Heavy-quarks + colour singlet at NNLO+PS with MiNNLO

Javier Mazzitelli

Based on works on: MiNNLO for QQ, with P. Monni, P. Nason, A. Ratti, E. Re, M. Wiesemann and G. Zanderighi MiNNLO for QQF with M. Wiesemann Zbb at NNLO+PS with V. Sotnikov and M. Wiesemann Soft function for QQ with S. Catani, S. Devoto and M. Grazzini Soft function for QQF with S. Devoto

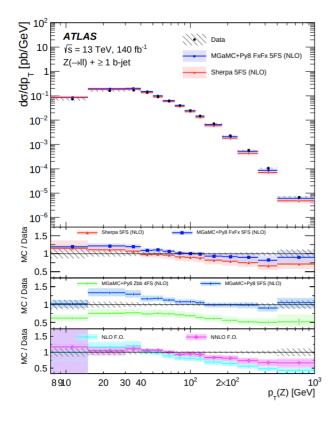
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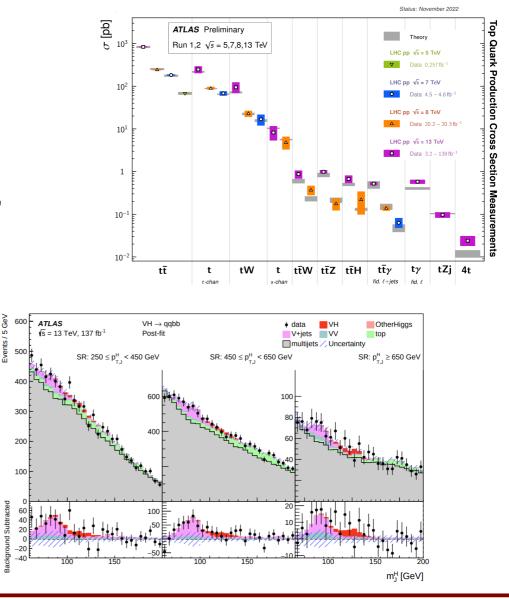


Ringberg 2024: 2nd Workshop on Tools for High Precision LHC Simulations

Heavy-quark (+colourless) production

- Huge number of very interesting signatures at the LHC involve heavy quarks
- Top quark of course...
- ... but not the only one! Heavy flavour production relevant in Higgs searches, BSM analyses, constraints to PDFs, heavy-flavour effects to other signatures (e.g. DY), and so on...





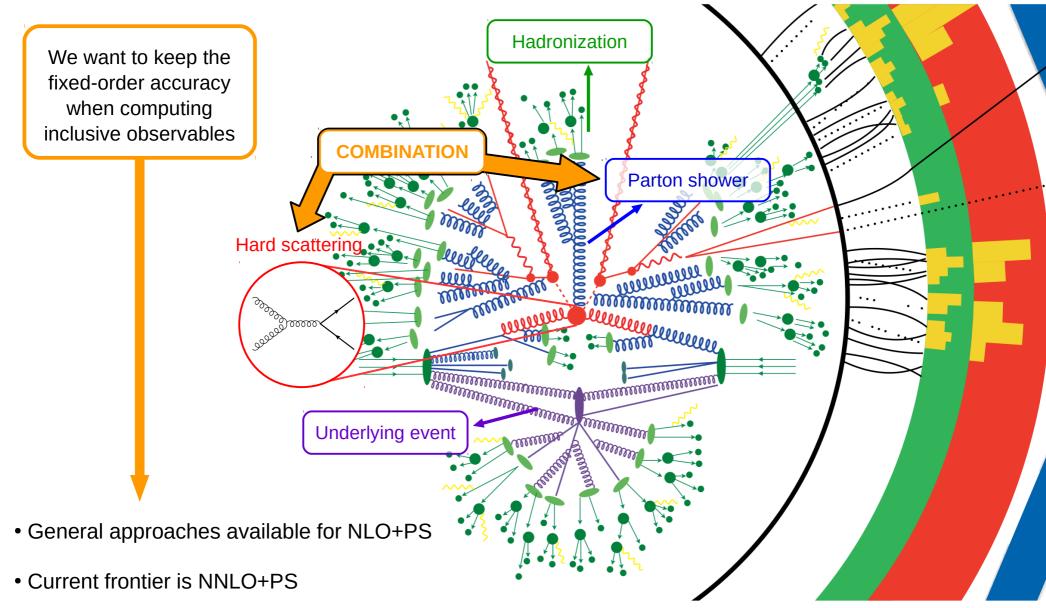
Accurate simulations for processes with heavy quarks are crucial to fully exploit their physics potential!

