Z boson production in association with bottom quarks at NNLO+PS

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in collaboration with Vasily Sotnikov and Marius Wiesemann [based on 2404.08598]



QCD@LHC, Freiburg, October 10th 2024

Motivation



- $m_b \sim 5 GeV$, not too big, not too small... both 4FS and 5FS are sensible choices
- When only large scales involved 5FS expected to perform better, while finite mass effects from 4FS are relevant at scales of O(m_b)
- Bottom-flavoured jets straightforwardly defined in 4FS
 [see talk by G. Stagnitto on
 flavour-sensitive jet algorithms]
- Both 4FS and 5FS known up to NLO+PS in QCD, also their combination in a variable flavour number scheme
- Significant differences between 4FS and 5FS at NLO, and tension between 4FS and data
- 4FS NLO predictions affected by large perturbative uncertainties

We aim to solve the tension by improving the 4FS predictions with the NNLO corrections, plus their matching to parton showers

Motivation

- It is also a very interesting project from a technical point of view:
 - Phenomenological application of one of the most complex two-loop amplitudes that can be obtained with current technology
 - First NNLO+PS generator for a genuine 2 → 3 QCD process
 - More importantly, it represents the first NNLO+PS for a process of the type heavy-quark+colourless



[dd]

 10^{3}

10

 10^{1}

 10^{-1}

ATLAS Preliminary

Run 1,2 √s = 5,7,8,13 TeV

Status: November 2022

√s = 13 Te\

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Quark Production

Cross

Section Measuremen

Outline

• NNLO+PS and heavy-quark production

• Extension to heavy-quark + colour singlet

• Z+bottom-pair production at NNLO+PS

• Summary and Outlook

Event generators

combining the high-energy scattering with PS and hadronization models are the cornerstone of experimental analyses



	F	F+j	F+2j
F@NNLO _{PS}	NNLO	NLO	LO

Non trivial task! Double counting between ME and shower, inclusion of virtual corrections, ...

NNLO+PS timeline

- NNLO+PS generators for colour-singlet production available for about 10 years
- Few years ago we extended the MiNNLO method to heavy-quark production
- First NNLO+PS generator for heavy-quark+colourless obtained earlier this year

Zbb, topic of this talk!



[timeline from M. Wiesemann, SM@LHC 23]

MiNNLO_{PS} for colour-singlet production

[Monni, Nason, Re, Wiesemann, Zanderighi]

- Derivation based on the connection between MiNLO' and q_T -resummation
- Starting point: low p_T factorization formula

$$d\sigma^{(\text{sing})} \sim d\sigma^{(0)}_{c\bar{c}} \times \exp\left[-S_c(b)\right] \times \left[HC_1C_2\right]_{c\bar{c};a_1a_2} \times f_{a_1}f_{a_2}$$



	F	F+j	F+2j
MiNLO'	NLO	NLO	LO
MiNNLO _{PS}	NNLO	NLO	LO

For details on the MiNNLO_{PS} colour-singlet derivation see the talk by S. Zanoli

- Numerically efficient, no reweighting involved (in variance to first MiNLO-based approaches)
- Applicable beyond 2 to 1 and, as we will see, even beyond colour singlet production

q_T resummation: color singlet

 $d\sigma^{(\text{sing})} \sim d\sigma^{(0)}_{c\bar{c}} \times \exp\left(-S_c\right) \times \left[HC_1C_2\right]_{c\bar{c};a_1a_2} \times f_{a_1}f_{a_2}$



Parton distribution functions

Collinear functions → hard-collinear emissions

Sudakov exponent \rightarrow soft and flavor diagonal emissions

Hard function \rightarrow hard process-dependent radiation

Resummed cross section physical (finite) when $p_T \rightarrow 0$

Can be computed at different logarithmic accuracies depending on which logs are included: LL: $\alpha_s^n L^{n+1}$ NLL: $\alpha_s^n L^n$ NNLL: $\alpha_s^n L^{n-1}$

Can also be 'matched' to the fixed order upon expansion in α_s :

NLL+NLO, NNLL+NLO, NNLL+NNLO

q_T resummation: heavy quark pairs

[1208.5774, 1307.2464, 1408.4564, 1806.01601]

Bold: operator in color space

 $|M\rangle$: vector in color space





Effects coming from soft emissions from the FS contained in operator $\pmb{\Delta}$

