Simultaneous Determination of Fragmentation Functions and Test on Momentum Sum Rule

Jun Gao

INPAC, Shanghai Jiao Tong University

based on 2305.14620 with ChongYang Liu, XiaoMin Shen, Bin Zhou
and 2401.02781 with ChongYang Liu, XiaoMin Shen, HongXi Xing, YuXiang Zhao

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INPAC INSTITUTE OF NUCLEAR AND PARTICLE PHYSICS

Outline

- 1. Introduction

- 2. Automation of fragmentation calculations at next-to-leading order

- 3. Global analysis of FFs to light charged hadrons

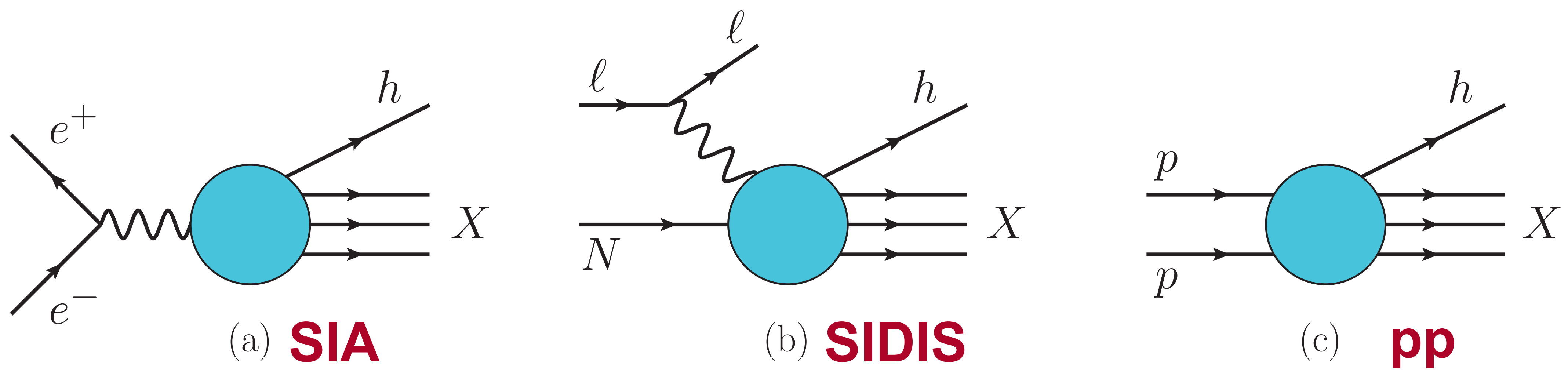
- 4. Summary

Single inclusive hadron production

- In its simplest form, fragmentation functions (FFs) describe number density of the identified hadron wrt the fraction of momentum of the initial parton it carries, as measured in single inclusive hadron production, e.g., from single-inclusive annihilation (SIA), semi-inclusive DIS (SIDIS), pp collisions

single inclusive hadron production/observable

[1607.02521]



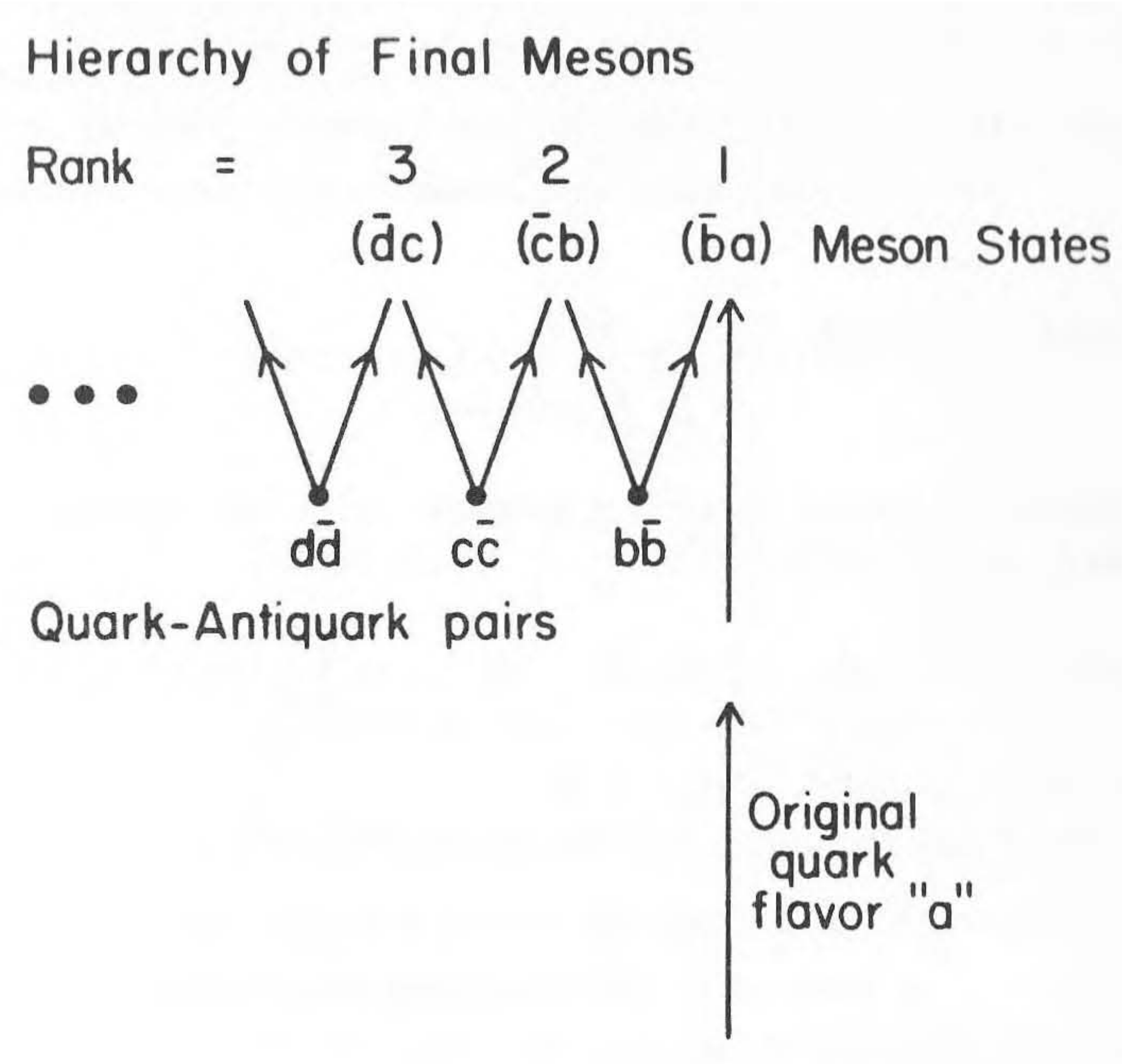
(a) **SIA** (b) **SIDIS** (c) **pp**

$$\frac{1}{\sigma_{\rm tot}}\,\frac{d\sigma^{e^+e^-\to hX}}{dz} = F^h(z,Q^2)\,, \quad z = \frac{2\,E_h}{\sqrt{s}}$$

exp. definition of unpolarized collinear FFs

other forms: polarized FFs, TMD FFs, di-hadron FFs

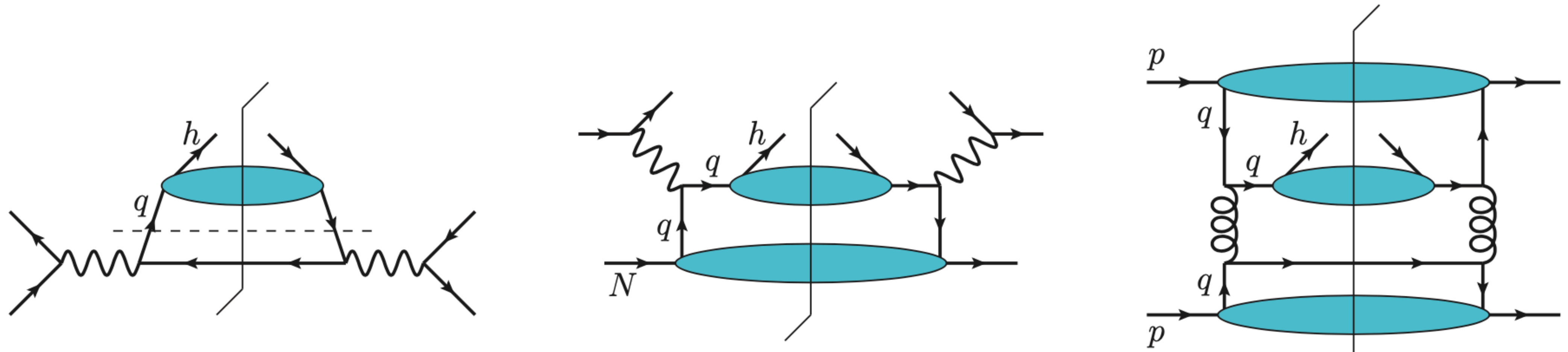
parton model **[Field&Feynman]**



distribution of momentum to mesons via creation of quark-antiquark pairs in cascade

QCD collinear factorization

- QCD collinear factorization ensures universal separation of long-distance and short-distance contributions in high energy scatterings involving initial/final state hadrons, and enables predictions on cross sections



