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# Automated calculation of Jet fragmentation at NLO in QCD

arxiv: 2305.14620

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第三届量子场论及其应用研讨会

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- 2** FMNLO Framework
- 3** Applications at LHC
- 4** Analysis of Fragmentation Function
- 5** Summary and Prospects



## Introduction



## FMNLO Framework



## Applications at LHC



## Analysis of Fragmentation Function

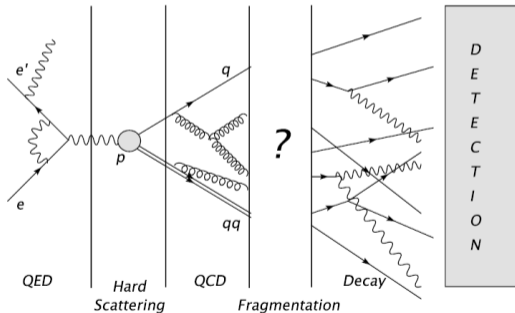


## Summary and Prospects

# Fragmentation Function



- $D_q^h(z, Q^2)$ : The number of hadrons of type  $h$  initiated by  $q$  with energy fraction  $z$  at scale  $Q$  per  $dz$  (R.Field)



# Experiments



## 1 Single Inclusive Annihilation(SIA)

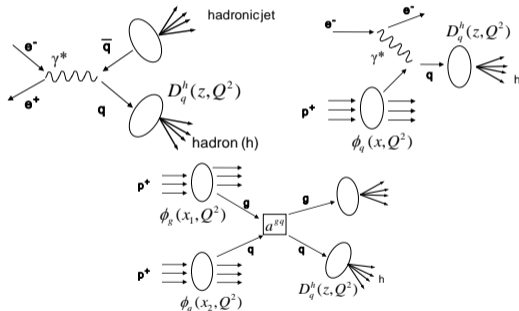
$$e^+e^- \rightarrow h + X$$

## 2 Semi-Inclusive Deep-Inelastic Scattering (SIDIS)

$$e^- + p \rightarrow h + X$$

## 3 Hadron Production

$$p + p \rightarrow h + X$$



# QCD factorization



## Factorization Theorem

$$\sigma(e^+e^- \rightarrow hX) = \hat{\sigma} \otimes FF \qquad \frac{d\sigma(e^+e^- \rightarrow hX)}{dz} = \sum_i \int_x^1 \frac{dz}{z} C_i\left(z, \alpha_s(\mu), \frac{q^2}{\mu^2}\right) D_i^h\left(\frac{x}{z}, \mu^2\right)$$

$$\sigma(e^-p \rightarrow hX) = \hat{\sigma} \otimes PDF \otimes FF$$

$$\sigma(pp \rightarrow hX) = \hat{\sigma} \otimes PDF \otimes PDF \otimes FF$$

## Sum rule

$$\sum_h \int_0^1 z D_{q(g)}^h(z, Q^2) = 1$$

## DGLAP evolution

$$\frac{d}{d \ln Q^2} \vec{D}^h(z, Q^2) = \hat{P} \otimes \vec{D}^h(Q^2)$$

$$\vec{D}^h = \begin{pmatrix} D_s^h \\ D_g^h \end{pmatrix}, D_s^h = \sum_q (D_q^h + D_{\bar{q}}^h), \hat{P} = \begin{pmatrix} P_{q \rightarrow qq} & 2n_f P_{q \rightarrow gq} \\ P_{g \rightarrow q\bar{q}} & P_{g \rightarrow gg} \end{pmatrix}$$

# Existing Global Analysis of FFs



- BKK, J. Binnewies, B. A. Kniehl and G. Kramer, 1995
- DSS, D. de Florian, R. Sassot and M. Stratmann, 2007
- KKP, B. A. Kniehl, G. Kramer and B. Pötter, 2000
- NNFF, V. Bertone, S. Carrazza, N.P. Hartland, E.R. Nocera, J. Rojo, 2017
- MAPFF, R. Abdul Khalek, V. Bertone, A. Khoukli, E. R. Nocera, 2022
- JAM, JAM Collaboration. N. Sato, C. Andres, J.J. Ethier, W. Melnitchouk, 2019



