#### Back-to-back azimuthal correlations in Z+jet events at 1 high transverse momentum in the TMD parton branching 2 method at next-to-leading order 3

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Abstract

Azimuthal correlations in Z+jet production at large transverse momenta are com-18 puted by matching Parton - Branching (PB) TMD parton distributions and showers with 19 NLO calculations via MCatNLO. The predictions are compared with those for dijet pro-20 duction in the same kinematic range. The azimuthal correlations  $\Delta \phi$  between the Z bo-21 son and the leading jet are steeper compared to those in dijet production at transverse 22 momenta  $\mathcal{O}(100)$  GeV, while they become similar for very high transverse momenta 23 24  $\mathcal{O}(1000)$  GeV. The different patterns of Z+jet and dijet azimuthal correlations can be used to search for potential *factorization - breaking* effects in the back-to-back region, which de-25 26 pend on the different color and spin structure of the final states and their interferences with the initial states. In order to investigate these effects experimentally, we propose to 27 measure the ratio of the distributions in  $\Delta \phi$  for Z+jet- and multijet production at low and 28 at high transverse momenta, and compare the results to predictions obtained assuming 29 30 factorization. We examine the role of theoretical uncertainties by performing variations of the factorization scale, renormalization scale and matching scale. In particular, we 31 32 present a comparative study of matching scale uncertainties in the cases of PB-TMD and collinear parton showers. 33

# **1** Introduction

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The description of jet production in association with a Z boson in hadron-hadron collisions 35 is an important test of predictions obtained in Quantum Chromodynamics (QCD), and pro-36 vides a relevant background to Higgs boson studies and to new physics searches. The asso-37 ciated Z boson plus jet production has been measured by CDF and D0 in proton-antiproton 38 collisions at a center-of-mass energy  $\sqrt{s} = 1.96$  TeV [1,2]. At the LHC the ATLAS and CMS 39 collaborations have published measurements in proton-proton (pp) collisions at a center-of-40 mass energy  $\sqrt{s} = 7$  TeV [3–5], 8 TeV [6] and 13 TeV [7,8]. Azimuthal correlations between 41 Z bosons and jets have been measured at 8 TeV [6] and 13 TeV [8]. 42 The distribution in the azimuthal angle  $\Delta \phi$  between the Z boson and the jet is an espe-43 cially sensitive observable, probing several aspects of QCD physics. At leading order in the 44 strong coupling  $\alpha_s$ , one has  $\Delta \phi = \pi$ . The smearing of this delta-like distribution is a mea-45 sure of higher order QCD radiation. In the region near  $\Delta \phi = \pi$ , this is primarily soft gluon 46 radiation, while in the region of small  $\Delta \phi$  it is primarily hard QCD radiation. The large- $\Delta \phi$ 47 region of nearly back-to-back Z boson and jet is influenced by both perturbative and non-48 perturbative QCD contributions. The relative significance of these contributions depends on 49 the scale of the transverse momentum imbalance between the boson and the jet. Importantly, 50 the resummation of soft multi-gluon emissions in the nearly back-to-back region probes the 51 transverse momenta of the initial state partons, which can be described by transverse mo-52 mentum dependent (TMD) [9] parton distribution functions (PDFs). Theoretical predictions 53 for Z boson + jet production including soft gluon resummation have recently been given in 54 Refs. [10–14]. 55 All the experimental measurements of boson-jet azimuthal correlations that have been 56

the jets of the order  $p_{\rm T} \approx \mathcal{O}(100)$  GeV. In this kinematical range, fixed-order perturbative 58 corrections beyond next-to-leading order (NLO) are sizeable, and at small  $\Delta \phi$  NLO calcu-59 lations are usually not sufficient for reliable predictions. For the large- $\Delta\phi$  region of nearly 60 back-to-back Z boson and jet, the boson-jet  $p_{\rm T}$  imbalance scale is of order a few GeV, which 61 is significantly influenced by both perturbative resummation and non-perturbative effects. 62 It is worth noting that all the experimental measurements performed up to now do not cover 63 the large  $\Delta \phi$ , nearly back-to-back region with sufficiently fine binning to investigate detailed 64 features of QCD. 65

<sup>66</sup> With the increase in luminosity at the LHC, it becomes possible to measure Z+jet pro-<sup>67</sup> duction in the high  $p_{\rm T}$  range, with  $p_{\rm T} \approx \mathcal{O}(1000)$  GeV. In this work, we observe that in this <sup>68</sup> kinematical range the resummation of soft gluons and TMD dynamics in the nearly back-<sup>69</sup> to-back region can be explored in a new regime, characterized by boson-jet  $p_{\rm T}$  imbalance <sup>70</sup> scales on the order of a few ten GeV. The large- $\Delta\phi$  region, involving deviations of the order <sup>71</sup> of the experimental angular resolution of about 1 degree from  $\Delta\phi = \pi$ , can be investigated <sup>72</sup> by analyzing jets with measurable transverse momenta.