In the colour singlet case, H is given by the (IR-subtracted) all-orders matrix element for $cc \rightarrow F$

$$H = \operatorname{Tr}(\mathbf{H}) \sim \langle \mathcal{M} | \mathcal{M} \rangle$$

In the tt case, the presence of the operator Δ leads to non-trivial color correlations

 $\operatorname{Tr}(\mathbf{H}\Delta) \sim \langle \mathcal{M} | \Delta | \mathcal{M} \rangle$

$$d\sigma^{(\text{sing})} \sim d\sigma_{c\bar{c}}^{(0)} \times \exp\left[-S_{c}(b)\right] \times \left[\text{Tr}(\mathbf{H}\Delta)C_{1}C_{2}\right]_{c\bar{c};a_{1}a_{2}} \times f_{a_{1}}f_{a_{2}}$$

$$\text{Tr}(\mathbf{H}\Delta) \sim \langle \mathcal{M} | \Delta | \mathcal{M} \rangle \qquad \text{IR regulated virtual corrections}$$

$$\Delta \sim \exp\left\{-\int_{b_{0}^{2}/b^{2}}^{M} \frac{dq^{2}}{q^{2}} \Gamma(\alpha_{s}(q))\right\}^{\dagger} \mathbf{D}(\alpha_{s}(b_{0}/b), \phi) \exp\left\{-\int_{b_{0}^{2}/b^{2}}^{M} \frac{dq^{2}}{q^{2}} \Gamma(\alpha_{s}(q))\right\}$$
Exponential of soft anomalous dimension matrix Operator leading to azimuthal correlations

- Soft anomalous dimension encodes logarithmic behavior of soft wide-angle emissions
- **D** encodes the azimuthal dependence of the constant terms, with $\langle D \rangle_{\Phi,av} = 1$
- Even for q_T azimuthally-averaged cross sections, D contributes in the gluon channel due to the interference with the collinear coefficient functions (starting at NNLO)
- All the ingredients for NNLL+NNLO resummation known except for **D**⁽²⁾
- $D^{(2)}$ contributes with a constant term at $O(\alpha_s^4)$ that vanishes upon azimuthal average
- Translation between virtual corrections and IR-regulated *M* highly non trivial! The correct finite part of subtraction operator needs to be explicitly computed

$$|\mathcal{M}\rangle = \left(1 - \tilde{\mathbf{I}}\right) |\mathcal{M}\rangle_{\text{unreg}}$$

Extending MiNNLO: from colour singlet to $Q\overline{Q}$

• MiNNLO method for colour singlet has the q_T resummation formula as starting point:

$$d\sigma^{(\text{sing})} \sim d\sigma^{(0)}_{c\bar{c}} \times \exp\left(-S_c\right) \times \left[HC_1C_2\right]_{c\bar{c};a_1a_2} \times f_{a_1}f_{a_2}$$

• But now we have to deal with the more complicated $Q\overline{Q}$ structure:

$$d\sigma^{(\text{sing})} \sim d\sigma_{c\bar{c}}^{(0)} \times \exp\left(-S_{c}\right) \times \left[\text{Tr}(\mathbf{H}\Delta)C_{1}C_{2}\right]_{c\bar{c};a_{1}a_{2}} \times f_{a_{1}}f_{a_{2}}$$

We can modify the $Q\overline{Q}$ factorization formula as long as we keep NNLO accuracy (and LL in view of the matching with the shower)

We can take it into a shape that resembles the colorless final state case

Connection to MiNNLO derivation becomes simpler

$$\operatorname{Tr}(\mathbf{H}\Delta) \sim \langle \mathcal{M} | \Delta | \mathcal{M} \rangle \longrightarrow$$
 "Sudakov" $\times \langle \mathcal{M} | \mathcal{M} \rangle + \text{h.o.}$

[[]JM, Monni, Nason, Re, Wiesemann, Zanderighi]

MiNNLO for $Q\overline{Q}$ in three steps

(1) Simplify the exponential of the soft anomalous dimension

$$\langle \mathcal{M} | \boldsymbol{\Delta} | \mathcal{M} \rangle \sim \langle \mathcal{M} | \boldsymbol{\Delta}_{\mathrm{NLL}} | \mathcal{M} \rangle - \int \frac{dq^2}{q^2} \frac{\alpha_s^2(q)}{(2\pi)^2} \langle \mathcal{M}^{(0)} | \boldsymbol{\Gamma}^{(2)} + \boldsymbol{\Gamma}^{(2)\dagger} | \mathcal{M}^{(0)} \rangle$$