[see talks by

Kenneth and Miha]

Event generators

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

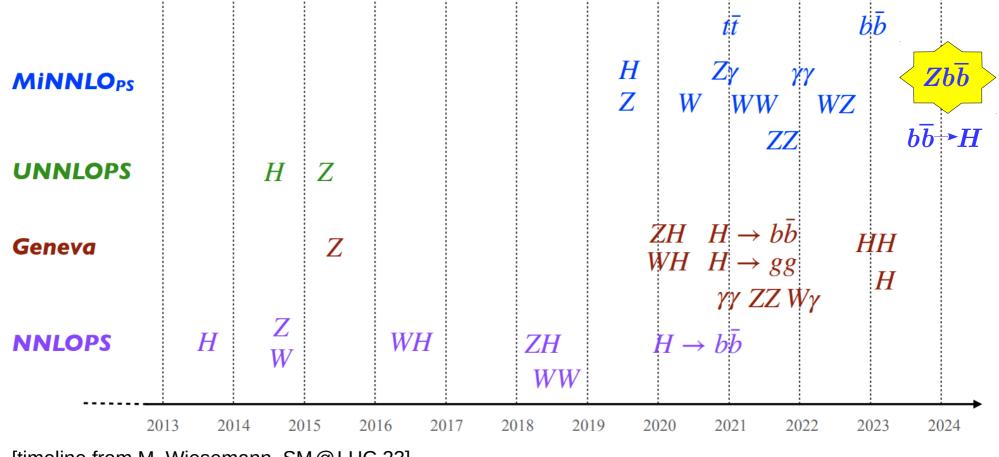


	F	F+j	F+2j
F@NNLO _{PS}	NNLO	NLO	LO

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
- We recently finished the first NNLO+PS generator for heavy-quark+colourless