Introduction



**FMNLO Framework**



Applications at LHC



Analysis of Fragmentation Function



Summary and Prospects



# Motivation for new computation framework



- The available processes of hard scattering are limited and are usually implemented case-by-case
- Interactions in the hard processes are usually constrained to be SM interaction
- Direct calculations at NLO are costly in computation time

# FMNLO



- 2305.14620(ChongYang Liu, XiaoMin Shen, Bin Zhou, Jun Gao)
- <https://fmnlo.sjtu.edu.cn/~fmnlo/>
- Based on hybrid scheme of NLO calculations
  - phase-space slicing of collinear regions
  - local subtraction methods
- Integrated with MG5\_aMC@NLO, any processes could be calculated. (SM and BSM)
  - $e^+e^- \rightarrow \gamma^* \rightarrow q\bar{q} \rightarrow hX$
  - $\mu^+\mu^- \rightarrow H \rightarrow gg \rightarrow hX$
  - $pp \rightarrow jj/Zj/\gamma j$
- Once the grid is generated by MG5\_aMC@NLO, it can be convoluted with FF to obtain observables within seconds
- With built-in BKK, KKP, DSS FF sets, more could be added.
- Linked to LHAPDF library, data sets on LHAPDF could be accessed easily.

# Theory Ingredients



$$\begin{aligned} \frac{d\sigma}{dp_{T,h}} = & \int dx \int dPS_m \left[ |M|_{B,m}^2 + |M|_{V,m}^2 + |\tilde{\mathcal{I}}_m^2 \right] \sum_{i=1}^m \delta(p_{T,h} - xp_{T,i}) D_{h/i}^0(x) \\ & + \int dx \int dPS_{m+1} \left[ |M|_{R,m+1}^2 \sum_{i=1}^{m+1} \delta(p_{T,h} - xp_{T,i}) D_{h/i}^0(x) - |\mathcal{I}_{m+1}^2 \sum_{\tilde{i}=1}^m \delta(p_{T,h} - xp_{T,\tilde{i}}) D_{h/\tilde{i}}^0(x) \right]. \end{aligned}$$

$|M|_B^2$ ,  $|M|_V^2$  and  $|M|_R^2$  represent square of matrix elements at leading order (LO), one-loop level and in real corrections, respectively.  $|\mathcal{I}_{m+1}^2$  denotes the local subtraction terms, and  $|\tilde{\mathcal{I}}_m^2 = \int PS_1 |\mathcal{I}_{m+1}^2$

# Theory Ingredients



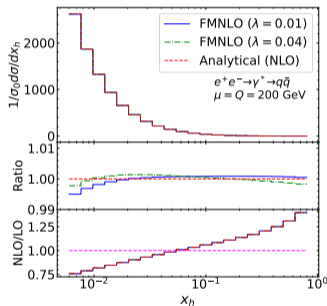
$$\begin{aligned}
 & \int dx \int dPS_{m+1} (\Theta(\lambda - C) + \Theta(C - \lambda)) \left[ |M|_{R,m+1}^2 \sum_{i=1}^{m+1} \delta(p_{T,h} - xp_{T,i}) D_{h/i}^0(x) - |\mathcal{I}|_{m+1}^2 \sum_{\bar{i}=1}^m \delta(p_{T,h} - x\bar{p}_{T,\bar{i}}) D_{h/\bar{i}}^0(x) \right] \\
 &= \int dx \int dPS_{m+1} \Theta(C - \lambda) \left[ |M|_{R,m+1}^2 \sum_{i=1}^{m+1} \delta(p_{T,h} - xp_{T,i}) D_{h/i}^0(x) - |\mathcal{I}|_{m+1}^2 \sum_{\bar{i}=1}^m \delta(p_{T,h} - x\bar{p}_{T,\bar{i}}) D_{h/\bar{i}}^0(x) \right] + |\tilde{\mathcal{J}}|_m^2
 \end{aligned}$$

- Two  $\Theta$  functions are inserted to partition into the unresolved and resolved collinear regions with a cutoff  $\lambda$ .
- The phase space integral of  $m + 1$ -body above the cutoff is free of infrared and collinear singularities and can be calculated numerically in four dimensions.
- The integral below the cutoff which contains collinear singularities can be factorized using the collinear approximations.