(a) **SIA** (b) **SIDIS** (c) **pp**

$$\frac{1}{\sigma_{\text{tot}}}\frac{d\sigma^{e^+e^-\to hX}}{dz} = \frac{1}{\sum_q e_q^2}\left(2F_1^h(z,Q^2)+F_L^h(z,Q^2)\right)$$

$$2F_1^h(z,Q^2) = \sum_q e_q^2\left(D_1^{h/q}(z,Q^2)+\frac{\alpha_s(Q^2)}{2\pi}\left(C_1^q\otimes D_1^{h/q}+C_1^g\otimes D_1^{h/g}\right)(z,Q^2)\right)$$

$$\frac{d^3\sigma^{\ell p\to \ell hX}}{dx\,dy\,dz} = \frac{2\pi\alpha_{\text{em}}^2}{Q^2}\left(\frac{1+(1-y)^2)}{y}\,2F_1^h(x,z,Q^2)+\frac{2(1-y)}{y}\,F_L^h(x,z,Q^2)\right)$$

$$\begin{aligned}2F_1^h(x,z,Q^2) &= \sum_q e_q^2\left(f_1^{q/p}D_1^{h/q}+\frac{\alpha_s(Q^2)}{2\pi}\left(f_1^{q/p}\otimes C_1^{qq}\otimes D_1^{h/q}\right.\right.\\ &\qquad \left.\left.+f_1^{q/p}\otimes C_1^{gq}\otimes D_1^{h/g}+f_1^{g/p}\otimes C_1^{qg}\otimes D_1^{h/q}\right)\right],\end{aligned}$$

- ❖ coefficient functions, hard scattering; infrared (IR) safe, calculable in pQCD, independent of the hadron
- ❖ FFs/PDFs, reveal inner structure of hadrons or parton-hadorn transition; NP origin, universal, e.g. DIS vs. pp collisions; fitted from data
- ❖ runnings of FFs/PDFs with μ_D/μ_f are governed by the DGLAP equation

unpolarized collinear FFs, operator definition

$$\begin{aligned}D_1^{h/q}(z) &= \frac{z}{4}\mathop{\sum\!\!\!\!\!\!\int}_X \int\frac{d\xi^+}{2\pi}\,e^{ik^-\xi^+}\,\mathrm{Tr}\Big[\langle 0|\,\mathcal{W}(\infty^+,\xi^+)\,\psi_q(\xi^+,0^-,\vec{0}_T)\,|P_h,S_h;X\rangle\\ &\quad\times\langle P_h,S_h;X|\,\bar{\psi}_q(0^+,0^-,\vec{0}_T)\,\mathcal{W}(0^+,\infty^+)\,|0\rangle\,\gamma^-\Big]\,.\end{aligned}$$

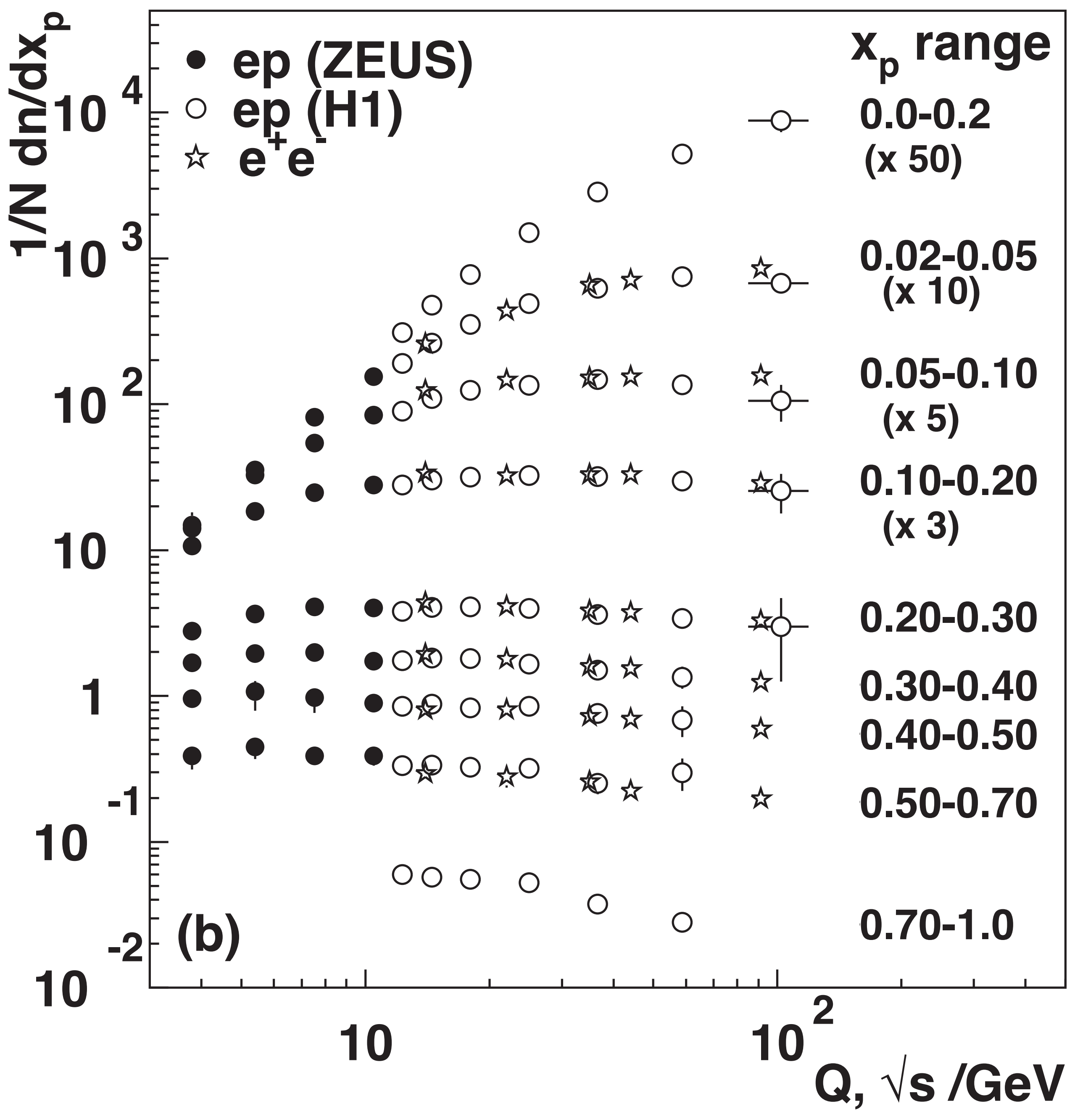
$$\frac{d}{d\ln\mu^2}D_1^{h/i}(z,\mu^2) = \frac{\alpha_s(\mu^2)}{2\pi}\sum_j\int_z^1\frac{du}{u}\,P_{ji}(u,\alpha_s(\mu^2))\,D_1^{h/j}\left(\frac{z}{u},\mu^2\right)$$

[Collins, Soper, Sterman]

Global data and phenomenological analysis

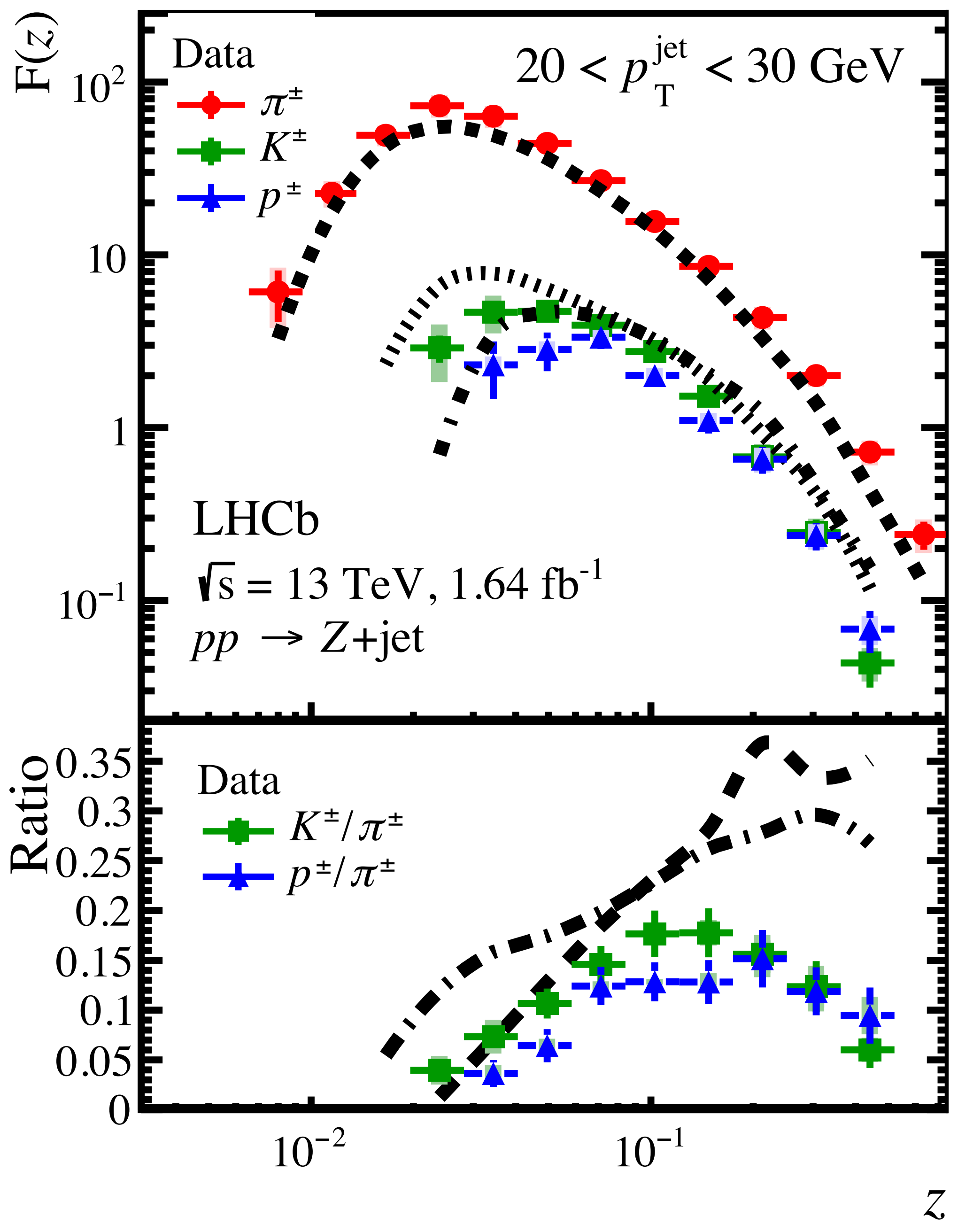
- Measurements are available from colliders SLAC, LEP, HERA, RHIC, LHC and fixed-target HERMES, COMPASS experiments for various charged hadrons as well as neutral hadrons; many groups provide phenomenological FFs from global analysis at NLO/NNLO in QCD

