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

in collaboration with S. Devoto, S. Kallweit, J. Mazzitelli, L. Rottoli and C. Savoini [*Phys.Rev.D* 107 (2023) 7, 074032, arXiv:2212.04954]



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Introduction



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[G. Salam @ ICHEP 2022]

Motivations

W+1bj and W+2bj interesting signatures

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



from VH(->bb) analysis [CMS:arXiv:1808.08242]

Postfit normalisation corrections

$Z(\nu\nu)H$	$W(\ell \nu)H$	$Z(\ell\ell)H$ low- p_T	$Z(\ell\ell)H$ high-p
1.04 ± 0.07	1.04 ± 0.07	—	—
2.09 ± 0.16	2.09 ± 0.16	_	—
1.74 ± 0.21	1.74 ± 0.21	—	—
0.95 ± 0.09	_	0.89 ± 0.06	0.81 ± 0.05
1.02 ± 0.17	—	0.94 ± 0.12	1.17 ± 0.10
1.20 ± 0.11	_	0.81 ± 0.07	0.88 ± 0.08
0.99 ± 0.07	0.93 ± 0.07	0.89 ± 0.07	0.91 ± 0.07







State of the art

NLO corrections (massless bottom quarks)

[Ellis, Veseli, 1999]

NLO corrections (massive bottom quarks)

[Febres Cordero, Reina, Wackeroth, 2006, 2009]

NLO corrections (4FS+5FS)

[Campbell, Ellis, Febres Cordero, Maltoni, Reina, Wackeroth, Willenbrock, 2009] [Campbell, Caola, Febres Cordero, Reina, Wackeroth,2011]

NLO+PS

[Oleari, Reina, 2011] [Frederix, Frixione, Hirschi, Maltoni, Pittau, Torrielli, 2011]

POWHEG+MiNLO

[Luisoni, Oleari, Tramontano, 2015]

Wbb + up to 3 jets

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



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Analytical Two-loop W+4 partons amplitude in Leading Colour Approximation (LCA) [Badger, Hartanto, Zoia, 2021] [Abreu, Febres Cordero, Ita, Klinkert, Page, Sotnikov, 2021] **NNLO corrections (massless bottom quarks)** First NNLO QCD calculation for [Hartanto, Poncelet, Popescu, Zoia, 2022] massless bottom quarks!

see talks by S. Zoia, G. Gambuti







Wbb @ NNLO with massless b quarks

First computation for Wbb @ NNLO with massless b quarks recently performed

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

Jet algorithm	$\sigma_{ m NNLO}$ [fb]	$K_{ m NNLO}$	
${ m flavour}{ m -}k_{ m T}$	$445(5)^{+6.7\%}_{-7.0\%}$	1.23	
flavour anti- $k_{ m T}$ (a=0.05)	$690(7)^{+10.9\%}_{-9.7\%}$	1.38	$O(50\%)$ when ι
flavour anti- $k_{\rm T}$ ($a = 0.1$)	$677(7)^{+10.4\%}_{-9.4\%}$	1.36	k_T algo
flavour anti- $k_{\rm T}$ (a = 0.2)	$647(7)^{+9.5\%}_{-8.9\%}$	1.33	







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Infrared safety and flavour tagging

Jet clustering algorithms consist in a sequence of two-to-one recombination steps. They are then completely defined once the binary distance d_{ii} and the beam distance d_{iB} are given. For the family of k_T algorithms

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

For parton level calculation (fixed order), infrared safety is a crucial requirement For observable sensitive to the flavour assignment, **infrared safety can be an issue**, usually associated **to gluon** splitting to quarks in the double soft limit (the problem starts at NNLO)



$$R_{ij}^2 = (y_i - y_j)^2 + (\phi_i - \phi_j)^2$$

this may lead to a flavour configuration different from the corresponding virtual one, spoiling KLN cancellation

cannot alter tagging

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Flavour aware jet algorithms: flavour k_T