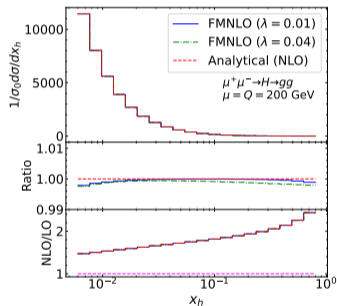
# Lepton Collisions



- Consider two processes
  - ①  $e^+e^- \rightarrow \gamma^* \rightarrow q\bar{q} \rightarrow hX$
  - ②  $\mu^+\mu^- \rightarrow H \rightarrow gg \rightarrow hX$
- Toy model
  - $x D_{h/i}(x, \mu) = N_i x^{-1/2} (1-x)^5$
  - $N_i = 1$  for  $q$  and  $\bar{q}$ ,  
 $N_i = 9/4$  for  $g$
- The deviation from analytical results are only a few per mille



(a)  $e^+e^- \rightarrow \gamma^* \rightarrow q\bar{q}$

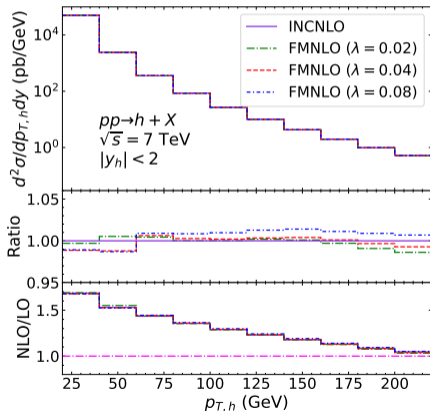


(b)  $\mu^+\mu^- \rightarrow H \rightarrow gg$

# Hadron Collisions



- $pp \rightarrow h + X$
- Comparison with INCNLO  
(Hadro-production program by PHOX)
- PDF: CTEQ6M NLO  
FF: BKK
- Agreement with numerical values





Introduction



FMNLO Framework



Applications at LHC



Analysis of Fragmentation Function

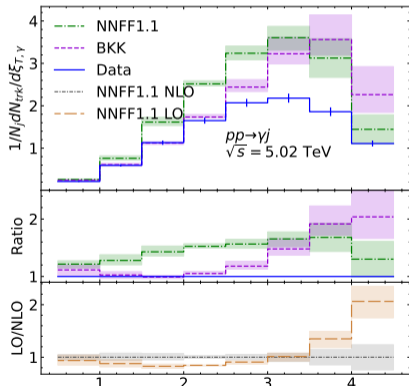


Summary and Prospects

# Isolated photon tagged jets



- arxiv: 1801.04895
- $pp \rightarrow \gamma j$
- $\xi_T^\gamma \equiv \ln[-p_{T,\gamma}^2 / (p_{T,\gamma} \cdot p_{T,h})]$
- Error bands indicate scale variations, which are obtained by taking the envelope of theory predictions of the 9 scale combinations of  $\mu_F/\mu_{F,0} = \mu_R/\mu_{R,0} = \{1/2, 1, 2\}$  and  $\mu_D/\mu_{D,0} = \{1/2, 1, 2\}$ .
- Experimental errors are represented by error bars

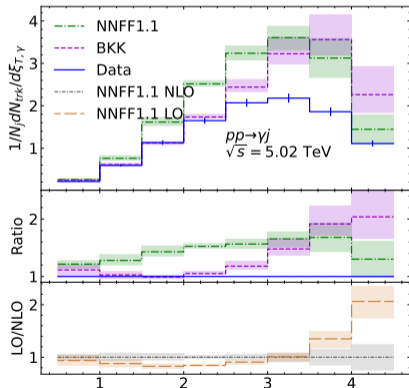




# Isolated photon tagged jets



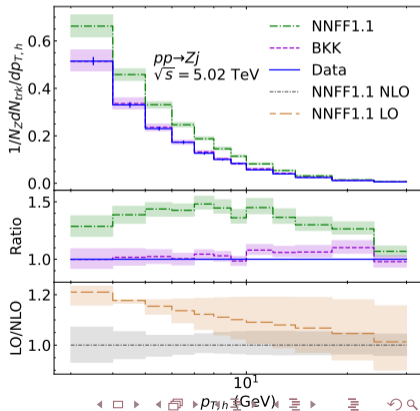
- BKK results closely resemble the experimental data and exhibit a good agreement in the lower  $\xi_T^\gamma$  region [0.5, 2.5], the discrepancy is large as  $\xi_T^\gamma$  increases
- The NNFF1.1 results match the experimental data in the lower and higher regions, deviations are large in the middle



