COMPARISON OF CMS MEASUREMENTS WITH PREDICTIONS AT NLO APPLYING THE PARTON BRANCHING METHOD AND PYTHIA

Fernando Guzman $o^{a,\dagger}$, Si Hyun Jeon $o^{b,\dagger}$, Hannes Jung $o^{c,\dagger}$ Danyer Pérez Adán $o^{c,\dagger}$, Markus Seidel $o^{d,\dagger}$ Sara Taheri Monfared $o^{c,\dagger}$

^aInstituto Superior de Tecnologías y Ciencias Aplicadas, La Habana, Cuba ^bBoston University, Boston, USA ^cDeutsches Elektronen-Synchrotron DESY, Hamburg, Germany ^dRiga Technical University, Riga, Latvia

FATEME ALMAKSUSI ^{©‡}, DANIEL BELMONTE PÉREZ ^{©‡} DORUKHAN BONCUKCU ^{©‡}, ALEKSANDR BOGER ^{©‡} EMMANUEL BOTERO OSORIO ^{©‡}, ISADORA BOZZA GALVÃO ^{©‡} JUAN ESTEBAN OSPINA HOLGUÍN ^{©‡}, BEHNAM FALAHI ^{©‡} FAEZE GAGONANI ^{©‡}, OMAR GONZÁLEZ ^{©‡} AÇELYA DENIZ GÜNGÖRDÜ ^{©‡}, ABDELHAMID HADDAD ^{©‡} MAHTAB JALALVANDI ^{©‡}, JOSUÉ DANIEL JARAMILLO ^{©‡} JESUS JIMENEZ ZEPEDA ^{©‡}, GLEB KUTYREV ^{©‡} NAZANIN ZAHRA NOROUZI ^{©‡}, NESTOR RAUL MANCILLA XINTO ^{©‡} HARITZ MENTASTE ^{©‡}, LUCAS JOHNNY MONTE TAMAYO ^{©‡} FERNANDA MORA REY ^{©‡}, INMACULADA MOYANO REJANO ^{©‡} VIBHA PADMANABHAN ^{©‡}, MAYVI PEDRAZA ^{©‡}, SWAPNIL RATHORE ^{©‡} QURATULAIN ZAHOOR ^{©‡}, HAOLIANG ZHENG ^{©‡}

> Received 27 March 2024, accepted 17 April 2024, published online 7 May 2024

In August 2023, more than 30 students joined the *Special Remote DESY Summer School* to work on projects of importance for the LHC experiments. In a dedicated initiative, analyses that had not been incorporated into the Rivet package were implemented and verified. Here, a brief description of the accomplished work is given, and a comparison of the measurements with predictions obtained from matched standard parton shower Monte Carlo event generators as well as with those obtained from Parton Branching TMDs with corresponding parton showers are presented.

 ${\rm DOI:} 10.5506/{\rm APhysPolBSupp.} 17.4\text{-}{\rm A1}$

[†] Supervisor

 $^{^{\}ddagger}$ Summer student

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1. Introduction

In August 2023, more than 30 students participated in the Special Remote DESY Summer School [1] to work on projects of importance for the LHC experiments. The Special Remote DESY Summer School was endorsed by IUPAP [2] and included in the program of the International Year of Basic Sciences for Sustainable Development (IYBSSD) [3]. The school was fully online, with virtual meeting sessions from 2–4 pm CEST, for students from the Far East it was late in the evening and for students from the Far West it was very early in the morning. A similar fully online school was held in 2021 [4].

The school in 2023 was held in the spirit of the IUPAP policy to open the channels for scientific cooperation across all political and other divides in the hope and expectation that enhanced scientific collaborations are an important means to develop improved understandings between different peoples that contributes to world peace.

The student projects were on coding, testing, and validating computer codes of experimental analyses that have been already published by the CMS Collaboration, but are not yet available in the Rivet (Robust Independent Validation of Experiment and Theory) package [5].

In the following, we describe briefly the analyses in the area of QCD jets and electroweak physics that have been developed here.

