D- and B-hadron production at NLO in the GM-VFN scheme vs. LHC data

Bernd Kniehl (Hamburg University)

kniehl@desy.de

in collaboration with G. Kramer, I. Schienbein, and H. Spiesberger

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OUTLINE

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6 $B$ mesons at the LHC

7 Summary
OVERVIEW

- One-particle inclusive production of heavy hadrons $H = D, B, \Lambda_c, \ldots$

- General-Mass Variable Flavour Number Scheme (GM-VFNS): [1]
  - Collinear logarithms of the heavy-quark mass $\ln \mu/m_h$ are subtracted and resummed
  - Finite non-logarithmic $m_h/Q$ terms are kept in the hard part/taken into account
  - Scheme guided by the factorization theorem of Collins with heavy quarks [2]

Ongoing effort to compute all relevant processes in the GM-VFNS at NLO:

- Available:
  - $e^+ + e^- \rightarrow (D^0, D^+, D^{*+}) + X$: FFs [3]
  - $\gamma + \gamma \rightarrow D^{*+} + X$: direct process [4]
  - $\gamma + \gamma \rightarrow D^{*+} + X$: single-resolved process [5]
  - $\gamma + p \rightarrow D^{*+} + X$: direct process [6]
  - $\gamma + p \rightarrow D^{*+} + X$: resolved process [7]
  - $p + \bar{p} \rightarrow (D^0, D^+, D^{*+}, D^+_s, \Lambda_c^+, B^0, B^+) + X$ [1]

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**Overview -Continued-**

Input for the computation: Fragmentation Functions (FFs) into heavy hadrons $H$

- FFs from fits to $e^+ e^-$ data from Z factories
- Include also $B$ factories → Switch from ZM to GM
- Use initial scale $\mu_0 = m$ (instead of $\mu_0 = 2m$) for consistency with PDFs → important for gluon fragmentation

<table>
<thead>
<tr>
<th>$H$</th>
<th>Data</th>
<th>Scheme</th>
<th>Reference</th>
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</thead>
<tbody>
<tr>
<td>$D^{*+}$</td>
<td>ALEPH, OPAL</td>
<td>ZM 2m</td>
<td>BKK, PRD58(1998)014014</td>
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<td>$D^0, D^+, D_s^+, \Lambda_c^+$</td>
<td>OPAL</td>
<td>ZM 2m</td>
<td>KK, PRD71(2005)094013</td>
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<td>$D^0, D^+, D_s^+, \Lambda_c^+$</td>
<td>OPAL</td>
<td>ZM m</td>
<td>KK, PRD74(2006)037502</td>
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<tr>
<td>$D^0, D^+, D_s^+$</td>
<td>Belle, CLEO, ALEPH, OPAL</td>
<td>GM m</td>
<td>KKKSc, NPB799(2008)34</td>
</tr>
<tr>
<td>$B^0, B^+$</td>
<td>OPAL</td>
<td>ZM 2m</td>
<td>BKK, PRD58(1998)034016</td>
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<tr>
<td>$B^0, B^+$</td>
<td>ALEPH, OPAL, SLD</td>
<td>ZM m</td>
<td>KKScSp, PRD77(2008)014011</td>
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</tbody>
</table>

**Goal:**
- Test pQCD formalism, scaling violations and universality of FFs in as many processes as possible
Fixed Order Perturbation Theory:

- finite collinear logs $\ln \frac{Q}{m_c}$ arise → can be kept in hard part
  Of course need exp. Input for $u, d, s, g$ PDFs at scale $Q_0^{(3)}$

Variable Flavour Number Scheme (VFNS):

- often large ratios of scales involved: multi-scale problems
  For $Q \gg m_c$: write $\ln \frac{Q}{m_c} = \ln \frac{Q}{\mu} + \ln \frac{\mu}{m_c}$, subtract $\ln \frac{\mu}{m_c}$ and resum $\ln \frac{\mu}{m_c}$ by introducing charm PDF at $Q_0^{(4)} \simeq m_c$ using a perturbative boundary condition
**GENERAL-MASS VARIABLE-FLAVOUR-NUMBER SCHEME**

