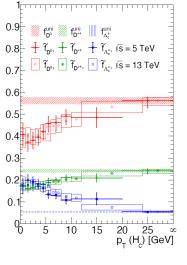
Nonuniversality of charm and beauty fragmentation and its impact on measurements at LHC and in neutrino (astro)physics

FH Particle Physics Discussion, DESY, 4.7.2025

Achim Geiser, DESY Hamburg

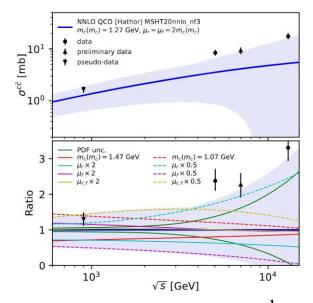


see also PhD thesis Y. Yang, DESY-Thesis-2024-013, in collaboration with Uni HH theory (S. Moch, O. Zenaiev)



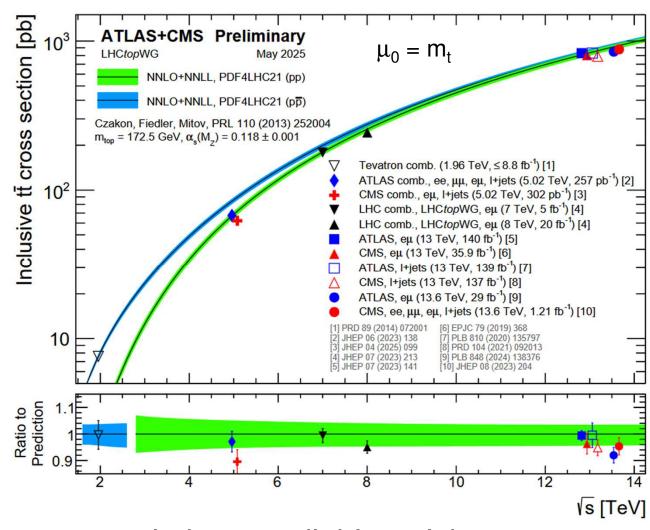
- Introduction/Motivation
- Evidence for charm and beauty fragmentation nonuniversality
- Phenomenological ddFONLL parametrization of charm nonuniversality
- Impact on total charm cross section measurements at LHC
- Extraction of m_c(m_c) and low-x PDF constraints at NNLO
- Potential impact on jet flavour tagging at LHC
- Potential impact on predictions for neutrino flux spectra from charm and beauty decays at LHC (e.g. for FASER), at fixed targets (e.g. SHIP) and in cosmic ray air showers (e.g. IceCube)

arXiv:2506.22616 subm. to JHEP



Teaser: measurements of total ttbar cross section

plethora of LHC results on total top cross section



produce the same for charm (and beauty)

(so far at LHC: only strong extrapolations available, relying on disproven charm fragmentation universality assumption)

-> need to treat nonuniversality

Why measure the total ccbar cross section?

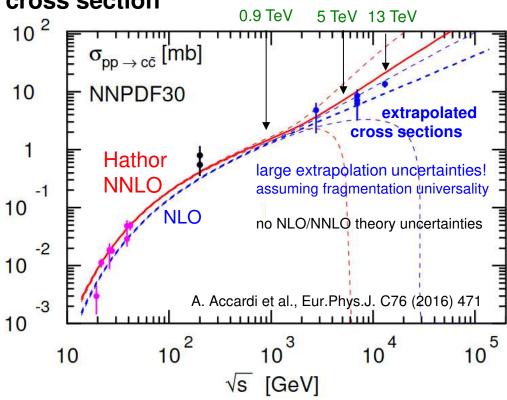
Total cross section has smallest theoretical pQCD uncertainty

- NNLO predictions available for total charm cross section

(differential cross sections: still only NLO+NLL)

 No theory dependence on fragmentation (or other nonperturbative effects)

> (see also D. d'Enterria, Moriond 2017)



treated in this contribution:

-> use measured double differential (p_T and y) single charm cross sections over largest possible phase space and

extrapolate/interpolate to total cross section

with "small" extrapolation factors

accounting for charm fragmentation nonuniversality (new)

Part 1

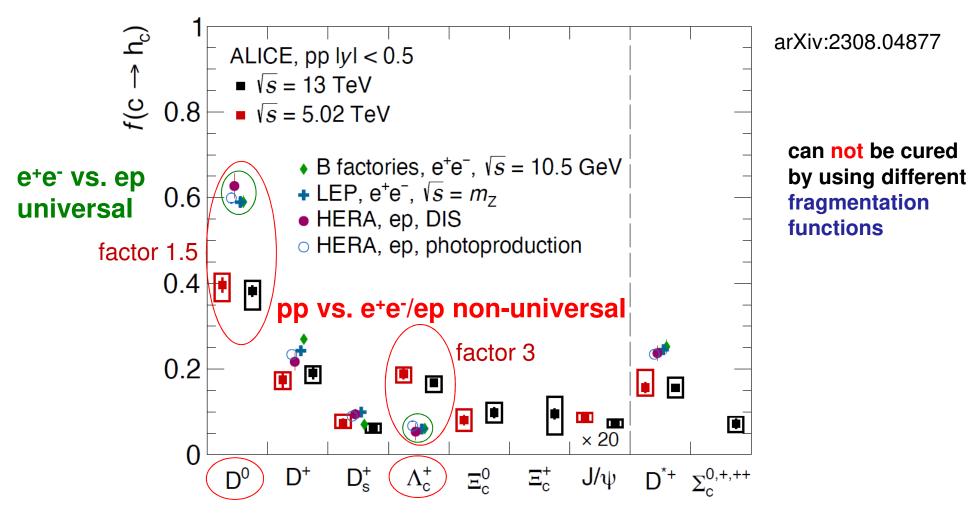
Evidence for nonuniversality of Charm and Beauty fragmentation in pp collisions

starts to accumulate from ~ 2016

attempt to review and parametrize it phenomenologically

Non-universality of charm fragmentation

Charm fragmentation fractions (p_T-integrated production fractions) in e⁺e⁻, ep, and pp

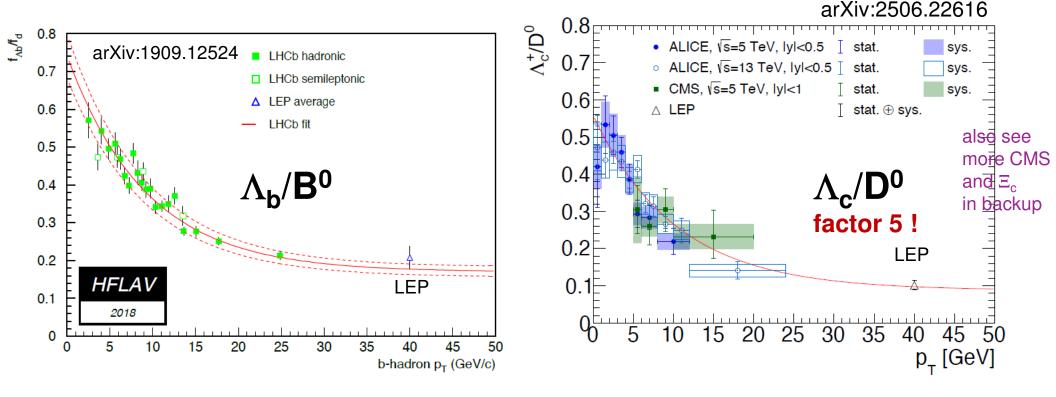


what about p_T and y dependence of production fractions?