Based on the above observation, in this paper we propose experimental investigations of 73 back-to-back azimuthal correlations in the  $p_T \approx \mathcal{O}(1000)$  GeV region, with a systematic scan 74 of the large- $\Delta \phi$  regime from this high  $p_{\rm T}$  region down to  $p_{\rm T} \approx \mathcal{O}(100)$  GeV – a regime which 75 is completely unexplored experimentally up to now. We present dedicated phenomenologi-76 cal studies of this  $\Delta \phi$  region as a function of  $p_{\rm T}$ , enabling one to explore boson-jet transverse 77 momentum imbalances from a jet scale of several ten GeV down to the few GeV scale. To 78 perform these studies, we use the Parton Branching (PB) approach [15,16] to TMD evolution, 79 matched to NLO calculations of Z+jet production with MADGRAPH5\_AMC@NLO [17]. 80 This approach has already been successfully applied, across a wide energy and mass range, 81 to the Z boson  $p_{\rm T}$  spectrum at the LHC [18] and the Drell-Yan (DY)  $p_{\rm T}$  spectrum at lower 82 fixed-target energies [19], so that the investigation of the same method in the Z+jet case is 83 compelling. The  $\Delta\phi$  correlation in the kinematical range proposed in this paper allows one 84 to study the interplay of perturbative and non-perturbative contributions to TMD dynamics 85 (see e.g. [20] for the DY case) as a function of both the boson-jet  $p_{\rm T}$  imbalance and the evolu-86 tion scale of the TMD distribution itself, of the order of the hard scale of the process, given 87 by the transverse momenta of the Z boson or the jet. 88

In a previous publication [21] we have investigated the  $\Delta \phi_{12}$  correlation in high- $p_{\rm T}$  dijet 89 events by applying TMD PDFs and parton shower together with NLO calculations of the 90 hard scattering process. In multijet events the azimuthal correlation between two jets has 91 been measured at the LHC by ATLAS and CMS [22–26]. The region of  $\Delta \phi_{12} \rightarrow \pi$  is of special 92 interest, since so-called factorization - breaking [27-29] effects could become important in the 93 case of colored final states. Multijet production is believed to be sensitive to such effects, as 94 well as vector boson + jet production [30]. In order to investigate factorization - breaking ef-95 fects, we propose to compare the theoretical description of the azimuthal correlation  $\Delta \phi_{12}$  in 96 multijet production with the one in Z+jet production. A thorough investigation of azimuthal 97 correlations in the back-to-back region in Z+jet events has been also performed in Ref. [10], 98 addressing the issue of factorization - breaking. 99

In this report we compare in detail high- $p_{\rm T}$  dijet and Z+jet production by applying the 100 PB TMD method [15, 16] at NLO. In Ref. [21] these PB TMD PDFs were applied to multijet 101 production at large transverse momenta. We apply the same method to the calculation of 102 Z+jet production. We propose to use the same kinematic region for the high- $p_{\rm T}$  dijet and 103 Z+jet production to allow a direct comparison of the measurements. At large enough  $p_{\rm T}$  the 104 mass of the Z-boson becomes negligible, and the different color and spin structure of the final 105 states might allow to observe factorization - breaking effects by comparing the measurements 106 to calculations assuming that factorization holds. 107

In the following, we start by describing the basic elements of the PB TMD method and the Z+jet calculation in Sec. 2. In Sec. 3 we present results for the Z+jet azimuthal correlations and compare them with the multijet case. We summarize in Sec. 4. In an appendix we discuss technical details on the use of MCatNLO+CASCADE3.

### 112 2 Basic elements of the calculation

In this section we first recall the salient features of the PB TMD approach, summarizing the main concepts of the approach and its applications; then we describe the calculation of Z+jet production by the PB TMD method matched with NLO matrix elements in MAD-GRAPH5\_AMC@NLO.