Outline

• NNLO+PS for heavy-quark production

• Extension to heavy-quark + colour singlet

• Z+bottom-pair production at NNLO+PS

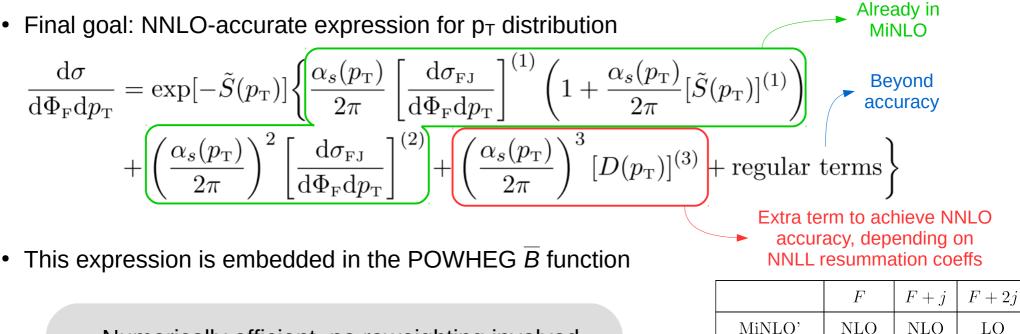
• Summary and Outlook

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

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



- 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

LO

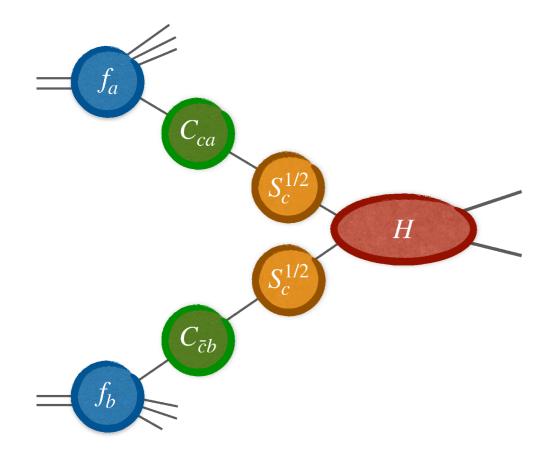
NNLO

MiNNLO_{PS}

NLO

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 :

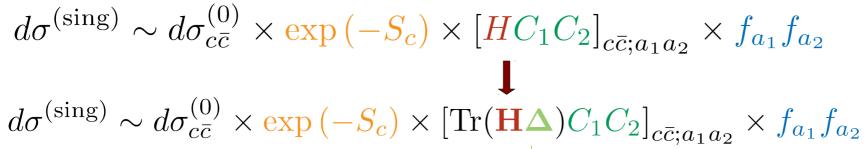
NLL+NLO, NNLL+NLO, NNLL+NNLO

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



(Ĉca S1/ H $C_{\bar{c}b}$

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" $\times \langle \mathcal{M} | \mathcal{M} \rangle + h.o.$

[[]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 arrived therefore to the desired expression keeping NNLO accuracy!

Computed by diagonalizing $\Gamma^{(1)}$ — Sum of complex exponentials

$$d\sigma^{(\text{sing})} \sim d\sigma^{(0)}_{c\bar{c}} \exp\left[-S_c''(b)\right] \left\langle \mathcal{M}^{(0)} \right| \exp\left[\int \frac{dq^2}{q^2} \frac{\alpha_s(q)}{2\pi} (\mathbf{\Gamma}^{(1)} + \mathbf{\Gamma}^{(1)\dagger})\right] \left| \mathcal{M}^{(0)} \right\rangle \left[\text{Tr}(\mathbf{H}\,\mathbf{D})C_1C_2\right]_{c\bar{c};a_1a_2}^{\phi} f_{a_1}f_{a_2}$$

Of the form
$$\sum_{i} \exp\left[-S(B \to B_i)\right]$$

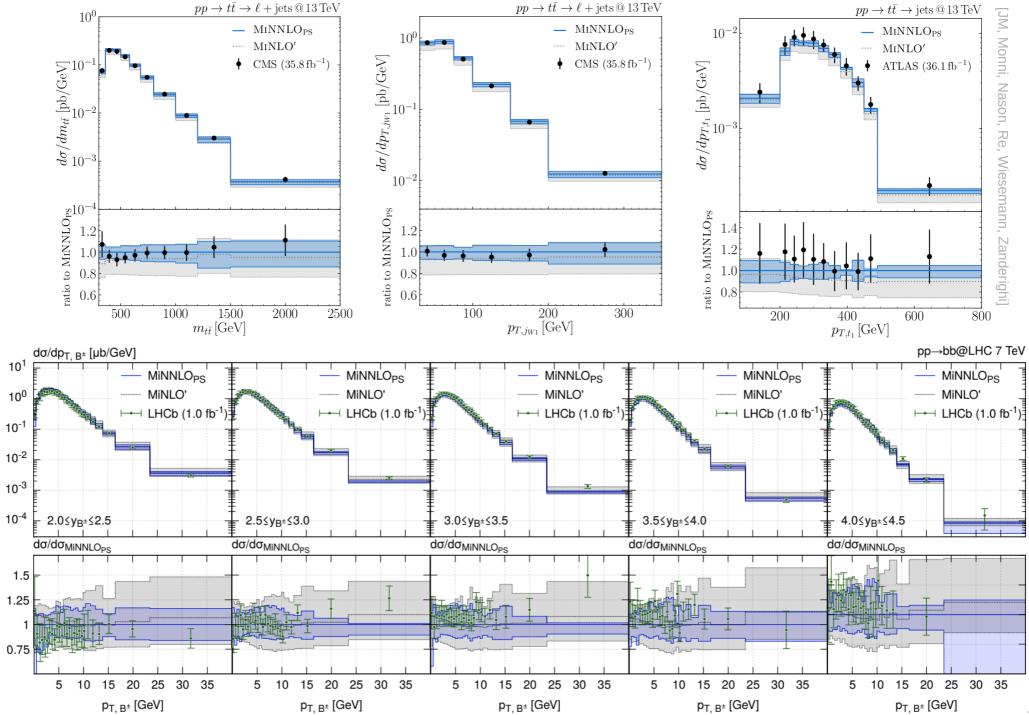
More precisely, each term is an 'usual' Sudakov form factor with an effective (complex) value of $B^{(1)}$ and $B^{(2)}$

