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Charm total cross sections with nonuniversal fragmentation treatment, part II

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Total charm-pair cross sections in pp collisions are interesting because they can be calculated to NNLO in QCD without any reference to fragmentation effects. On the other hand, the fiducial differential charm cross sections from which the total cross sections must be extrapolated are currently known to NLO+NLL at most (e.g. FONLL), and must be treated for known effects of nonuniversal charm fragmentation.
A new procedure using the FONLL framework as input for an empirical parametrization of the data in both shape and normalization, with all its parameters actually fitted to data, is used to derive so-called data-driven FONLL (ddFONLL) parametrizations which can be used to extrapolate the differential cross sections to total cross sections with minimal bias. This includes an empirical treatment of all known non-universal charm fragmentation effects, in particular for the baryon-to-meson ratio as a function of transverse momentum.
The total charm-pair cross sections obtained in this way, which supersede all previous ones obtained using the assumption of charm-fragmentation universality, are consistent with NNLO predictions, and allow first studies of their sensitivity e.g. to the charm-quark mass and/or the NNLO gluon PDF at very low transverse momentum fractions x.

Introduction

The theory of Quantum-Chromo-Dynamics (QCD) is a well-established part of the Standard Model of particle physics, which describes most of the processes occurring in pp collisions at LHC rather well. Predictions for charm production are particularly challenging since, due to the closeness of the charm quark mass, $m_c \sim 1.5$ GeV, to the nonperturbative QCD scale, $\Lambda_{QCD} \sim 0.3$ GeV, the convergence of the perturbative series is slow, resulting in large theoretical uncertainties. In addition, nonperturbative effects enter the hadronization of charm quarks into charm hadrons, the entities actually measurable in detectors. Recently, it was established[1,2,3,4] (Fig. 1) that the corresponding charm fragmentation effects are non-universal, i.e. can not simply be transferred from $e^+ e^-$ and ep measurements to pp measurements and may be dependent on kinematics. Finding an appropriate treatment of this non-universality[5] is one of the central themes of this contribution. For space reasons, only the most important parts of the information already given in a similar writeup[6] , of which this writeup can be considered to be a follow-up, are given here, and are amended by additional information. More details can be found there, and full details are available meanwhile in a thesis writeup[7] . Since the results were presented at the conference, the method has also already been applied by CMS to preliminary measurements at 7 TeV[8] .

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Measuring the total cross section for charm-quark-antiquark pair production, $\sigma_{c\bar{c}}^{\mathrm{tot}}$, almost[a] identical to the total summed and integrated cross section for the prompt production of charm hadrons H_c containing a single charm quark c (not $\bar{c}$), $\sigma_{H_c}^{\mathrm{all}}$, is of particular interest since the corresponding theoretical predictions are currently the only pp charm cross sections calculable at next-to-next-to-leading order (NNLO) in QCD, and do furthermore not depend upon charm fragmentation. As we will demonstrate, they can thus be used to derive constraints on genuine QCD parameters such as the charm-quark mass m_c and the proton parton density functions (PDFs), at NNLO. For such measurements, differential H_c distributions measured in limited kinematic ranges (fiducial cross sections) and for a restricted set of H_c final states need to be extrapolated to the total cross section, under certain constraints concerning their shape and normalization in unmeasured regions. Furthermore, the possibly phase space dependent relative contributions of different H_c final states (nonuniversality) need to be accounted for.

In this contribution we will describe how such shape, normalization and nonuniversality constraints can be obtained in an entirely data driven way, based on a theory-inspired parametrization of the multi-differential cross sections, and fully accounting for charm nonuniversality effects, without attempting to rely on any particular nonuniversal charm fragmentation model. Since space is limited, we will extensively refer to previous writeups[5,6] where applicable.

An alternative approach for 5 TeV pp data only, relying on a specific colour reconnection model, can be found in [9].

2 FONLL vs. ddFONLL calculations

The highest order calculations available so far for differential charm-production cross sections are based on the massive next-to-leading order (NLO) plus massless next-to-leading-log (NLL) approach, also known as general mass variable flavour number scheme, one example of which, exploited here, is the FONLL[10] approach. By construction, the NLL part of this calculation becomes significant only at high values of charm transverse momentum ($p_{Tc} \gg m_c$), such that, since the total cross section is dominated by the low p_T contribution, NLO massive fixed order calculations without resummation could also be used instead for this purpose.