### 117 2.1 PB TMD method

The PB approach [16] provides a formulation for the evolution of TMD parton distributions 118 in terms of perturbatively calculable Sudakov form factors and real-emission splitting ker-119 nels, with angular ordering phase space constraints and with non-perturbative distributions 120 at the initial scale of the evolution to be determined from fits to experiment. This formulation 121 uses a soft-gluon resolution scale  $z_M$  [15] to separate resolvable and non-resolvable branch-122 ings. An important feature of the PB TMD evolution equation [16] concerns its collinear 123 limits: upon integration over all transverse momenta, the PB TMD evolution equation re-124 turns the DGLAP [31–34] equation for resolution scale  $z_M \rightarrow 1$ , while it coincides with 125 the CMW [35, 36] coherent branching equation for angular-ordered  $z_M$  [37]. The PB TMD 126 method is based on the "unitarity" picture [38] of parton evolution usually employed in 127 parton showering Monte Carlo (MC) algorithms [39,40]. The PB evolution equation for the 128 TMD distributions is matched by a corresponding TMD parton shower for the spacelike par-129 ton cascade, generated by "backward evolution" [41]. A significant difference with respect to 130 ordinary parton showers is that in the PB TMD method TMD distributions are defined and 131 determined from fits to experimental data, which places constraints on fixed-scale inputs 132 to evolution, while in ordinary parton showers instead nonperturbative physics parameters 133 and showering parameters are tuned. No MC tuning is performed in the PB TMD case. 134 The NLO PB collinear and TMD parton distributions were obtained in Ref. [42] from QCD

<sup>135</sup> The NLO PB collinear and TMD parton distributions were obtained in Ref. [42] from QCD <sup>136</sup> fits to precision DIS data from HERA [43] using the xFitter analysis framework [44,45]. Two

different sets, PB-NLO-2018-Set 1 and PB-NLO-2018-Set 2, were obtained, with PB-NLO-137 2018-Set 1 corresponding at collinear level to HERAPDF 2.0 NLO [43]. In PB-NLO-2018-Set 2 138 the transverse momentum (instead of the evolution scale in Set 1) is used as the scale in the 139 running coupling  $\alpha_s$  which corresponds to the angular ordering of soft gluon emissions in the 140 initial-state parton evolution [36,37,46,47]. It has been shown in [18,19] that Set 2 provides a 141 better description of experimental measurements for the Z - boson spectrum at small low- $p_{\rm T}$ . 142 Also, it has been shown in [21] that the transverse momentum scale in the running coupling 143  $\alpha_{\rm s}$  is important for a good description of data on di-jet angular correlations. In this paper we 144 will concentrate on Set 2 only. 145 In Fig. 1 we show the TMD PDF distributions for up quarks and gluons at x = 0.01

In Fig. 1 we show the TMD PDF distributions for up quarks and gluons at x = 0.01and  $\mu = 100$  and 1000 GeV for PB-NLO-2018-Set 2. The transverse momentum distribution of gluons is broader than that of quarks, due to gluon self-coupling and the different color factors. In Fig. 1 also the uncertainties of the distributions, as obtained from the fit [42], are shown. The differences in the transverse momentum spectra of quarks and gluons will show

up in differences in azimuthal correlation distributions.

PB-NLO-HERAI+II-2018-set2, x = 0.01, µ = 100 GeV PB-NLO-HERAI+II-2018-set2, x = 0.01, μ = 1000 GeV xA(x,k,u) ×A(x,k,μ) aluor aluon 10 10 10-10-10-10 TMDplotter 2.2.4 TMDplotter 2.2.4 10 10-10 10 10 10 1.2 ĭ.2 1. 1. 0.9 0.9 08 0.8 10  $10^{2}$ 10 10 10 10 k, [GeV] k, [GeV]

Figure 1: TMD parton density distributions for up quarks and gluons of PB-NLO-2018-Set 2 as a function of  $k_{\rm T}$  at  $\mu = 100$  and 1000 GeV and x = 0.01. In the lower panels show the full uncertainty of the TMD PDFs, as obtained from the fits [42].

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The PB TMD evolution equation resums Sudakov logarithms. Current calculations in the PB TMD approach are performed with leading-logarithm (LL) and next-to-leading-logarithm (NLL) accuracy. The accuracy can be systematically improved, and the extension to next-tonext-to-leading logarithmic (NNLL) accuracy is being studied. In this respect, the approach can be compared [48] with analytic resummation methods [49, 50]. The extraction of TMD distributions from the PB TMD fits described above could be compared with extractions, such as [51, 52], based on [49, 50]. The TMDlib tool [53, 54] is designed as an aid for such
studies. On the other hand, while analytic resummation approaches apply to the inclusive
transverse momentum spectrum, the PB TMD approach works at exclusive level and can be
applied to make predictions not only for the inclusive spectrum but also for the structure of
the final states.

