PROCEEDINGS OF SCIENCE

Jet fragmentation calculation at NLO with general-purpose Monte Carlo generators

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Observables for single-inclusive hadron productions can be calculated by convolution of process-dependent partonic cross sections and universal fragmentation functions (FFs) at leading power in QCD factorization theory. The FMNLO framework is proposed to perform such calculations in an automated way at next-to-leading order (NLO) in QCD using general-purpose Monte Carlo generators. In this talk, we present the basic idea of FMNLO, which relies on a combination of the phase-space slicing method and local subtraction methods. Additionally, with the help of interpolation techniques, FMNLO is also a promising tool for fits of FFs. We present the outcomes of a new NLO fit of FFs to unidentified charged hadrons using LHC measurements, with particular sensitivity to the gluon FF.

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1. Introduction

The fragmentation functions (FFs) are the counterparts of parton distribution functions (PDFs) in the final state, and describe the probabilities to find hadrons inside the partons [1]. The FFs play important roles in QCD factorization theory. Observables of single-inclusive hadron production can be written as convolution of partonic matrix elements (MEs) and FFs (and also PDFs in presence of initial-state hadrons) at leading power in QCD factorization theory [2]. As an example, the energy fraction $x_h \equiv 2E_h/\sqrt{s}$ of hadron h in single inclusive annihilation (SIA) $e^+e^- \to h + X$ can be written as

$$\frac{d\sigma}{dx_h} = \sum_{i=q,\bar{q},g} \int_0^1 \frac{dz}{z} C_i^0(x/z, \epsilon) D_{h/i}^0(z, \epsilon). \tag{1}$$

The infrared (IR) divergences in the partonic coefficient functions C_i^0 can be absorbed into the bare FFs

$$D_{h/i}^0(x, \epsilon) = D_{h/i}(x, \mu_D) + \left(\frac{\mu_R^2}{\mu_D^2}\right)^{\epsilon} \frac{\alpha_s(\mu_R)}{2\pi} \frac{1}{\epsilon} P_{ji}^{+(0)} \otimes D_{h/j}(x, \mu_D) \tag{2}$$

where $D_{h/i}$ are the renormalized FFs, $P_{ji}^{+(0)}$ are the time-like splitting functions, and μ_R, μ_D are the renormalization scale and fragmentation scale, respectively.

The FFs are universal non-perturbative objects and can be extracted from measurements. The partonic MEs, on the other hand, are process-dependent. However, processes with available analytic partonic results at next-to-leading order (NLO) are limited, and are usually implemented case-by-case. Also, analytical results with various selection criteria may not be available. In Ref. [3] we overcome these limitations by combining general-purpose Monte Carlo (GPMC) generators and FFs. Our prescription, FMNLO, has been implemented with MG5_aMC@NLO [4, 5], which is a powerful tool for automated NLO calculation for various processes, with convenient facilities of imposing various cuts, and reconstructing jets. In this talk, we present the basic idea of FMNLO, and shows its applications in NLO fit of FFs to unidentified charged hadrons.

2. The framework

One of the key point of combining GPMC generators and FFs is the treatment of IR divergence. To deal with IR divergence, GPMC generators generally adopt local subtraction schemes such as dipole formalism or FKS formalism [6–9]. However, for fragmenting measurements, where one of the final state hadron is identified, there are additional collinear divergence, whose local subtraction may not be implemented in GPMC generators. In Ref. [3], we proposed another approach to single out these IR divergences by imposing additional slicing of phase space. Our method is to a large extent independent of the details of the local subtraction schemes, and can be easily implemented in GPMC generators.

The basic idea of our framework is dividing the $m + 1$ body phase space (for real corrections and the corresponding local subtraction terms) into two regions. In the first region, all final state partons are well separated, and all IR divergences are canceled between the real MEs and the local subtraction terms. In the second region, two final state partons are collinear, and if one of them fragments into the tagged hadron, there are remaining IR divergences. Fortunately, the MEs in the

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collinear region factorize into Born MEs and splitting kernels, and we can partially carry out the phase space integral in this region analytically. Finally, we find the integral in the collinear region of the $m+1$ body phase space can be written as an integral in Born (m-body) phase space, and in this way, the IR divergences are singled out and can be correctly absorbed into the FFs. (see Ref. [3] for more details).