Details of some theory aspects of the data driven FONLL (ddFONLL) approach used here, previously referred to as "modified FONLL", are given in a previous report[5]. In a nutshell, the FONLL theory, including its charm fragmentation extension, is modified to ddFONLL by replacing the fixed "universal" fragmentation fraction $f_{H_c}^{\mathrm{uni}}$ obtained from e^+e^- and/or ep collisions by a p_T-dependent hadron-production fraction $\tilde{f}_{H_c}(p_T)$ directly obtained from measurements at LHC (Fig. 1),

$$d\sigma_{H_c}^{\mathrm{FONLL}} = f_{H_c}^{\mathrm{uni}} \cdot \left(d\sigma_{pp\to c}^{\mathrm{FONLL}} \otimes D_{c\to H_c}^{\mathrm{NP}} \right) \quad \to \quad d\sigma_{H_c}^{\mathrm{ddFONLL}} = \tilde{f}_{H_c}(p_T) \cdot \left(d\sigma_{pp\to c}^{\mathrm{FONLL}} \otimes D_{c\to H_c}^{\mathrm{NP}} \right) \quad (1)$$

while the FONLL parametrizations of the quark-level differential cross sections $d\sigma_{pp\to c\bar{c}}^{\mathrm{FONLL}}$ and the parametrization of the nonperturbative fragmentation function $D_{c\to H_c}^{\mathrm{NP}}$, here using the Kartvelishvili[11] parametrization, remain unchanged. The other change is that, instead of treating the FONLL QCD parameters μ_f and μ_r (factorization and renormalization scales) and m_c (charm pole mass) as external QCD parameters, they are empirically left to float freely, to be fitted from data, separately for each pp center-of-mass energy. The same is true for the Kartvelishvili parameter α_K. In contrast to FONLL, ddFONLL is therefore no longer a QCD theory prediction, rather a theory-inspired parametrization of the pp data at a given center of mass energy. For the PDFs, the CTEQ6.6 set[12], not relying on pp charm fragmentation universality as input, is used, including uncertainties consistent with the PROSA[13] low-x gluon parametrization of the rapidity dependence (only) of LHC charm data in different regions of p_T (see Fig. 2 left, also see

[a]Hadron states containing a $c\bar{c}$ pair or more than one c quark contribute only about 1% to the total charm cross section and are hence neglected here.

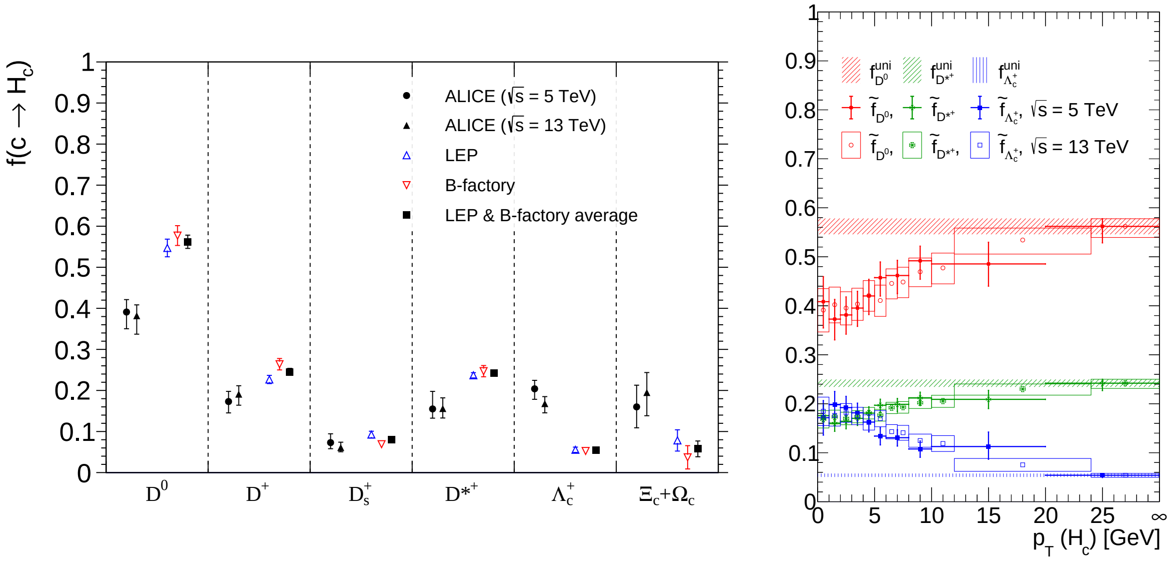

Figure 1 – Integrated fragmentation fractions f (left) and differential hadron fractions $\tilde{f}$ as a function of p_T (right) at 5 and 13 TeV, for different charm hadron final states, compiled from [1,2,3,4,14].

previous explanations[5]). In the limit $\tilde{f}(p_T) \equiv f^{\rm uni}$ (e.g. for e^+e^- or ep, or at large transverse momenta), the standard FONLL parametrization is fully recovered, i.e. the approach remains fully consistent with all successful previous e^+e^- and ep FONLL applications and high p_T charm jet applications by definition.