single incl. production of unidentified charged hadrons (SIA & SIDIS)



[Particle data group]

Jet fragmentation to light charged hadrons (LHCb)



[2208.11691]

$$z = \frac{\mathbf{p}_{\rm had}\cdot\mathbf{p}_{\rm jet}}{|\mathbf{p}_{\rm jet}|^2}, \quad F(z) = \frac{1}{N_{Z+{\rm jet}}}\frac{{\rm d}N_{\rm had}(z)}{{\rm d}z}$$

global analysis

- major groups/families include BKK, AKK, HKNS, DSS, NNFF, MAPFF, JAM etc.
- mostly done at NLO in QCD since exact NNLO coefficient functions only known recently for SIDIS
- different determination can be quite different due to selection of data sets as well as theory treatments, not converge as well as the case of PDF fits

[1607.02521 for a review]

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FMNLO (fragmentation at NLO in QCD)

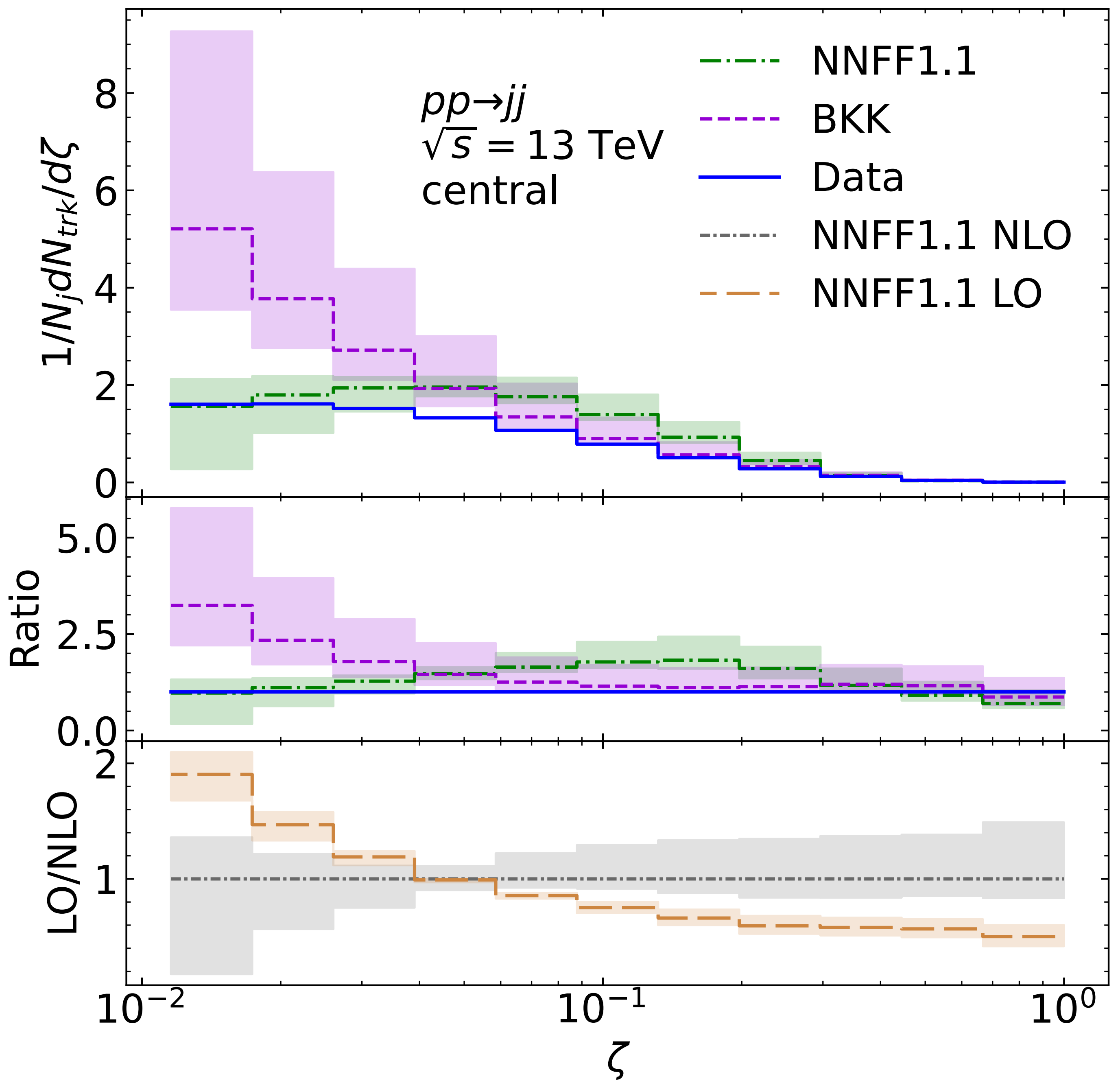
- FMNLO is a program for automated and fast calculations of fragmentation cross sections of arbitrary processes. It is based on a hybrid scheme of phase-space slicing method and local subtraction method, accurate to NLO in QCD

- automation of fragmentation calculations for arbitrary hard processes at NLO, within SM and BSMs via MG5_aMC@NLO

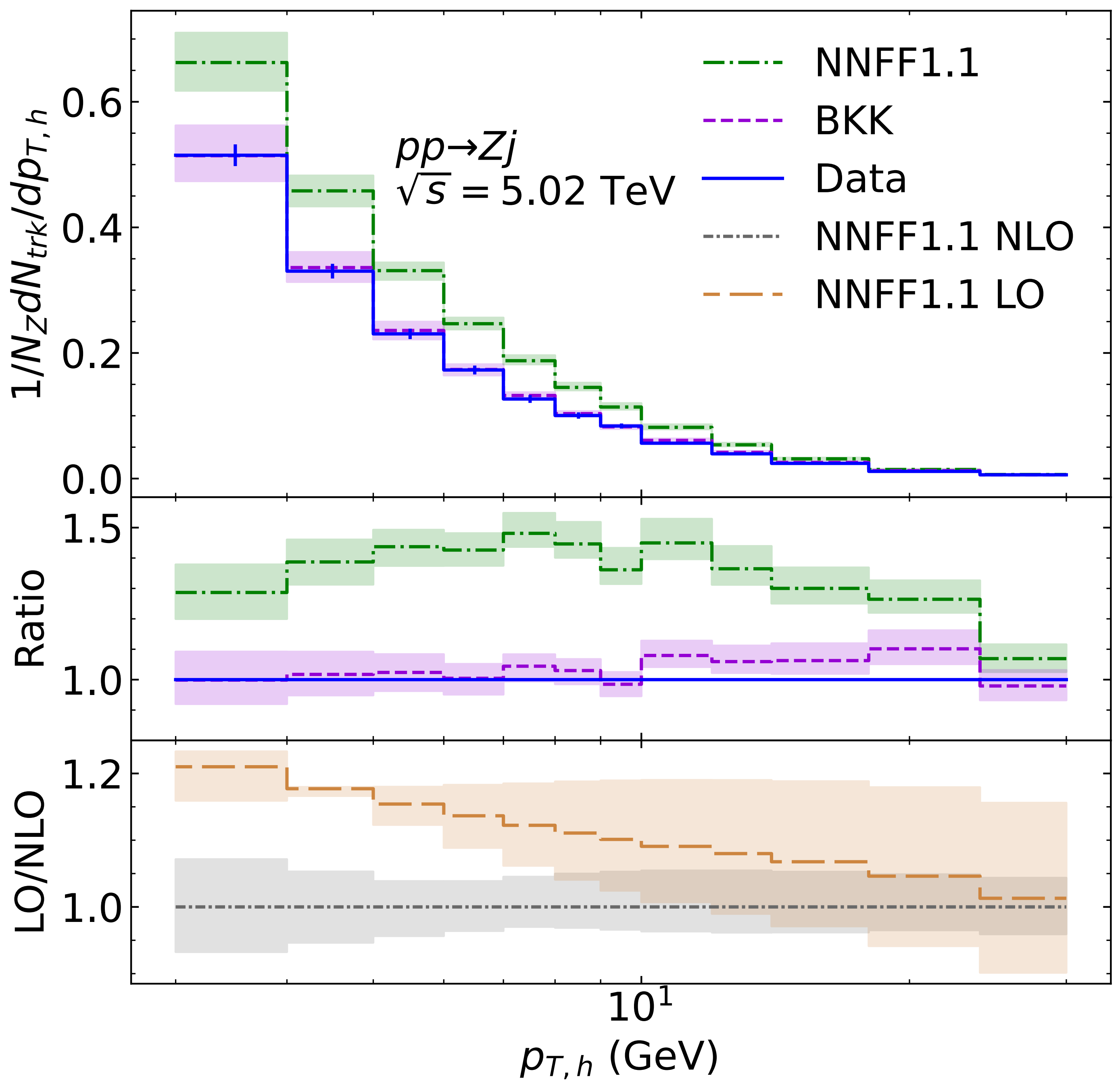
- fast convolution algorithms of partonic cross sections with FFs without repeating the time consuming MC integrations