Now all the ingredients are free from IR divergence and can be calculated numerically in four-dimensional spacetime with Monte Carlo method. As an example, the differential distribution in the energy fraction x_h carried by the tagged hadron h in SIA can be schematically written as

$$\frac{d\sigma}{dx_h} = \sum_{i=1}^{m} \int \frac{dx_i}{x_i} \left[\frac{d\sigma_m^{(0)}}{dx_i} + \frac{d\tilde{\sigma}_m^{(1)}}{dx_i} \right] D_{h/i}(x_h/x_i, \mu_D) + \sum_{i=1}^{m+1} \int \frac{dx_i}{x_i} \left[\frac{d\tilde{\sigma}_{m+1}^{(1)}}{dx_i} \right] D_{h/i}(x_h/x_i, \mu_D)$$
$$+ \sum_{i=1}^{m} \int \frac{dx_i}{x_i} \left[\frac{\alpha_S(\mu_R)}{2\pi} \frac{d\sigma_m^{(0)}}{dx_i} \right] \left(\bar{D}_{h/i}(x_h/x_i, \mu_D) + \tilde{D}_{h/i}(x_h/x_i, \mu_D) \right), \quad (3)$$

where $d\sigma_m^{(0)}/dx_i$ is the LO partonic differential cross section with respect to the energy fraction carried by the i-th parton. The $d\tilde{\sigma}_m^{(1)}/dx_i$ and $d\tilde{\sigma}_{m+1}^{(1)}/dx_i$ are NLO partonic MEs and local subtraction terms in m- and $(m+1)$- body phase space, respectively. $\bar{D}$ and $\tilde{D}$ are convolutions of the original FFs D with some process-independent functions (see Ref. [3] for details).

3. The FMNLO program

Our framework has been interfaced to MG5_aMC@NLO. The corresponding code, FMNLO, is publicly available. In our code, the master formula Eq. (3) is boosted with the interpolation techniques. Especially, the most time-consuming part is the calculation of the partonic MEs and local subtraction terms, corresponding to the terms in squared brackets of Eq. (3). They are calculated once and stored in tables using histograms in MG5_aMC@NLO. These tables can be convoluted with different sets of FFs very quickly, which is very useful if we want to compare theoretical predictions of different sets of FFs or perform a fit of FFs.

We have validated our scheme and codes for both leptonic collisions and pp collisions. For leptonic collisions, the FMNLO predictions have been checked by analytic calculation at NLO in QCD. For pp collisions, we find good agreement between FMNLO and the INCNLO program [10]. Finally, we have verified the stability of FMNLO predictions with different choices of the phase space slicing parameter.

4. A new NLO fit of FFs to unidentified charged hadrons

Our code, FMNLO, has been used to perform a fit of unidentified charged hadron FFs at NLO in QCD. We only use hadronic collisions data from the ATLAS Collaboration [11, 12] and the CMS Collaboration [13–15], including parton fragmentation measurements in association with either an isolated photon or a Z boson, and parton fragmentation measurements in dijet events. In this demonstration study, we assume all quark FFs to unidentified charged hadrons are equal at the initial scale $Q_0 = 5$ GeV, and parameterize the quark FFs and gluon FFs as

$$xD_{h/i}(x, Q_0) = a_{i,0} x^{\alpha_i} (1-x)^{\beta_i} \left(1 + a_{i,1} x + a_{i,2} x^2\right). \quad (4)$$

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Experiments	N_{pt}	$\chi^2(/N_{pt})$, **NLO**	$\chi^2(/N_{pt})$, **NLO**$_{w/o\ th.}$	$\chi^2(/N_{pt})$, **LO**$_{w/o\ th.}$
CMS γ	5	11.3(2.27)	28.8(5.76)	48.5(9.71)
ATLAS γ	7	17.8(2.55)	18.8(2.68)	40.5(5.78)
CMS Z	11	16.2(1.47)	24.8(2.25)	906.9(82.4)
ATLAS Z	9	47.5(5.27)	48.1(5.34)	348.8(38.8)
ATLAS central jets	141	98.1(0.69)	112.9(0.79)	833.7(5.83)
ATLAS forward jets	141	76.4(0.53)	98.0(0.68)	855.6(5.98)
Total	318	267.4(0.84)	331.2(1.04)	3034.0(9.54)

Table 1: The χ^2 of individual data sets and their sum from our nominal NLO fit and alternative fits at NLO and LO without theoretical uncertainties.

So there are 10 free parameters in the fit. The DGLAP evolution of the FFs are carried out by the HOPPET program [16]. The CT14 NLO parton distribution functions [17] are used for initial hadrons.