Non-universality of charm fragmentation vs. p_T

Both beauty and charm baryon to meson production ratios in pp collisions exhibit strong p_T dependence,

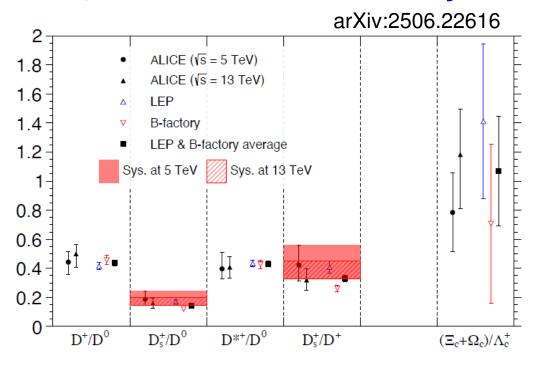
asymptotically approaching `universal' LEP e+e- values at high p_T

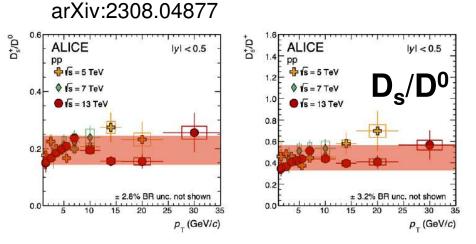


-> strategy (data driven! directly use measurements): treat baryon to meson production fractions vs p_T as non-universal treat asymptotic high p_T limit as universal

(Non-)universality of charm fragmentation vs. p_T

Study meson/meson and baryon/baryon ratios





no significant p_T dependence!

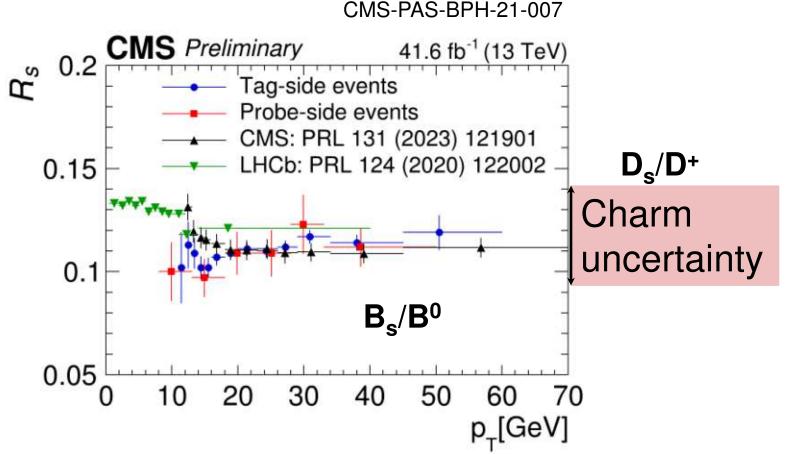
assign systematic uncertainties for potential small deviations, as e.g. known for B_s/B^0 (next slide)

no significant initial state dependence!

-> strategy (data driven!):
treat meson-to-meson and baryon-to-baryon production ratios as universal
(both integrated and as function of p_T, within uncertainties)

Non-universality of Bs, Ds fragmentation

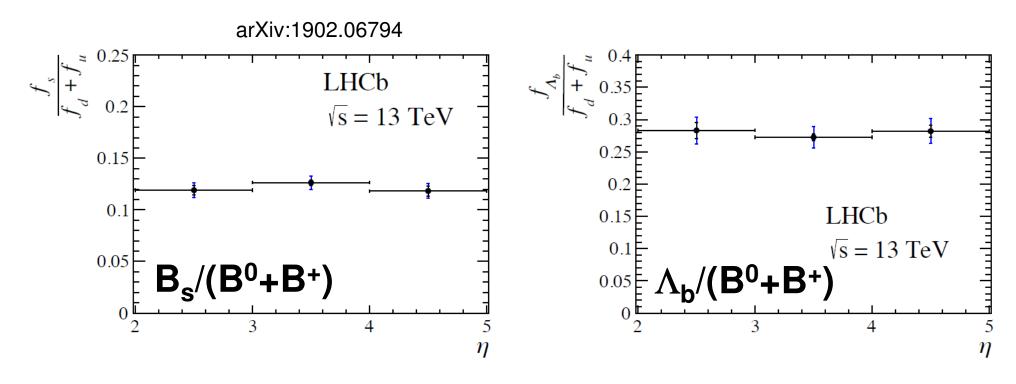
Study meson/meson ratios



-> uncertainty on meson-to-meson ratio for charm covers measured effect for beauty

(Non-)universality of charm and beauty fragmentation vs. (pseudo)rapidity

Neither beauty meson-to-meson nor baryon-to-meson production ratios in pp collisions exhibit noticeable rapidity (y) dependence



-> strategy (data driven!):

treat charm production fractions as universal in rapidity (within unc.)
-> can use ALICE measurements of p_T dependence at all rapidities

Will be consistency-checked with charm data later

Non-universality of charm fragmentation

represent nonuniversality
in terms of p_T-dependent
charm hadron production fractions
taken directly from data
(no functional parametrization)

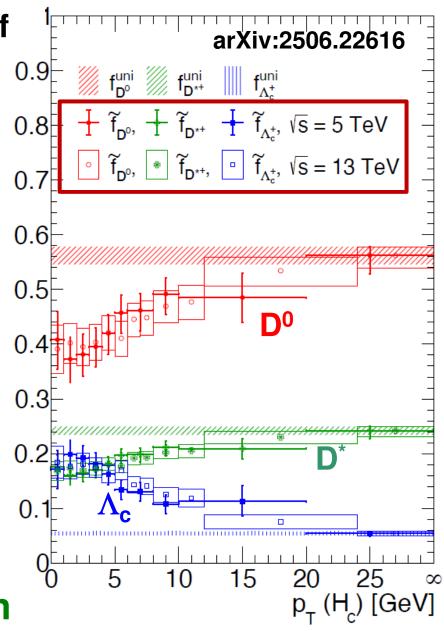
So far, treat 5 and 13 TeV measurements separately.

Consistent, so possibly combine in the future.