- future goal/generalizations: transverse observables, NNLO corrections

QCD inclusive dijets at LHC



Z-boson tagged jet



🔥 **News**

2023.05: 🎉🎉 FMNLOv1.0 first release of `FMNLO` interfaced with `MG5_aMC@NLO`.

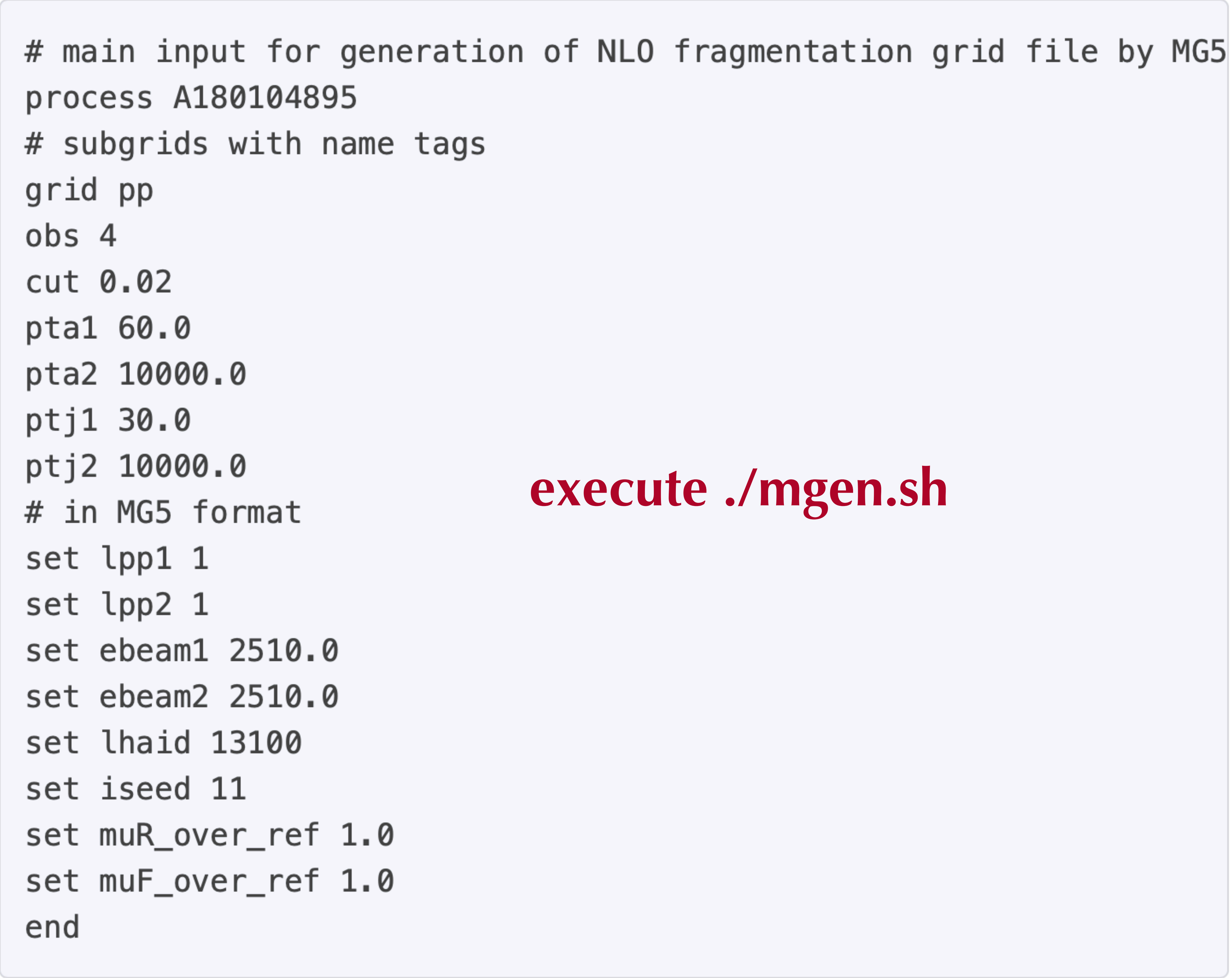
https://fmnlo.sjtu.edu.cn/~fmnlo/

[JG, Liu, Shen, Zhou, 2305.14620]

FMNLO (fragmentation at NLO in QCD)

- A two step tutorial for usage of FMNLO: 1, generation of an interpolation table for hard coefficient functions; 2, fast convolution with arbitrary FFs and arbitrary binning of the experimental distribution

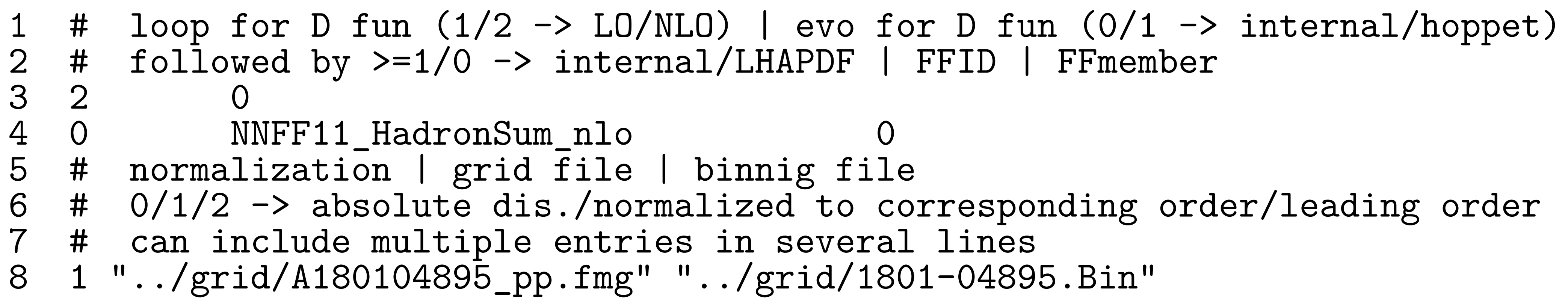
create a MG5 module for a hard scattering process and set parameters in proc.run



```
# main input for generation of NLO fragmentation grid file by MG5
process A180104895
# subgrids with name tags
grid pp
obs 4
cut 0.02
pta1 60.0
pta2 10000.0
ptj1 30.0
ptj2 10000.0
# in MG5 format
set lpp1 1
set lpp2 1
set ebeam1 2510.0
set ebeam2 2510.0
set lhaid 13100
set iseed 11
set muR_over_ref 1.0
set muF_over_ref 1.0
end
```