Theoretically sounded but problematic for data/theory comparison

- parton level)
- anti-*k_T* is de-facto the jet algorithm used in all analysed for its properties

• experimentally, jet reconstruction and flavour assignment are performed at the particle level (not at the





Flavour aware jet algorithms: flavour k_T

Theoretically sounded but problematic for data/theory comparison

- **unfolding corrections** can be **sizeable**: ~ 12 % Z + b jet as estimated at NLO+PS accuracy



• requires to unfold the experimental data to the theory calculation performed with the flavour k_T algorithm

[Gauld, Gehrmann–De Ridder, Glover, Huss, Majer, 2020]







Flavour aware jet algorithms: flavour anti-*k*_{*T*}

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

ur anci- K_T ai

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

$$\mathcal{S}_{ij} = 1 - \theta(1 - \kappa) \cos\left(\frac{\pi}{2}\kappa\right), \qquad \kappa = \frac{1}{a} \frac{k_{T,i}^2 + k_{T,j}^2}{2k_{T,max}^2}$$
$$\mathcal{S}_{ij} \sim E^4 \implies d_{ij}^{(F)} \sim E^2$$

the suppression factor overcompensates the divergent behaviour of d_{ij} in the double soft limit: in this way, both conditions 1 and 2 hold

does not vanish in the double soft limit





Flavour aware jet algorithms: flavour anti-*k*_T

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

"LAVOUT ANGU-NT AUJURATION

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

$$\mathcal{S}_{ij} = 1 - \theta(1 - \kappa) \cos\left(\frac{\pi}{2}\kappa\right), \qquad \kappa = \frac{1}{a} \frac{k_{T,i}^2 + k_{T,j}^2}{2k_{T,max}^2}$$

Parameter *a* control the turning on of the suppression factor: in the limit $a \rightarrow 0$, 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

does not vanish in the double soft limit





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Flavour aware jet algorithms: new ideas

Recently, the problem has triggered a lot of activity in the theoretical community!

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 flavourblind jet algorithms

Requires flavour information of many particles in the event



[Caletti, Larkoski, Marzani, Reichelt, 2022]

[Gauld, Huss, Stagnitto, 2022]

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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, 2022]







Flavour aware jet algorithms: massive calculation

Massive bottom quarks

- quark mass is the physical IR regulator: physical suppression in the double-soft limit

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

Caveat

- Calculation with massive quarks is challenging

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

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





Outline

- Methodology: slicing formalism
- Methodology: two-loop virtual amplitude
- Phenomenological results
- Conclusions

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Infrared singularities

Class of contributions entering the NNLO corrections



KLN theorem and collinear factorisation ensure the cancellation of singularities for any infrared safe observables, but virtuals, real-virtual and reals live on different phase spaces and are separately divergent ... Subtraction/Slicing scheme required!





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q_T -subtraction formalism

Cross section for the production of a triggered final state F at N^kLO

All emission unresolved; approximate the cross section with its singular part in the soft and/or collinear limits

q_T resummation

- expand to fixed order
- $\mathcal{O}(\alpha_s^k)$ ingredient required



$$\int d\sigma_{N^{k}LO} = \mathcal{H} \otimes d\sigma_{LO} + \int \left[d\sigma_{N^{k-1}LO}^{R} - d\sigma_{N^{k}LO}^{CT} \right]_{q_{T} > q_{T}^{\text{cut}}} + \mathcal{O}\left((q_{T}^{\text{cut}})^{\ell} \right)$$

1 emission always resolved $F + j @ N^{k-1}LO$

complexity of the calculation reduced by one order!