Reminder:

meson/meson ratios remain universal baryon/baryon ratios remain universal rapidity dependence remains universal high p_T limit remains universal

Use this for phenomenological approach



Part 2

arXiv:2506.22616

main contributor: Y.Yang

Phenomenological ddFONLL approach to treatment of nonuniversality of charm fragmentation in pp collisions for total cross section extrapolations

ddFONLL code and procedures available on public gitlab repository https://gitlab.cern.ch/ddfonll/charm-total-cross-section/. for use by third parties

FONLL (NLO+NLL) QCD theory predictions vs. data driven FONLL (ddFONLL)

standard FONLL theory:

charm quark level
$$d\sigma_{pp\to c\bar{c}}^{\rm FONLL} = f_i f_j \otimes d\hat{\sigma}_{ij\to c\bar{c}}$$
PDFs massive NLO + massless NLL matrix elements

perturbative QCD parameters:

charm hadron level

$$d\sigma_{H_c}^{\text{FONLL}} = f_{H_c}^{\text{uni}} \cdot (d\sigma_{pp \to c\bar{c}}^{\text{FONLL}} \otimes D_{c \to H_c}^{NP})$$
universal

fragmentation fraction. a number, e.g. from e⁺e⁻, ep

fragmentation function e.g. Kartvelishvili, from LEP

single parameter: α_κ

data driven FONLL (ddFONLL): arXiv:2311.07523

arXiv:2506.22616

for treatment of PDFs. see backup

arXiv:1205.6344

$$d\sigma_{H_c}^{\mathsf{ddFONLL}} = \underbrace{\tilde{f}_{H_c}\left(p_T\right)} \cdot \left(d\sigma_{pp \to c\bar{c}}^{\mathsf{FONLL}} \otimes D_{c \to H_c}^{NP}\right)$$

all parameters, including QCD scales, fitted to data (χ^2 minimization)

04.07.25 A. Geiser, FH Part. Phys. Discussion

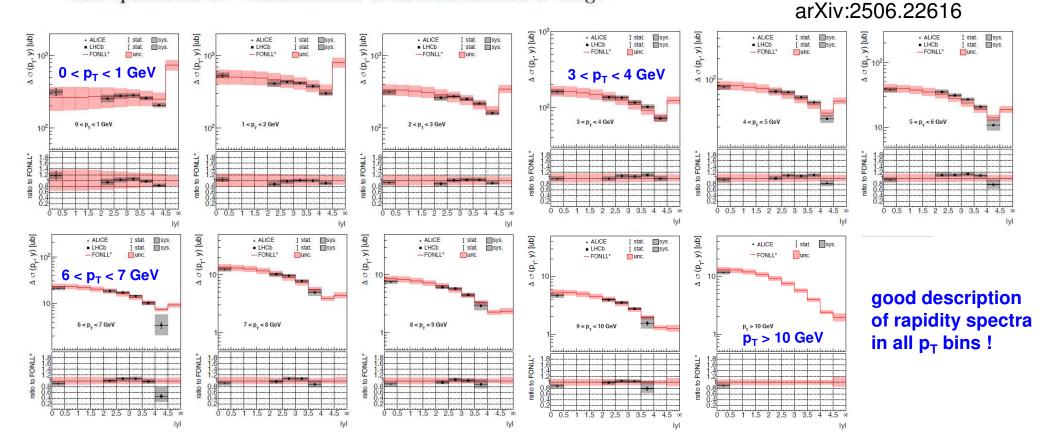
Application to published 13 TeV ALICE+LHCb D⁰ data

arXiv:2506.22616

D^0 CROSS SECTION IN FULL KINEMATIC RANGE

same for 5 TeV in backup

✓ Data constrained FONLL with total uncertainty (CTEQ6.6 PDF $\oplus \tilde{f} \oplus (\mu_f, \mu_r, m_c, \alpha_K)$) gives good descriptions for D^0 measurements in the full kinematic range



-> strategy for extrapolation to total charm cross section: use data whenever available, otherwise ddFONLL data constrained band

Extrapolated total pp charm pair cross section

arXiv:2506.22616

13 TeV:

phase space extrapolation factor ~1.9

$$\sigma_{c\bar{c}}^{\rm tot}(13~{\rm TeV}) = 17.43^{+0.56}_{-0.53}({\rm data})^{+0.76}_{-0.78}(\tilde{f})^{+1.47}_{-1.22}({\rm PDF})^{+0.24}_{-0.18}(\mu_f, \mu_r, m_c, \alpha_K)^{+2.05}_{-1.19}(f_{D^0}^{pp})~{\rm mb}$$

~ 1/4 of total inelastic cross section!

5 TeV: (arXiv:2311.07523)

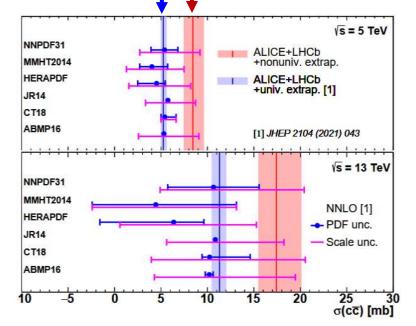
phase space extrapolation factor ~1.8

$$\sigma_{c\bar{c}}^{\text{tot}}(5 \text{ TeV}) = 8.43_{-0.25}^{+0.25}(\text{data})_{-0.42}^{+0.40}(\tilde{f})_{-0.56}^{+0.67}(\text{PDF})_{-0.12}^{+0.13}(\mu_f, \mu_r, m_c, \alpha_K)_{-0.65}^{+0.88}(f_{D^0}^{pp}) \text{ mb}$$

assuming universality

this work (~50% increase)

NNLO QCD theory

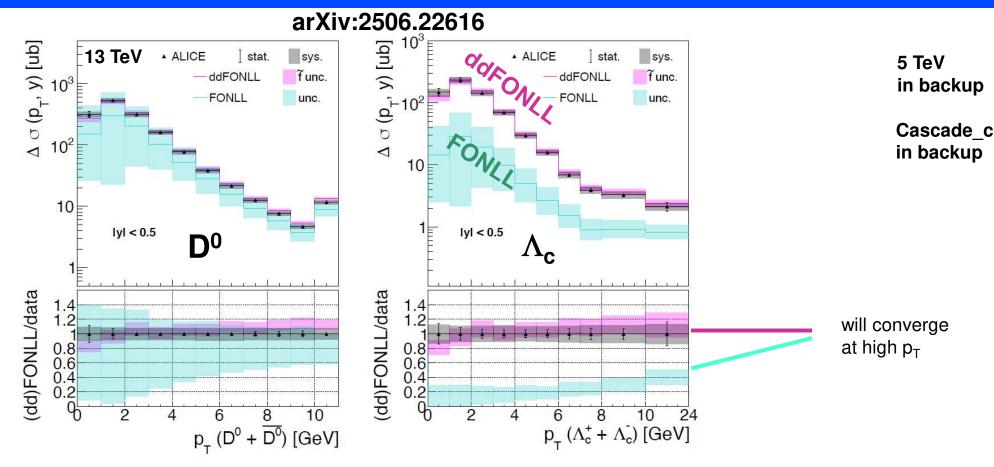


-> treatment of charm fragmentation nonuniversality has significant impact on total cross section results! consistent with upper edge of NNLO band

ddFONLL code and procedures available on public gitlab repository for use by third parties

Adapted from M. Garzelli et al., arXiv:2009.07763, JHEP 04 (2021) 043)

