Hadroproduction of open heavy flavour for PDF analyses

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Based on Helenius, Paukkunen, JHEP 1805 (2018) 196

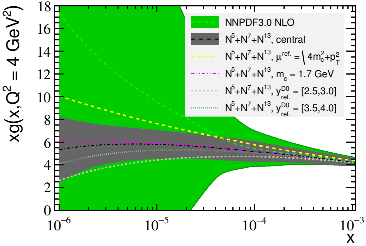
JYVÄSKYLÄN YLIOPISTO

SUOMEN AKATEMIA

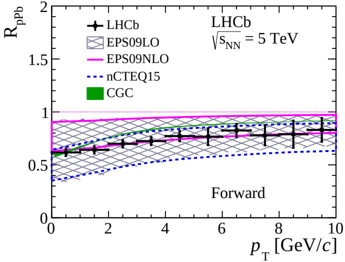
Open heavy-flavour measurements promising PDF constraints

- The potential of D (and B) meson production as a PDF constraint has been actively discussed [GAULD, ROJO, PRL 118, 072001 ; PROSA, EPJ C75, 396 ; KUSINA ET.AL. PRL 121,052004]

reduction of NNPD3.0 gluon uncertainty upon including LHCb D-meson data



large y nuclear modification in p-Pb from LHCb [JHEP 10 (2017) 090]

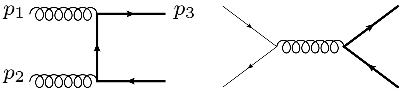


- Theoretical description typically based on fixed-order QCD (e.g. the MNR code [Mangano et.al. NP B373, 295]), FONLL [CACCIARI ET.AL. JHEP 9805, 007], or Powheg+Pythia [Frixione et.al. JHEP 0709, 126]
- Here, we discuss a novel implementation of the full **general-mass variable-flavour-number scheme (GM-VFNS)** treatment

Fixed-flavour-number scheme (FFNS)

- In FFNS, the heavy quarks are produced in three partonic processes

$$g + g \to Q + X, \quad q + \overline{q} \to Q + X, \quad q + g \to Q + X$$



+ NLO diagrams

$$\frac{d\sigma(h_1 + h_2 \to \mathrm{Q}/\overline{\mathrm{Q}} + X)}{dp_{\mathrm{T}}\,dy} = \sum_{ij} \int_{x_1^{\min}}^{1} dx_1 \int_{x_2^{\min}}^{1} dx_2$$

$$f_i^{h_1}(x_1, \mu^2_{\mathrm{fact}}) \quad \frac{d\hat{\sigma}^{ij\to \mathrm{Q}/\overline{\mathrm{Q}}+X}(\tau_1, \tau_2, m^2, \mu^2_{\mathrm{ren}}, \mu^2_{\mathrm{fact}})}{dp_{\mathrm{T}}\,dy} \quad f_j^{h_2}(x_2, \mu^2_{\mathrm{fact}})$$

where $\quad \tau_1 \equiv \frac{p_1 \cdot p_3}{p_1 \cdot p_2} = \frac{m_{\mathrm{T}} e^{-y}}{\sqrt{s} x_2}, \ \tau_2 \equiv \frac{p_2 \cdot p_3}{p_1 \cdot p_2} = \frac{m_{\mathrm{T}} e^{y}}{\sqrt{s} x_1}, \ m_{\mathrm{T}} = \sqrt{p_{\mathrm{T}}^2 + m^2}$

- FFNS cross sections behave as $\sim \log(p_{\mathrm{T}}^2/m^2)$ in the $p_{\mathrm{T}} \to \infty$ limit

Fixed-flavour-number scheme (FFNS)