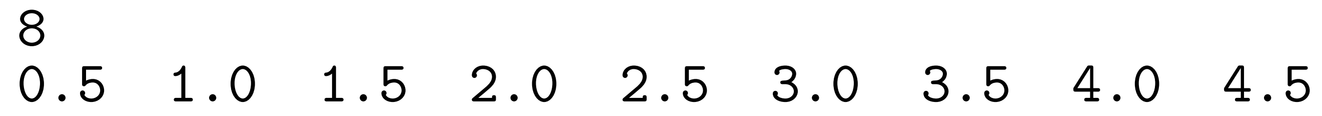
execute ./mgen.sh

setup parameters for cross section calculations



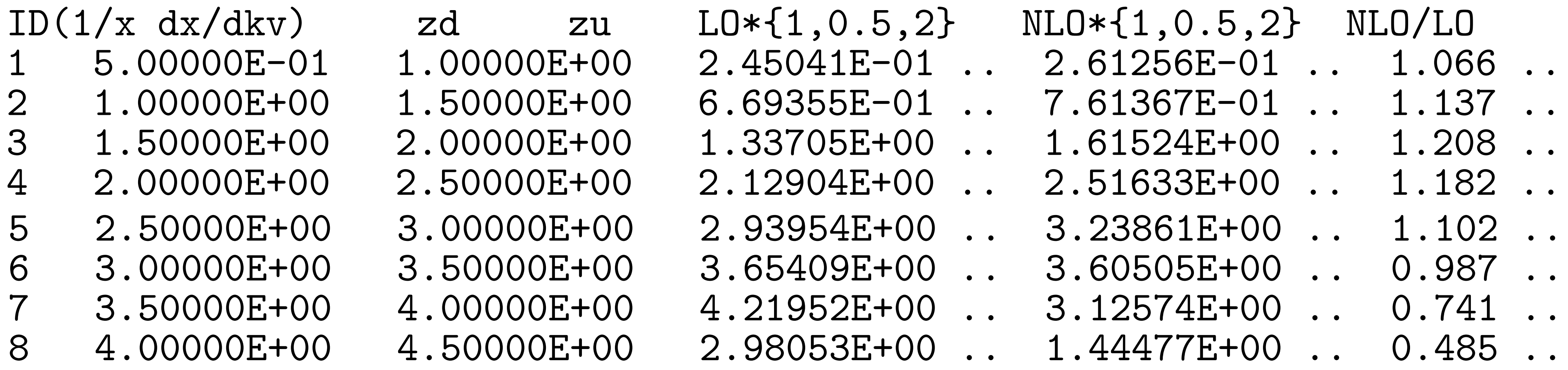
```
#  loop for D fun (1/2 -> LO/NLO) | evo for D fun (0/1 -> internal/hoppet)
#  followed by >=1/0 -> internal/LHAPDF | FFID | FFmember
2        0
0        NNFF11_HadronSum_nlo            0
#  normalization | grid file | binnig file
#  0/1/2 -> absolute dis./normalized to corresponding order/leading order
#  can include multiple entries in several lines
1 "../grid/A180104895_pp.fmg" "../grid/1801-04895.Bin"
```

example of binning



```
8
0.5  1.0  1.5  2.0  2.5  3.0  3.5  4.0  4.5
```

cross section output **execute ./fmnlo**



```
ID(1/x dx/dkv)     zd        zu      LO*{1,0.5,2}   NLO*{1,0.5,2}  NLO/LO
1    5.00000E-01  1.00000E+00  2.45041E-01 ..  2.61256E-01 ..  1.066 ..
2    1.00000E+00  1.50000E+00  6.69355E-01 ..  7.61367E-01 ..  1.137 ..
3    1.50000E+00  2.00000E+00  1.33705E+00 ..  1.61524E+00 ..  1.208 ..
4    2.00000E+00  2.50000E+00  2.12904E+00 ..  2.51633E+00 ..  1.182 ..
5    2.50000E+00  3.00000E+00  2.93954E+00 ..  3.23861E+00 ..  1.102 ..
6    3.00000E+00  3.50000E+00  3.65409E+00 ..  3.60505E+00 ..  0.987 ..
7    3.50000E+00  4.00000E+00  4.21952E+00 ..  3.12574E+00 ..  0.741 ..
8    4.00000E+00  4.50000E+00  2.98053E+00 ..  1.44477E+00 ..  0.485 ..
```

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Global analysis of FFs

- Establishing a new framework on global analysis of fragmentation functions to identified charged hadrons, including charged pion, kaon and proton, using most recent data from SIA, SIDIS, and pp collisions

parametrization of FFs to charged pion/kaon/proton at an initial scale (Q=5 GeV):

$$zD_i^h(z, Q_0) = z^{\alpha_i^h}(1-z)^{\beta_i^h} \exp\left(\sum_{n=0}^{m} a_{i,n}^h (\sqrt{z})^n\right)$$

parton-to-π^+	favored	α	β	a_0	a_1	a_2	d.o.f.
u	Y						5
$\bar{d} \simeq u$	Y	-	-		-	-	1
$\bar{u} = d$	N					x	4
$s = \bar{s} \simeq \bar{u}$	N	-				x	3
$c = \bar{c}$	N					x	4
$b = \bar{b}$	N					x	4
g	N		F				4

parton-to-K^+	favored	α	β	a_0	a_1	a_2	d.o.f.
u	Y					x	4
$\bar{s} \simeq u$	Y	-	-		-	x	1
$\bar{u}=d=\bar{d}=s$	N					x	4
$c = \bar{c}$	N					x	4
$b = \bar{b}$	N					x	4
g	N		F			x	3

parton-to-p	favored	α	β	a_0	a_1	a_2	d.o.f.
$u = 2d$	Y					x	4
$\bar{u} = \bar{d} = s = \bar{s}$	N				x	x	3
$c = \bar{c}$	N					x	4
$b = \bar{b}$	N					x	4
g	N		F			x	3

- a joint determination of FFs to charged pion, kaon and proton at NLO in QCD (63 parameters) including estimation of uncertainties with Hessian sets
- apply a strong selection criteria on the kinematics of fragmentation processes to ensure validity of LT factorization and perturbative calculations ($z>0.01$ and $E_h/p_{T,h}>4$ GeV)
- including theory uncertainties (residual scale variations) into the covariance matrix
- use fast interpolation techniques for calculations of cross sections which largely increase efficiency of the global fit

[JG, CY Liu, XM Shen, HX Xing, YX Zhao, 2401.02781]

Selection of data

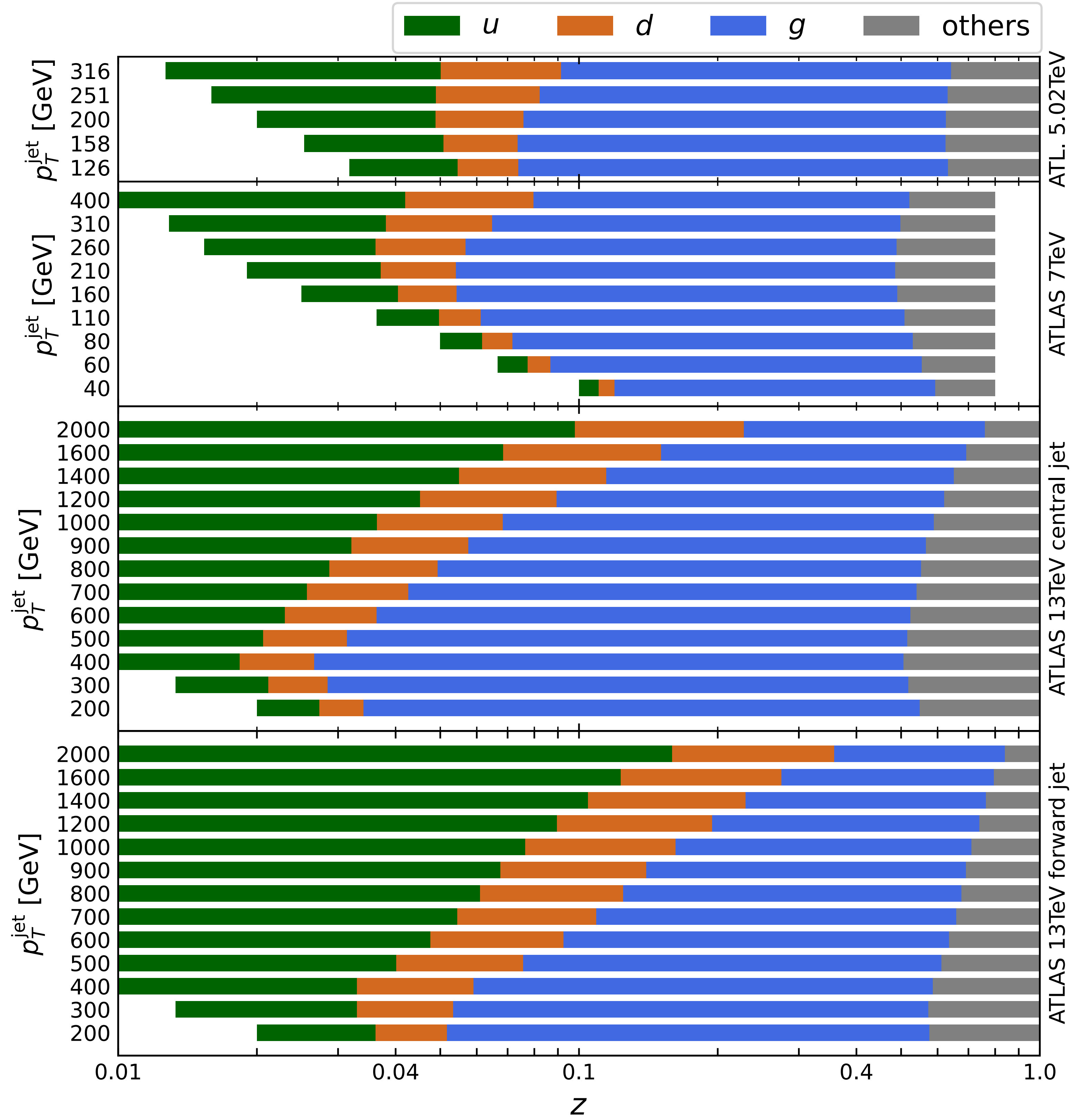
- For the first time the jet fragmentation data from LHC have been incorporated into the global analysis of FFs to light charged hadrons, including from processes of incl. jet, dijet, Z or photon tagged jet productions, due to the development of FMNLO