Performance illustration on 13 TeV ALICE data



FONLL: a priori prediction with full uncertainty, with `classical' universality assumption, PDF unc. and 7-point scale variation **ddFONLL:** fit to ALICE+LHCb D⁰ data (next slide), here $\tilde{f}_{D^0}(p_T)$ unc. only (w/o fitted $\mu_{\rm f}, \mu_{\rm r}, m_{\rm c}, \alpha_{\rm K}$ uncertainties and PDF uncertainties),

+ `postdiction' for Λ_c data (full uncertainty ~50% larger, mainly PDFs)

ddFONLL "QCD" fit parameters

arXiv:2506.22616

4-dimensional "fit" of ALICE + LHCb double differential D⁰ data (χ^2 scan)

Reminder: now phenomenological parameters (no longer a priori pQCD)

$$\mu_0 = \operatorname{sqrt}(m_c^2 + p_{Tc}^2)$$

	5 TeV	13 TeV
factorization scale μ_f	1.0-2.0 μ_0 (1.68)	1.19-1.52 μ_0 (1.41)
renormalization scale μ_r	$0.34 \text{-} 0.87 \; \mu_0 \; (0.48)$	$0.29 - 0.48 \mu_0$ (0.37)
charm `pole' mass m _c	1.3-1.9 GeV (1.7)	1.7-2.1 GeV (1.9)
Kartvelishvili fragm. par. α_{K}	6-25 (9)	5-9 (6)

... but all in `reasonable' QCD parameter range.

factorization scale prefers to be on the higher side

renormalization scale prefers to be on the low side

(compare arXiv:1506.07519 and arXiv:0711.1983 for theoretical arguments)

pole mass is on the higher side (but still consistent with pole mass obtained from running mass)

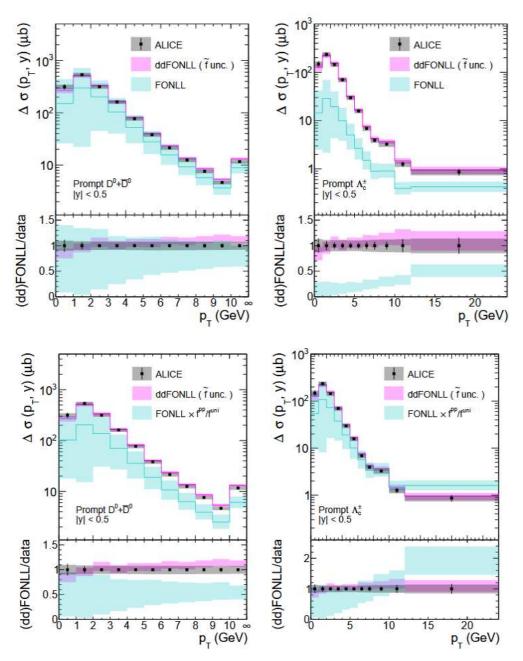
`average' fragmentation parameter comes out consistent with LEP value of 6.1

use 5 TeV fit parameters to `estimate' 0.9 TeV cross section: (not a measurement,

$$\sigma_{c\bar{c}, \text{pseudo}}^{\text{tot}}(0.9 \text{ TeV}) = 1.67 \pm 0.24 \text{ mb}$$

but use as proxy later)

External alternative proposal: FONLL rescaling Check on 13 TeV ALICE D 0 and Λ_c data



arXiv:2506.22616

ddFONLL vs. default FONLL

In clear disagreement with baryon data

ddFONLL vs. FONLL rescaled to measured average fragmentation fractions

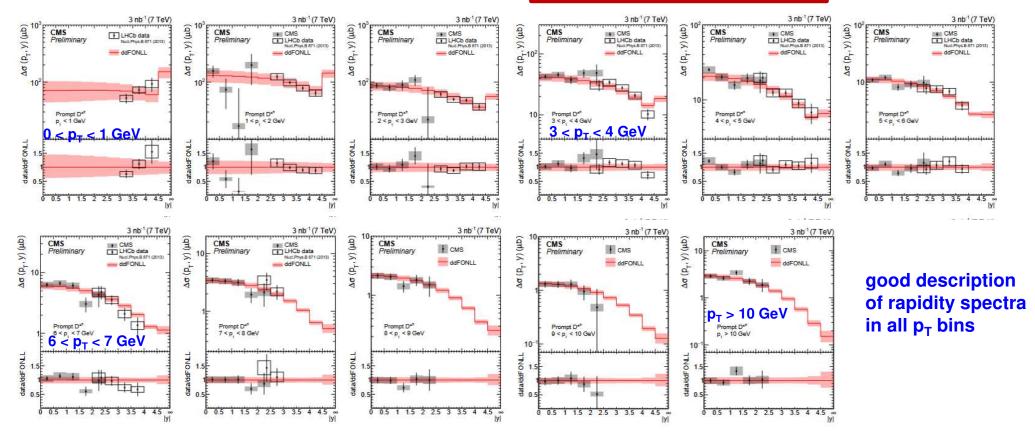
Better, but not really good enough.

Tension with data in particular at high p_T . Inconsistency with LEP at high p_T .

ddFONLL application to 7 TeV CMS+LHCb D* data



larger rapidity coverage, extrapolation factor 1.4



again use data whenever available, otherwise ddFONLL data constrained band -> extrapolated total pp charm cross section at 7 TeV:

$$\sigma_{\rm c\overline{c},tot} = 9.39^{+0.74}_{-0.74}({\rm data})^{+0.31}_{-0.32}(\tilde{f})^{+0.64}_{-0.51}({\rm PDF})^{+0.30}_{-0.41}(\mu_f,\mu_r,m_c,\alpha_K)^{+0.83}_{-1.07}(f^{\rm pp})\,{\rm mb}$$

Part 3

arXiv:2506.22616

main contributor: O. Zenaiev

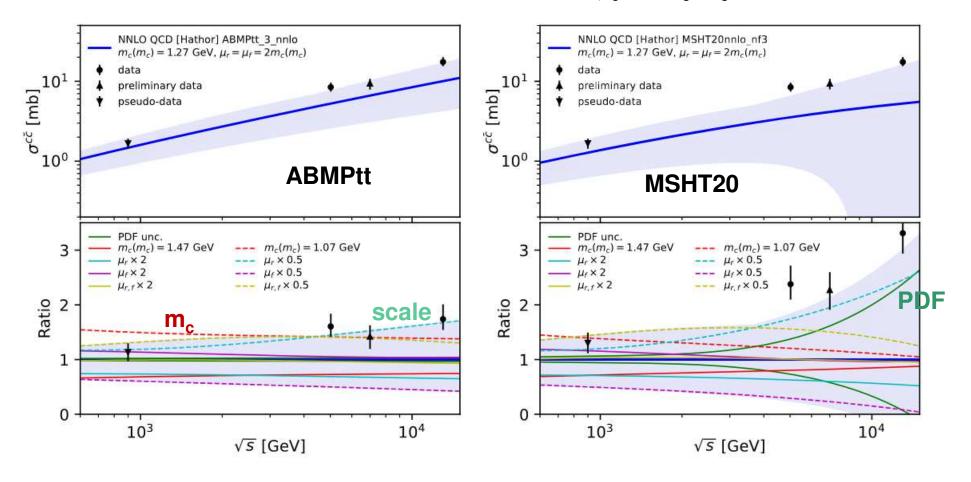
NNLO QCD interpretation of resulting parton level total cross sections (a priori no fragmentation effects)