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$$\int d\sigma_{N^k LO} = \mathscr{H} \otimes d\sigma_{LO} + \int \left[d\sigma_{N^k LO} + \int d\sigma_{N^k LO} \right] d\sigma_{N^k LO} = \mathscr{H} \otimes d\sigma_{N^k LO} + \int \left[d\sigma_{N^k LO} + \int d\sigma_{N^k LO} \right] d\sigma_{N^k LO} + \int d\sigma_{N^k LO} + \int$$

All ingredients for $Wb\bar{b} + j$ @ NLO available:

Required matrix elements implemented in public libraries such as OpenLoops2 [Buccioni, Lang, Lindert, Maierhöfer, Pozzorini, Zhang, Zoller '19]

Local subtraction scheme available, for example dipole subtraction [Catani, Seymour, '98] [Catani, Dittmaier, Seymour, Trocsanyi '02]

Automatised implementation in the MATRIX framework, which relies on the efficient multi-channel Monte Carlo integrator MUNICH [Grazzini, Kallweit, Wiesemann '17] [Kallweit in preparation]

 $\left[\sigma_{N^{k-1}LO}^{R} - d\sigma_{N^{k}LO}^{CT}\right]_{q_{T} > q_{T}^{cut}} + \mathcal{O}\left((q_{T}^{cut})^{\ell}\right)$



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$$\int d\sigma_{N^{k}LO} = \mathscr{H} \otimes d\sigma_{LO} + \int \left[d\sigma_{N^{k-1}LO}^{R} - d\sigma_{N^{k}LO}^{CT} \right]_{q_{T} > q_{T}^{\text{cut}}} + \mathcal{O}\left((q_{T}^{\text{cut}})^{\mathscr{C}} \right)$$

H contains virtual correction after subtraction of IR singularities and contribution of soft/collinear origin

• Beam functions



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

> see talks by B. Mistlberger, G. Vita





$$\int d\sigma_{N^{k}LO} = \mathcal{H} \otimes d\sigma_{LO} + \int \left[d\sigma_{N^{k-1}LO}^{R} - d\sigma_{N^{k}LO}^{CT} \right]_{q_{T} > q_{T}^{\text{cut}}} + \mathcal{O}\left((q_{T}^{\text{cut}})^{\ell} \right)$$

H contains virtual correction after subtraction of IR singularities and contribution of soft/collinear origin

- Soft function



The resummation formula shows a **richer structure** because of additional soft singularities

- Soft logarithms controlled by the **transverse momentum anomalous dimension** Γ_t known up to NNLO [Mitov, Sterman, Sung, 2009], [Neubert, et al 2009]
- Hard coefficient gets a **non-trivial** colour structure (matrix in colour-space)
- Non trivial azimuthal correlations



$$\int d\sigma_{N^{k}LO} = \mathcal{H} \otimes d\sigma_{LO} + \int \left[d\sigma_{N^{k-1}LO}^{R} - d\sigma_{N^{k}LO}^{CT} \right]_{q_{T} > q_{T}^{\text{cut}}} + \mathcal{O}\left((q_{T}^{\text{cut}})^{\ell} \right)$$

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The resummation formula shows a **richer structure** because of additional soft singularities

 q_T subtraction formalism extended to the case of **heavy** quarks production [Catani, Grazzini, Torre, 2014]

Successful employed for the computation of NNLO QCD corrections to the production of

- a top pair [Catani, Devoto, Grazzini, Kallweit, Mazzitelli, Sargsyan 2019]
- a **bottom pair** production [Catani, Devoto, Grazzini, Kallweit, Mazzitelli, 2021]



$$\int d\sigma_{N^{k}LO} = \mathcal{H} \otimes d\sigma_{LO} + \int \left[d\sigma_{N^{k-1}LO}^{R} - d\sigma_{N^{k}LO}^{CT} \right]_{q_{T} > q_{T}^{\text{cut}}} + \mathcal{O}\left((q_{T}^{\text{cut}})^{\mathscr{C}} \right)$$

H contains virtual correction after subtraction of IR singularities and contribution of soft/collinear origin





The resummation formula shows a **richer structure** because of additional soft singularities

