Predictions for Z-boson production in association with a $b$-jet at $\mathcal{O}(\alpha_s^3)$

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Fixed-order predictions are provided for the associated production of a Z-boson and a $b$-jet at $\mathcal{O}(\alpha_s^3)$ in perturbative QCD, obtained by combining a massless next-to-next-to-leading order and a massive next-to-leading order calculation. These predictions require a jet algorithm which leads to an infrared-safe definition of jet-flavour for massless quarks, for which we use the flavour-$k_T$ algorithm. A comparison to CMS data obtained in pp collisions at a centre-of-mass energy of 8 TeV is performed, which is first unfolded to account for an incompatible choice of jet algorithm. To quantify the agreement of the central prediction and data, a chi-squared is computed for the pseudorapidity and transverse-momentum distributions of the leading $b$-jet: $\chi^2/N_{\text{dat}}(\alpha_s^3, p_{T,b}) = 21.6/14$, $\chi^2/N_{\text{dat}}(\alpha_s^3, \eta_b) = 8.96/8$.

INTRODUCTION

The precise measurement of processes involving jets with identified flavour is of high phenomenological relevance at the LHC. Processes where a vector boson is produced in association with a flavoured jet are of particular interest due to the high production rate and clean experimental signature. Such measurements provide an important testing ground for perturbative QCD calculations involving flavoured jets, and can also be used to extract information on the flavour structure of protons. These processes also constitute the dominant background for measurements of the associated production of a (hadronically decaying) Higgs and vector boson. Theory predictions for these processes are currently available to next-to-leading order (NLO) accuracy matched to a Parton Shower (PS). However, in order to fully exploit the potential of current and prepare for more accurate future measurements, it is imperative to have more precise predictions at our disposal.

The purpose of this work is to fill this gap by presenting a precise calculation for flavoured-jet observables related to the process $pp \rightarrow Z + b$-jet. This is achieved by computing the next-to-next-to-leading order (NNLO) contribution to the massless (differential) cross-section for the process $pp \rightarrow Z + b$-jet, and by combining this with the corresponding massive computation for the production of a $Z + bb$ final state, up to the third order in the strong coupling, i.e at $\mathcal{O}(\alpha_s^3)$. Specifically, we perform an expansion of both massless and massive cross-section computations, and substitute the coefficient of the massless computation with that of the massive one at all orders at which it is known. The resulting prediction is fully differential, accounts for mass corrections up to $\mathcal{O}(\alpha_s^3)$ exactly, and additionally includes a resummation of the initial state logarithms associated to the heavy quark up to next-to-next-to-leading logarithmic accuracy (NNLL).

This method, often referred to as ‘FONLL’, has previously been applied to the description of exclusive flavoured hadron final states. QCD inclusive processes, inclusive cross-sections for several processes, as well as differential predictions of flavoured jets. An algorithm to apply this method in the context of multijet merging with Parton Showers was also recently developed. See also where these (and alternative) techniques have been developed. Here we extend this work by applying the method to fully differential (flavoured-jet) observables based on a massless NNLO calculation.

The computation of fixed-order flavoured-jet observables as described above must necessarily be performed with an algorithm that leads to an infrared-safe definition of jet flavour. However, the only available LHC data for this process have been presented for flavour-tagged jets which have been reconstructed with the anti-$k_T$ algorithm. The main issue with jet algorithms of this type is related to how wide-angle soft quark-antiquark pairs are clustered as part of the prediction. There is a possibility that only one of these (flavoured) soft quarks is clustered into a hard jet, altering its flavour, and thus rendering the definition of jet flavour sensitive to soft physics. Such a definition is not infrared safe, and for massless quarks the prediction is not finite. Therefore a direct comparison to data is not possible. To overcome this problem, we have performed an unfolding procedure to correct the data, which allows for a consistent comparison between theoretical predictions and data at the
level of infrared-safe observables.

In the following, we provide details of the ingredients of the calculation, before providing a comparison to available (unfolded) data from the CMS collaboration in pp collisions at $\sqrt{s} = 8$ TeV. We conclude with a discussion on the prospects of direct comparisons between perturbative QCD predictions and future LHC measurements.