- Parton-level calculations folded with $\mathrm{Q} \to h_3$ **fragmentation functions** $D_{Q\to h_3}(z)$
- The fragmentation variable z not unique for massive objects. A possible choice is

$$z \equiv \frac{E_{\mathrm{hadron}}}{E_{\mathrm{parton}}} \quad \text{(in hadronic c.m. frame)}$$

which leads to

$$\frac{d\sigma(h_1 + h_2 \to h_3 + X)}{dP_{\mathrm{T}}dY} = \sum_{ij} \int_{z^{\min}}^{1} \frac{dz}{z} \int_{x_1^{\min}}^{1} dx_1 \int_{x_2^{\min}}^{1} dx_2$$

$$f_i^{h_1}(x_1, \mu^2_{\mathrm{fact}}) \quad \frac{d\hat{\sigma}^{ij\to \mathrm{Q}+X}(\tau_1,\tau_2,m^2,\mu^2_{\mathrm{ren}},\mu^2_{\mathrm{fact}})}{dp_{\mathrm{T}}dy} \quad f_j^{h_2}(x_2, \mu^2_{\mathrm{fact}}) \quad D_{Q\to h_3}(z)$$

where the partonic and hadronic variables are related as

$$p_{\mathrm{T}}^2 = \frac{M_{\mathrm{T}}^2 \cosh^2 Y - z^2 m^2}{z^2}\left(1 + \frac{M_{\mathrm{T}}^2 \sinh^2 Y}{P_{\mathrm{T}}^2}\right)^{-1} \xrightarrow{P_{\mathrm{T}}\to\infty} \left(\frac{P_{\mathrm{T}}}{z}\right)^2$$

$$y = \sinh^{-1}\left(\frac{M_{\mathrm{T}} \sinh Y}{P_{\mathrm{T}}} \frac{p_{\mathrm{T}}}{m_{\mathrm{T}}}\right) \xrightarrow{P_{\mathrm{T}}\to\infty} Y$$

where $M_{\mathrm{T}} = \sqrt{P_{\mathrm{T}}^2 + M_{h_3}^2}$ is the hadronic transverse mass

Fixed-flavour-number scheme (FFNS)

- FFNS approach tends to undershoot the LHCb data by a factor of two at high p_{T}

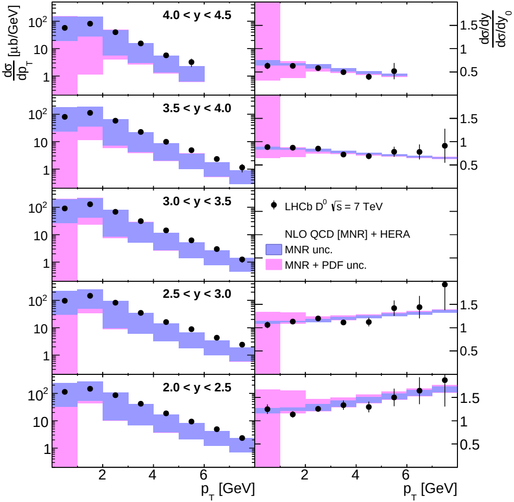
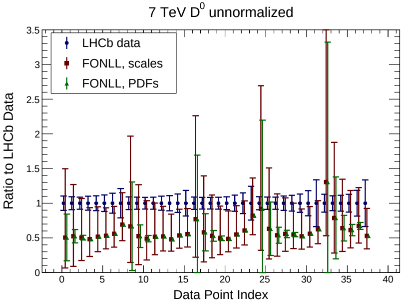


Fig. from [Zenaiev EPJ C77, 151]

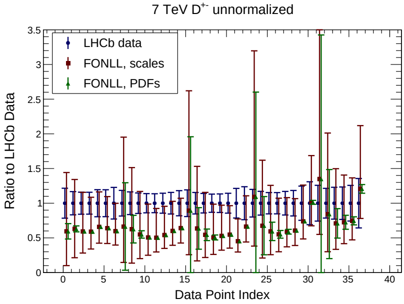
Fixed-flavour-number scheme (FFNS)

- Also FONLL [Cacciari et.al. JHEP 9805, 007] ($\approx$ FFNS at small p_{T}) systematically below the data

[Gauld et.al. JHEP 1511, 009]



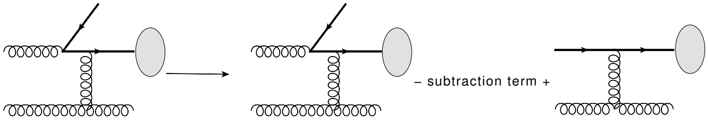
[Gauld et.al. JHEP 1511, 009]