Non trivial ingredient

- **Two-loop soft function** for heavy-quark (back-toback Born kinematic) [Catani, Devoto, Grazzini, Mazzitelli,2023]
- Recently generalised to arbitrary kinematics [Devoto, Mazzitelli in preparation]



$$\int d\sigma_{N^{k}LO} = \mathcal{H} \otimes d\sigma_{LO} + \int \left[d\sigma_{N^{k-1}LO}^{R} - d\sigma_{N^{k}LO}^{CT} \right]_{q_{T} > q_{T}^{\text{cut}}} + \mathcal{O}\left((q_{T}^{\text{cut}})^{\ell} \right)$$

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The resummation formula shows a **richer structure** because of additional soft singularities

Once the corresponding two-loop amplitude is available, the framework allows the calculation of the NNLO correction to the production of **a massive** heavy-quark pair and a generic color singlet process

• First application: $t\bar{t}H$ [Catani, Devoto, Grazzini, Kallweit, Mazzitelli, Savoini, **2023**]

see talk by C. Savoini



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Two-loop virtual amplitude



5-point amplitude with 1 massive particle current state of the art, more massive legs out of reach!





Two-loop virtual amplitude



But mp is the smallest scale in the game, exploit the hierarchy!

Use MASSIFICATION to relate the massive amplitude to the massless one up to power corrections of the mass

5-point amplitude with 1 massive particle current state of the art, more massive legs out of reach!







Massification procedure in a nutshell

Amplitude factorisation in massless QCD

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

Jet function: collinear contributions



[Catani, 1998][Sterman, Tejeda-Yeomans, 2003]

Soft function: coherent soft radiation

Hard function: shortdistance dynamics





Massification procedure in a nutshell

Amplitude factorisation in massless QCD

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

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

$$|\mathscr{M}^{[p],(m)}\rangle = \mathscr{F}^{[p]}\left(\frac{Q^2}{\mu^2}, \frac{m_i^2}{\mu^2}\alpha_S(\mu^2), \epsilon\right) \times \mathscr{F}^{[p]}\left(\frac{Q^2}{\mu^2}, \frac{m_i^2}{\mu^2}\alpha_S(\mu^2), \epsilon\right) = \prod_i \mathscr{F}^i\left(\frac{Q^2}{\mu^2}, \frac{Q^2}{\mu^2}, \frac{Q^2}{$$



[Catani, 1998][Sterman, Tejeda-Yeomans, 2003]

 $\mathcal{S}^{[p]}\left(\{k_i\}\frac{Q^2}{\mu^2}, \alpha_S(\mu^2), \epsilon\right) \times |\mathcal{H}^{[p]} > + \mathcal{O}\left(\frac{m^2}{Q^2}\right)$ $\left(\frac{m_i^2}{\mu^2}\alpha_S(\mu^2),\epsilon\right) = \prod_i \left(\mathscr{F}^i\left(\frac{Q^2}{\mu^2},\frac{m_i^2}{\mu^2}\alpha_S(\mu^2),\epsilon\right)\right)^{1/2}$ space-like massive form factor





Massification procedure in a nutshell

Master formula of "massification"

$$|\mathscr{M}^{[p],(m)}\rangle = \prod_{i} \left[Z_{[i]}\left(\frac{m^{2}}{\mu^{2}}, \alpha_{s}(\mu^{2}), \epsilon\right) \right]^{1/2} \times |\mathscr{M}^{[p]}\rangle + \mathcal{O}\left(\frac{m^{2}}{Q^{2}}\right)$$
$$Z_{[i]}\left(\frac{m^{2}}{\mu^{2}}, \alpha_{s}(\mu^{2}), \epsilon\right) = \mathscr{F}^{i}\left(\frac{Q^{2}}{\mu^{2}}, \frac{m^{2}_{i}}{\mu^{2}}, \alpha_{s}(\mu^{2}), \epsilon\right) \left[\mathscr{F}^{i}\left(\frac{Q^{2}}{\mu^{2}}, 0, \alpha_{s}(\mu^{2}), \epsilon\right) \right]^{-1}$$