Factorization formula was the starting point for color-singlet MiNNLO

Now we have a sum of colorless-final-state-like factorization formulas

Follow MiNNLO color-singlet derivation for each of them and arrive to MiNNLO for $Q\overline{Q}$

$Q\overline{Q}$ production at NNLO+PS



ΓJN,

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 $d\sigma/d^2q_T$
- Only new soft singularities \rightarrow integrate the (subtracted) **soft current**

E.g. at NLO:

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

Soft function for Q

$$\mathbf{h}(\alpha_{\rm S}) = 1 + \frac{\alpha_{\rm S}}{2\pi} \left(h_{34}^{(1)} \mathbf{T}_3 \cdot \mathbf{T}_4 + h_{33}^{(1)} C_F \right)$$

$$\mathbf{h}(\alpha_{\rm S}) = 1 + \frac{\alpha_{\rm S}}{2\pi} \left(h_{34}^{(1)} \mathbf{T}_3 \cdot \mathbf{T}_4 + h_{33}^{(1)} C_F \right)$$

$$\mathbf{Analytic results}$$

$$\mathbf{Numerical results}$$

$$+ \left(\frac{\alpha_{\rm S}}{2\pi} \right)^2 \left(h_{34}^{(2)} \mathbf{T}_3 \cdot \mathbf{T}_4 + h_{13}^{(2)} \mathbf{T}_1 \cdot \mathbf{T}_3 + h_{14}^{(2)} \mathbf{T}_1 \cdot \mathbf{T}_4 + h_{23}^{(2)} \mathbf{T}_2 \cdot \mathbf{T}_3 + h_{24}^{(2)} \mathbf{T}_2 \cdot \mathbf{T}_4 \right)$$

$$+ \left(h_{3434}^{(2)} \mathbf{T}_3 \cdot \mathbf{T}_4 \mathbf{T}_3 \cdot \mathbf{T}_4 + h_{3433}^{(2)} \mathbf{T}_3 \cdot \mathbf{T}_4 C_F + h_{3333}^{(2)} C_F^2 \right) + \mathcal{O}(\alpha_{\rm S}^3)$$
Contributions connecting two different massive legs
Contributions coming from the square of the NLO result, afterwards azimuthally averaged