- Very similar situation when FFNS is matched to parton shower (e.g. Powheg+Pythia, aMC@NLO) [Gauld et.al. JHEP 1511, 009]

From FFNS to GM-VFNS heuristically

- Initial-state $\log(p_{\mathrm{T}}^2/m^2)$ terms in FFNS:



(a) (a) (b) (c)

- In GM-VFNS these are resummed to contributions involving the **heavy-quark PDF** $f_Q^{h_1}$

$$(\mathrm{c}): \int \frac{dz}{z} dx_1 dx_2 \; f_Q^{h_1}(x_1, \mu^2_{\mathrm{fact}}) \; \frac{d\hat{\sigma}^{Qg\to Q+X}(\tau_1,\tau_2)}{dp_{\mathrm{T}}dy} \; f_g^{h_2}(x_2, \mu^2_{\mathrm{fact}}) \; D_{Q\to h_3}(z)$$

- The addition of $Qg \to Q + X$ channel must be compensated by the **subtraction term** (b), which is the above expression with the heavy-quark PDF to first order in α_s,

$$f_Q(x, \mu^2_{\mathrm{fact}}) = \left(\frac{\alpha_s}{2\pi}\right) \log\left(\frac{\mu^2_{\mathrm{fact}}}{m^2}\right) \int_x^1 \frac{\mathrm{d}\ell}{\ell} P_{qg}\left(\frac{x}{\ell}\right) f_g(\ell, \mu^2_{\mathrm{fact}}) + \mathcal{O}(\alpha_s^2)\,.$$

- (a)+(b)+(c) finite in $p_{\mathrm{T}} \to \infty$ limit

From FFNS to GM-VFNS heuristically

- In GM-VFNS $d\hat{\sigma}^{Qg\to \mathrm{Q}+X}$ is ambiguous. The only requirement is that

$$\boxed{\frac{d\hat{\sigma}^{Qg\to \mathrm{Q}+X}(\tau_1,\tau_2)}{dp_{\mathrm{T}}dy}} \xrightarrow{p_{\mathrm{T}}\to\infty} \boxed{\frac{d\hat{\sigma}^{qg\to \mathrm{q}+X}(\tau_1,\tau_2)}{dp_{\mathrm{T}}dy}}\Bigg|_{m=0} \qquad (\mathrm{q} = \text{light quark})$$

- **SACOT scheme** [Kniehl et.al PRD71, 014018]: Ignore all mass dependence

$$d\hat{\sigma}^{Qg\to \mathrm{Q}+X}(\tau_1,\tau_2) \equiv d\hat{\sigma}^{qg\to \mathrm{q}+X}(\tau_1^0,\tau_2^0)$$

$$\tau_1^0 = \tau_1\big|_{m=0} = \frac{p_{\mathrm{T}}e^{-y}}{\sqrt{s}x_2}, \ \tau_2^0 = \tau_2\big|_{m=0} = \frac{p_{\mathrm{T}}e^{y}}{\sqrt{s}x_1},$$

- Since $d\hat{\sigma}^{qg\to \mathrm{q}+X}/d^3p \xrightarrow{p_{\mathrm{T}}\to 0} \left(\tau_{1,2}^0\right)^{-n}$

$$d\sigma/dP_{\mathrm{T}} \xrightarrow{P_{\mathrm{T}}\to 0} \pm\infty, \ \textbf{diverges towards low } P_{\mathrm{T}}\textbf{!}$$

- Can be “saved” by enforcing the factorization scale $\mu = m_Q$ until $P_{\mathrm{T}} \gg 0$ [Kniehl et.al. EPJ C75, 140].