History & Remarks

- The formula retrieves mass logarithms and constant terms !
- Consistent with previous results for NNLO QED correction to Bhabha scattering
- Successfully employed to derive and cross check results for $q\bar{q} \rightarrow Q\bar{Q}$ and $gg \rightarrow Q\bar{Q}$ amplitudes
- Recently extended to the case of two different external masses ($M \gg m$) see talks by M. Rocco and Y. Ulrich

[Glover, TauskandJ, VanderBij, 2001] [Penin 2005-2006] [Czakon, Mitov, Moch, 2007] [Engel, Gnendiger, Signer, Ulrich 2019]







Massification procedure for Wbb

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

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

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

• 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 :

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











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Massification procedure for Wbb

$$\mathscr{M}^{[p],(m)} = \prod_{i \in \{\text{all legs}\}} \left($$

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



additional process dependent terms and have been excluded from the definition of the $Z_{r_i}^{(m|0)}$

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

• Starting from two loops, contributions from heavy quarks loops (lh and hh) arise. Their description requires





Massification procedure for Wbb

$$\mathscr{M}^{[p],(m)} = \prod_{i \in \{\text{all legs}\}} \left($$

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additional process dependent terms and have been excluded from the definition of the $Z_{r_{i}}^{(m|0)}$

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

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

• Starting from two loops, contributions from heavy quarks loops (lh and hh) arise. Their description requires





WQQAmp: a massive C++ implementation

We have implemented the one-loop and two-loop amplitudes of [Abreu et al, 2022] in a C++ library for the efficient numerical evaluation of the **massive amplitudes**

WbbAmp

see talk by D. Chicherin [Chicherin, Sotnikov, Zoia 2021]

PentagonFunctions-cpp

evaluation of pentagons functions

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

massive phase space point mapped into a massless one (the mapping reduces to the identity in the massless limit)

Massification

[Buccioni, Lang, Lindert, Maierhöfer, Pozzorini, Zhang, Zoller, 2019]



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

 $|M_0|^2$

Finite remainder defined subtracting the IR poles as defined in [Ferroglia, Neubert, **Pecjac, Yang, 2009**]

 $\mathcal{O}(4s)$ per phase space point





WQQAmp: a massive C++ implementation

We have implemented the one-loop and two-loop amplitudes of [Abreu et al, 2022] in a C++ library for the efficient numerical evaluation of the **massive amplitudes**

We have recently fixed a bug of the library impacting the finite remainder of the two-loop amplitude. Phenomenological results mildly affected, in the following we will report the updated ones









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- Methodology: slicing formalism
- Methodology: two-loop virtual amplitude
- Phenomenological results



• **fiducial**: inspired by ATLAS $VH(\rightarrow b\bar{b})$ **boosted** analysis [ATLAS:arXiv:2007.02873]

$$p_{T,\ell} > 25 \text{ GeV}$$
 $|\eta_{\ell}| < 2.5$ $p_T^W > 150 \text{ GeV}$
Jet selection
 $p_{T,j} > 20 \text{ GeV}$ and $|\eta_{\ell}| < 2.5$ or
 $p_{T,j} > 30 \text{ GeV}$ and $2.5 < |\eta_{\ell}| < 4.5$

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

4-flavour scheme (4FS), $m_b=4.92$ GeV G_{μ} -scheme, CKM diagonal anti- k_T (and k_T) algorithm with R = 0.4NNPDF30 as 0118 nf 4(LO)NNPDF31 as 0118 nf 4 (NLO, NNLO)





Behaviour of the perturbative series and scale choice

• A priori, the use of a fixed scale is physically **not very** well motivated

 $\sigma(pp \to W(\ell^+ \nu_e)b\overline{b})$ [fb], $\sqrt{s} = 13.6 \,\text{TeV}$







Behaviour of the perturbative series and scale choice

- A priori, the use of a fixed scale is physically not very well motivated
- Naively, a dynamic scale as H_T would be a better choice. However, it leads to a poor perturbative convergence with no overlap between NLO and **NNLO** within their uncertainties bands

