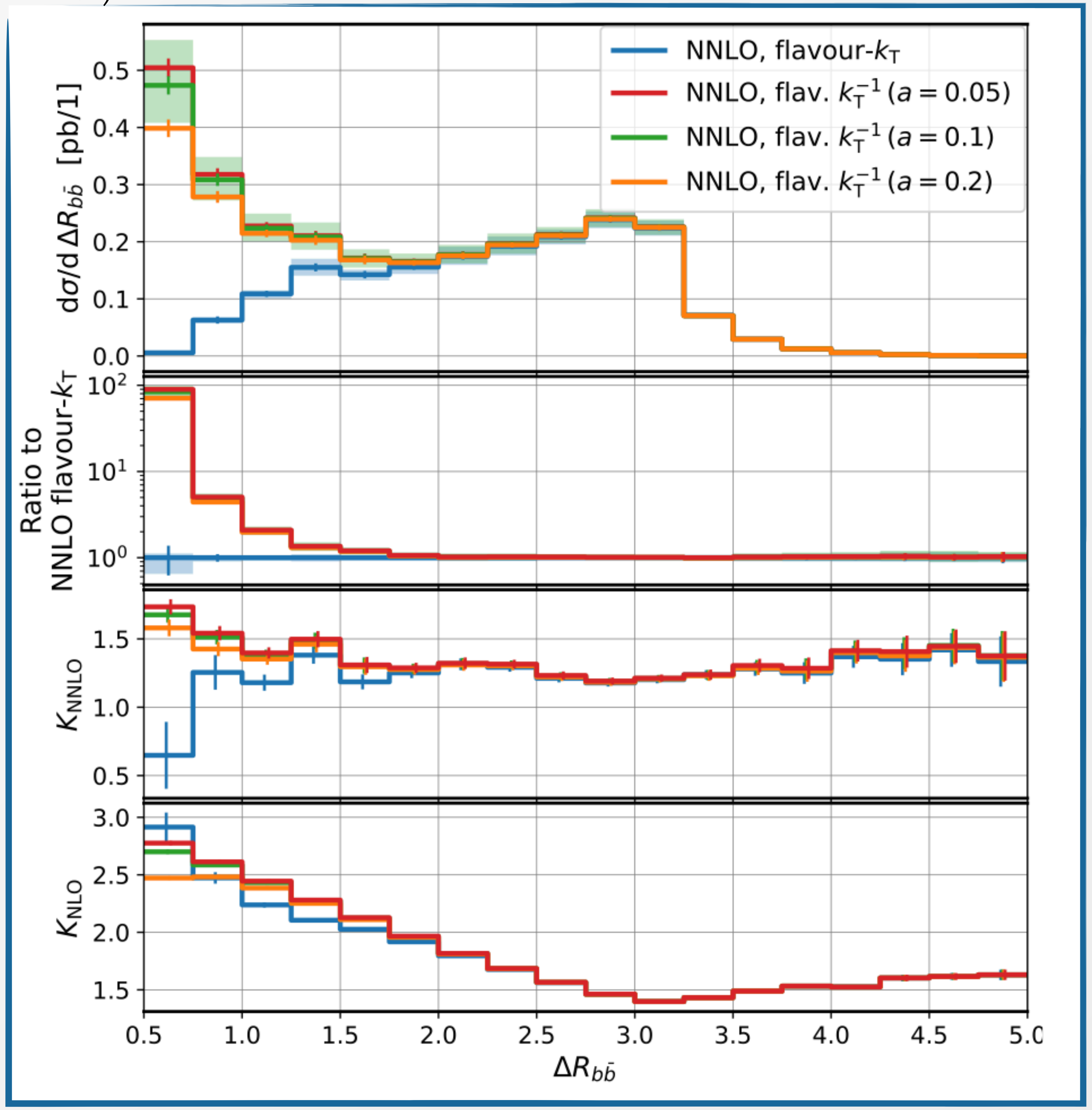
$$\text{NLO 4FS: } 468 \text{ fb} \xrightarrow{1,2} 481 \text{ fb} \xrightarrow{3} 493 \text{ fb}$$

Comparison with HPPZ: fiducial cross sections

Flavour k_T favours the clustering of the two bottom quarks in the same jet, leading to a suppression at small ΔR_{bb} (largely due to the modified definition of beam distances, already at LO)

- At NLO, flavour anti k_T reproduces standard anti k_T in the limit $a \to 0$. At NNLO cannot be arbitrarily small because of the infrared problem
- HPPZ choice: $a \in [0.05, 0.2]$





Comparison with HPPZ: differential distributions

Other distributions display similar pattern of the higher-order corrections

The process features two dominant configurations: **gluon splitting** and **t-channel** enhancement (back-to-back bottom quarks and back-to-back leptons)