Now straight perturbative QCD at NNLO

Total charm pair cross section vs. sqrt(s), NNLO

Hathor, full NNLO QCD, 3 flavour, running mass, $\mu_0 = 2m_c(m_c)$

arXiv:2506.22616



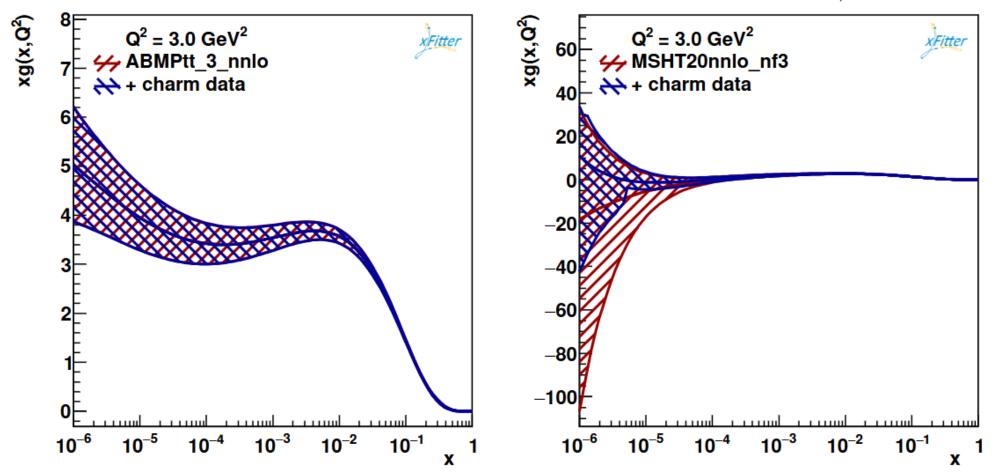
Sensitivity to NNLO PDFs at low x (~10⁻⁵), in particular at 13 TeV Sensitivity to $m_c(m_c)$. Perfect description by ABMPtt with $\mu_r = \frac{1}{2} \mu_0$

First such direct constraint estimates from LHC pp collisions at NNLO

Include total charm cross sections in PDF fit (profiling)

arXiv:2506.22616

Hathor, full NNLO QCD, 3 flavour, running mass, μ_0 = $2m_c(m_c)$, μ_r = $\frac{1}{2}$ $\mu_{0,}$ no scale variations



Strong reduction of uncertainty on NNLO gluon pdf at low x (x < 10^{-4}) for MSHT20. Central value becomes "more physical".

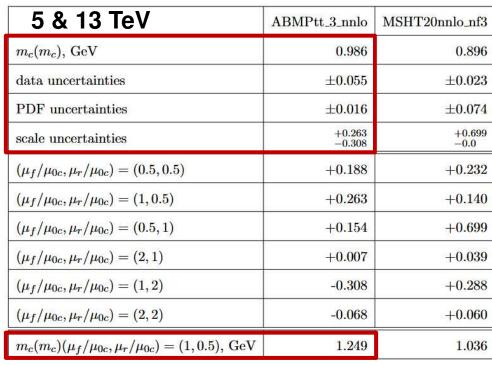
Small effect for ABMPtt (already constrained more by parametrization)

The two become more similar.

Sensitivity to m_c(m_c)



Hathor, full NNLO QCD, 3 flavour, running mass, $\mu_0 = 2m_c(m_c)$, 7-point scale variation



$$m_c(m_c) = 0.986^{+0.269}_{-0.313} \text{ GeV}$$

PDG: $m_c(m_c) = 1.2730 \pm 0.0028 \text{ GeV}$

Result consistent with PDG, but uncertainty ~factor 100 larger.

Still, first NNLO determination at LHC. Confirms that perturbative QCD continues to work down to scale m_c at LHC energies (within large but understood scale uncertainties).

1750

1500

■ Total unc.

∙Data unc.

→ Scale unc.

→ PDF unc.

 $\sqrt{s} = 0.9 \text{ TeV}$

 $\sqrt{s} = 5.02 \text{ TeV}$

 $\sqrt{s} = 7 \text{ TeV}$

 $\sqrt{s} = 13$ TeV

 $\sqrt{s} = 5.02.13$ TeV

PDG2025 $m_c(m_c) = 1273.0 \pm 2.8 \text{ MeV}$

750 1000 1250

 $m_c(m_c)[MeV]$

ABMPtt 3 nnlo

MSHT20nnlo nf3

ABMPtt_3_nnlo F MSHT20nnlo_nf3

ABMPtt 3 nnlo

ABMPtt 3 nnlo

MSHT20nnlo nf3

ABMPtt 3 nnlo

MSHT20nnlo nf3

250

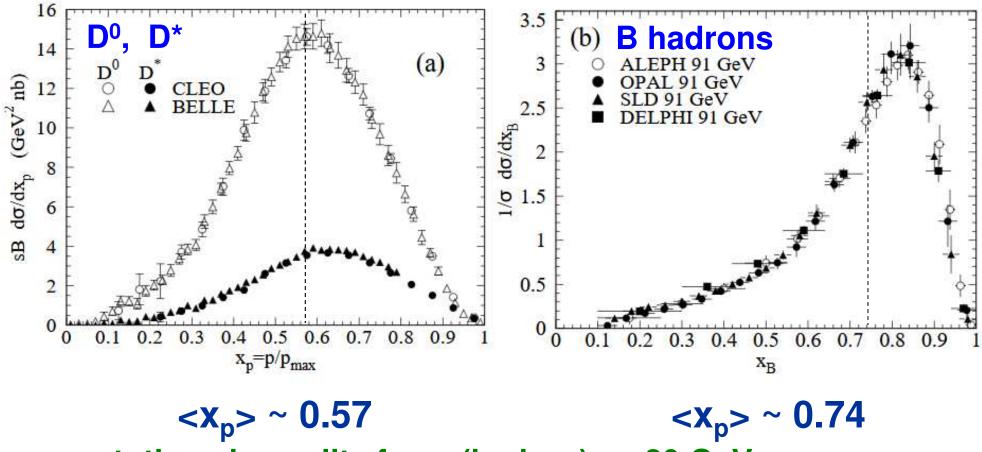
Part 4

Potential effect on flavor tagging of LHC jets (preliminary)