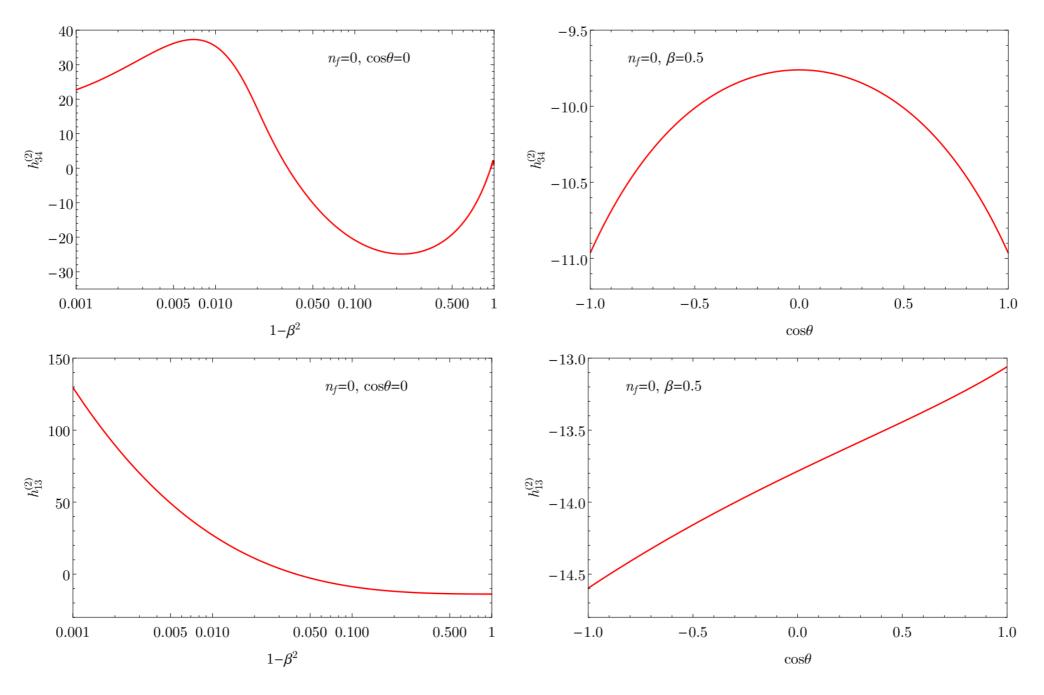
- Numerical integration: at most two-fold integrals, performed in MATHEMATICA
- Numerical results pre-computed and implemented in 2-dimensional grid:

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

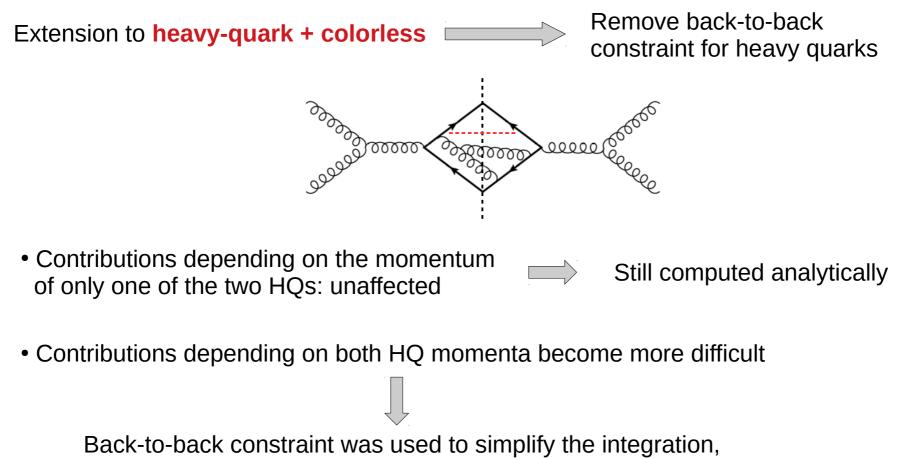
- Grids afterwards fitted using a spline approximation
- Uncertainties connected to all of this procedure are negligible
- Note: many pieces of h_{34} we know analytically, but the evaluation of MPLs was slow, so those bits are also directly included in the numerical grids

Soft function for $Q\overline{Q}$

From [Catani, Devoto, Grazzini, JM, 2301.11786], see also [Angeles-Martinez, Czakon, Sapeta 1809.01459]