LHC measurements for hadron inside jet measurements (jet fragmentation)

exp.	$\sqrt{s}$(TeV)	luminosity	hadrons	final states	R_j	cuts for jets/hadron	observable	$N_{\rm pt}$
ATLAS[60]	5.02	25 $\rm pb^{-1}$	$h^\pm$	$\gamma+j$	0.4	$\Delta\phi_{j,\gamma} > \frac{7\pi}{8}$	$\frac{1}{N_{\rm jet}}\frac{dN_{\rm ch}}{dp_{T,h}}$	6
CMS[61]	5.02	27.4 $\rm pb^{-1}$	$h^\pm$	$\gamma+j$	0.3	$\Delta\phi_{j,\gamma} > \frac{7\pi}{8}, \Delta R_{h,j} < R_j$	$\frac{1}{N_{\rm jet}}\frac{dN_{\rm ch}}{d\xi}$	4
ATLAS[62]	5.02	260 $\rm pb^{-1}$	$h^\pm$	$Z+h$	no jet	$\Delta\phi_{h,Z} > \frac{3}{4}\pi$	$\frac{1}{n_Z}\frac{dN_{\rm ch}}{dp_{T,h}}$	9
CMS[63]	5.02	320 $\rm pb^{-1}$	$h^\pm$	$Z+h$	no jet	$\Delta\phi_{h,Z} > \frac{7}{8}\pi$	$\frac{1}{n_Z}\frac{dN_{\rm ch}}{dp_{T,h}}$	11
LHCb[64]	13	1.64 $\rm fb^{-1}$	$\pi^\pm, K^\pm, p/\bar{p}$	$Z+j$	0.5	$\Delta\phi_{j,\gamma} > \frac{7\pi}{8}, \Delta R_{h,j} < R_j$	$\frac{1}{n_Z}\frac{dN_{\rm ch}}{d\zeta}$	20
ATLAS[65]	5.02	25 $\rm pb^{-1}$	$h^\pm$	inc. jet	0.4	-	$\frac{1}{N_{\rm jet}}\frac{dN_{\rm ch}}{d\zeta}$	63
ATLAS[66]	7	36 $\rm pb^{-1}$	$h^\pm$	inc. jet	0.6	$\Delta R_{h,j} < R_j$	$\frac{1}{N_{\rm jet}}\frac{dN_{\rm ch}}{d\zeta}$	103
ATLAS[67]	13	33 $\rm fb^{-1}$	$h^\pm$	dijet	0.4	$p_T^{\rm lead}/p_T^{\rm sublead} < 1.5$	$\frac{1}{N_{\rm jet}}\frac{dN_{\rm ch}}{d\zeta}$	280

- LHC measurements on hadron inside jet provide essential inputs for u/d/g flavor separation with wide kinematic coverages, both in energy scale Q and in momentum fraction z
- In dijets or inclusive jets production, low p_T and central (high p_T and forward) jets are mostly initiated by g(u-quark); Z or photon tagged jets are more likely from u/d quarks

kinematic/flavor coverage (LO) for ATLAS jet fragmentation



Selection of data

- Other data include ratios of inclusive production rates of different hadrons measured in pp collisions, single incl. hadron production from SIA (w/wo heavy-flavor tagging) mostly at Z-pole, and incl. hadron production in SIDIS from HERA and COMPASS, for identified or unidentified charged hadrons

incl. hadron production at RHIC and LHC (pp)

exp.	$\sqrt{s_{NN}}$(TeV)	# events (million)	$p_{T,h}$	hadrons	observable	$N_{\rm pt}$
ALICE[58]	13	40-60(pp)	$[2, 20]$ GeV	$\pi, K, p,\ K^0_S$	$K/\pi, p/\pi, K^0_S/\pi$	49
ALICE[58]	7	150(pp)	$[3, 20]$ GeV	π, K, p	13TeV/7TeV for π, K, p	37
ALICE[57]	5.02	120(pp)	$[2, 20]$ GeV	π, K, p	$K/\pi, p/\pi$	34
ALICE[56]	2.76	40(pp)	$[2, 20]$ GeV	π, K, p	$K/\pi, p/\pi$	27
STAR[68]	0.2	14(pp)	$[3, 15]$ GeV	π, K, p, K^0_S	$K/\pi,\ p/\pi^+,\ \bar{p}/\pi^-,\ K^0_S/\pi,\ \pi^-/\pi^+,\ K^-/K^+$	60

incl. hadron production at Z-pole (SIA)

exp.	$\sqrt{s}$	lum.(n_Z)	final states	hadrons	$N_{\rm pt}$
OPAL[51]	m_Z	780 000	$Z \to q\bar{q}$	$\pi^\pm, K^\pm$	20
ALEPH[52]	m_Z	520 000	$Z \to q\bar{q}$	$\pi^\pm, K^\pm, p(\bar{p})$	42
DELPHI[53]	m_Z	1 400 000	$Z \to q\bar{q}$	$\pi^\pm, K^\pm, p(\bar{p})$	39
			$Z \to b\bar{b}$	$\pi^\pm, K^\pm, p(\bar{p})$	39
SLD[77]	m_Z	400 000	$Z \to q\bar{q}$	$\pi^\pm, K^\pm, p(\bar{p})$	66
			$Z \to b\bar{b}$	$\pi^\pm, K^\pm, p(\bar{p})$	66
			$Z \to c\bar{c}$	$\pi^\pm, K^\pm, p(\bar{p})$	66
TASSO[75]	34GeV	77 pb^{-1}	inc. had.	$\pi^\pm, K^\pm, p(\bar{p})$	3
TASSO[75]	44GeV	34 pb^{-1}	inc. had.	$\pi^\pm, \pi^0$	5
TPC[76]	29GeV	70 pb^{-1}	inc. had.	$\pi^\pm, K^\pm$	12
OPAL[54]	201.7GeV	433 pb^{-1}	inc. had.	$h^\pm$	17
DELPHI[55]	189GeV	157.7 pb^{-1}	inc. had.	$\pi^\pm, K^\pm, p(\bar{p})$	9

incl. hadron production at HERA and COMPASS (SIDIS)

exp.	$\sqrt{s}$(GeV)	luminosity	kinematic cuts	hadrons	obs	$N_{\rm pt}$
H1[69]	318	44 pb^{-1}	$Q^2 \in$[175,20000] GeV^2	$h^\pm$	$D \equiv \frac{1}{N}\frac{dn_{h^\pm}}{dx_p}$	16
H1[70]	318	44 pb^{-1}	$Q^2 \in$[175,8000] GeV^2	$h^\pm$	$A \equiv \frac{D^+ - D^-}{D^+ + D^-}$	14
ZEUS[71]	300,318	440 pb^{-1}	$Q^2 \in$[160,40960] GeV^2	$h^\pm$	D	32
COMPASS06[72, 73]	17.3	540 pb^{-1}	$x \in [0.14, 0.4], y \in [0.3, 0, 5]$	π, K, h	$\frac{dM^h}{dz}$	124
COMPASS16[74]	17.3	-	$x \in [0.14, 0.4], y \in [0.3, 0, 5]$	π, K, p	$\frac{dM^h}{dz}$	97

Quality of the fit

- A best-fit with good agreements to the global data sets (1370 points in total) are found, χ^2/N well below 1; individual agreements to the 138 sub-datasets are also tested, motivating usage of a tolerance $\Delta\chi^2 \sim 2$ in determination of Hessian uncertainties

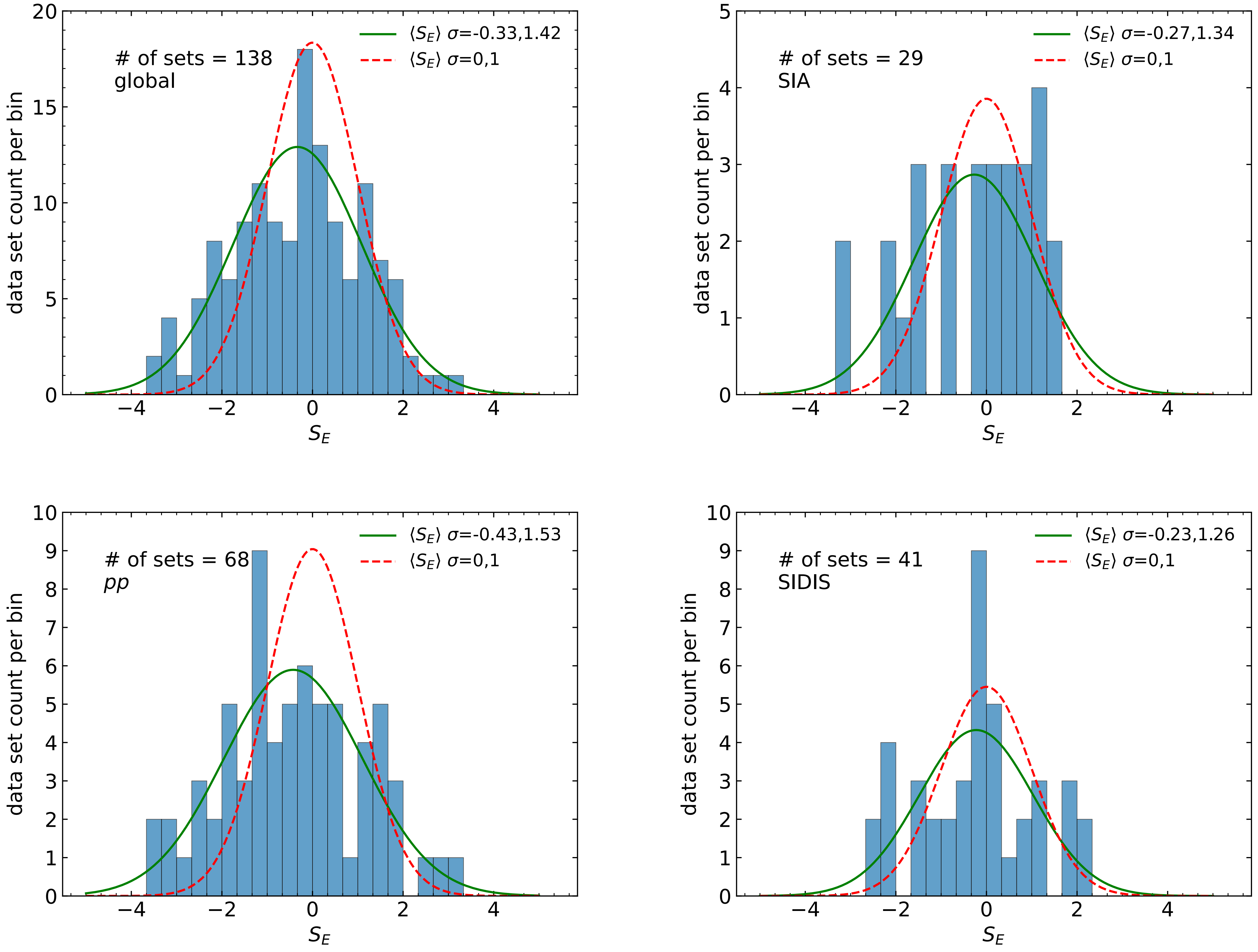
[CTEQ-TEA]