By minimizing the log-likelihood function, we find the best-fit parameters for the quark and gluon FFs. The error sets of FFs are generated with the iterative Hessian approach. The overall agreement between the NLO prediction from our fit and the data is summarized in Table 1. Numbers in parentheses correspond to χ^2 divided by the number of data points. The total χ^2 of our nominal fit is 267.4 for 318 data points. We find very good agreement to ATLAS dijet measurements. The agreement to CMS Z+jet measurement is also good while it is much worse for the ATLAS Z+jet measurement. The bad agreement of LO fit indicates the necessity of inclusion of NLO corrections.

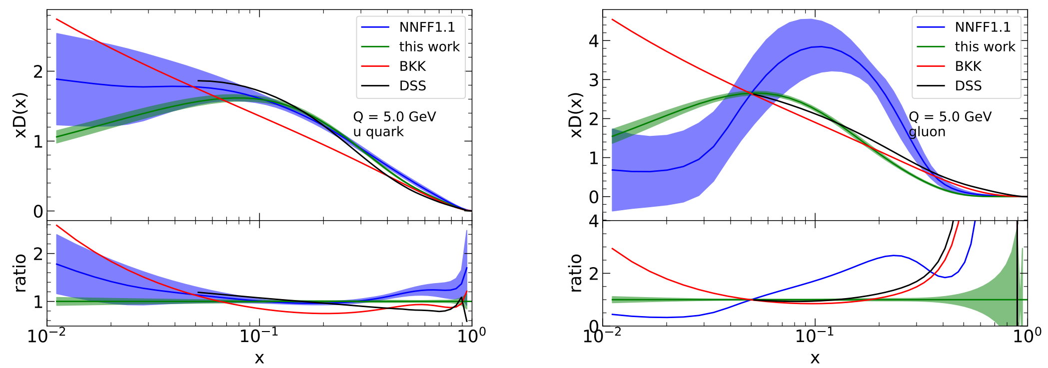

Figure 1: The u-quark (left panel) and gluon (right panel) fragmentation functions to unidentified charged hadron at $Q_0 = 5$ GeV from our nominal NLO fit as a function of the momentum fraction x. They are compared to the NNFF1.1, BKK and DSS results. The colored bands indicate the uncertainties as estimated with the Hessian (MC) method for our (NNFF1.1) fit.

Finally, we compare our FFs to those from NNFF1.1 [18], BKK [19] and DSS [20] at the scale of 5 GeV in Fig. 1. For u quark FF, we find good agreement for momentum fraction x between 0.1 and 0.3, but in the small x region, we observe a large deviation. For gluon FF, we find notable disparities, especially for $x > 0.5$, the ratio of NNFF gluon FF to our fit has a sudden and pronounced increase. The disparities, together with the large uncertainties of gluon FF, emphasize

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the need for additional constraints and data to improve the accuracy of the gluon FF fit.

5. Conclusions

We present a prescription for combining general-purpose Monte Carlo generators and fragmentation functions (FFs) at NLO in QCD. This framework is based on a combination of phase-space slicing and the local subtraction methods, and has been interfaced to MG5_aMC@NLO. The corresponding code, FMNLO, is now publicly available [3]. FMNLO can be used as an automated tool for theoretical predictions of fragmentation measurements, especially for those with jet reconstruction or various cuts.

By utilizing FMNLO, we perform a new fit of FFs to unidentified charged hadrons. As compared with fits of FFs to unidentified charged hadron in literature, we include new hadron-in-jet data from ATLAS and CMS. These data provide direct access to the momentum fraction dependence of FFs and are sensitive to the gluon FFs. We observe some tension between the gluon FF of our result and that of NNFF1.1, indicating the necessities of additional constraints and data in gluon FF fit, which will be presented in an upcoming work.

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References

[1] A. Metz and A. Vossen, *Parton Fragmentation Functions*, *Prog. Part. Nucl. Phys.* **91** (2016) 136–202 [1607.02521].

[2] J. C. Collins, D. E. Soper and G. F. Sterman, *Factorization of Hard Processes in QCD*, *Adv. Ser. Direct. High Energy Phys.* **5** (1989) 1–91 [hep-ph/0409313].

[3] C. Liu, X. Shen, B. Zhou and J. Gao, *Automated calculation of jet fragmentation at NLO in QCD*, *JHEP* **09** (2023) 108 [2305.14620].