A framework to compute theoretical predictions combining the PB TMD resummation 163 with fixed-order NLO matrix elements in MADGRAPH5\_AMC@NLO has been developed 164 in [18,19]. The predictions [18] have been successfully compared with LHC measurements of 165 Z boson  $p_{\rm T}$  and  $\phi^*$  distributions [55–57]. Predictions by this method have also been success-166 ful in describing [19] DY  $p_{\rm T}$  spectra at lower masses and energies [58–61]. The significance 167 of this result is enhanced by the recent observation [62] that fixed-order NNLO corrections 168 are not extremely large in the kinematic region of the data. This framework has also been 169 applied to di-jet production [21], and predictions for di-jet correlations have been found in 170 good agreement with LHC measurements [25,26]. We will employ this framework for Z+jet 171 production in the next subsection. 172

As a method which is applicable at the level of exclusive final states, the PB TMD approach can be used in the context of multi-jet merging algorithms. A TMD multi-jet merging method has been developed in [63]. Its application to Z boson + multi-jets production [63,64] illustrates that transverse momentum recoils in the initial-state showers [65–67] influence significantly the theoretical systematics associated with the merging parameters. In the present paper, we will concentrate on the Z+jet back-to-back region, rather than the multi-jet production region, and we will therefore not use the TMD merging procedure.

Recently, the PB TMD evolution equation has been generalized to include TMD splitting functions [68,69], defined through high-energy factorization [70]. This generalization is important particularly for processes sensitive to TMD distributions at small values of longitudinal momentum fractions x. In this paper we consider processes at mid to large x and we do not consider it in the following.

### **2.2** Calculation of Z+jet distributions

The process Z+jet at NLO is calculated with MADGRAPH5\_AMC@NLO using the collinear PB-NLO-2018-Set 2, as obtained in Ref. [42] applying  $\alpha_s(M_Z) = 0.118$ . The matching of NLO matrix elements with PB TMD parton distributions is described in Refs. [18,19,41]. The extension to multijet production is illustrated in Ref. [21]. Predictions are obtained by processing the MADGRAPH5\_AMC@NLO event files in LHE format [71] through CASCADE3 [41] for an inclusion of TMD effects in the initial state and for simulation of the corresponding parton shower (labeled MCatNLO+CAS3 in the following).

Fixed order NLO Z+jet production is calculated with MADGRAPH5\_AMC@NLO in a procedure similar to the one applied for dijet production described in [21] (labeled MCatNLO(fNLO)). For the MCatNLO mode, the HERWIG6 [72, 73] subtraction terms are calculated, as they are best suited for the use with PB - parton densities, because both apply the same angular ordering condition. The use HERWIG6 subtraction terms together with <sup>198</sup> CASCADE3 is justified in appendix Section 5 for final state parton shower as well as initial <sup>199</sup> and final state showers by a comparison of the predictions obtained with CASCADE3 and <sup>200</sup> with HERWIG6. The matching scale  $\mu_m$  = SCALUP limits the contribution from PB-TMDs <sup>201</sup> and TMD showers.

In the calculations, the factorization and renormalization scales are set to  $\mu = \frac{1}{2} \sum_{i} p_{T,i}$ , where the index *i* runs over all particles in the matrix element final state. This scale is also used in the PB-TMD parton distribution  $\mathcal{A}(x, k_T, \mu)$ . The scale uncertainties of the predictions are obtained from variations of the scales around the central value in the 7-point scheme avoiding extreme cases of variation.



Figure 2: Transverse momentum spectrum of the Z+jet-system  $p_{T,Zj}$  (left) and  $\Delta \phi_{Zj}$  distribution (right). The predictions are shown for fixed NLO (MCatNLO(fNLO), the (unphysical) distribution at LHE-level and after inclusion of PB-TMDs (MCatNLO+CAS3).