  $\Longrightarrow$ wiggles in the P_{T} spectra

From FFNS to GM-VFNS heuristically

- In GM-VFNS $d\hat{\sigma}^{Qg\to \mathrm{Q}+X}$ is ambiguous. The only requirement is that

$$\boxed{\frac{d\hat{\sigma}^{Qg\to \mathrm{Q}+X}(\tau_1,\tau_2)}{dp_\mathrm{T}dy}} \xrightarrow{p_\mathrm{T}\to\infty} \boxed{\frac{d\hat{\sigma}^{qg\to \mathrm{q}+X}(\tau_1,\tau_2)}{dp_\mathrm{T}dy}}\Bigg|_{m=0} \qquad (\mathrm{q} = \text{light quark})$$

- **FONLL scheme** [Cacciari et.al. JHEP 9805 007]: Introduce a damping factor

$$d\hat{\sigma}^{Qg\to \mathrm{Q}+X}(\tau_1,\tau_2) \equiv \left[\frac{p_T^2}{p_T^2+c^2m^2}\right] d\hat{\sigma}^{qg\to \mathrm{q}+X}(\tau_1^0,\tau_2^0), \quad c \sim 5$$

$$\tau_1^0 = \tau_1\big|_{m=0} = \frac{p_\mathrm{T}e^{-y}}{\sqrt{s}x_2}, \; \tau_2^0 = \tau_2\big|_{m=0} = \frac{p_\mathrm{T}e^{y}}{\sqrt{s}x_1},$$

- Since $d\hat{\sigma}^{qg\to \mathrm{q}+X}/d^3p \xrightarrow{p_\mathrm{T}\to 0} \left(\tau_{1,2}^0\right)^{-n}$

$d\sigma/dP_\mathrm{T} \xrightarrow{P_\mathrm{T}\to 0} 0$, **consistently with the data, thanks to the damping factor**

From FFNS to GM-VFNS heuristically

- In GM-VFNS $d\hat{\sigma}^{Qg\to \mathrm{Q}+X}$ is ambiguous. The only requirement is that

$$\boxed{\frac{d\hat{\sigma}^{Qg\to \mathrm{Q}+X}(\tau_1,\tau_2)}{dp_{\mathrm{T}}dy}} \xrightarrow{p_{\mathrm{T}}\to\infty} \boxed{\frac{d\hat{\sigma}^{qg\to \mathrm{q}+X}(\tau_1,\tau_2)}{dp_{\mathrm{T}}dy}}\Bigg|_{m=0} \quad (\mathrm{q} = \text{light quark})$$

- **SACOT-m_{T} scheme**: $d\hat{\sigma}^{Qg\to \mathrm{Q}+X}(\tau_1,\tau_2) \equiv d\hat{\sigma}^{qg\to \mathrm{q}+X}(\tau_1,\tau_2)$

  $Qg \to \mathrm{Q} + X$ process involves $\overline{\mathrm{Q}}$ in the X state (implicitly) so the kinematics should be that of the $\mathrm{Q}\overline{\mathrm{Q}}$ production

$$\tau_1 = \frac{m_{\mathrm{T}}e^{-y}}{\sqrt{s}x_2}, \quad \tau_2 = \frac{m_{\mathrm{T}}e^{y}}{\sqrt{s}x_1},$$

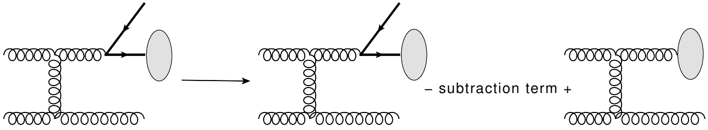
  - Since $d\hat{\sigma}^{qg\to \mathrm{q}+X}/d^3p \xrightarrow{p_{\mathrm{T}}\to 0} (\tau_{1,2})^{-n}$

$$d\sigma/dP_{\mathrm{T}} \xrightarrow{P_{\mathrm{T}}\to 0} 0,$$ **consistently with the data, ok**

  - The same underlying idea as in the SACOT-χ scheme used by CTEQ for DIS [Guzzi et.al. PRD86, 053005]

From FFNS to GM-VFNS heuristically

- Final-state $\log(p_\mathrm{T}^2/m^2)$ terms in FFNS:



- In GM-VFNS these logs are resummed to the **gluon FF** $D_{g\to h_3}(z,\mu^2_\mathrm{frag})$

$$\int \frac{dz}{z} dx_1 dx_2 \; f_g^{h_1}(x_1,\mu^2_\mathrm{fact}) \; \frac{d\hat\sigma^{gg\to g+X}(\tau_1,\tau_2)}{dp_\mathrm{T}dy} \; f_g^{h_2}(x_2,\mu^2_\mathrm{fact}) \; D_{g\to h_3}(z,\mu^2_\mathrm{frag})$$

- Compensate with a **subtraction term** using the $\mathcal{O}(\alpha_s)$ expression for the gluon-to-h_3 FF

$$D_{g\to h_3}(x,\mu^2_\mathrm{frag}) = \left(\frac{\alpha_s}{2\pi}\right)\log\left(\frac{\mu^2_\mathrm{frag}}{m^2}\right)\int_x^1 \frac{\mathrm{d}\ell}{\ell} P_{qg}\left(\frac{x}{\ell}\right) D_{Q\to h_3}(\ell)$$

- The presence of $Q\overline{Q}$ in the final state is again implicit in $gg\to g+X$ channel — use the massive $\tau_{1,2}$ here as well.

From FFNS to GM-VFNS heuristically

- The final expression in GM-VFNS:

Includes ALL partonic subprocesses (unlike FFNS)

$$\frac{d\sigma(h_1+h_2\to D^0+X)}{dP_{\rm T}dY} = \sum_{ijk}\int_{z^{\rm min}}^{1}\frac{dz}{z}\int_{x_1^{\rm min}}^{1}dx_1\int_{x_2^{\rm min}}^{1}dx_2$$

$$f_i^{h_1}(x_1,\mu^2_{\rm fact})\ \frac{d\hat\sigma^{ij\to k}(\tau_1,\tau_2,m,\mu^2_{\rm ren},\mu^2_{\rm fact},\mu^2_{\rm frag})}{dp_{\rm T}dy}\ f_j^{h_2}(x_2,\mu^2_{\rm fact})\ D_{k\to h_3}(z,\mu^2_{\rm frag})$$

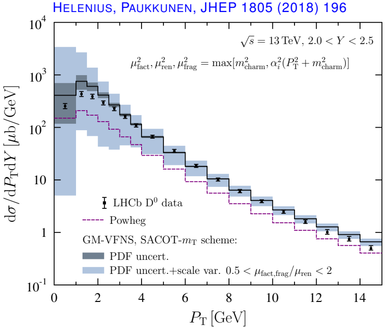
Scale-dependent, universal FFs

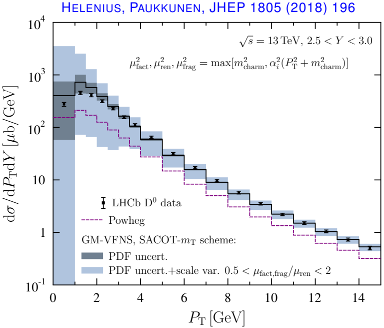
Coefficient functions up to $\mathcal{O}(\alpha_s^3)$ behave as FFNS at low $p_{\rm T}$, as zero-mass $\overline{\rm MS}$ matrix elements at high $p_{\rm T}$

- SACOT-$m_{\rm T}$ scheme implemented to INCNLO code [Aversa et.al. Nucl.Phys. B327, 105] interfaced with MNR $Q\overline{Q}$ routines [Mangano et.al. Nucl.Phys. B373, 295].
- In the following, we apply this to D-meson production in p-p with NNPDF3.1NLO (pch) [Eur.Phys.J. C77 (2017), 663] PDFs and KKKS08 [Kneesch et.al. Nucl.Phys. B799 (2008) 34] FFs.
- Comparison to Powheg+Pyhtia setup: NLO partonic $c\bar{c}$ events from Powheg [Frixione et.al. JHEP 0709, 126] showered/hadronized with Pythia v8.230 [Sjöstrand et.al. Compt.Phys.Comm. 191, 159], used e.g. in [Klasen et.al. JHEP 1408 (2014) 109; Gauld et.al. JHEP 1511, 009].