Soft function for $Q\overline{Q}$ + colour singlet

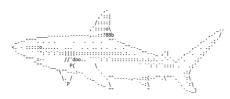


both of the pieces computed fully analytically as for the pieces that needed numerical integration in the last steps

We have to numerically perform up to 4-fold integrations

• Change of approach: go for on-the-fly evaluation, to avoid having to deal with a complicated 6-dimensional grid

Soft function for Heavy quark production in ARbitrary Kinematics



- C++ library for on-the-fly evaluation of soft function
- Numerical integration using VEGAS from gsl
- Most complicated parts: four-fold integrals
- Validated against independent MATHEMATICA implementation
- About 1 second per phase space point

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!

[see talk by Simone]



[Catani, JM et al. 2210.07846]

ttW

 $b\overline{b}W$

[Buonocore, JM et al. 2212.04954]

[Devoto, JM, in prep]

MiNNLO_{PS} formalism for $Q\overline{Q}F$ ready to go, 'only' needed ingredient are the process-dependent two loop corrections

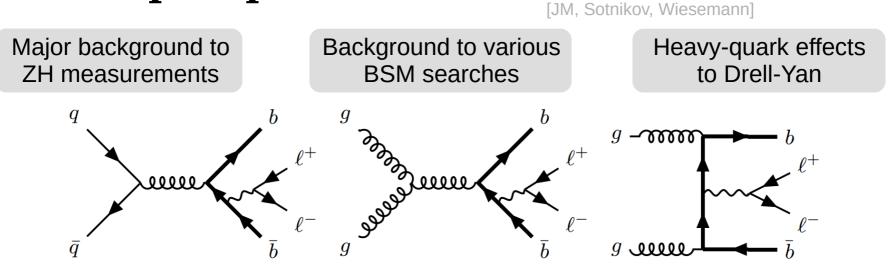
[Buonocore, JM et al. 2306.16311]

$Zb\overline{b}$ 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]

Z+bottom-pair production at NNLO+PS



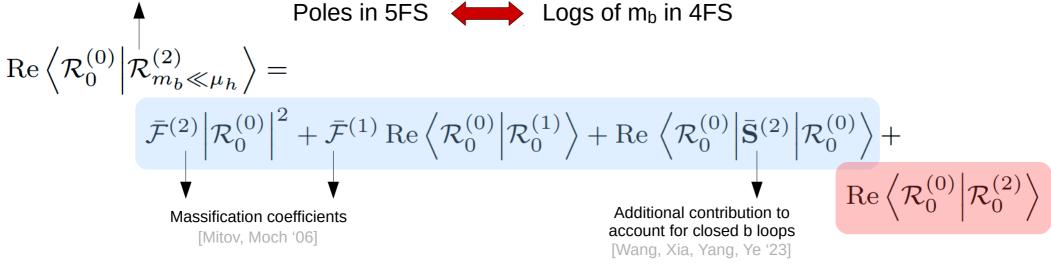
- $m_b \sim 5$ GeV, not too big, not too small... both 4FS and 5FS are sensible choices
- When only large scales involved 5FS expected to perform better, while finite mass effects from 4FS are relevant at scales of O(m_b)
- Bottom-flavoured jets straightforwardly defined in 4FS
- Both 4FS and 5FS known 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 improve the 4FS predictions by computing for the first time the NNLO corrections, and match them to parton showers with the MiNNLO method

Two-loop corrections

- Full corrections (five-point two-loop amplitudes with massive b's) out of reach
- We rely on massless amplitudes and apply a 'massification' procedure

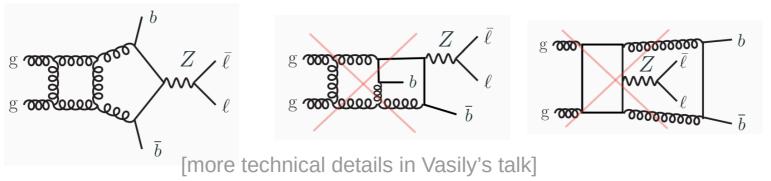
2-loop finite reminder



- 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 $\ell = e, \mu, m_b = 4.92 \text{GeV}, \text{NNPDF31}$
- 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