DETAILS OF THE CALCULATION

In this work we are interested in the prediction of flavoured-jet observables for the process $pp \to Z + b$-jet at $\mathcal{O}(\alpha_s^3)$. We here wish to combine the computation performed in a scheme where the $b$-quark is treated as a massless parton (5fs) with that where mass effects of the $b$-quark are included exactly (4fs). Schematically, the combined cross-section is

$$d\sigma^{\text{FONLL}} = d\sigma^{5fs} + (d\sigma^{4fs}_{m_b} - d\sigma^{4fs}_{m_b \rightarrow 0}), \quad (1)$$

where $d\sigma^{5fs}$ is the massless 5fs prediction, $d\sigma^{4fs}_{m_b}$ is the massive 4fs prediction, and $d\sigma^{4fs}_{m_b \rightarrow 0}$ is the prediction obtained in the massless limit of the 4fs. It is further understood that each of these predictions has an expansion in terms of perturbative coefficients. The computation of all terms in Eq. (1) will be performed with parton distribution functions (PDFs) and $\alpha_s$ defined in the 5fs, and as a consequence it is necessary to re-write the contributions in parenthesis in terms of 5fs inputs. This can be achieved by applying the relevant $n_f$-dependent scheme corrections to the perturbative coefficients—see for example Eq. (3.15)–(3.16) of [6].

Massless calculation. The computation of $d\sigma^{5fs}$ at $\mathcal{O}(\alpha_s^3)$ requires the NNLO QCD calculation of the process $pp \to Z + \text{jet}$ in the 5fs. This has been computed for the first time in this work, based on the calculation of the process $pp \to Z + \text{jet}$ [40]. This previous computation, which is agnostic to the flavour of the out-going jet, was performed with the NNLOJET framework [40] and uses the antenna subtraction method [41–49] to obtain fully differential cross-section predictions after the analytical cancellation of all infrared divergences.

The main difference is that the computation of flavour sensitive observables for the $Z + b$-jet process requires the complete flavour and momentum information of all physical (squared) matrix elements and subtraction terms. This was not available previously in the $Z+\text{jet}$ calculation, but has been incorporated into the NNLOJET framework, allowing for the computation of flavoured-jet observables. See [50] for an overview of this procedure.

Massive calculation. To obtain the massive contribution $d\sigma^{4fs}_{m_b}$ at $\mathcal{O}(\alpha_s^3)$, originally computed in [51]–[52] for $Z + b\bar{b}$ production at NLO level, we use the automated framework aMC@NLO [53] [54] which has been operated with a number of external libraries [55]–[59].

Zero-mass limit. When taking the zero-mass limit of the massive coefficient, terms multiplied by power-corrections of the form $m_b^2/Q^2$ vanish, while finite and logarithmically divergent terms without such a pre-factor remain. These latter contributions are already included within $d\sigma^{5fs}$, and therefore must be subtracted from the massive coefficient to avoid double counting according to Eq. (1). Note that here we only discuss the presence of logarithmic divergences that can be associated to initial-state splittings, as the application of an infrared-safe (flavoured) jet algorithm will remove those divergences associated with final-state splittings.

The finite terms which are present in the zero-mass limit can be obtained from the 5fs massless computation discussed above by neglecting all $b$-quark initiated contributions, and by applying the necessary scheme corrections. The computation of the logarithmically divergent contributions can instead be performed in the following way. First, an expression for the $b$-quark PDF expanded up to $\mathcal{O}(\alpha_s^2)$ using the matching coefficients given in [8] should be obtained. This PDF is then convoluted with the massless partonic cross-section of the massless 5fs calculation (also expanded in $\alpha_s$), and the resultant terms of the convolution up to $\mathcal{O}(\alpha_s^3)$ are kept. The computation of these logarithmic corrections is performed with a specially tailored Monte Carlo programme, which includes the expressions for both the matching coefficients of [8] and the massless partonic cross-section up to $\mathcal{O}(\alpha_s^2)$.