Comparison with the LHCb 13 TeV data

- LHCb p-p cross sections well reproduced by the SACOT-m_{T} approach





PDF = NNPDF3.1NLO (pch)
FF = KKKS08

- Sizable theory uncertainties at low p_{T}: scale and PDF uncertainties shown, others (scheme dependence, fragmentation variable z,...) more difficult to estimate
- Powheg+Pyhtia setup down by a factor of two with a large scale uncertainty (very similar to FONLL/FFNS)

Comparison with the LHCb 13 TeV/5 TeV data

- Ratios between different c.m. energies

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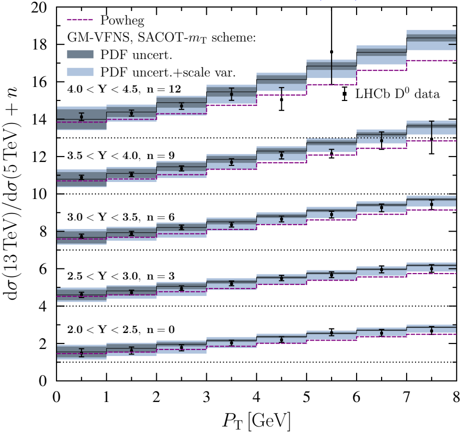


PDF = NNPDF3.1NLO (pch)

FF = KKKS08

- GM-VFNS consistent with the data — reduced scale uncertainties
- Powheg+Pyhtia gives systematically weaker P_T dependence

Main difference between Powheg+Pyhtia and GM-VFNS?

- **Powheg+Pyhtia setup:**

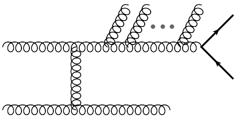
  — Powheg: Provides partonic NLO $c\bar{c}$ events defining the hardest emission scale

  — Pythia: Generates parton shower for the Powheg events below the hardest emission scale and hadronizes the event.

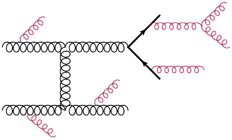
  — Allows for a fully exclusive description of final state

Powheg+Pyhtia setup does **not** account for the possibility that the sole $c\bar{c}$ is created during the shower

Resummed in GM-VFNS via gluon FFs



Extra radiation from the incoming/outgoing partons added by the Pythia shower



Forward-direction x_2 distributions

- The forward LHCb D-meson measurements in p-p probe PDFs at very small x_2

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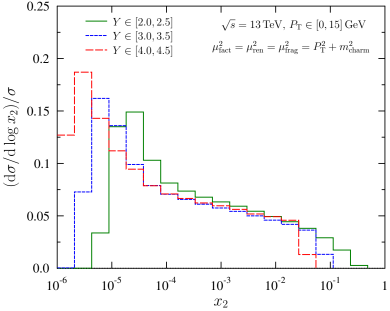

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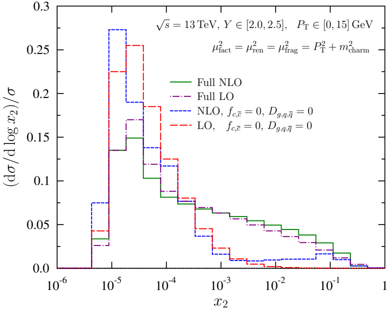


- The **long tails** in GM-VFNS towards large x weaken the small-x sensitivity
- FFNS-based NLO calculations (MNR, Powheg, FONLL at low p_T) largely lack these large-x contributions

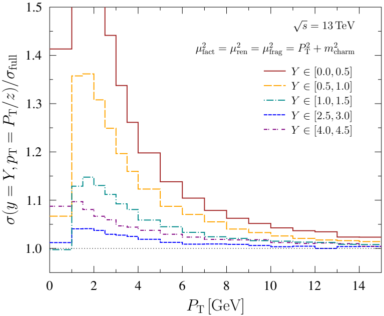
$\Longrightarrow$ **Bias the sensitivity to overly small x!**

Massive vs. massless fragmentation variable

- The "massive" vs. "massless" fragmentation variable makes a significant difference

massive: $z \equiv \frac{E_{\mathrm{hadron}}}{E_{\mathrm{parton}}}$ (in hadronic c.m. frame)