Same kind of term generated by B⁽²⁾

Can be absorbed in a modified $B^{(2)}$ coefficient! \blacktriangleleft

(2) Write the remaining factor in a 'factorized' form

This mismatch can also be absorbed (up to NNLO) in an additional redefinition of $B^{(2)}$

(3) Compute the remaining exponential in a basis in which $\Gamma^{(1)}$ is diagonal Sum of complex exponentials

Absorbe in a redefinition of B⁽¹⁾, which is now complex (done for each term in the sum)

• We therefore arrived to the "Sudakov" $\times \langle \mathcal{M} | \mathcal{M} \rangle + h.o.$

shape we were after, keeping NNLO accuracy

[JM, Monni, Nason, Re, Wiesemann, Zanderighi]



[JM, Ratti, Wiesemann, Zanderighi]

Extending MiNNLO: from $Q\overline{Q}$ to $Q\overline{Q}F$

Analytic expression for **H**⁽⁰⁾ matrix General implementation based on OpenLoops tree_colbasis

General implementation for $\langle D^{(1)*}G^{(1)} \rangle$ contribution (also numerical)

Extension of the calculation of soft contributions at low \boldsymbol{p}_{T} to general kinematics

. . . .

These contributions determine the exact subtraction operator in $|\mathcal{M}\rangle = \left(1 - \tilde{\mathbf{I}}\right) |\mathcal{M}\rangle_{\mathrm{unreg}}$

- I operator can be extracted from computation of $d\sigma/d^2q_{\scriptscriptstyle T}$
- Only new soft singularities wrt color singlet \rightarrow integrate the (subtracted) **soft current**

E.g. at NLO:

$$-\mathbf{J}(k)^{2}_{sub} = \sum_{J=3,4} \left[\frac{p_{J}^{2}}{(p_{J}\cdot k)^{2}} \mathbf{T}_{J}^{2} + \sum_{i=1,2} \left(\frac{p_{i}\cdot p_{J}}{p_{J}\cdot k} - \frac{p_{1}\cdot p_{2}}{(p_{1}+p_{2})\cdot k} \right) \frac{2\mathbf{T}_{i}\cdot\mathbf{T}_{J}}{p_{i}\cdot k} \right] + \frac{2p_{3}\cdot p_{4}}{(p_{3}\cdot k)(p_{4}\cdot k)} \mathbf{T}_{3}\cdot\mathbf{T}_{4}$$



• Numerical results pre-computed and implemented in 2-dimensional grid:

 $\left\{\beta = \sqrt{1 - \frac{4m^2}{s}}, \ \cos\theta\right\} \longrightarrow 5000 \text{ points optimized for t}\bar{t} \text{ production}$

- Grids afterwards fitted using a spline approximation, negligible uncertainties
- Note: many pieces of h_{34} we know analytically, but the evaluation of MPLs was slow, so those bits are also directly included in the numerical grids



Soft function for $Q\overline{Q}$ +colourless

Soft function for Heavy quark production in ARbitrary Kinematics





ttH

[Catani, JM et al. 2210.07846]

Extension to heavy-quark + colorless of equivalent $Q\overline{Q}$ calculations

Q Calculations atani, Devoto, Grazzini, JM, 2301.11786], e also [Angeles-Martinez, Czakon, Sapeta 1809.01459]

Implies removing back-to-back constraint for heavy quarks

New approach (on-the-fly) vs old results (grid+interpolation)

- C++ library for on-the-fly evaluation of soft function
- Most complicated pieces involve four-fold integrals integrated with VEGAS
- Validated against independent MATHEMATICA implementation
- About 1 second per phase space point typically enough for needed accuracy

Not a big problem for applications, but needs to be included in last stage via reweighting technique

This new development allowed not only for NNLO+PS for $Q\overline{Q}F$, but also to extend the q_T -subtraction method for this class of processes!

ttW



bbW

Soft function for Q\overline{Q}+colourless

Soft function for Heavy quark production in ARbitrary Kinematics





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Implies removing back-to-back constraint for heavy quarks

New approach (on-the-fly) vs old results (grid+interpolation)

C++ library for on-the-fly evaluation of soft function

Thanks to these developments the MiNNLO_{PS} formalism for

processes of the type $Q\overline{Q}F$ is ready to be used with full generality,

'only' needed ingredient are the process-dependent two loop corrections

Not a big problem for applications, but needs to be included in last stage via reweighting technique

This new development allowed not only for NNLO+PS for $Q\overline{Q}F$, but also to extend the q_T -subtraction method for this class of processes!