In Fig. 2 we show the distributions of the transverse momentum of the Z+jet system, 207  $p_{T,Z_i}$ , and the azimuthal correlation in the Z+jet system,  $\Delta \phi_{Z_i}$ , for a fixed NLO calcula-208 tion, for the full simulation including PB-TMD PDFs and parton showers as well as for the 209 MCatNLO calculation at the level where subtraction terms are included without addition 210 from parton shower (LHE-level). We require a transverse momentum  $p_{\rm T} > 200$  GeV for the 211 Z boson and define jets with the anti- $k_{\rm T}$  jet-algorithm [74], as implemented in the FASTJET 212 package [75], with a distance parameter of R=0.4. The effect of including PB-TMD PDFs 213 and parton showers can be clearly seen from the difference to the fixed NLO and LHE-level 214 calculations. 215

In the low  $p_{T,Zj}$  region one can clearly see the expected steeply rising behavior of the fixed NLO prediction. In the  $\Delta \phi_{Zj}$  distribution one can observe the limited region for fixed NLO at  $\Delta \phi_{Zj} < 2/3\pi$ , since at most two jets in addition to the Z boson appear in the calculation. At large  $\Delta \phi_{Zj}$ , the fixed NLO prediction rises faster than the full calculation including resummation via PB-TMDs and parton showers. In the following we concentrate on the large  $\Delta \phi_{Zj}$  region.

# Back-to-back azimuthal correlations in Z+jet and multijet pro duction

We now present predictions, obtained in the framework described above, for Z+jet and multijet production.\* The selection of events follows the one of azimuthal correlations  $\Delta \phi_{12}$  in the back-to-back region ( $\Delta \phi_{12} \rightarrow \pi$ ) in multijet production at  $\sqrt{s} = 13$  TeV as obtained by CMS [26]: jets are reconstructed with the anti- $k_{\rm T}$  algorithm [74] with a distance parameter of 0.4 in the rapidity range of |y| < 2.4. We require either two jets with  $p_{\rm T}^{\rm leading} > 200$  GeV or a Z boson and a jet as leading or subleading objects with a transverse momentum  $p_{\rm T}^{\rm leading} > 200$  GeV.

<sup>231</sup> We consider distributions of the azimuthal correlation between the Z boson and the lead-<sup>232</sup> ing jet,  $\Delta \phi_{\text{Zj}}$ , for  $p_{\text{T}}^{\text{leading}} > 200 \text{ GeV}$  as well as for the very high  $p_{\text{T}}$  region of  $p_{\text{T}}^{\text{leading}} > 1000$ <sup>233</sup> GeV.

The calculations are performed with MCatNLO+CAS3 using PB-NLO-2018-Set 2 as the collinear and TMD parton densities with running coupling satisfying  $\alpha_s(m_Z) = 0.118$  and PB-TMD parton shower.



Figure 3: Predictions of the azimuthal correlation  $\Delta \phi_{Zj}(\Delta \phi_{12})$  for Z+jet and multijet processes in the back-to-back region for  $p_T^{\text{leading}} > 200 \text{ GeV}$  (left) and  $p_T^{\text{leading}} > 1000 \text{ GeV}$  (right) obtained from MCatNLO+CAS3. Shown are the uncertainties obtained from scale variation (as described in the text). The measurements of dijet correlations as obtained by CMS [26] are shown as data points, for comparison.

In Fig. 3, the prediction for the azimuthal correlations  $\Delta \phi_{Zj}$  for Z+jet production in the back-to-back region is shown.<sup>†</sup> We also show, for comparison, the prediction of azimuthal correlations  $\Delta \phi_{12}$  for multijet production in the same kinematic region, compared to the measurement of dijet production obtained by CMS [26]. We observe that the distribution

<sup>\*</sup>A framework based on CCFM evolution [76] was described in [77,78] for multi-jet and vector boson + jet correlations.

<sup>&</sup>lt;sup>+</sup>Predictions for the region of small  $\Delta \phi$  require including the contribution of higher parton multiplicities, e.g. via multi-jet merging [63].

of azimuthal angle  $\Delta \phi_{Zj}$  in Z+jet-production for  $p_T^{\text{leading}} > 200 \text{ GeV}$  is more strongly correlated towards  $\pi$  than the distribution of angle  $\Delta \phi_{12}$  in multijet production. This difference is reduced for  $p_T^{\text{leading}} > 1000 \text{ GeV}$ .

Differences in  $\Delta \phi$  between Z+jet and multijet production can result from the different flavor composition of the initial state and therefore different initial state transverse momenta and initial state parton shower, as well as from differences in final state showering since both processes have a different number of colored final state partons. Effects coming from factorization - breaking, interference between initial and final state partons, will depend on the final state structure and the number of colored final state partons.