	$\mid \sigma_{\rm total} \; [{\rm pb}]$	ratio to NLO
NLO+PS $(m_{b\bar{b}\ell\ell})$ MINLO' $(m_{b\bar{b}\ell\ell})$ MINNLOPS $(m_{b\bar{b}\ell\ell})$	$ \begin{vmatrix} 32.21(0)^{+16.4\%}_{-13.4\%} \\ 22.33(1)^{+28.2\%}_{-17.9\%} \\ 51.23(4)^{+17.3\%}_{-12.4\%} \end{vmatrix} $	$1.000 \\ 0.693 \\ 1.591$
$\frac{1}{\text{NLO+PS } (H_T/2)}$ $\frac{1}{\text{MINNLO}_{PS} (H_T/2)}$	$ \begin{vmatrix} 40.14(1)^{+18.9\%} \\ -15.0\% \\ 58.70(4)^{+19.0\%} \\ -13.1\% \end{vmatrix} $	$1.000 \\ 1.462$

• 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 around 5% (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	$p_{\rm T}(\text{leading}) > 35 \text{GeV}, p_{\rm T}(\text{subleading}) > 25 \text{GeV}, \eta < 2.4$		
Zboson	$71 < m_{\ell\ell} < 111 { m GeV}$		
Generator-level b jet	b hadron jet, $p_{ m T}$ $>$ 30 GeV, $ \eta $ $<$ 2.4		

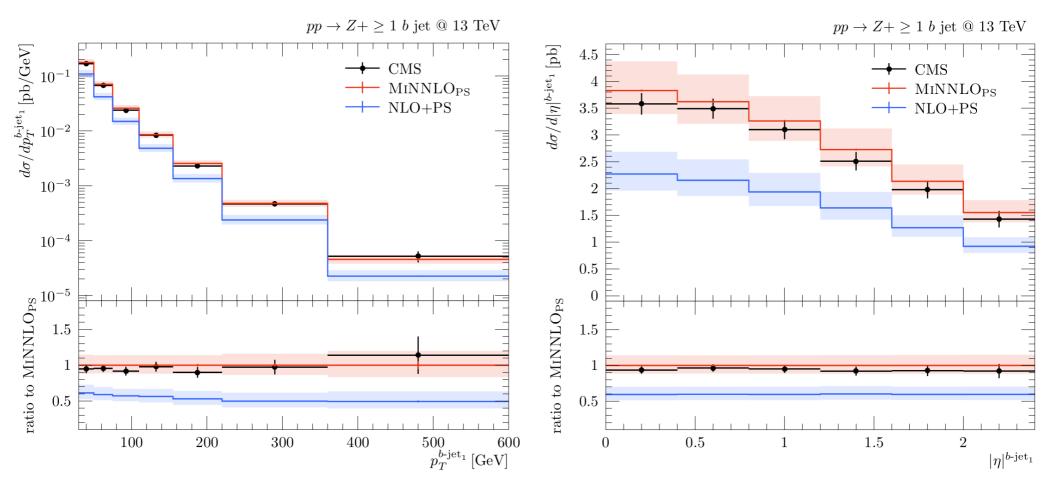
• We compute fiducial cross sections at NLO+PS and NNLO+PS in the 4FS, and compare to CMS measurement and to NLO+PS in the 5FS

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)	6.85 ± 0.98	0.80 ± 0.11
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