This ddFONLL approach implies the following assumptions [6]:

- The p_T dependence of $\tilde{f}$ asymptotically approaches LEP e^+e^- values[15] at high p_T, i.e. at high p_T (> 25 GeV), charm fragmentation universality is fully recovered.
- As motivated by measurements[16], there is no strong non-universal rapidity dependence of $\tilde{f}$, and any potential small residual dependencies are absorbed into the global $\tilde{f}$ uncertainties. This assumption is also verified a posteriori by the fits to data [5,6,7].
- Non-universal effects in the nonperturbative fragmentation function D^{NP} at a given pp center-of-mass energy are small enough such that the approximation of treating them as factorizable w.r.t. $\tilde{f}$ in Eq. (1) (p_T-dependent reshuffling of final state charm hadron fractions) holds well enough within current $\tilde{f}$ and freely fitted α_K uncertainties. This assumption is also verified a posteriori by the fits on data.
- For pp, all ddFONLL parameters except the PDFs may be $\sqrt{s}$ dependent.

A further simplification made, again based on measurements, is

- While the baryon-to-meson H_c ratios are strongly p_T dependent[2,3,4,5,6], the meson-to-meson and baryon-to-baryon ratios remain p_T independent[17,6]. Known small deviations from this assumption, e.g. for hadrons containing strange vs. u or d quarks[18,6], are absorbed into the global $\tilde{f}$ uncertainties. Again, this approach is also verified a posteriori on data.

This is further exemplified by the resulting ddFONLL 'prediction' for the Cascade$_c$ final state, which is compared to ALICE data and to a prediction from the specific PYTHIA colour reconnection model [9] in Fig. 2 right.

3 Fit Results

The results of fitting the free ddFONLL parameters μ_f, μ_r, m_c and α_K to 5 and 13 TeV D^0 data[2,19] were already shown previously[5,6]. Very good agreement with data was obtained, reflected by the χ^2 S-factor for the 4D fit coming out very close to 1 [7]. The fit parameters are given in table 1, and show consistency between 5 and 13 TeV. In both cases, the fitted α_K

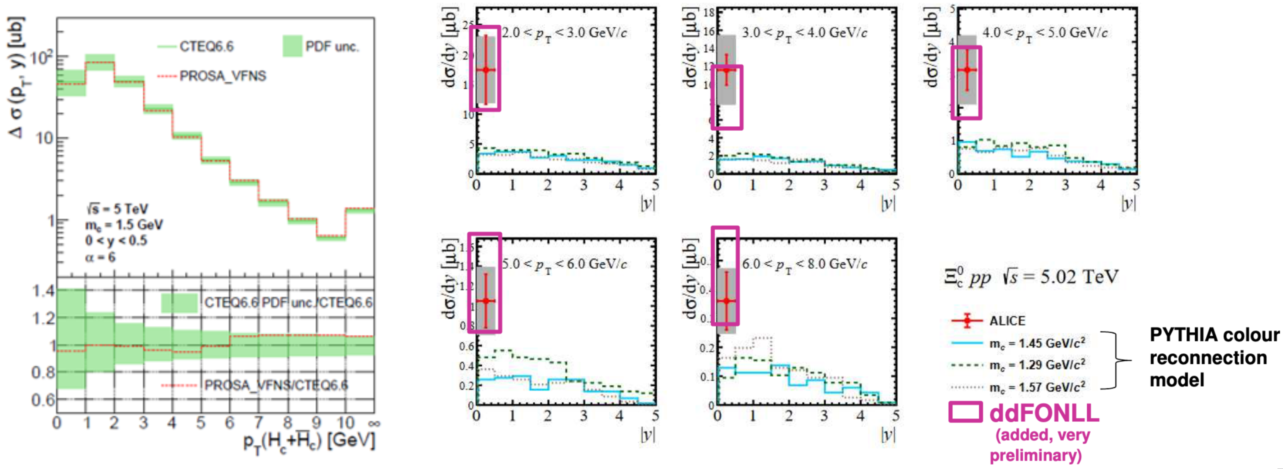

Figure 2 – left: Comparison of the CTEQ and PROSA PDFs. right: Ξ_c^0 cross sections as a function of $|y|$; the figures were adapted from [9].