Jet algorithm. It is essential for fixed-order computations to be applied to observables which are insensitive to both the dynamics of soft and collinear physics. To this end, we use the flavour-$k_T$ algorithm originally proposed in [52]. As compared to standard jet algorithms, the clustering procedure for this algorithm must have both the flavour and momentum information of the input particles. First, the flavour of pseudo(jets) is defined by the net flavour of its constituents, assigning $+1$ ($-1$) if a flavoured quark (antiquark) is present. Second, the definition of the distance measure of this algorithm (which determines the clustering outcome) depends on the flavour of the pseudojet being clustered. These steps are necessary to avoid situations where soft quarks can alter the flavour of a jet, as described above. In addition, the net flavour criterion also ensures that jets which contain (quasi)collinear quark pairs are not assigned an overall flavour based on such splittings. More details can be found in [14]–[32].

COMPARISON WITH 8 TeV CMS DATA

In this Section we perform a comparison of the $Z + b$-jet CMS data at 8 TeV provided in [37], and validate our implementation of Eq. (1). Before doing so we summarise the numerical set-up, and present details on the unfolding procedure which is applied to this data to make a consist-
ent comparison with our theoretical predictions possible.

**Numerical inputs.** All predictions are provided with the NNPDF3.1 NNLO PDF set \([60]\) with \(\alpha_s(M_Z) = 0.118\) and \(n_f^{\text{max}} = 5\), where both the PDF and \(\alpha_s\) values are accessed via LHAPDF \([61]\). The results are obtained using the \(G_{\mu}\)-scheme with the following values for the input parameters: \(M_Z^\text{\mu} = 91.1876\ \text{GeV}\), \(\Gamma_Z^\text{\mu} = 2.4952\ \text{GeV}\), \(M_W^\text{\mu} = 80.385\ \text{GeV}\), \(\Gamma_W^\text{\mu} = 2.085\ \text{GeV}\), and \(G_{\mu} = 1.16638 \times 10^{-5}\ \text{GeV}^{-2}\). Including also the universal corrections to the \(\rho\) parameter when determining the numerical values of \(\alpha\) and \(\sin^2 \theta_W\) as in \([62]\), leads to \(\alpha_{\text{eff.}} = 0.007779\) and \(\sin^2 \theta_W,\text{eff.} = 0.2293\). An uncertainty due to the impact of missing higher-order corrections is assessed in the predictions by varying the values of \(\mu_F\) and \(\mu_R\) by a factor of two around the central scale \(\mu_0 \equiv E_{T,Z}\), with the additional constraint that \(\frac{1}{2} \leq \mu_F/\mu_R \leq 2\). The scales are treated as correlated between the coefficients appearing in Eq. \((1)\). We follow the specific setup of the flavour-\(k_T\) algorithm adopted in \([50]\), where a value of \(\alpha = 2\) is used and a beam distance measure that includes a sum over both QCD partons as well as the reconstructed gauge boson is introduced.

**Unfolding.** As already highlighted, the fixed-order prediction for a flavoured-jet cross-section as defined in Eq. \((1)\) must be performed with an infrared-safe definition of jet flavour. However, there is no data available for the process \(pp \rightarrow Z + b\text{-jet} (or in fact any process) which uses such a definition of jet flavour. Instead, the current experimental approach is to first reconstruct anti-\(k_T\) jets, and then identify the flavour of these jets after the reconstruction process—see for example \([63,65]\). To address this issue, we have computed a non-perturbative correction to the CMS data \([37]\) as described below.

This data has been presented for anti-\(k_T\) \(b\)-jets, with a flavour assignment based on whether the jet contains \(B\)-hadron decay products and the additional requirement that \(\Delta R(B,\text{jet}) < 0.5\). To correct this data to the level of flavour-\(k_T\) jets, we apply an unfolding procedure with the RooUnfold \([66]\) package using the iterative Bayes method \([67]\). The input to this procedure is a theoretical model for the original data using both the anti-\(k_T\) algorithm (which is measured) and the flavour-\(k_T\) algorithm (which we wish to unfold to).

This model is provided with an NLO+PS prediction for \(Z + b\text{-jet}\) using aMC@NLO \([54]\) interfaced to Pythia8.243 \([85]\), which uses the set of numerical inputs as defined above. For the central value, we use a 5fs prediction of \(Z + \text{jet}\), where the \(b\)-jet contribution of this sample is extracted. The benefit of this approach is that the fragmentation component (e.g. \(g \rightarrow b\bar{b}\)) is resummed by the PS. To assess the uncertainty of this procedure, the unfolding is repeated taking into account the impact of scale variations in the model. Additionally, the whole procedure is repeated with a 4fs prediction, and the envelope of all of these results is assigned as an uncertainty. Finally, the unfolding procedure was also performed with a bin-by-bin unfolding method, which led to almost identical results for the considered distributions.