We first investigate the role of initial state radiation and the dependence on the trans-250 verse momentum distributions coming from the TMD PDFs, which gives a large contribu-251 tion to the decorrelation in  $\Delta \phi$ . The k<sub>T</sub>-distribution obtained from a gluon TMD PDF is 252 different from the one of a quark TMD PDF as shown in Fig. 1 for x = 0.01 and scales of 253  $\mu = 200(1000)$  GeV. In Fig. 4 we show the probability of gg, qg and qq initial states (q stands 254 for quark and antiquark) as a function of  $p_{\rm T}^{\rm leading}$  for Z+jet and multijet production obtained 255 with MCatNLO+CAS3. At high  $p_{\rm T}^{\rm leading} > 1000$  GeV the qq channel becomes important for 256 both Z+jet and multijet final states, while at lower  $p_{\rm T}^{\rm leading} > 200$  GeV the gg channel is domi-257 nant in multijet production, leading to larger decorrelation effects, since gluons radiate more 258 compared to quarks.



Figure 4: The probability of gg, qg and qq initial states in Z+jet and multijet production (q stands for quark and antiquark) as a function of  $p_{T}^{\text{leading}}$ . The predictions are calculated with MCatNLO+CAS3.

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The role of final state radiation in the correlation in  $\Delta \phi_{12}$  distributions is more difficult 260 to estimate, since the subtraction terms for the NLO matrix element calculation also depend 261 on the structure of the final state parton shower. In order to estimate the effect of final state 262 shower we compare a calculation of the azimuthal correlations in the back-to-back region 263 obtained with MCatNLO+CAS3 with the one obtained with MCatNLO+PYTHIA8 (Fig. 5). 264 For the calculation MCatNLO+PYTHIA8 we apply the PYTHIA8 subtraction terms in the 265 MADGRAPH5\_AMC@NLO calculation, use the NNPDF3.0 [79] parton density and tune 266 CUETP8M1 [80]. 267

As shown in Fig. 5, the distributions are different because of the different parton shower in CASCADE3 and PYTHIA8, but the ratio of the distributions for Z+jet and multijet produc-



Figure 5: Predictions for the azimuthal correlation  $\Delta \phi_{Zj}(\Delta \phi_{12})$  in the back-to-back region for Z+jet and multijet production obtained with MCatNLO+CAS3 (left column) and MCatNLO+PYTHIA8 (right column). Shown are different regions in  $p_T^{\text{leading}} > 200 \text{ GeV}$  (upper row) and  $p_T^{\text{leading}} > 1000 \text{ GeV}$ (lower row). The bands show the uncertainties obtained from scale variation (as described in the text).

tion are similar: Z+jet-production gives a steeper (more strongly correlated) distribution at low  $p_{\rm T}^{\rm leading}$ , while at high  $p_{\rm T}^{\rm leading}$  the distributions become similar in shape. We conclude, that the main effect of the  $\Delta\phi$  decorrelation comes from initial state radiation, and the shape of the  $\Delta\phi$  decorrelation in the back-to-back region becomes similar between Z+jet and dijet processes at high  $p_{\rm T}^{\rm leading}$  where similar initial partonic states are important.

The matching scale  $\mu_m$  limits the hardness of parton-shower emissions, and is thus typically a non-negligible source of variation in matched calculations (see e.g. [81] for a detailed

discussion). It is thus interesting to assess the robustness of the previous findings under 277 variations of the matching scale. Assessing matching scale variations in both an angular-278 ordered shower - such as CASCADE3 - and a transverse-momentum-ordered shower -279 such as PYTHIA8 – additionally tests the *interpretation* of the matching scale. In transverse-280 momentum ordered showers, the matching scale sets the maximal transverse momentum of 28 the first shower branchings, while branchings beyond the first emission are not explicitly af-282 fected by the matching scale. In an angular-ordered shower, however, the matching scale is 283 applied as "veto scale" to avoid larger transverse momenta for any branching, i.e. the match-284 ing scale directly affects all branchings. The result of changing the matching scale to half or 285 twice the central value is shown in Fig. 6. As expected, the value of the matching scale has 286 an impact on the prediction (~ 5%). This is particularly apparent when  $\mu_m$  is used to set 287 the maximal transverse momentum of the first emission in PYTHIA8. Overall, we find that 288 interpreting the matching scale as veto scale in CASCADE3 leads to apparently more robust 289 predictions. Interestingly, the matching scale uncertainty becomes smaller for higher- $p_{\rm T}^{\rm leading}$ 290 jet configurations in CASCADE3. The size of the matching scale variation is comparable to 291 scale variations, and should thus be carefully studied when designing uncertainty estimates. 292 In dijet production the measurements are rather well described with predictions obtained 293 with MCatNLO+CAS3, as shown in Fig. 3 and discussed in detail in Ref. [21]. Only in the 294 very high  $p_{\mathrm{T}}^{\mathrm{leading}}$  region, a deviation from the measurement is observed, which could be 295 perhaps interpreted as coming from a violation of factorization. It is therefore very important 296 to measure  $\Delta \phi$  distributions in other processes, where factorization is expected to hold. 297 In order to experimentally probe effects which could originate from factorization - break-298