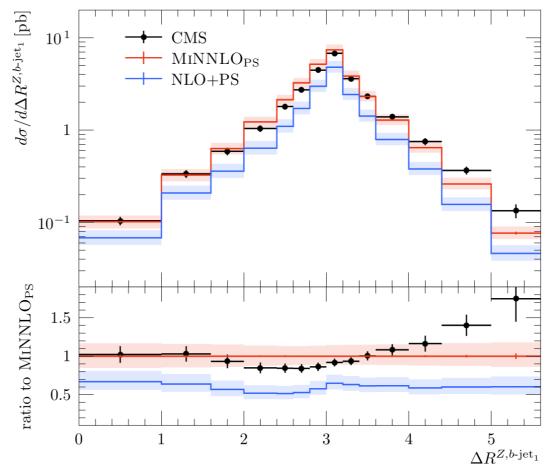
Differential distributions: Z+1b-jet



- 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

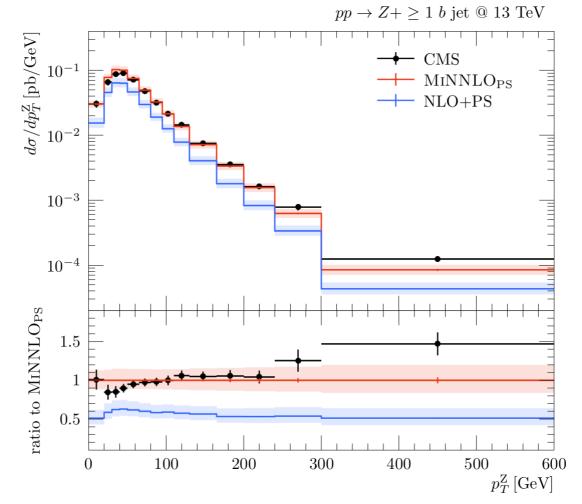


 $pp \rightarrow Z + \ge 1 \ b \text{ jet } @ 13 \ \text{TeV}$

- 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
- Simlar trend found in 5FS, though less pronounced
- Could be connected to large log(m_b) contributions

[JM, Sotnikov, Wiesemann]

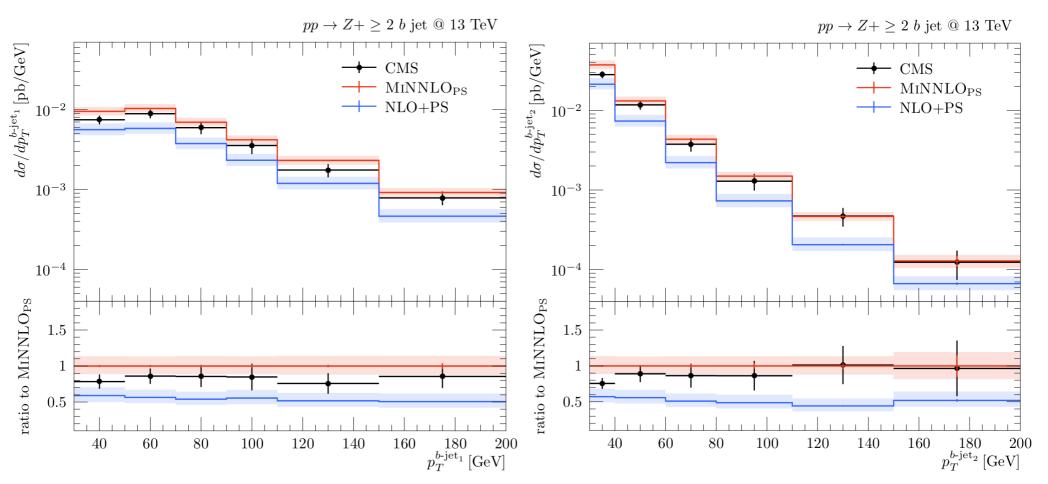
Differential distributions: Z+1b-jet



- Z-boson transverse momentum distribution well described by NNLO+PS within uncertainties
- Much improved description of shape compared to NLO+PS
- Prediction undershoots data in the last bins
- Would be good to test our results against the recent ATLAS measurement [2403.15093]

[see tension shown in Miha's talk]

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!