# Z tagged jets



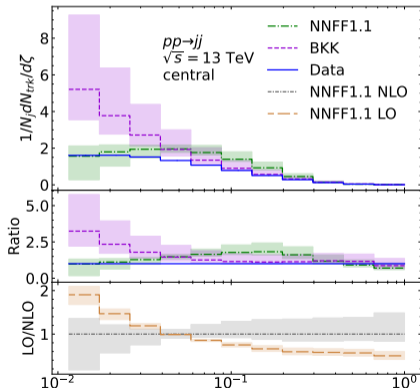
- arxiv: 2103.04377
- $pp \rightarrow Zj$
- In most regions, the experimental data lies within the error band of the BKK results.
- NNFF1.1 results show a greater discrepancy, particularly in the middle region



# QCD Inclusive dijets



- arxiv: 1906.09254
- $pp \rightarrow jj$
- $\zeta = p_{T,h}/p_{T,j}$
- Both the NNFF1.1 and BKK results fit well in the high  $\zeta$  region, but BKK lies more closely with experimental data
- In lower  $\zeta$  region (the first three bins), NNFF1.1 predictions exhibit a closer resemblance.





Introduction



FMNLO Framework



Applications at LHC



Analysis of Fragmentation Function



Summary and Prospects

# Data Selection



## Selected Data Sets

- Publications within 5 years
- Focused on  $pp$  collisions
- Exclude momentum fraction  $x < 0.01$  as it requires higher-order corrections

Experiments	lum.	observables	$N_{pt}$	Range
CMS 5.02 TeV	$27.4 \text{ pb}^{-1}$	$1/N_j dN_{trk}/d\xi_T^\gamma$	8(5)	$\xi_T^\gamma \in [0.5, 4.5]$
ATLAS 5.02 TeV	$25 \text{ pb}^{-1}$	$1/N_j dN_{trk}/dp_{T,h}$	10(7)	$p_{T,h} \in [1, 100] \text{ GeV}$
CMS 5.02 TeV	$320 \text{ pb}^{-1}$	$1/N_Z dN_{trk}/dp_{T,h}$	14(11)	$p_{T,h} \in [1, 30] \text{ GeV}$
ATLAS 5.02 TeV	$160 \text{ pb}^{-1}$	$1/N_Z d^2 N_{trk}/dp_{T,h} d\Delta\phi$	15(9)	$p_{T,h} \in [1, 60] \text{ GeV}$
ATLAS 13 TeV	$33 \text{ fb}^{-1}$	$1/N_j dN_{trk}/d\zeta$ (central)	261(143)	$\zeta \in [0.002, 0.67]$
ATLAS 13 TeV	$33 \text{ fb}^{-1}$	$1/N_j dN_{trk}/d\zeta$ (forward)	261(143)	$\zeta \in [0.002, 0.67]$

# Framework of fitting



- Parameterization

$$xD_{h/i}(x, Q_0) = a_{i,0}x^{\alpha_i}(1-x)^{\beta_i} \left( 1 + \sum_{n=1}^p a_{i,n}x^n \right)$$

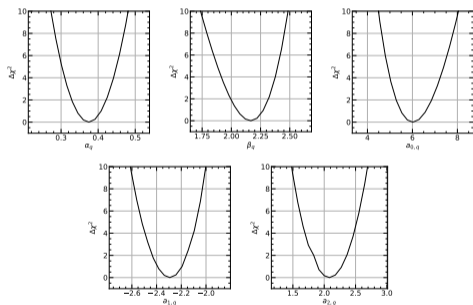
- No flavor separation
- $Q_0 = 5 \text{ GeV}$
- $p = 2, n_f = 5$
- Fitting quality: Log-likelihood Function

$$\chi^2(\{\alpha, \beta, a_n\}, \{\lambda\}) = \sum_{k=1}^{N_{\text{pt}}} \frac{1}{S_k^2} \left( D_k - T_k - \sum_{\mu=1}^{N_\lambda} \sigma_{k,\mu} \lambda_\mu \right)^2 + \sum_{\mu=1}^{N_\lambda} \lambda_\mu^2$$