	$\sqrt{s} = 5$ TeV	$\sqrt{s} = 13$ TeV
μ_f/μ_0	1.68 (1.00 - 2.00)	1.41 (1.19 - 1.52)
μ_r/μ_0	0.48 (0.34 - 0.93)	0.37 (0.29 - 0.48)
m_c [GeV]	1.7 (1.3 - 1.9)	1.9 (1.7 - 2.1)
α_K	9 (6 - 28)	6 (5 - 9)

Table 1: The best parameters used for the ddFONLL parametrization. The parentheses indicate the ranges of the uncertainty parameters, which were used to calculate so-called χ^2 uncertainties of ddFONLL.

parameters are also consistent with those expected from the asymptotic agreement with LEP. For illustration, the result of the 13 TeV ddFONLL parametrization obtained from the fit is also shown in Fig. 3 for the comparison to ALICE D^0 and Λ_c assuming charm fragmentation universality. Both the shape and normalization of both distributions are well described by ddFONLL while standard FONLL fails in both shape and normalization for the Λ_c case. A very similar comparison is also available for the 5 TeV case[5,7]. These results are fully consistent with all the explicit and implicit ddFONLL assumptions stated above (a posteriori verification).

Using the measurements for all bins in which measurements are available (not shown here, see [5,6]), and the ddFONLL data parametrization in all others, the resulting 5 TeV and 13 TeV total charm-pair production cross sections are obtained to be

$$\sigma_{c\bar{c}}^{\mathrm{tot}}(5\ \mathrm{TeV}) = 8.43^{+0.25}_{-0.25}(\mathrm{data})^{+0.40}_{-0.42}(\tilde{f})^{+0.67}_{-0.56}(\mathrm{PDF})^{+0.13}_{-0.12}(\mu_f, \mu_r, m_c, \alpha_K)^{+0.65}_{-0.88}(f^{pp}_{D^0})[\mathrm{mb}] \quad (2)$$

$$= 8.43^{+1.05}_{-1.16}(\mathrm{total})\ \mathrm{mb}. \quad (3)$$

$$\sigma_{c\bar{c}}^{\mathrm{tot}}(13\ \mathrm{TeV}) = 17.43^{+0.56}_{-0.53}(\mathrm{data})^{+0.69}_{-0.78}(\tilde{f})^{+1.47}_{-1.22}(\mathrm{PDF})^{+0.24}_{-0.18}(\mu_f, \mu_r, m_c, \alpha_K)^{+1.19}_{-2.05}(f^{pp}_{D^0})[\mathrm{mb}] \quad (4)$$

$$= 17.43^{+2.10}_{-2.57}(\mathrm{total})\ \mathrm{mb}. \quad (5)$$

in which $f^{pp}_{D^0}$ refers to the integrated D^0 fragmentation fraction measured at 5 TeV or 13 TeV, respectively. The respective extrapolation factors for unmeasured phase space are about 1.8 and 1.9. In Fig. 4 these total cross sections are compared to previous determinations[14] still based on the charm fragmentation universality assumption, and to NNLO predictions. The complete treatment of charm fragmentation nonuniversality significantly increases the extracted total charm cross sections, and therefore replaces all previous such determinations. The measurements are still consistent with the NNLO predictions, but now situated towards the upper edge of the NNLO theory uncertainty band.

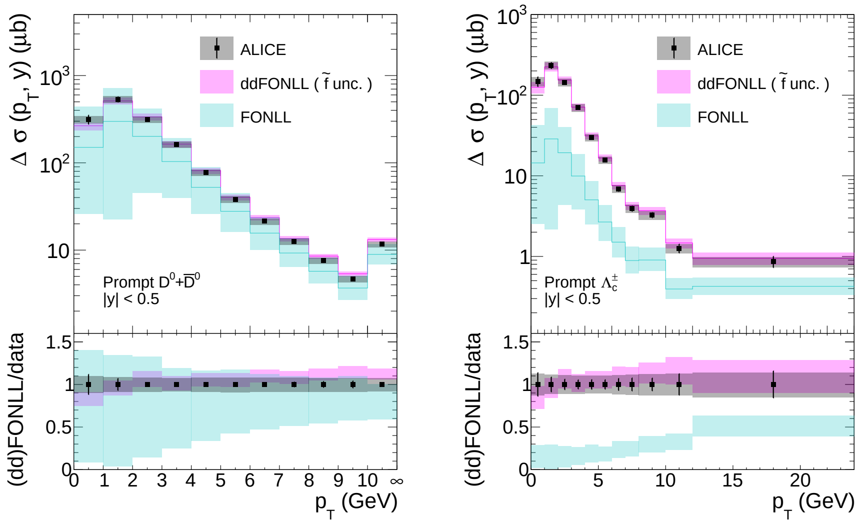

Figure 3 – Result of the fitted 13 TeV ddFONLL parametrization for D^0 (left) and Λ_c (right), compared to ALICE data[2] and to the standard FONLL prediction. Only the $\tilde{f}$ uncertainties are shown here for the ddFONLL case.