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

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

 $\sigma(pp \to W(\ell^+ \nu_e)b\bar{b})$ [fb], $\sqrt{s} = 13.6 \,\text{TeV}$





Behaviour of the perturbative series and scale choice

- A priori, the use of a fixed scale is physically not very well motivated
- Naively, a dynamic scale as H_T would be a better choice. However, it leads to a poor perturbative convergence with no overlap between NLO and NNLO within their uncertainties bands
- On the contrary, the choice of a fixed scale leads to a better perturbative convergence, suggesting a preference for smaller scales

 $\sigma(pp \to W(\ell^+ \nu_e)b\bar{b})$ [fb], $\sqrt{s} = 13.6 \,\text{TeV}$









Behaviour of the perturbative series and scale choice

- well motivated
- NNLO within their uncertainties bands
- better perturbative convergence, suggesting a preference for smaller scales
- "multi-scale" nature of the process



 $\sigma(pp \to W(\ell^+ \nu_e)b\bar{b})$ [fb], $\sqrt{s} = 13.6 \,\text{TeV}$



Wbb phenomenology: fiducial cross sections

Results

- Reference scale: $\sqrt{H_T \cdot m_{bb}}/2$
- Large NLO K-factors $K_{\rm NLO} \gtrsim 3$
- Relative large positive NNLO corrections, $K_{\rm NNLO} \sim 1.5$
- More reliable theory uncertainties estimated by s variations with a reduction to the 15 - 20% level

Other theoretical uncertainties are subdominant:

- Variation of bottom mass: $m_b = 4.2 \,\text{GeV} \implies \delta \sigma_{\text{NNLO}} / \sigma_{\text{NNLO}} = +2\%$
- Impact of massification estimated at NLO: $|\delta(\Delta \sigma_{\text{NLO}})/\Delta \sigma_{\text{NLO}}^{exact}| = 3\%$
- correction

	order	$\sigma^{bin~I}_{ m fid}[{ m fb}]$	$\sigma_{ m fid}^{bin~II}[m fb]$
	LO	$35.49(1)^{+25\%}_{-18\%}$	$8.627(1)^{+25}_{-18}$
	NLO	$137.20(5)^{+34\%}_{-23\%}$	$37.24(1)^{+38\%}_{-24\%}$
scale	NNLO	$198.9(8)^{+17\%}_{-15\%}$	$55.90(7)^{+19\%}_{-17\%}$
-			

• The part of the two-loop virtual amplitude computed in LCA contributes at the 2% level of the full NNLO





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Wbb phenomenology: *m*_{*bb*} differential distribution

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





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Comparison with HPPZ

Selection cuts

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

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

$p_{T,j} > 25 {\rm GeV}$	η_ℓ	< 2.4
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HPPZ $\alpha_{\rm s}$ and PDF scheme 5FS flavour k_T and flavour anti-k_T Jet clustering algorithm algorithm (R=0.5) NNPDF31_as_0118 (LO, NLO, pdf sets NNLO)

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

[CMS:arXiv:1608.07561]

Reference scale

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

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

This work

4FS

k_T and anti-k_T algorithm (R=0.5)

NNPDF30_as_0118_nf_4(LO) NNPDF31 as 0118 nf 4 (NLO, NNLO)





Comparison with HPPZ: fiducial cross sections

order	$\sigma^{ m 4FS}[{ m fb}]$	$\sigma_{a=0.05}^{\mathrm{5FS}}\left[\mathrm{fb} ight]$	$\sigma_{a=0.1}^{5\mathrm{FS}}$ [fb]	$\sigma^{\mathrm{5FS}}_{a=0.2}\mathrm{[fb]}$
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	$649.9(1.6)^{+12.6\%}_{-11.0\%}$	$690(7)^{+10.9\%}_{-9.7\%}$	$677(7)^{+10.4\%}_{-9.4\%}$	$647(7)^{+9.5\%}_{-9.4\%}$