overall agreement: χ^2 breakdown to sub-groups for the best-fit

Experiments	N_{pt}	χ^2	χ^2/N_{pt}
ATLAS jets †	446	350.8	0.79
ATLAS Z/γ+jet †	15	31.8	2.12
CMS Z/γ+jet †	15	17.3	1.15
LHCb Z+jet	20	30.6	1.53
ALICE inc. hadron	147	150.6	1.02
STAR inc. hadron	60	42.2	0.70
pp sum	703	623.3	0.89
TASSO	8	7.0	0.88
TPC	12	11.6	0.97
OPAL	20	16.3	0.81
OPAL (202 GeV) †	17	24.2	1.42
ALEPH	42	31.4	0.75
DELPHI	78	36.4	0.47
DELPHI (189 GeV)	9	15.3	1.70
SLD	198	211.6	1.07
SIA sum	384	353.8	0.92
H1 †	16	12.5	0.78
H1 (asy.) †	14	12.2	0.87
ZEUS †	32	65.5	2.05
COMPASS (06I)	124	107.3	0.87
COMPASS (16p)	97	56.8	0.59
SIDIS sum	283	254.4	0.90
Global total	1370	1231.5	0.90

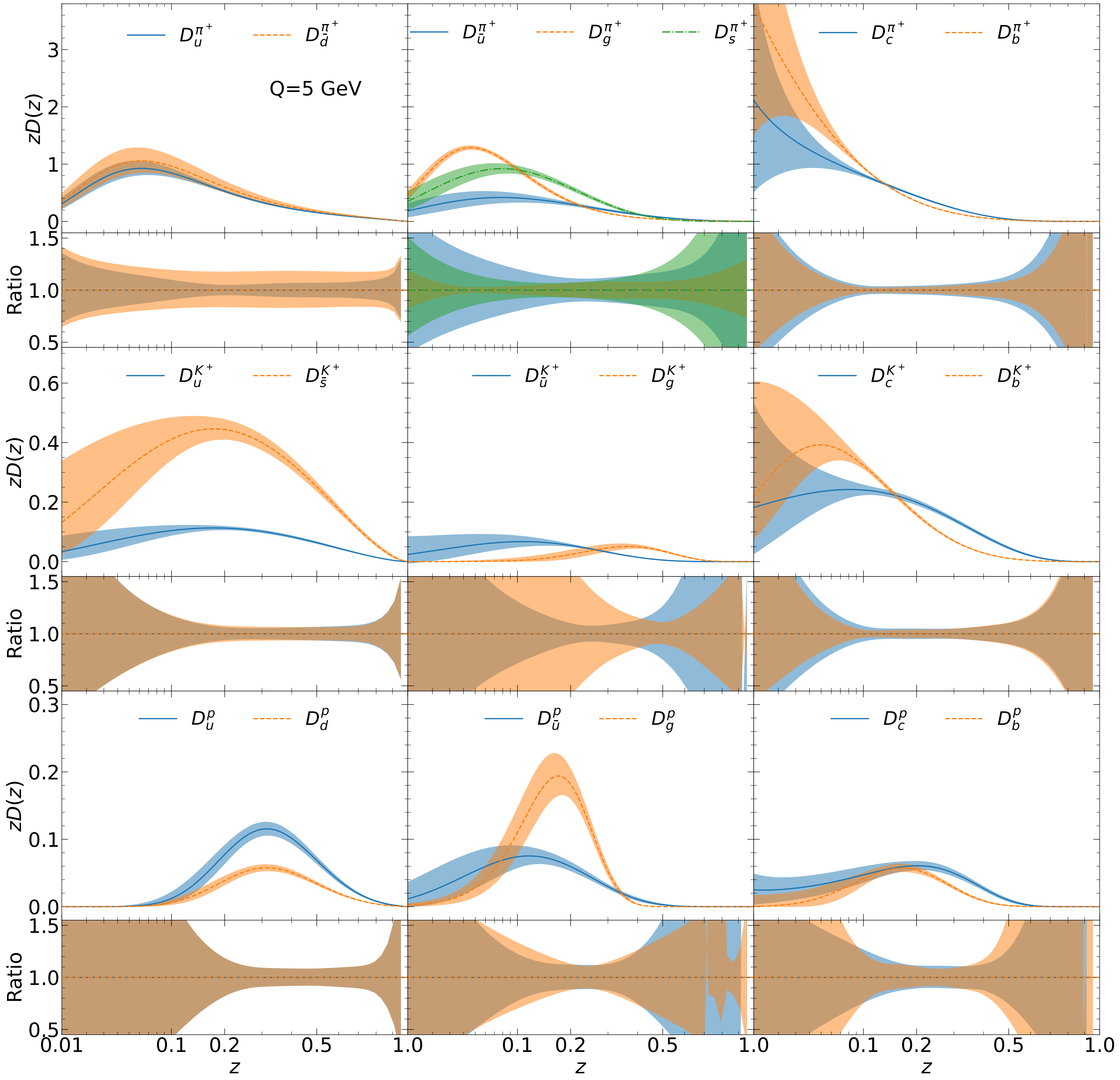
individual agreement: distributions of the effective Gaussian variable

$$S_E = \frac{(18N_{pt})^{3/2}}{18N_{pt}+1}\left\{\frac{6}{6-\ln(\chi^2/N_{pt})} - \frac{9N_{pt}}{9N_{pt}-1}\right\}$$



FFs to light charged hadrons

- We arrive at a best-fit of the charged pion, kaon and proton FFs together with 126 Hessian error FFs, two for each of the eigenvector direction; FFs are generally well constrained in the region with z~0.1-0.7



FFs (positive charge) vs. momentum fraction

- our results show an uncertainty of 3%, 4% and 8% for FFs of gluon to pion at z=0.05, 0.1 and 0.3, respectively
- similarly an uncertainty of 4%, 4% and 7% for FFs of u-quark to pion, kaon and proton at z=0.3, respectively
- FFs of heavy-quarks are well constrained for z between 0.1~0.5 due to the tagged SIA events at Z-pole measurements
- a preference for larger FFs of s quark to pion possibly due to decays of short-lived strange hadrons
- high precision of gluon FFs is mostly due to the data of jet fragmentation from the LHC