[4] J. Alwall, R. Frederix, S. Frixione, V. Hirschi, F. Maltoni, O. Mattelaer, H. S. Shao, T. Stelzer, P. Torrielli and M. Zaro, *The automated computation of tree-level and next-to-leading order differential cross sections, and their matching to parton shower simulations*, *JHEP* **07** (2014) 079 [1405.0301].

[5] R. Frederix, S. Frixione, V. Hirschi, D. Pagani, H. S. Shao and M. Zaro, *The automation of next-to-leading order electroweak calculations*, *JHEP* **07** (2018) 185 [1804.10017]. [Erratum: JHEP 11, 085 (2021)].

[6] S. Catani and M. H. Seymour, *The Dipole formalism for the calculation of QCD jet cross-sections at next-to-leading order*, *Phys. Lett. B* **378** (1996) 287–301 [hep-ph/9602277].

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[7] S. Catani, S. Dittmaier, M. H. Seymour and Z. Trocsanyi, *The Dipole formalism for next-to-leading order QCD calculations with massive partons*, *Nucl. Phys. B* **627** (2002) 189–265 [hep-ph/0201036].

[8] S. Frixione, Z. Kunszt and A. Signer, *Three jet cross-sections to next-to-leading order*, *Nucl. Phys. B* **467** (1996) 399–442 [hep-ph/9512328].

[9] S. Frixione, *A General approach to jet cross-sections in QCD*, *Nucl. Phys. B* **507** (1997) 295–314 [hep-ph/9706545].

[10] M. Werlen, "INCNLO-direct photon and inclusive hadron production code website." Version 1.4. http://lapth.cnrs.fr/PHOX_FAMILY.

[11] **CMS** Collaboration, A. M. Sirunyan *et. al.*, *Observation of Medium-Induced Modifications of Jet Fragmentation in Pb-Pb Collisions at $\sqrt{s_{NN}}$ = 5.02 TeV Using Isolated Photon-Tagged Jets*, *Phys. Rev. Lett.* **121** (2018), no. 24 242301 [1801.04895].

[12] **CMS** Collaboration, A. M. Sirunyan *et. al.*, *Using Z Boson Events to Study Parton-Medium Interactions in Pb-Pb Collisions*, *Phys. Rev. Lett.* **128** (2022), no. 12 122301 [2103.04377].

[13] **ATLAS** Collaboration, M. Aaboud *et. al.*, *Comparison of Fragmentation Functions for Jets Dominated by Light Quarks and Gluons from pp and Pb+Pb Collisions in ATLAS*, *Phys. Rev. Lett.* **123** (2019), no. 4 042001 [1902.10007].

[14] **ATLAS** Collaboration, G. Aad *et. al.*, *Medium-Induced Modification of Z-Tagged Charged Particle Yields in Pb + Pb Collisions at 5.02 TeV with the ATLAS Detector*, *Phys. Rev. Lett.* **126** (2021), no. 7 072301 [2008.09811].

[15] **ATLAS** Collaboration, G. Aad *et. al.*, *Properties of jet fragmentation using charged particles measured with the ATLAS detector in pp collisions at $\sqrt{s} = 13$ TeV*, *Phys. Rev. D* **100** (2019), no. 5 052011 [1906.09254].

[16] G. P. Salam and J. Rojo, *A Higher Order Perturbative Parton Evolution Toolkit (HOPPET)*, *Comput. Phys. Commun.* **180** (2009) 120–156 [0804.3755].

[17] S. Dulat, T.-J. Hou, J. Gao, M. Guzzi, J. Huston, P. Nadolsky, J. Pumplin, C. Schmidt, D. Stump and C.-P. Yuan, *New parton distribution functions from a global analysis of quantum chromodynamics*, *Physical Review D* **93** (feb, 2016).

[18] **NNPDF** Collaboration, V. Bertone, N. P. Hartland, E. R. Nocera, J. Rojo and L. Rottoli, *Charged hadron fragmentation functions from collider data*, *Eur. Phys. J. C* **78** (2018), no. 8 651 [1807.03310].

[19] J. Binnewies, B. A. Kniehl and G. Kramer, *Neutral kaon production in e^+e^-, ep, and $p\bar{p}$ collisions at next-to-leading order*, *Phys. Rev. D* **53** (Apr, 1996) 3573–3581.

[20] D. de Florian, R. Sassot and M. Stratmann, *Global analysis of fragmentation functions for protons and charged hadrons*, *Phys. Rev. D* **76** (Oct, 2007) 074033.

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