2. New Rivet plugins

Several published results obtained with the CMS experiment at the LHC that were not yet implemented in the Rivet package were investigated, ranging from jet production at $\sqrt{s} = 7$ TeV, and heavy flavor production to measurements involving the electroweak (EW) bosons γ , W, Z at $\sqrt{s} = 13$ TeV. The theoretical predictions at leading order (LO), obtained with PYTHIA 8 [6–8], using the CUETM1 tune [9] to fix a number of free parameters sensitive to the treatment of the underlying event, were used to validate the implementation of the different analyses into the Rivet package, and to compare the obtained results with those shown in the original publications.

The following analyses were studied:

- CMS_2010_I878118 Prompt and non-prompt J/ψ production in pp collisions at $\sqrt{s} = 7$ TeV [10] (Mayvi Pedraza Monzon, Supervisor: F. Guzman);
- CMS_2011_I944755 J/ψ and ψ_{2S} production in pp collisions at $\sqrt{s} = 7 \ TeV$ [11] (Shijie Zhang, Supervisor: H. Jung);

- CMS_2011_I895742 Measurement of the differential dijet production cross section in proton-proton collisions at $\sqrt{s} = 7$ TeV [12] (Josué Daniel Jaramillo Arroyave, Fernanda Mora Rey, Supervisor: H. Jung);
- CMS_2012_I1093951 Measurement of the inclusive cross section $\sigma(pp \rightarrow b\bar{b}X \rightarrow \mu\mu X' \text{ at } \sqrt{s} = 7 \text{ TeV } [13]$ (Faeze Gagonani, Nestor Raul Mancilla Xinto, Supervisor: H. Jung);
- CMS_2015_I1345159 Distributions of topological observables in inclusive three- and four-jet events in pp collisions at $\sqrt{s} = 7$ TeV [14] (Dorukhan Boncukcu, Açelya Deniz Güngördü, Supervisor: H. Jung);
- CMS_2015_I1359450 Measurement of the Z boson differential cross section in transverse momentum and rapidity in proton-proton collisions at 8 TeV [15] (Emmanuel Botero Osorio, Jesus Jimenez Zepeda, Nazanin Zahra Norouzi, Juan Esteban Ospina, Swapnil Rathore, Supervisor: S. Taheri Monfared);
- CMS_2015_I1410826 Measurement of the inclusive jet cross section in pp collisions at $\sqrt{s} = 2.76$ TeV [16] (Vibha Padmanabhan, Quratulain Zahoor, Supervisor: H. Jung);
- CMS_2016_I1485195 Measurement of the total and differential inclusive B^+ hadron cross sections in pp collisions at $\sqrt{s} = 13$ TeV [17] (Lucas Tamayo, Supervisor: H. Jung);
- CMS_2019_I1757506 Study of J/ψ meson production inside jets in pp collisions at $\sqrt{s} = 8$ TeV [18] (Behnam Falahi, Supervisor: H. Jung);
- CMS_2021_I1876550 Measurement of prompt open-charm production cross sections in proton-proton collisions at $\sqrt{s} = 13$ TeV [19] (Fateme Almaksusi, Haoliang Zheng, Supervisor: H. Jung);
- CMS_2021_I1869513 Measurement of the electroweak production of $Z\gamma$ and two jets in proton-proton collisions at $\sqrt{s} = 13$ TeV and constraints on anomalous quartic gauge couplings [20] (Daniel Belmonte, Haritz Mentaste, Omar González, Supervisor: Si Hyun Jeon);
- CMS_2021_I1876311 Measurements of the electroweak diboson production cross sections in proton-proton collisions at $\sqrt{s} = 5.02$ TeV using leptonic decays [21] (Cristina Ruiz González, Inmaculada Moyano Rejano, Supervisor: Si Hyun Jeon);

- CMS_2021_I1949191 Measurement of the inclusive and differential WZ production cross sections, polarization angles, and triple gauge couplings in pp collisions at $\sqrt{s} = 13$ TeV [22] (Mahtab Jalalvandi, Supervisor: D. Pérez Adán);
- CMS_2021_I1992937 Measurement of the production cross section for Z + b jets in proton-proton collisions at $\sqrt{s} = 13$ TeV [23] (Caue E. Sousa, Gleb Kutyrev, Aleksandr Boger, Isadora Bozza Galvão, Abdelhamid Haddad, Supervisor: D. Pérez Adán).