Test on momentum sum rule

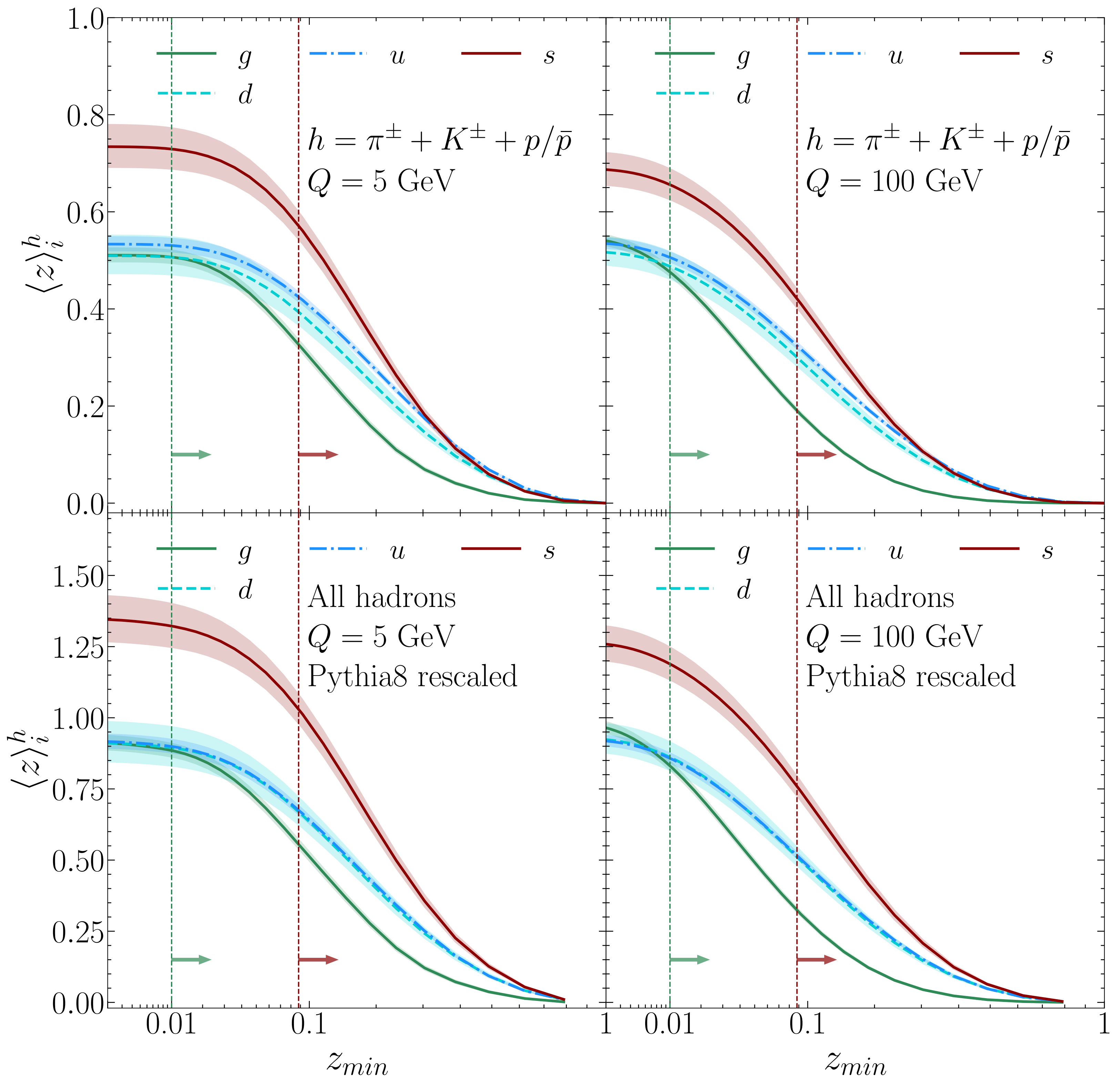
- FFs have the interpretation of number densities of hadrons and satisfy various fundamental sum rules as derived from first principle, including momentum sum rule, charge sum rule, etc.; momentum sum rules are tested with the extracted FFs and find consistency

momentum sum rule: $$\sum_h \int_0^1 dz z D_i^h(z, Q) = 1$$

with finite cutoff: $$\langle z \rangle_i^h = \int_{z_{min}}^1 dz z D_i^h(z, Q)$$

mom.	$g(z > 0.01)$	$u(z > 0.01)$	$d(z > 0.01)$	$s(z > 0.088)$
π^+	$0.200^{+0.008}_{-0.008}$	$0.262^{+0.017}_{-0.016}$	$0.128^{+0.020}_{-0.019}$	$0.161^{+0.013}_{-0.013}$
K^+	$0.018^{+0.004}_{-0.003}$	$0.058^{+0.005}_{-0.004}$	$0.019^{+0.004}_{-0.004}$	$0.015^{+0.002}_{-0.002}$
p	$0.035^{+0.006}_{-0.005}$	$0.044^{+0.004}_{-0.004}$	$0.022^{+0.002}_{-0.002}$	$0.015^{+0.002}_{-0.002}$
π^-	$0.200^{+0.008}_{-0.008}$	$0.128^{+0.020}_{-0.019}$	$0.299^{+0.054}_{-0.049}$	$0.161^{+0.013}_{-0.013}$
K^-	$0.018^{+0.004}_{-0.003}$	$0.019^{+0.004}_{-0.004}$	$0.019^{+0.004}_{-0.004}$	$0.205^{+0.014}_{-0.013}$
$\bar{p}$	$0.035^{+0.006}_{-0.005}$	$0.019^{+0.003}_{-0.003}$	$0.019^{+0.003}_{-0.003}$	$0.015^{+0.002}_{-0.002}$
Sum	$0.507^{+0.014}_{-0.013}$	$0.531^{+0.015}_{-0.013}$	$0.506^{+0.042}_{-0.037}$	$0.572^{+0.029}_{-0.028}$

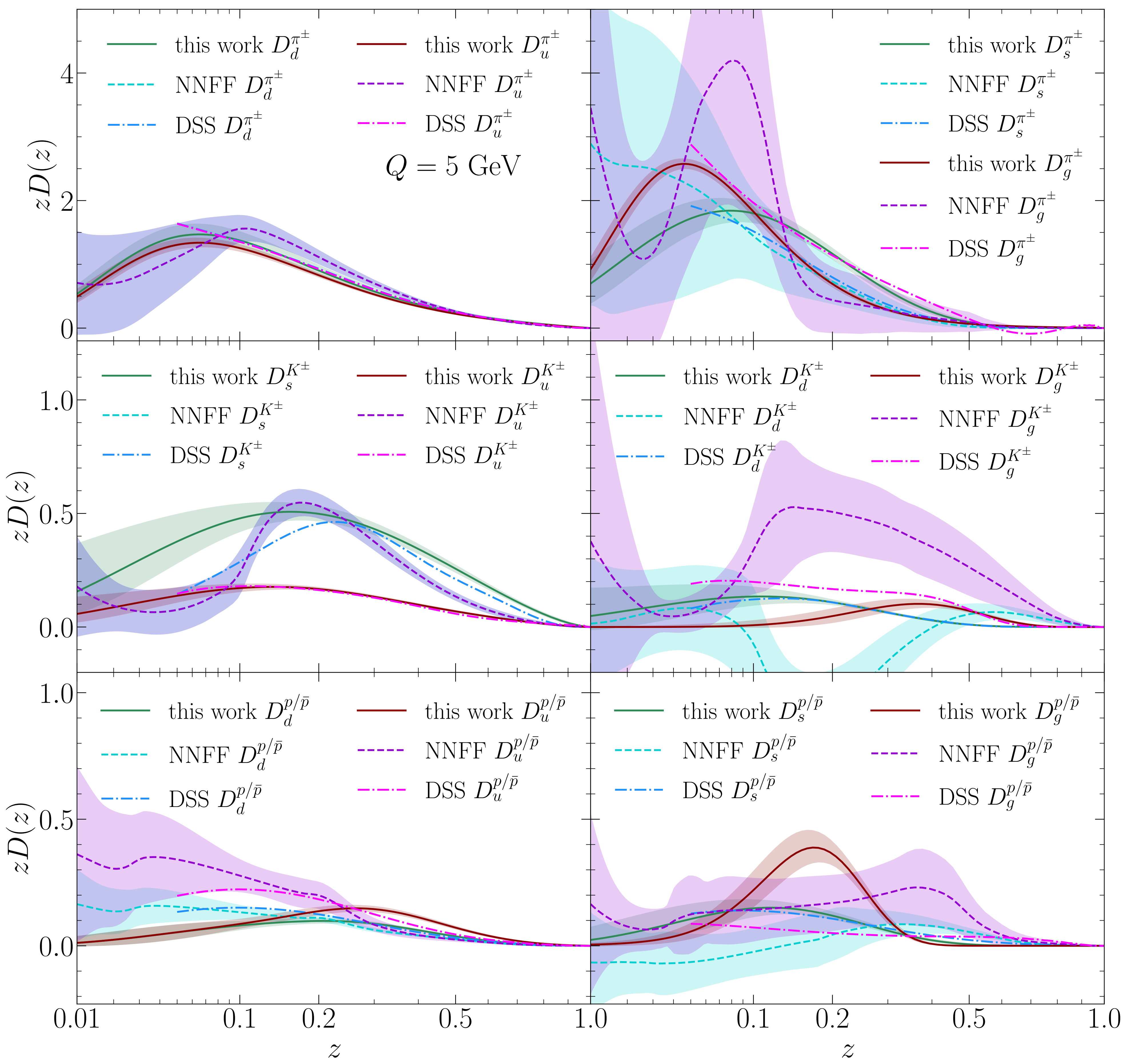
momentum carried by individual/all light charged hadrons at Q=5 GeV



total momentum vs. cutoff: light charged hadron; all hadrons (scaled from PYTHIA8)

Comparison to other determinations

- ✦ Our new extractions on FFs are compared to previous determinations from other groups (DSS and NNFF) for the charge-summed pion, kaon and proton; discrepancies are found and further investigations will be needed



FFs (charge-summed) vs. momentum fraction

- ❖ We find general agreement between ours and DSS for FFs of u and d quarks to pion, and of u quark to kaon
- ❖ however, discrepancies are found for FFs to protons and for FFs of gluon to all three charged hadrons
- ❖ NNFFs show larger uncertainties in general and can become negative in some kinematic regions
- ❖ future benchmark works involving different groups will be needed for investigation on discrepancies

[DSS21, DSS17, DSS07, NNFF1.0]

Summary

- Fragmentation functions (FFs) are essential non-perturbative inputs for precision calculations of hadron production cross sections in high energy scattering from first principle of QCD

- FMNLO is a program for automated and fast calculations of fragmentation processes at NLO in QCD is now publicly available, which is desirable for global analysis of FFs providing much improved efficiency and capability for arbitrary hard processes

- We perform a joint global analysis of FFs to identified charged hadrons, including charged pion, kaon and proton, at NLO in QCD, using most recent data from SIA, SIDIS, and pp collisions; constraints on gluon FFs are much improved and discrepancies are found wrt. previous determinations

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Thank you for your attention!