**Fiducial cross-section.** In Fig. \(1\) the cross-section predictions for the process \(pp \rightarrow Z + b\text{-jet}\) are shown within the fiducial region defined according to: \(p_{T,b} > 20\ \text{GeV}, |\eta_b| < 2.4,\) and \(M_{b,\ell} \in [71,111]\ \text{GeV}\). The \(b\)-jets are reconstructed with the flavour-\(k_T\) algorithm with \(R = 0.5\), with the additional constraint of \(\Delta R(b,\ell) > 0.5\). As discussed above, this matches the fiducial region of the data \([37]\) with the exception of the choice of the jet clustering algorithm.

The cross-section defined according to Eq. \((1)\) is labelled as ‘FONLL’, and predictions are shown at both \(O(\alpha_s^2)\) and \(O(\alpha_s^3)\) as a function of \(m_b\) (as it arises explicitly in the parenthesis on the r.h.s. of Eq. \((1)\)). The filled band indicates the uncertainty due to scale variation alone, and these predictions are then compared to the corresponding 5fs scheme predictions at each respective order. It is found that these two predictions coincide in the limit \(m_b \rightarrow 0\), which demonstrates that both the finite zero-mass and the logarithmically divergent terms have been correctly subtracted from the massive computation, thus providing an important cross-check of our implementation of Eq. \((1)\).

The physical prediction is obtained for the \(b\)-quark mass as indicated by the dashed vertical line at \(m_b^{\text{phys.}} = 4.92\ \text{GeV}\). At \(O(\alpha_s^2)\), the FONLL prediction is \(\sigma_{\text{FONLL}}(m_b^{\text{phys.}} = 4.92\ \text{GeV}) = 3.477_{-0.081}^{+0.081}\) (scales) pb. As compared to \(O(\alpha_s^3)\), a large reduction in the scale uncertainty of the prediction and a small negative shift on the central value is observed. Furthermore, it is found that the inclusion of mass corrections at \(O(\alpha_s^3)\) leads to a negative correction \((\approx -3\%)\). The impact of the mass corrections is as large as the scale uncertainty, which underpins the importance of including such corrections as part of a pre-
To compare this prediction to data, we perform the unfolding procedure for the fiducial cross-section region defined in [37], finding a correction of $c = 0.878^{+0.006}_{-0.009}$. It is found that the main contribution to this correction is the subtraction of a ‘fake’ rate from the data, corresponding to situations where an event which passes the fiducial selection when the anti-$k_T$ clustering is used, but does not pass the same selection when instead the flavour-$k_T$ clustering is employed. Applying this correction to the data gives $\sigma_{F_{\text{CMS}}, f-k_T} = 3.119 \pm 0.212^{+0.021}_{-0.032} \text{pb}$, where the first uncertainty is that of the original measurement and the second one due to the unfolding procedure. With respect to the central value of the FONLL $O(\alpha_s^3)$ prediction, conservatively taking only the experimental uncertainty into account, the agreement with the unfolded data is $1.69 \sigma$. In addition to the scale uncertainty shown in Fig. 1, an uncertainty due to PDF and variation of $\alpha_s(M_Z) = 0.118 \pm 0.001$ has also been assessed (at NLO), which gives $\delta \sigma(\text{PDF}, \alpha_s) = \pm 0.074 \text{ pb}$. The uncertainty of the prediction and unfolded data overlap when these additional sources of uncertainty are taken into account.

**Differential distributions.** As part of the measurement [37], a number of differential observables for the process $pp \rightarrow Z + b$-jet were considered. Here we have chosen to focus on the transverse momentum of the leading $b$-jet ($p_{T,b}$) as well as the absolute pseudorapidity of the leading $b$-jet ($\eta_b$). A more extensive study will be considered in a future work.