3. Comparison with predictions

While predictions at leading order (LO) obtained with PYTHIA 8 were used to test and validate the coded analyses, we present here a comparison of theoretical predictions obtained at next-to-leading (NLO) in the strong coupling $\alpha_{\rm s}$.

At NLO, the MadGraph5 aMC@NLO package [24] was used to calculate the hard process and supplement the partonic processes with parton shower and hadronization. We use the NLO Parton Branching (PB) collinear and the transverse momentum dependent (TMD) parton distributions as obtained in Ref. [25] from QCD fits to precise DIS (Deep Inelastic Scattering) data from HERA [26] using the xFitter analysis framework [27, 28]. We cross-check the results with predictions using the NNPDF31 collinear parton distributions [29]. We apply the Parton Branching transverse momentum distributions (TMD) PB-NLO-2018-Set 2 together with the TMD parton shower for the initial state as implemented in CASCADE3 [30] (labelled MCatNLO+CAS3) as well as a standard parton shower obtained with PYTHIA 8 (labelled MCatNLO+PYTHIA 8). The NLO hard process is calculated with appropriate subtraction terms for the use with CASCADE3 and PYTHIA 8. We use μ_{def} as factorization and renormalization scale $\mu_{\text{def}} = \mu_{\text{R,F}} = \frac{1}{2} \sum_{i} \sqrt{m_i^2 + p_{\text{T},i}^2}$, where the index *i* runs over all particles in the matrix element final state.

Since some measurements are performed at very small transverse momenta, special care has to be taken to avoid instabilities of the NLO cross section as well as to avoid too large negative cross sections. We apply a taming factor for the scale $\mu_{\rm R,F}$

$$\mu = \mu_{\rm R,F} = \mu_{\rm def}^2 + \mu_0^2 \,, \tag{1}$$

with μ_{def} being the default scale and μ_0 being a free parameter to avoid too small scales. We found the $\mu_0 = 20$ GeV leads to stable results for jet production with a transverse momentum down to $p_{\text{T}} \sim 10$ GeV.

In Fig. 1, we show a comparison of the cross section as a function of the leading jet $p_{\rm T}$ calculated with and without the taming factor of Eq. (1). We do not observe any significant change in the cross section at larger $p_{\rm T}$, however, applying Eq. (1), we are able to use an NLO calculation for jet production down to $p_{\rm T} \sim 10$ GeV.

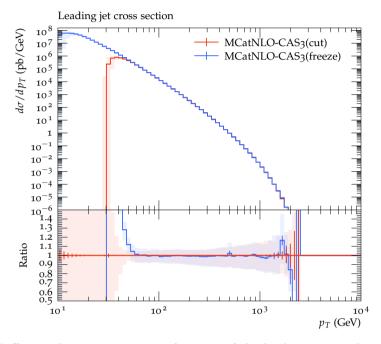


Fig. 1. Differential cross section as a function of the leading jet $p_{\rm T}$ obtained with MCatNLO+CAS3 applying the freeze of the scale (see Eq. (1)) and with a cutoff of $p_{\rm T} > 30$ GeV.

The theoretical uncertainty is estimated by independent variation of the factorization and renormalization scales by a factor of two up and down, avoiding the extreme combinations (7-point variation) and it is shown by the band in the figures.

In all predictions, we do not consider effects from multiparton interactions.

3.1. Comparison to QCD measurements

In Figs. 2–4, we compare measurements from CMS with predictions obtained from MCatNLO+CAS3 and MCatNLO+PYTHIA 8 using dijet production at NLO. The aim of this comparison is to check for differences in predictions from MCatNLO+CAS3 and MCatNLO+PYTHIA 8 since both predictions are based on different assumptions for higher-order corrections in the form of parton showers. In general, we observe a rather good agreement between the two different predictions.

In Fig. 2, inclusive jet cross sections are shown. The calculations give very similar predictions since inclusive jet and dijet production is largely sensitive to the collinear parton distributions. Also the prediction using NNPDF31 agrees well with the others.