Back to fragmentation issues

Charm and beauty fragmentation functions from e+e-

PDG 2024: fraction of quark (jet) momentum carried by heavy hadron



asymptotic universality for $p_T(hadron) > \sim 20 \text{ GeV}$

-> asymptotic universality of beauty jet fragmentation for p_{Tjet} >~ 27 GeV charm jet fragmentation for p_{Tiet} >~ 35 GeV

beauty fragmentation function from ttbar b-jets

CMS-PAS-TOP-18-012: fraction of quark (jet) momentum carried by B hadron

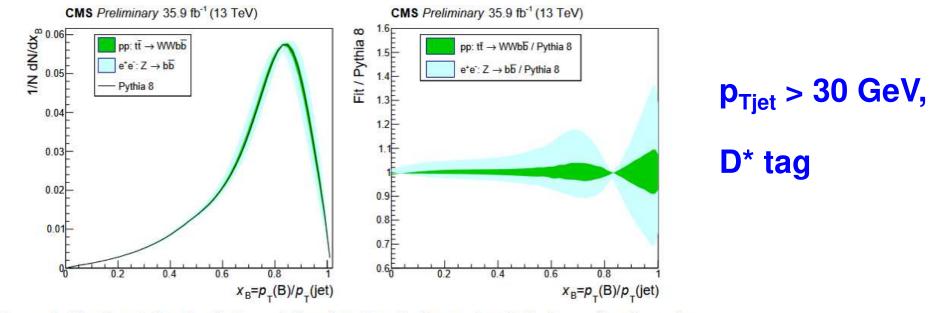


Figure 4: The Lund–Bowler fragmentation function for b quarks plotted as a function of x_b . The left panel shows the comparison of the result from this analysis (green), the result obtained from the data at the Z pole (light blue), and the current default function from PYTHIA 8 (black line). The right panel shows the value of the fitted functions divided by the PYTHIA 8 calculation.

b-jet fragmentation in ttbar events consistent with LEP (and with PYTHIA parameterization derived from LEP)

-> b-tagging for p_{Tiet} > 30 GeV presumably unaffected ☺

p_{Tjet} > 20 GeV might need a bit of further study

Charm jet tagging (very preliminary)

No "easy" clean charm jet reference sample -> situation less obvious

In contrast to beauty,

- **'stable'** charm hadrons have very different branching fractions and lifetimes -> change of meson/baryon composition with p_T can significantly affect the charm jet tagging efficiency:
- * Semileptonic branching fractions vary between 4% (Λ_c) and 16% (D+); applying p_T-dependent ddFONLL rescaling reduces average semileptonic charm branching fraction by ~16 %
- -> may affect jet lepton tag
- * Decay $c\tau$ varies between 60 μ (Λ_c) and 310 μ (D+)
- -> change of composition may affect Jet secondary vertex tag (not quantified)
- -> may indirectly also affect bg. to hadronic τ tag?
- -> c-tagging for p_{Tjet} > 40 GeV presumably safe © p_{Tjet} > 20 GeV, with possibly charm baryon enhancement by up to ~factor 2(?) should definitely be studied further

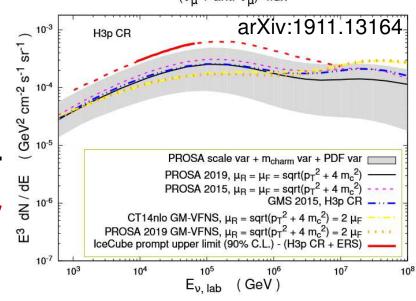
Part 5

Potential effect on neutrino spectra from charm decay (very preliminary)

Still to be quantified more precisely, but, along with semileptonic branching fraction, the low p_T charm baryon enhancement may reduce the neutrino rate from charm decays by O(16%) on average

by O(16%) on average.

Low-p_T-dominated forward production, such as for forward neutrino detection at LHC (e.g. FASER), in fixed target collisions (like e.g. for SHIP) or in cosmic ray air showers (like in IceCube) might be affected even more strongly (up to twice).



Neutrino rate from beauty decays presumably less affected, since semileptonic branching fractions similar for different b hadron types.

Summary, conclusions and outlook

Evidence for nonuniversality of charm and beauty fragmentation in pp collisions has been accumulated since ~2016. None of the physics models trying to account for that (not discussed here) were fully successful.

Was little accounted for so far concerning practical consequences

arXiv:2506.22616

(dd)FONLL/data

A novel fully data-based phenomenological approach, ddFONLL has been worked out to integrate the established nonuniversality of charm fragmentation and its uncertainty into the extrapolation of total charm pair cross sections at LHC.

-> total charm cross sections increase by O(50%) w.r.t. those still assuming universality. Repository for external use available.

Results are still in reasonable agreement with NNLO QCD expectations (near upper edge)

Comparison of sqrt(s) dependence with NNLO QCD theory gives insights on pQCD (multi-scale problem), constraints on PDFs, and charm quark mass, from hadronic collisions at NNLO.

Outlook:

ddFONLL method can be directly extended to beauty production and pA collisions, while remaining fully consistent with FONLL treatment of past or future charm/beauty results in e⁺e⁻ or ep collisions or very high p_T jets by construction.

Can also be extended to differential NNLO+NNLL (when available), to predictions of semileptonic decay neutrino spectra, and to modifications of charm (and b?) tagging of low p_T jets.

 $p_{\perp} (\Lambda_c^+ + \Lambda_c^-) [GeV]$

Final messages

A surprisingly simple purely phenomenological and data driven parametrization of charm fragmentation nonuniversality (slide 10) can reestablish consistency between all known charm measurements in pp collisions at LHC,

as well as with previous and future e⁺e⁻ and ep measurements.

Perturbative QCD at parton level remains valid down to the scale m_c, even at LHC energies.

Further applications/extensions can be expected.

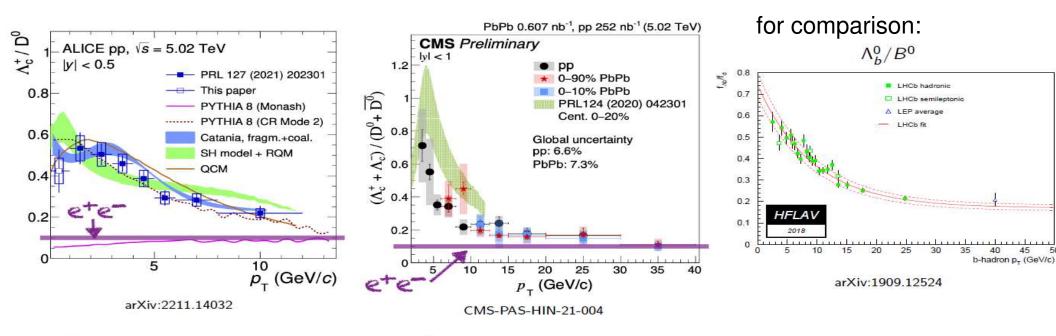
Backup

Non-universality of charm fragmentation

From slides Y.Yang at EPS 2023

 p_T DEPENDENT Λ_c^+/D^0 MEASUREMENTS

pp non-universal!