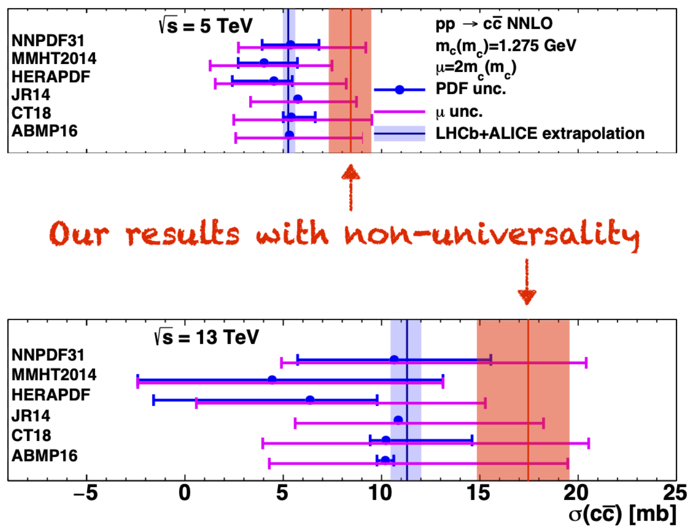

Figure 4 – Comparison of measured total charm-pair cross sections at 5 TeV and 13 TeV (red bands) to previous determinations[14] (blue bands) and to NNLO predictions with various PDF sets including theory uncertainties (points with bars). Plots adapted from [14].

CMS is able to measure D^* final states also at 0.9 TeV[20]. Since no cross section results are available so far at this energy, and in order to be able to evaluate the future sensitivity to the $\sqrt{s}$ dependence, we use our ddFONLL prediction for 0.9 TeV as a proxy for a potential future measurement.

Very preliminary studies of the sensitivity of these predictions to the MSbar charm quark mass, shown in Fig. 5, indicate that the mass preferred by the data is consistent with the world average and can be constrained with an uncertainty of order 200 MeV by these measurements. This uncertainty is still significantly larger than corresponding constraints e.g. from QCD fits of *ep* data[21], but a first step towards such a constraint from *pp* data at NNLO, and at least a very important consistency check. Furthermore, depending on the stiffness of the low-x PDF parametrization, these same studies indicate a significant potential for contraining the gluon distribution at very low x at NNLO, in an x region where data constraints[13] were so far possible only at NLO.

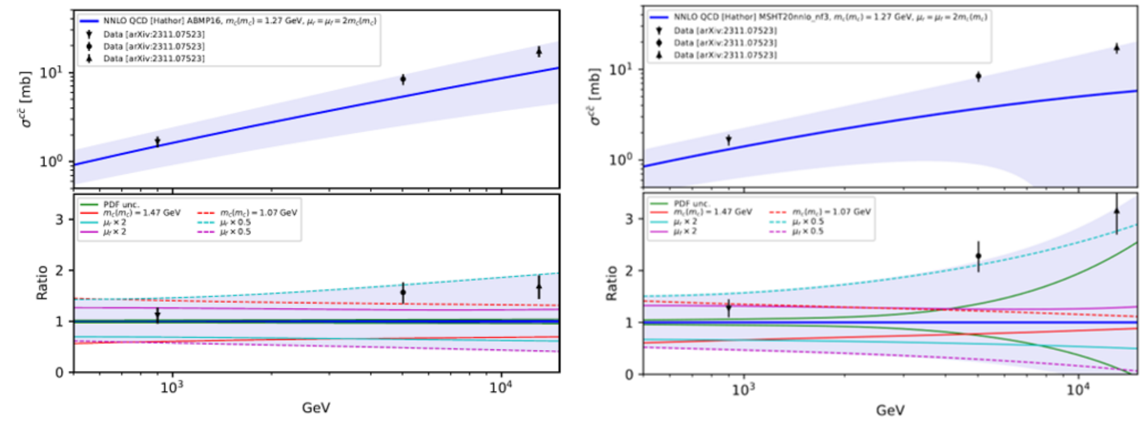

Figure 5 – Comparison of measured total charm-pair cross sections at 5 TeV and 13 TeV, and the proxy at 0.9 TeV (points) to NNLO fixed flavour predictions with ABMP16_3_nnlo[22] (left) and MHST20nnlo_nf3[23] (right) PDF sets, including theory uncertainties and their breakdown (bands and lines).

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