<sup>295</sup> ing in the back-to-back region we propose to measure the ratio of distributions in  $\Delta \phi_{Zj}$  for <sup>300</sup> Z+jet and  $\Delta \phi_{12}$  for multijet production at low and very high  $p_T^{\text{leading}}$ , and compare the mea-<sup>301</sup> surement with predictions assuming that factorization holds. The number of colored partons <sup>302</sup> involved in Z+jet and multijet events is different, and deviations from factorization will de-<sup>303</sup> pend on the structure of the colored initial and final state. In order to minimize the effect of <sup>304</sup> different initial state configurations, a measurement at high  $p_T^{\text{leading}}$ , could hint more clearly <sup>305</sup> possible factorization - breaking effects.

In Ref. [10] a detailed study on Z+jet azimuthal correlations is reported, applying TMDfactorization and the "winner-takes-all" jet recombination scheme, with the aim to reduce potential factorization breaking contributions. We have checked, that our main results remain unchanged when the "winner-takes-all" jet recombination scheme is applied, only in the last bin of the  $\Delta \phi_{Zj}$  distributions the cross section is reduced.

# **311 4 Summary and conclusions**

We have investigated azimuthal correlations in Z+jet production and compared predictions with those for multijet production in the same kinematic range. The predictions are based on PB-TMD distributions with NLO calculations via MCatNLO supplemented by PB-TMD parton showers via CASCADE3. The azimuthal correlations  $\Delta \phi_{Zj}$ , obtained in Z+jet production



Figure 6: The dependence on the variation of the matching scale  $\mu_m$  in predictions for the azimuthal correlation  $\Delta\phi_{\rm Zj}(\Delta\phi_{12})$  in the back-to-back region. Shown are predictions obtained with MCatNLO+CAS3 (left column) and MCatNLO+PYTHIA8 (right column) for  $p_{\rm T}^{\rm leading} > 200 \,\text{GeV}$  (upper row) and  $p_{\rm T}^{\rm leading} > 1000 \,\text{GeV}$  (lower row). The predictions with different matching scales  $\mu_m$  varied by a factor of two up and down are shown.

are steeper compared to those in multijet production ( $\Delta \phi_{12}$ ) at transverse momenta  $\mathcal{O}(100)$ GeV, while they become similar for very high transverse momenta,  $\mathcal{O}(1000)$  GeV, which is a result of similar initial parton configuration of both processes.

In Z+jet production the color and spin structure of the partonic final state is different compared to the one in multijet production, and differences in the azimuthal correlation patterns can be used to search for potential factorization - breaking effects, involving initial and final state interferences. In order to experimentally investigate those effects, we propose to measure the ratio of the distributions in  $\Delta \phi_{Zj}$  for Z+jet- and  $\Delta \phi_{12}$  for multijet production at low and at very high  $p_T^{\text{leading}}$ , and compare the measurements to predictions obtained assuming that factorization holds.

We have studied the matching scale dependence in the PB-TMD predictions and compared it with the case of NLO-matched calculations based on the PYTHIA8 collinear shower. We find that variations of the matching scale lead to more stable predictions in the PB-TMD

case, with the relative reduction of the matching scale theoretical uncertainty becoming more pronounced for increasing  $p_{\rm T}^{\rm leading}$  transverse momenta.

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# **5** Appendix: Comparison of CASCADE3 and HERWIG6

The calculations presented here apply the MCatNLOmethod using HERWIG6 (H6) subtraction terms, as implemented in MADGRAPH5\_AMC@NLO. The NLO accuracy of the calculations is preserved by construction, since the use of PB-TMD distributions and TMD shower, as ordinary parton showers, does not change the inclusive cross section.