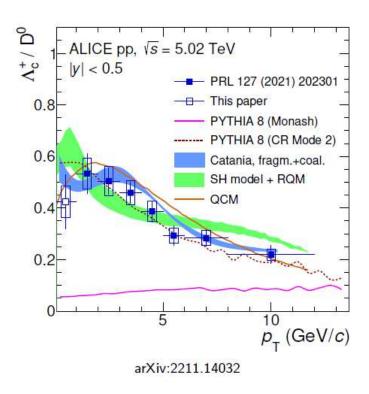
- ✓ clear p_T dependence observed on Λ_c^+/D^0 measurements from pp→ asymptotically close to e^+e^- value, $0.10^{+0.01}_{-0.01}$ (as like observed on Λ_b^0/B^0)
- -> strategy (data driven!):

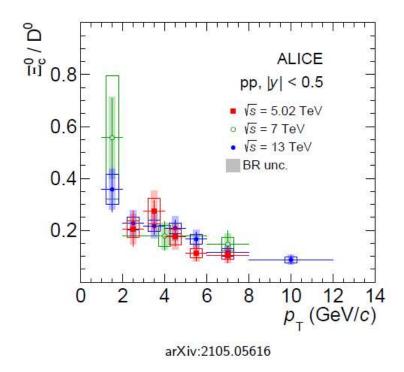
treat baryon to meson production fractions vs p_T as non-universal treat asymptotic high p_T limit as universal

Baryon to baryon ratio

From slides Y.Yang at EPS 2023

$$\Lambda_c^+/D^0$$
 and Ξ_c^0/D^0 measurement





 \checkmark no significant p_T dependence observed for baryon-to-baryon

FONLL (NLO+NLL) QCD theory predictions and PROSA/CTEQ PDFs

From slides Y.Yang at EPS 2023

constrained by

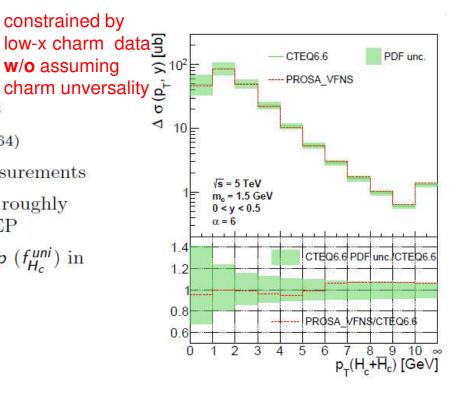
CHARM HADRON PRODUCTION IN pp COLLISIONS

Hadron cross section $(d\sigma_{H_c})$ given by convolutions of perturbative cross section $(d\hat{\sigma}_{ij\to c\bar{c}})$ and non-perturbative functions $(f_i, f_j, D_{c \to H_c}^{NP})$:

$$d\sigma_{H_c} \propto d\sigma_{pp \to c\bar{c}} \otimes D_{c \to H_c}^{\rm NP}, \quad d\sigma_{pp \to c\bar{c}} = f_i f_j \otimes d\hat{\sigma}_{ij \to c\bar{c}}$$

- $\checkmark d\hat{\sigma}_{ij\to c\bar{c}}$ given at NLO+NLL (FONLL) in QCD
 - \rightarrow has scales $(\mu_f \text{ and } \mu_r)$ and pole mass (m_c) uncertainties charm unversality \hat{g}
- \checkmark PDFs f_i and f_i of initial states determined from measurements
 - → used CTEQ6.6 as a proxy of PROSA_VFNS (arXiv:1911.13164)
- \checkmark fragmentation function $(D_{c\to H_c}^{\rm NP})$ for final states also from measurements
 - \rightarrow used Kartvelishvili function having a single parameter α_K , roughly constrained not to be too far off the one extracted from LEP
- \checkmark normalization given by a fragmentation fraction from $e^+e^-/ep~(f_{H_c}^{uni})$ in universality assumption
 - → original FONLL theory (arXiv:1205.6344):

$$d\sigma_{H_c}^{\rm FONLL} = f_{H_c}^{uni} \cdot (d\sigma_{pp \to c\bar{c}}^{\rm FONLL} \otimes D_{c \to H_c}^{NP})$$



-> strategy (data driven "theory"):

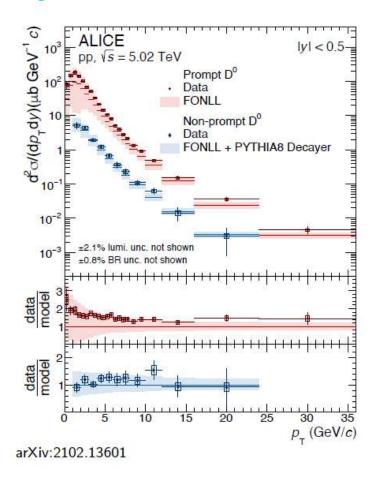
modify phenomenologically to include nonunversality and fit to data (within uncertainties)

Application to published 5 TeV ALICE+LHCb charm data

From slides Y.Yang at EPS 2023

Extrapolating D^0 measurements at 5 TeV

Input measurements:



phenomenol. modified and $d\sigma_{H_c}^{\rm FONLL\ with\ \tilde{\it f}}$ to find best description of data with 4 free parameters $(\mu_f,\,\mu_r,\,m_c$ and $\alpha_K)$:

$$\chi^2 = \sum_{\text{data bins}} \frac{(\text{FONLL} - \text{data})^2}{\text{statistical unc.}^2 + \text{systematic unc.}^2}$$

 \rightarrow i.e., finding μ_f^b , μ_r^b , m_c^b and α_K^b of the least χ^2

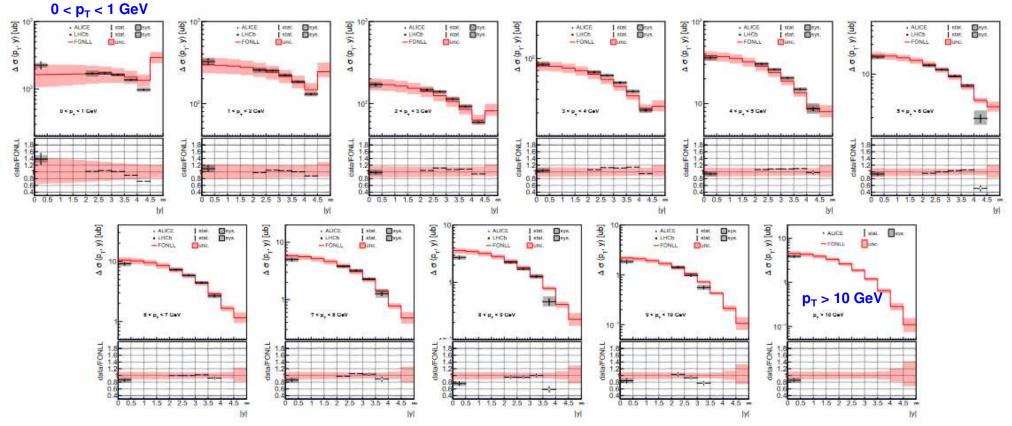
✓ use to extrapolate D⁰ measurements at 5 TeV from LHC