Remarks

- $m_b \in [4.2, 4.92]$, at the 2% level
- below due to the different flavour scheme

• The parameter a of the flavour anti k_T algorithm plays a role similar to m_h in our massive calculation • Uncertainty estimated by varying $a \in [0.05, 0.2]$ amounts to 7 %; smaller uncertainty estimated by varying

• General **agreement within scale variations**, but the massive calculation performed in the 4FS **systematically**







Comparison with HPPZ: jet clustering algorithms

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







Conclusions

Thanks to the progress in

- subtraction scheme: the calculation of soft function for arbitrary kinematics allows to use the q_T subtraction formalism for the production of a coloured massive final state + a colour singlet system, as ttH and Wbb
- **QCD five-point scattering amplitude:** calculation of analytical amplitudes one massive + 4 partons in the leading colour (non planar topology within the reach in the near future)

we have completed the first calculation of Wbb production in NNLO QCD in the 4FS (massive b-quarks):

- for the missing massive amplitude, we rely on an approximation based on the massification procedure of the corresponding massless amplitude
- NNLO QCD radiative corrections **crucial for precision phenomenology**
- our calculation minimises ambiguities related to flavour tagging allowing for a more direct comparison to data

Outlooks

- matching to parton shower to reach NNLO+PS accuracy
- extension to other processes



BACKUP

Standard
$$k_T$$
 algorithm $d_{ij} = \min\left(k_{T,j}^2\right)$

Flavour aware k_T algorithm (usually flavour information available at each step of the clustering procedure

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

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

r
$$k_T$$

$$_{i}, k_{T,j}^{2}$$
 $R_{ij}^{2}, d_{iB} = k_{T,i}^{2}$
 $\alpha = 2$: condition 1 automatically satisfied

S



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

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)

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

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

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



Intro: slicing methods: q_T subtraction formalism for massive final states

Resolution variable (for example in Drell-Yan)

 q_T := transverse momentum of the dilepton final state Q := invariant mass of the dilepton final state

Final state must be massive!

Initial-state radiation

For $q_T/Q > 0$ one emission is always resolved





Intro: slicing methods: *q*_T subtraction formalism for massive final states

• <u>Massive final state</u> linear (m = 1) power corrections due to final-state emission



► <u>At NNLO</u>: linear (m=1) + log enhancement

analytical insight for inclusive cross section in pure QED

$$= -\frac{3\pi}{8} \frac{\alpha}{2\pi} r_{\text{cut}} \left[\frac{6(5-\beta^2)}{3-\beta^2} + \frac{-47+8\beta^2+3\beta^4}{\beta(3-\beta^2)} \log \frac{1+\beta}{1-\beta} \right]$$

$$= \sqrt{1-\frac{4m^2}{s}} \qquad \text{[LB, Grazzini, Tramontano, 2019]}$$

in general we have to rely on an extrapolation procedure!



Ingredients: two-loop massless amplitudes

Two-loop helicity virtual amplitudes for W boson and four partons available in the Leading-colour approximation (LCA)

- analytical expressions obtained within the framework of numerical unitary (using numerical samples)
- the results are expressed in terms of a basis of **one-mass pentagon functions** [Chicherin, Sotnikov, Zoia 2021]
- off-shell W boson including its leptonic decay
- publicly available <u>http://www.hep.fsu.edu/~ffebres/W4partons</u>
- analytical expressions of the one-loop amplitudes up to $\mathcal{O}(\epsilon^2)$ available in LCA

some complications

- Amplitudes provided as analytical expressions that can be processed in Mathematica; this is not suitable for on-the-fly numerical evaluation for Monte Carlo integration
- Rather long algebraic expressions akin to numerical round-off errors
- Reference process is $u\bar{b} \rightarrow \bar{b}de^+\nu_{\rho}$. Initial-final state crossing involves in general analytic continuation

