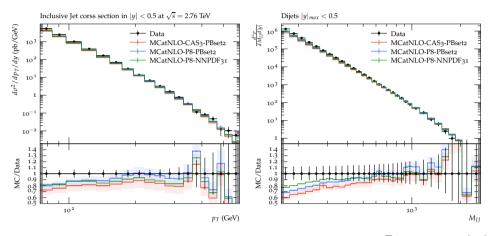


Fig. 2. Differential cross section as a function of the jet $p_{\rm T}$ at $\sqrt{s} = 2.76$ TeV [16] (left) and as a function of the dijet mass M_{JJ} at $\sqrt{s} = 7$ TeV [12] (right) obtained with MCatNLO+CAS3 and MCatNLO+PYTHIA 8 using PB-NLO-2018-Set 2. For comparison also shown is MCatNLO+PYTHIA 8 with NNPDF31.

In the following distributions, the effect of TMD parton densities and parton shower is investigated. In Fig. 3 (left), the invariant mass distribution of four-jet events with a $p_{\rm T}$ of the leading jet of 190 $< p_{\rm T} < 300$ GeV is shown. The four-jet mass distribution is sensitive to the parton shower since in the dijet matrix element at NLO at most three jets are produced, and therefore the fourth jet comes from the parton shower. In Fig. 3 (right), the particle content of jet evolution is investigated by a measurement of the energy of J/ψ mesons inside jets with a transverse momentum of $p_{\rm T} >$ 25 GeV at $\sqrt{s} = 8$ TeV. The predictions are in good agreement with the measurements.

Next, heavy flavor production is studied. In Fig. 4, measurements of charm and bottom production are shown. Since heavy quarks are not only produced in the hard matrix element, but also during the jet evolution, we use the zero-mass-variable-flavour-number scheme (ZMVFS) for the calculation (which allows charm or bottom quarks to be produced from light parton matrix elements). However, a drawback of ZMVFS is that the ma-

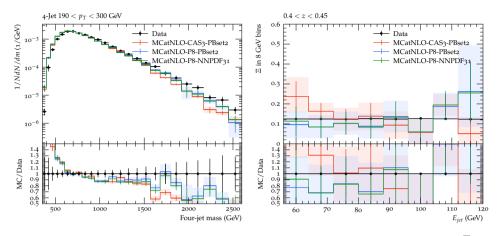


Fig. 3. Normalized distribution for x_3 in high- p_T three-jet events at $\sqrt{s} = 7$ GeV [14] (left) and the normalized distribution of energy of J/ψ mesons inside jets at $\sqrt{s} = 8$ GeV [18] (right) obtained with MCatNLO+CAS3 and MCatNLO+PYTHIA 8 using PB-NLO-2018-Set 2. For comparison also shown is MCatNLO+PYTHIA 8 with NNPDF31.

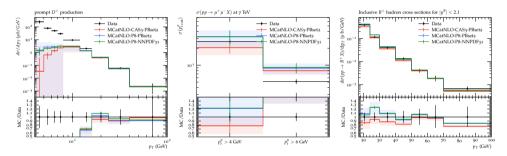


Fig. 4. Differential cross section as a function of $p_{\rm T}$ for D^* production at $\sqrt{s} = 13$ TeV [19] (left), the total cross section for $\sigma(pp \rightarrow b\bar{b}X \rightarrow \mu\mu X')$ at $\sqrt{s} = 7$ TeV as a function of the $p_{\rm T}$ cut (middle) [13], and the differential cross section for B^+ mesons at $\sqrt{s} = 13$ TeV [17] (right) obtained with MCatNLO+CAS3 and MCatNLO+PYTHIA 8 using PB-NLO-2018-Set 2. For comparison also shown is MCatNLO+PYTHIA 8 with NNPDF31.

trix element becomes divergent for small $p_{\rm T}$ (since all partons are treated massless), and therefore a $p_{\rm T}$ cut-off has to be applied. For NLO calculations with subtraction terms (in the MCatNLO framework), we found that we need to freeze the scale μ for low $p_{\rm T}$. With the procedure described in Eq. (1), we are able to use ZMVFS at NLO down to $p_{\rm T} = 10$ GeV. One can clearly see the effect of this lower- $p_{\rm T}$ cut in the distributions of the transverse momentum of heavy flavoured mesons in Fig. 4. Apart from the

low- $p_{\rm T}$ region, which is affected by the $p_{\rm T}$ cut, the predictions agree rather well with the measurements and only small differences between the different parton shower approaches are observed.