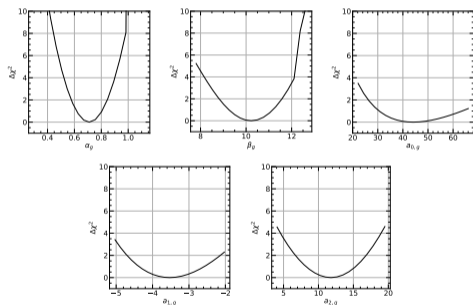
# LM scan



Profile of total  $\chi^2$  change from scans on individual parameters with other parameters freely varying.



(a) LM scan of quarks



(b) LM scan of gluon

# Results



Best fit results and LM Scan on Individual parameters (68% Confidence Level)

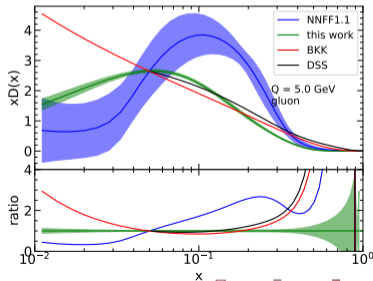
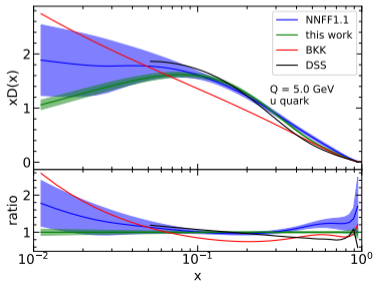
<b>quark</b>	$\alpha$	$\beta$	$a_0$	$a_1$	$a_2$	$\langle x \rangle$
best-fit	0.375	2.166	6.016	-2.292	2.083	0.586
unc.(scan)	+0.03 -0.03	+0.11 -0.12	+0.55 -0.56	+0.10 -0.10	+0.18 -0.20	--
unc.(Hessian)	+0.03 -0.03	+0.09 -0.10	+0.45 -0.44	+0.08 -0.08	+0.16 -0.16	+0.007 -0.008
<b>gluon</b>	$\alpha$	$\beta$	$a_0$	$a_1$	$a_2$	$\langle x \rangle$
best-fit	0.710	10.224	44.080	-3.527	11.786	0.510
unc.(scan)	+0.09 -0.16	+1.09 -0.91	+19.54 -13.54	+0.95 -0.85	+3.54 -3.60	--
unc.(Hessian)	+0.09 -0.10	+0.91 -0.93	+18.9 -14.1	+0.92 -0.83	+3.32 -3.52	+0.011 -0.012



# Comparison of FF



- Uncertainties and deviations of different FF sets at small  $x$  region are large
- FF sets of quarks exhibit good agreements in  $x > 0.1$  except BKK
- Deviation of  $D_g^h$  from different FF sets is large, more constraints are required
- The error band in our nominal fit is tight. On one hand, LHC data restricts gluon FF well. On the other hand, it's due to our chosen form of parameterization and error estimation method.





Introduction



FMNLO Framework



Applications at LHC



Analysis of Fragmentation Function



Summary and Prospects

# Summary and Prospects



## Summary

- In this presentation, we propose a new framework for the calculation of differential cross section combining general-purpose Monte-Carlo generators with fragmentation functions (FFs) at NLO in QCD
- Its numerical stability is validated in cases of lepton collisions and hadron collisions
- It is further applied on the predictions of hadron cross section on LHC and the results are compared with experimental data
- With the framework and data on LHC, Fragmentation Function fit is obtained and compared with existing FF sets

## Prospects

- Include more experimental data points
- Detailed analysis with respect to Fragmentation Function fit, including different forms of parametrization, range of kinematic cuts and scale choices
- Include identified charged hadron
- Extend precision of calculation to NNLO



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谢谢