The $p_{T,b}$ distribution is shown in Fig. 2, where the absolute cross-section is shown in the upper panel, the ratio to data in the central panel, and the ratio to the NLO 5fs prediction in the lower panel. The FONLL predictions are provided at the physical $b$-quark mass, and the uncertainty due to scale variation is shown. The central result of the unfolded CMS data is indicated with black error bars, and the additional uncertainty due to the input model of the unfolding procedure is overlaid with a grey crossed fill. In the lower panel, we have included the central (N)NLO predictions in the 5fs scheme to indicate the relevance of the mass corrections. A large reduction in the scale uncertainties for this distribution are observed at $O(\alpha_s^3)$. The impact of the mass corrections is most relevant at small values of $p_{T,b}$, where they approximately amount to $-4\%$, while for large $p_{T,b}$ they essentially vanish. This behaviour is naively expected as a scale set by the power corrections is of the form $m_b^2/p_{T,b}^2$. Reasonable agreement with the data is found, although there is a tendency for the data to prefer a smaller normalisation.

To better quantify this agreement, we have computed the $\chi^2$ for this observable with respect to the central FONLL predictions, finding $\chi^2/N_{\text{dat}}(\alpha_s^3, p_{T,b}) = 24.9/14$ and $\chi^2/N_{\text{dat}}(\alpha_s^3, p_{T,b}) = 21.6/14$. This is an underestimate of the agreement as no correlations have been included in this test—they are not publicly available—and only the experimental (inner) uncertainty of the unfolded data has been used to be conservative. The latter choice is particularly relevant at large $p_{T,b}$ values, where the uncertainty on the modelling of the unfolding (outer) is relevant. In this region, the unfolding is sensitive to the modelling of events where the $Z$ boson recoils against a jet which originated from a hard $g \rightarrow b \bar{b}$ splitting.

The corresponding Figure for the $|\eta_b|$ distribution is shown in Fig. 3. As before, the $O(\alpha_s^3)$ corrections are essential for improving the precision of the theory predictions. These mass corrections are negative, and range from $-2\%$ at central pseudorapidities to $-4\%$ in the forward region. The mass corrections are observed to be most important for the $q\bar{q}$-induced channel, and therefore become more important at larger pseudorapidity values where the relative contribution of this channel increases. These corrections are important for improving the description of the data, particularly at central pseudorapidity values where the absolute cross-section is largest. Performing the chi-squared test as above leads to $\chi^2/N_{\text{dat}}(\alpha_s^3, |\eta_b|) = 15.1/8$ and $\chi^2/N_{\text{dat}}(\alpha_s^3, |\eta_b|) = 8.96/8$, therefore finding agreement between the most precise theoretical prediction and the unfolded data.

**DISCUSSION AND CONCLUSIONS**

In this work, we have performed a precision calculation for observables related to the process $pp \rightarrow Z+b$-jet. This has been achieved by combining a massless NNLO and a massive NLO computations at $O(\alpha_s^3)$. This is the first
time that such a matching has been performed with a fully differential NNLO massless computation. The predictions exhibit greatly reduced uncertainties and open the door for precision studies involving flavoured jets. The benefit of this approach is that the contribution to the cross-section which arises from collinear initial-state splittings of the form $g \rightarrow b\bar{b}$, can be conveniently resummed by PDF evolution as part of the massless calculation. This approach is suitable for all processes where these type of logarithmic corrections dominate the cross-section. At the same time, the impact of finite $b$-quark mass effects can easily be incorporated. As a consequence of using a massless calculation, it becomes necessary to use an infrared-safe definition of jet flavour, which does not align with the current choice made by experimentalists.

To tackle this issue, we have taken the approach to unfold the experimental data which allows for a consistent comparison between the precise theoretical computation and data. We have found reasonable agreement for the comparison between the precise theoretical computation and the experimental data which allows for a consistent comparison between the precise theoretical computation and data. This approach is suitable for all processes where these type of logarithmic corrections dominate the cross-section. At the same time, the impact of finite $b$-quark mass effects can easily be incorporated. As a consequence of using a massless calculation, it becomes necessary to use an infrared-safe definition of jet flavour, which does not align with the current choice made by experimentalists.

Figure 3: As in Fig. 2, now for the absolute psudorapidity distribution of the leading flavour-$k_T$ $b$-jet.