Application to published 5 TeV ALICE+LHCb charm data

From slides Y.Yang at EPS 2023

D^0 CROSS SECTION IN FULL KINEMATIC RANGE

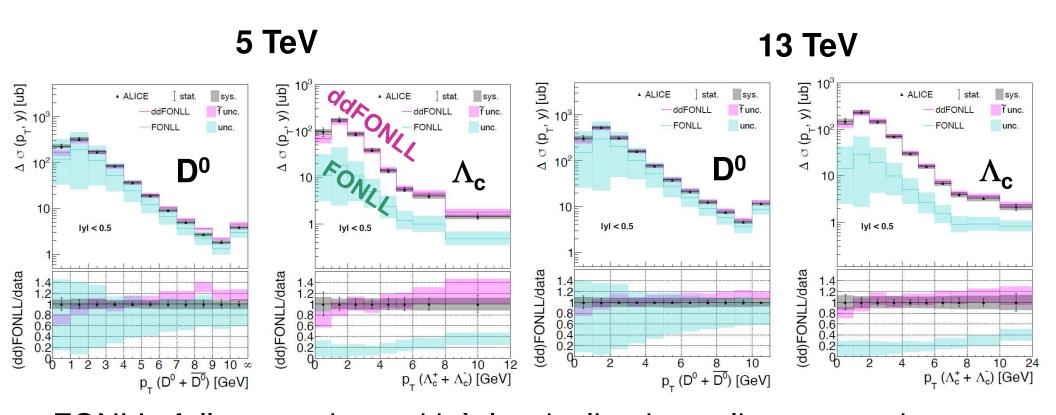
✓ Data constrained FONLL with total uncertainty (CTEQ6.6 PDF \oplus \tilde{f} \oplus (μ_f , μ_r , m_c , α_K)) gives good descriptions for D^0 measurements in the full kinematic range (as a function of p_T in backup)



-> strategy:

use data whenever available, otherwise data constrained theory

Performance illustration on 5 + 13 TeV ALICE data



FONLL: full uncertainty, with `classical' universality assumption ddFONLL: f uncertainty only (for cross check)

Cascade_c at 5 TeV

plot adapted from arXiv:2311.11426

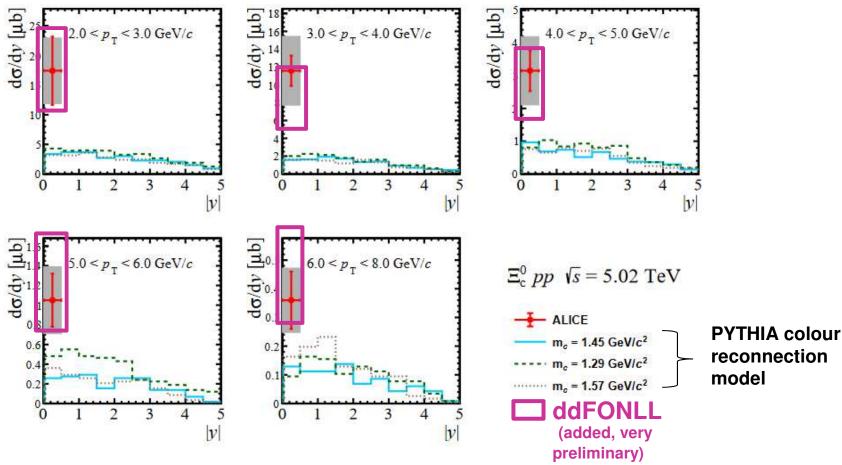
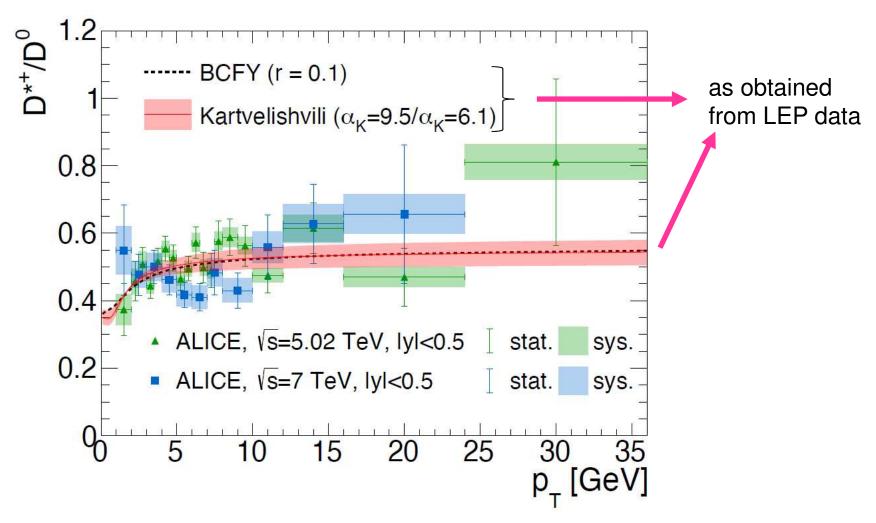


Figure 11: Measured Ξ_c^0 cross section as a function of rapidity compared with PYTHIA simulations with the bands corresponding to a 1σ variation around the optimum.

ddFONNL also works for Cascade_c!

D* vs. D⁰ fragmentation



LHC data consistent with LEP -> universality holds for D*/D

-> ddFONLL for D⁰ can be translated into ddFONLL for D* (e.g. future 0.9 TeV measurements)

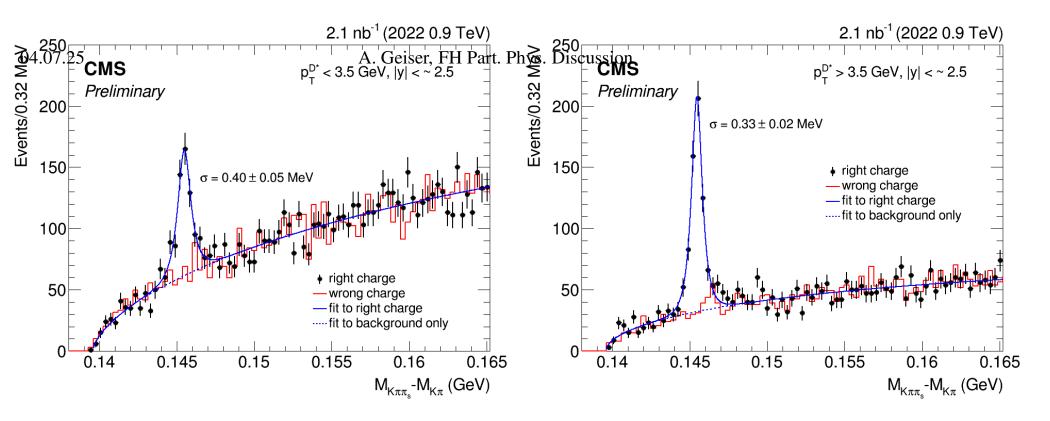
Charm cross sections at 0.9 TeV?

CMS-DP-2022-024

$$D^* p_T < 3.5 \text{ GeV}$$

$$D^* |y| < \sim 2.5$$

$$D^* p_T > 3.5 \text{ GeV}$$



no cross sections available so far, but would like to have proxy for QCD studies -> use plain ddFONLL applied to 0.9 TeV FONLL with 5 TeV fit parameters, expect:

 $\sigma_{\text{tot}}(\text{ccbar}) = 1.7^{+0.24}_{-0.24}(\text{total})\text{mb}.$

not a measurement!