[Catani, JM et al. 2210.07846] [Buonocore, JM et al. 2306.1



$\mathbf{Z}\mathbf{b}\overline{\mathbf{b}}$ production

- NLO 5FS [Campbell, Ellis, Keith, Maltoni, Willenbrock '03]
- NLO 4FS [Febres Cordero, Reina, Wackeroth '08,'09] (see also [Campbell, Ellis, Keith '00])
- NLO+PS in MadGraph5 aMC@NLO [Frederix, Frixione, Hirschi, Maltoni, Pittau, Torrielli '11] (+ multi-jet merging in 5FS)
- NLO+PS in Sherpa [Krauss, Napoletano, Schumann '16] (+ multi-jet merging in 5FS)
- NLO+PS combination 4FS + 5FS [Höche, Krause, Siegert '19] (see also [Forte, Napoletano, Ubiali '18])
- NNLO in 5FS one b-jet [Gauld, Gehrmann-De Ridder, Glover, Huss, Majer '20]

NEW: First NNLO and NNLO+PS computation in 4FS [JM, Sotnikov, Wiesemann]

Two-loop corrections

• Full corrections (five-point two-loop amplitudes with massive b's) out of reach

Poles in 5FS \leftarrow Logs of m_b in 4FS

• We rely on massless amplitudes and apply a 'massification' procedure Re

2-loop finite reminder

(-(0)) = (2)

Recently applied as well to Wbb production [Buonocore, JM et al. '23]

$$\operatorname{Re}\left\langle \mathcal{R}_{0}^{(\circ)} \left| \mathcal{R}_{m_{b} \ll \mu_{h}}^{(\circ)} \right\rangle = \left[\overline{\mathcal{F}}^{(2)} \left| \mathcal{R}_{0}^{(0)} \right|^{2} + \overline{\mathcal{F}}^{(1)} \operatorname{Re}\left\langle \mathcal{R}_{0}^{(0)} \left| \mathcal{R}_{0}^{(1)} \right\rangle + \operatorname{Re}\left\langle \mathcal{R}_{0}^{(0)} \left| \overline{\mathbf{S}}^{(2)} \right| \mathcal{R}_{0}^{(0)} \right\rangle + \left[\operatorname{Re}\left\langle \mathcal{R}_{0}^{(0)} \right| \mathcal{R}_{0}^{(2)} \right\rangle \right] \right]$$

$$\operatorname{Massification coefficients}_{[\operatorname{Mitov, Moch '06]}} \left[\operatorname{Mitov, Moch '06]} \right]$$

- Log-enhanced terms (blue) obtained without approximations
- Massless two-loop reminder (red) computed from analytic results

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

- Obtained in the leading colour approximation $(1/N_c^2 \text{ corrections})$
- No contributions with Z coupling to closed quark loop (negligible at NLO)



Setup of the calculation

- 13TeV collisions, bb $\ell\ell$ final state with ℓ =e, μ , m_b=4.92GeV, NNPDF31
- MiNNLO central scale setting: $\mu_R = \mu_F = m_{bb\ell\ell} e^{-L}$, $Q = m_{bb\ell\ell}/2$ Born coupling central scale: $\mu_R^{(0)} = m_{bb\ell\ell}$
- Modified log L = log(Q/p_T) for $p_T < Q/2$, L = 0 for $p_T > Q$, interpolation in between
- Showering with Pythia8, using Monash tune Hadronization, multi-parton interactions and QED shower included
- OpenLoops for tree and one-loop amplitudes, including color- and spin-correlated
- Two-loop amplitudes from analytic results
 - Large expressions O(1Gb)

elaborate numerical stability checks and rescue system through higher precision

Evaluation of special functions through PentagonFunctions++

[Chicherin, Sotnikov, Zoia '21]

Total cross section

- We compute the total cross section only with a cut 66GeV < $m_{\ell\!\ell}$ < 116GeV
- We implemented an NLO+PS generator in the 4FS for comparison
- We compare as well with MiNLO' results (MiNNLO without $D^{(\geq 3)}$ terms)
- Only for these numbers: hadronization, MPI and QED shower are turned off