3.2. Comparison to onium processes

Measurements of J/ψ production have been performed in [10, 11]. We use the CASCADE Monte Carlo event generator [30–32] in stand-alone mode with internally implemented processes based on $k_{\rm T}$ -factorization with the unintegrated gluon density JH-2013-set1 [33]. Prompt J/ψ and $\psi(2S)$ are calculated within the colour singlet model, as well as χ_c production for feeddown to J/ψ . A description of the calculation is given in Ref. [34]. The nonprompt production J/ψ is generated using $g^*g^* \rightarrow b\bar{b}$ with subsequent decay to J/ψ via the hadronization package PYTHIA 6. In Fig. 5, we show the double differential cross section for prompt J/ψ production [10] as well as the cross section for prompt $\psi(2S)$ production [11]. A reasonable description of the measurements with the predictions based on $k_{\rm T}$ -factorization is achieved.

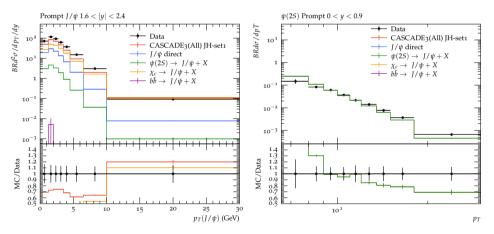


Fig. 5. Double differential cross section for J/ψ production at $\sqrt{s} = 7$ TeV [10] (left), and for $\psi(2S)$ production [11] (right) compared with predictions from CAS-CADE3.

3.3. Comparison to electroweak processes

In this section, we compare measurements of electroweak processes with predictions from MCatNLO+CAS3 and MCatNLO+PYTHIA 8 (with the same settings for parton densities and parton showers as in the earlier section) using DY production at NLO.

In Fig. 6 (left), the transverse momentum of Z bosons at $\sqrt{s} = 8$ TeV is shown. The calculations give similar predictions. At larger $p_{\rm T}$ the predictions fall below the measurements, since at larger $p_{\rm T}$ higher-order corrections become important.

In Fig. 6 (right), the cross section as a function of the azimuthal angle $\Delta \phi$ between a *b* jet and the *Z* boson in *Z* + *b* events at $\sqrt{s} = 13$ is shown. Here, we compare predictions obtained with inclusive *Z* boson production at NLO with the measurements and the difference of the predicted cross section to the measurement, especially at small $\Delta \phi$, can be attributed to higher-order hard jet radiation, which is not included in the simulation. Small differences between the parton shower and the TMD predictions can be observed.

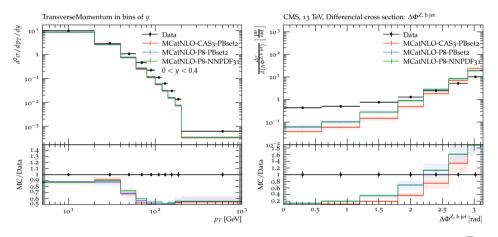


Fig. 6. Differential cross section as a function of $p_{\rm T}$ for Z production at $\sqrt{s} = 8$ TeV [15] (left) and as a function of the azimuthal angle $\Delta \phi$ between a b jet and the Z boson in Z+b events at $\sqrt{s} = 13$ TeV [23] (right) obtained with MCatNLO+CAS3 and MCatNLO+PYTHIA 8 using PB-NLO-2018-Set 2. For comparison also shown is MCatNLO+PYTHIA 8 with NNPDF31.

In Fig. 7 (left), the total cross section of ZZ production as a function of \sqrt{s} as measured in [21] is compared with predictions obtained from calculations obtained with a hard process of $pp \rightarrow ZZ + X$ at NLO with MCatNLO+CAS3 and MCatNLO+PYTHIA 8.