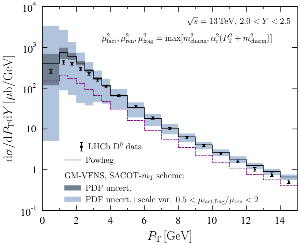
massless: $y^{\mathrm{parton}} = Y^{\mathrm{hadron}};\ p_{\mathrm{T}}^{\mathrm{parton}} = P_{\mathrm{T}}^{\mathrm{hadron}}/z$

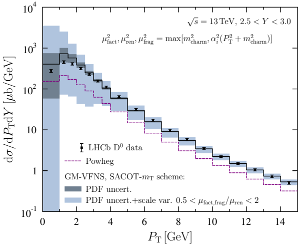


- Not only a multiplicative "front factor" — shifts the sampled $x_{1,2}$ regions
- Similar effect seen in e.g. the AKK08 fit of proton FFs [Nucl.Phys. B803, 42]
- Present also in FFNS/FONLL approaches — different modelling in Pythia

Summary

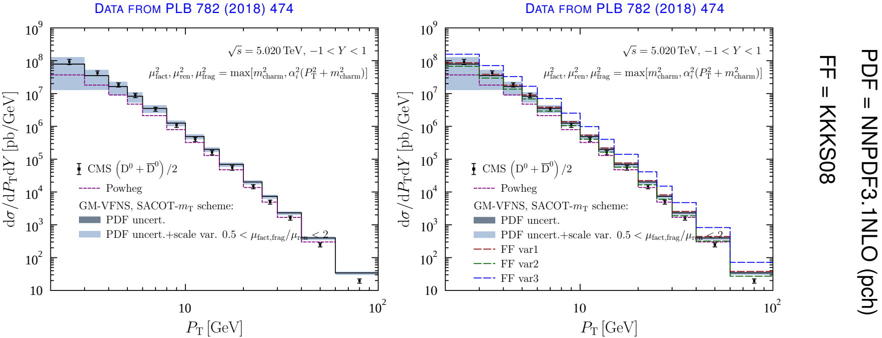
- Introduced a novel GM-VFNS scheme — SACOT-$m_{\rm T}$ — for heavy-flavoured meson production in hadron colliders
  - Resolves the difficulty of $p_{\rm T} \rightarrow 0$ limit of the naive SACOT scheme in a physically motivated manner
  - Yields an excellent agreement with the LHCb p-p data
- Paves the way for consistently using D- (and B-meson) data in global GM-VFNS PDF and FF fits.
  - For the moment full NLO level — parts of the NNLO known
- Significant theory uncertainty at low $p_{\rm T}$ from the ambiguous fragmentation variable
  - A minimum $p_{\rm T}$ cut, ($\sim 3\,{\rm GeV}$?) might be in order to reduce the potential bias in PDF fits





Comparison with the mid-rapidity CMS 5 TeV data

- At $P_\mathrm{T} \gtrsim 20\,\mathrm{GeV}$, GM-VFNS tends to overshoot the CMS data — good agreement at low P_T

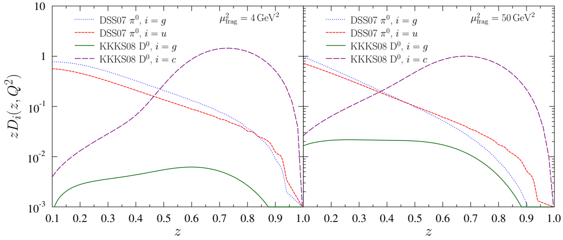


- Powheg+Pyhtia seems to do better at $P_\mathrm{T} \gtrsim 20\,\mathrm{GeV}$ — $\log(p^2_\mathrm{T}/m^2) \gtrsim 5$, so beware...

- At $P_\mathrm{T} \gtrsim 20\,\mathrm{GeV}$ the largest uncertainty in GM-VFNS is the FF variation (KKKS08 constrained by e^+e^- only)

Bonus material

- KKKS08 fragmentation functions



- z distributions at $Y = 0$