	$\sigma_{ m total} \; [m pb]$	ratio to NLO
NLO+PS $(m_{b\bar{b}\ell\ell})$ MINLO' $(m_{b\bar{b}\ell\ell})$ MINNLO _{PS} $(m_{b\bar{b}\ell\ell})$	$\begin{array}{c c} 31.86(1)^{+16.3\%}_{-13.3\%} \\ 22.33(1)^{+28.2\%}_{-17.9\%} \\ 50.58(4)^{+16.8\%}_{-12.2\%} \end{array}$	$1.000 \\ 0.701 \\ 1.588$
NLO+PS $(H_T/2)$ MINNLO _{PS} $(H_T/2)$	$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	$1.000 \\ 1.393$

• Very large NNLO corrections of O(50%) for both scale choices

NLO prediction and uncertainty estimation are not reliable!

- No reduction of scale uncertainties and no overlap with NLO band
- MiNLO' unphysical do to uncompensated log(m_b) fixed by two-loop virtuals
- Massless finite reminder contributes at few percent level (LCA uncertainties negligible)

Comparison to LHC measurements

• We compare to a recent measurement of Z+b-jets by CMS [CMS, 2112.09659]

Object	Selection
Dressed leptons	$p_{\rm T}$ (leading) > 35 GeV, $p_{\rm T}$ (subleading) > 25 GeV, $ \eta < 2.4$
Zboson	$71 < m_{\ell\ell} < 111{ m GeV}$
Generator-level b jet	b hadron jet, $p_{\mathrm{T}} > 30 \mathrm{GeV}$, $ \eta < 2.4$

• We compute fiducial cross sections at NLO+PS and NNLO+PS in the 4FS, and compare to CMS measurement and to NLO+PS in the 5FS

Obtained with MadGraph5, taken from CMS paper

$\sigma_{\rm fiducial} ~[{\rm pb}]$	$ Z+\geq 1 b$ -jet	$Z+\geq 2$ b-jets
NLO+PS $(5FS)$	7.03 ± 0.47	0.77 ± 0.07
NLO+PS (4FS)	4.08 ± 0.66	0.44 ± 0.08
$MINNLO_{PS}$ (4FS)	6.72 ± 0.91	0.79 ± 0.10
CMS	6.52 ± 0.43	0.65 ± 0.08

- Tension with data at NLO+PS in the 4FS, lifted with inclusion of NNLO corrections
- Excellent agreement between NNLO+PS (4FS) and NLO+PS (5FS) predictions

Differential distributions: Z+1b-jet



- NLO+PS normalization is completely off, p_{T} shape not well described either
- NNLO+PS is in remarkable agreement with data, both normalization and shape
- Theory uncertainties are still larger than experimental ones in most bins

[JM, Sotnikov, Wiesemann]

Differential distributions: Z+1b-jet



 $pp \rightarrow Z + \geq 1 \ b \text{ jet } @ 13 \text{ TeV}$

- Region of large separation between Z and leading b-jet in η - ϕ plane not well described
- Originates from region with large rapidity separation, also not well described
- Similar trend found in 5FS, though less pronounced
- Could be connected to large log(m_b) contributions

Differential distributions: Z+2b-jet



- Normalization of NNLO+PS slightly overshoots data, as seen at fiducial level for \geq 2b jet
- Still in good agreement within the uncertainties
- Experimental uncertainties are considerably larger due to lower statistics

Summary

- We have further extended the MiNNLO_{PS} method
- Our formalism is now ready to provide NNLO+PS for processes of the type $Q\overline{Q}$ +F
- Only process-dependent ingredient: two-loop amplitudes
- We finished the first application: $Zb\overline{b}$ at NNLO+PS
- Double-virtuals obtained through 'massification' procedure
- Most complicated final state simulated at NNLO+PS to date
- Huge improvement w.r.t. NLO+PS, good agreement with 5FS predictions and data

Outlook

- Further studies on $Zb\overline{b}$:
 - More detailed analysis of 4FS vs 5FS
 - Comparison to NNLO fixed-order
 - Dependence on shower settings
- Public release of the event generator
- Development of NNLO+PS generators for $Q\overline{Q}F$: $t\overline{t}H$, $t\overline{t}W$, $b\overline{b}H$, $b\overline{b}W$, ...

Thanks!