LCA and Massification

- contributions
- sizeable $C_F / (N_C / 2) \sim 0.89$ and $(C_F / (N_C / 2))^2 \sim 0.8$

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

with **OpenLoops2**

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• we have carried out the massification procedure in LCA to explicitly check the cancellation of the poles • however, in this way we are artificially introducing **spurious miscancellation** between real and virtual

• moreover, the terms introduced with the massification, being enhanced by large logarithms of μ^2/m^2 , are generally the dominant contributions and the difference between Full Colour and Leading Colour can be





WQQAmp: a massive C++ implementation

Dealing with the complications

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 (<u>https://github.com/lecopivo/OptimizeExpressionToC</u>)

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 (we found this step to be crucial)
- automatised generation of C++ source files for each block
- handling of numerical instabilities a posteriori with a simple rescue system (at integration stage)

Crossing

- simple permutation of the momenta in the algebraic coefficients
- 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]



Validation and checks

- two-loop massless amplitudes (stability) digits), apart for some points where it badly fails (simple rescue system)
- one-loop amplitudes in LCA **available in MCFM**, which allows to extract the LCA
- · Poles cancelled! Yang, 2009] (in LCA)

the C++ (double precision) code reproduces the massless results obtained with (quad precision) Mathematica for different phase space points and crossing of the amplitudes within the single floating-precision (7-9

we have tested both the massless and massive amplitudes against the independent implementation

the IR singularities of the massive amplitude agree with the ones predicted in [Ferroglia, Neubert, Pecjac,





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WQQAmp: a massive C++ implementation

WORKFLOW in a NUTSHELL

Evaluation of One-Loop bare amplitudes and Two-Loop Remainders





Wbb phenomenology (inclusive): total cross section

Behaviour of the perturbative series

• fixed scale

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

• dynamic scale

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

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

• qualitative similar results



Wbb phenomenology (inclusive): total cross section

Behaviour of the perturbative series

- Very large NLO corrections ($K_{\rm NLO} \sim 5$), due to opening of the quark-gluon channel. LO uncertainties bands completely unreliable
- **Starting from NNLO**, one start to see the convergence of the perturbative series with a reduction of both Kfactors ($K_{NNLO} \sim 1.6$) and theoretical uncertainties (scale variations), which are more reliable

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

order	$\sigma_{ m incl}[m pb]$
LO	$18.270(2)^{+28\%}_{-20\%}$
NLO	$60.851(7)^{+31\%}_{-21\%}$
NNLO	$96.91(8)^{+21\%}_{-17\%}$





Comparison with HPPZ: fiducial cross sections

order	$\sigma^{ m 4FS}[{ m fb}]$	$\sigma_{a=0.05}^{\mathrm{5FS}}\left[\mathrm{fb} ight]$	$\sigma^{\mathrm{5FS}}_{a=0.1} \mathrm{[fb]}$	$\sigma^{ m 5FS}_{a=0.2}[{ m fb}]$
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

- Use same running coupling and PDF set of the 5FS calculation
- Add the extra factor (due to the conversion between \overline{MS} and decoupling schemes): $-\alpha_s \frac{2T_R}{3\pi} \ln \frac{\mu_R^2}{m^2} \sigma_{q\bar{q}}^{\text{LO}}$ 2. No corrective term for pdfs at this order
- Take the massless limit $m_b \rightarrow 0$ 3.



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





Comparison with HPPZ: jet clustering algorithms

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

- because of the infrared problem





Comparison with HPPZ: additional 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)





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Comparison with HPPZ: r_{cut} dependence





 $d\sigma_{N^{k}LO} = \mathscr{H} \otimes d\sigma_{LO} + \left[d\sigma_{N^{k-1}LO}^{R} - d\sigma_{N^{k}LO}^{CT} \right]_{q_{T}/O > r_{\text{out}}} + \mathcal{O}(r_{\text{cut}}^{\ell})$

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 $\mathcal{O}(1\%)$ $\rightarrow \mathcal{O}(0.2\%)$ at the level of the total cross section