In Fig. 7 (right), the jet multiplicity in WZ events is shown. The hard process is calculated in the $WZ \rightarrow l\nu l^+ l^-$ mode with MadGraph5_aMC@NLO. Differences coming from the different parton showers can be observed in the jet multiplicity.

In Fig. 8, the cross section for $Z\gamma jj$ at $\sqrt{s} = 13$ TeV [20] as a function of the leading jet $p_{\rm T}$ is shown for events in the EW phase space (left) and in the full EW+QCD phase space (right). For the prediction, the hard process



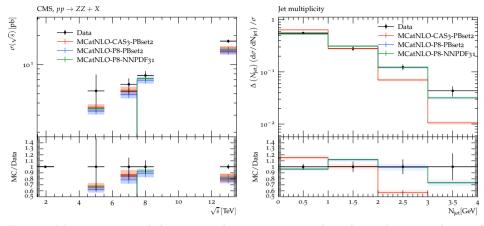


Fig. 7. Measurements di-boson production compared with predictions obtained with MCatNLO+CAS3 and MCatNLO+PYTHIA 8 using PB-NLO-2018-Set 2. The total cross section for ZZ production as a function of \sqrt{s} (left) [21] and jet multiplicity for WZ production at $\sqrt{s} = 13$ TeV [22] (right) are presented. For comparison also shown is MCatNLO+PYTHIA 8 with NNPDF31.

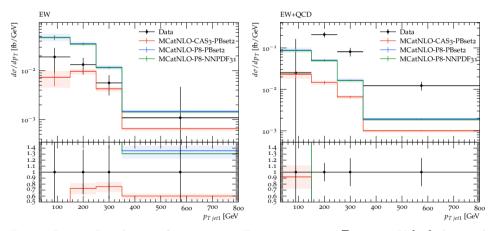


Fig. 8. Jet $p_{\rm T}$ distribution for events in $Z\gamma jj$ events at $\sqrt{s} = 13$ TeV [20] obtained with MCatNLO+CAS3 and MCatNLO+PYTHIA 8 using PB-NLO-2018-Set 2. Left: distribution for events in the EW phase space. Right: distribution of events in the full EW+QCD phase space.

generated is Z + 2 jet at NLO, the photon is radiated as part of the finalstate parton shower, thus representing only the pure QCD phase space. A significant difference between the predictions of MCatNLO+CAS3 and MCatNLO+PYTHIA 8 is observed, which can be attributed to the treatment of high- p_T photon radiation in the parton shower.

4. Conclusion

During August 2023, students from different countries joined the *Special Remote DESY Summer School* investigating analyses performed by the CMS experiment at the LHC. Several analyses in the QCD and electroweak area were implemented into the **Rivet** analysis frame for easy comparison with predictions of Monte Carlo event generators.

The analyses were validated by comparing the results of simulations with the ones described in the original publications. The results presented here use the newly coded Rivet plugins to perform a comparison of predictions obtained with MCatNLO+CAS3 based Parton Branching transverse momentum dependent (PB-TMD) parton distributions with the corresponding parton shower and with MCatNLO+PYTHIA 8 applying collinear parton densities and parton showers. The hard processes were generated with MCatNLO at NLO with the collinear parton density PB-NLO-2018-Set 2 (and for comparison NNPDF31). It is observed that the difference between predictions obtained with different collinear parton densities is very small, however in some distributions, differences are observed between the conventional parton shower in PYTHIA 8 and the TMD-based parton shower (and TMD distributions) in MCatNLO+CAS3.

The comparisons presented here are the first systematic comparisons of predictions based on MCatNLO+CAS3 and MCatNLO+PYTHIA 8 applying the same collinear parton densities, and therefore contribute to a better understanding of the differences between predictions based on TMD parton densities and conventional parton showers.

The very successful cooperation and collaboration of students with different backgrounds contribute significantly to the Science4Peace idea.

We are grateful to Andy Buckley and Christian Gütschow from the Rivet team for their support and advice before, during and after the Summer School. Help and support was also received from Achim Geiser on onium production as well as from Patrick Connor on jet production analyses in CMS.

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