Since HERWIG6 (H6) subtraction terms are used in the MCatNLO+CAS3 calculations, 339 we investigate here in detail the contribution of the parton shower used in CASCADE3. We 340 compare predictions obtained with MCatNLO+CAS3 with the corresponding ones obtained 341 with MCatNLO+H6, using the same LHE files used for the predictions in this paper. We 342 study the jet distributions obtained with the anti- $k_{\rm T}$  algorithm with distance parameter 0.4 343 in Z+jet events with  $p_{\rm T} > 30$  GeVand  $|\eta| < 5$ . We compare distributions of the first and 344 second jet in Z+jet events: the first (highest  $p_{\rm T}$ ) jet is part of the lowest order process, while 345 the second (highest  $p_{\rm T}$ ) jet is the real correction and therefore subject to subtraction terms 346 (keeping in mind that the highest  $p_{\rm T}$  jet in an NLO calculation can also come from the real 347 correction). 348

In H6 the allowed region of z for a branching  $q \rightarrow qg$  in the shower is  $Q_q/Q < z < 1 - Q_g/Q$  (e.g. A.2.2 in Ref. [82]), with  $Q_q = m_q + \text{VQCUT}$  and  $Q_g = m_g + \text{VGCUT}$ , and  $m_q, m_g$ being the quark and gluon effective masses, and VQCUT, VGCUT the minimum virtuality parameters.

First we investigate final state parton showers. In CASCADE3, the PYTHIA6 final state shower is used (since the PB - method has not yet been applied for final state radiation), with the angular ordering veto condition. Since final state radiation is independent of parton densities, a direct comparison of MCatNLO+CAS3 and MCatNLO+H6, using the same LHE files, while only simulating final state radiation, is possible. In Fig. 7 we show a comparison of predictions for the transverse momentum of the first two highest  $p_{\rm T}$  jets in Z+jet events (using identical LHE files).

The uncertainty coming from different parameter settings in the H6 final state parton shower is estimated by changing the light quark masses from the default to 0.32 GeV(Rmas = 0.32, labelled as  $m_l$ ) and VQCUT, VGCUT from the default to 0.1(1.5), labelled as  $Vc_l(Vc_h)$ , respectively (the lowest values chosen are those for which H6 is still working).

In Fig. 8 comparison is shown for the pseudorapidity  $\eta$  of the first two highest  $p_{\rm T}$  jets. Within the variation of the parameters, the prediction of MCatNLO+CAS3 agrees with the one of MCatNLO+H6, justifying the application of the PYTHIA6 final state parton shower algorithm.

Next we investigate the contribution of PB - TMD PDFs and the PB - TMD parton shower in the initial state and compare the predictions with the ones from H6. Since in H6 the initial state parton shower cannot be applied alone, but only in combination with the final state shower, we perform a similar calculation also with CASCADE3. In Fig. 9 we show a comparison of MCatNLO+CAS3 and MCatNLO+H6 predictions (including the same parameter variations for H6 as for the final state shower) for the transverse momentum of the first two highest  $p_{\rm T}$  jets. In Fig. 10 the corresponding comparison is shown for the pseudorapidity dis-



Figure 7: Comparison of predictions obtained with MCatNLO+CAS3 and MCatNLO+H6 for Z+jet obtained with MCatNLO. Shown are predictions using only final state parton shower. The band of MCatNLO+CAS3 shows the uncertainties obtained from scale variation (as described in the text).



Figure 8: Comparison of predictions obtained with MCatNLO+CAS3 and MCatNLO+H6 for Z+jet obtained with MCatNLO. Shown are predictions using only final state parton shower. The band of MCatNLO+CAS3 show the uncertainties obtained from scale variation (as described in the text).

tributions. The transverse momentum distributions agree well within the uncertainties coming from parameter variations, while for the  $\eta$ -distributions some differences in the very forward/backward regions are seen. However, one can see, that a variation of VQCUT, VGCUT

<sup>378</sup> has an significant effect especially in the forward/backward region. Since these parameters

are very different from the ones used in PB TMD PDFs and the PB - TMD shower, we con clude that the use of H6 subtraction terms in MCatNLO is consistent with the use of PB TMD PDFs, PB - TMD initial state parton shower, as applied in MCatNLO+CAS3.



Figure 9: Comparison of predictions obtained with MCatNLO+CAS3 and MCatNLO+H6 for Z+jet obtained with MCatNLO. Shown are predictions using initial and final state parton shower. The band of MCatNLO+CAS3 show the uncertainties obtained from scale variation (as described in the text).

381



Figure 10: Comparison of predictions obtained with MCatNLO+CAS3 and MCatNLO+H6 for Z+jet obtained with MCatNLO. Shown are predictions using initial and final state parton shower. The band of MCatNLO+CAS3 show the uncertainties obtained from scale variation (as described in the text).

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