Two basic approaches:

- Fixed Order Perturbation Theory (FFNS)
- Parton Model (ZM-VFNS)

Interpolating scheme combining the good features:

- Parton Model with quark masses (GM-VFNS, ACOT)

**Glossary:**

- ZM: Zero Mass
- GM: General Mass
- VFNS: Variable Flavour Number Scheme
- FFNS: Fixed Flavour Number Scheme
Our theoretical basis for $p\bar{p} \rightarrow D^* X$

Factorization Formula:

$$d\sigma(p\bar{p} \rightarrow D^* X) = \sum_{i,j,k} \int dx_1 \, dx_2 \, dz \, f_i^p(x_1) \, \bar{f}_j^{\bar{p}}(x_2) \times \hat{\sigma}(ij \rightarrow kX) \, D_k^{D^*}(z) + \mathcal{O}(\alpha_s^{n+1}, (\frac{\Lambda}{Q})^p)$$

$Q$: hard scale, $p = 1, 2$

- $d\sigma(\mu_F, \mu'_F, \alpha_s(\mu_R), \frac{m_h}{p_T})$: hard scattering cross sections free of long-distance physics $\rightarrow m_h$ kept
- PDFs $f_i^p(x_1, \mu_F), \bar{f}_j^{\bar{p}}(x_2, \mu_F)$: $i, j = g, q, c \quad [q = u, d, s]$
- FFs $D_k^{D^*}(z, \mu'_F)$: $k = g, q, c$

$\Rightarrow$ need short distance coefficients including heavy quark masses

### List of Subprocesses: GM-VFNS

#### Only light lines

<table>
<thead>
<tr>
<th></th>
<th>Process</th>
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<tbody>
<tr>
<td>1</td>
<td>$gg \rightarrow qX$</td>
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<td>$qg \rightarrow gX$</td>
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<tr>
<td>4</td>
<td>$qg \rightarrow qX$</td>
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<td>$q\bar{q} \rightarrow gX$</td>
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<tr>
<td>6</td>
<td>$q\bar{q} \rightarrow qX$</td>
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<tr>
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<td>$qg \rightarrow \bar{q}X$</td>
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<td>$qq \rightarrow qX$</td>
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<td>12</td>
<td>$q\bar{q} \rightarrow q'X$</td>
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<td>$q\bar{q} \rightarrow gX$</td>
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<td>14</td>
<td>$q\bar{q} \rightarrow qX$</td>
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<td>15</td>
<td>$qq' \rightarrow gX$</td>
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<tr>
<td>16</td>
<td>$qq' \rightarrow qX$</td>
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#### Heavy quark initiated ($m_Q = 0$)

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<td>$QQ \rightarrow gX$</td>
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<td>$QQ \rightarrow QX$</td>
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<td>12</td>
<td>$Q\bar{Q} \rightarrow qX$</td>
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<td>13</td>
<td>$Q\bar{q} \rightarrow gX$, $q\bar{Q} \rightarrow gX$</td>
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<td>$Qg \rightarrow gX$, $qq \rightarrow gX$</td>
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<td>16</td>
<td>$Qg \rightarrow QX$, $qq \rightarrow qX$</td>
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#### Mass effects: $m_Q \neq 0$

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<tr>
<td>8</td>
<td>$qg \rightarrow \bar{Q}X$</td>
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<td>9</td>
<td>$qg \rightarrow QX$</td>
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<td>-</td>
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<tr>
<td>12</td>
<td>$q\bar{q} \rightarrow QX$</td>
</tr>
</tbody>
</table>

⊕ Charge conjugated processes
ADOPTED PROCEDURE –CONTINUED–

- Compare $m \to 0$ limit of massive calculation with massless $\overline{\text{MS}}$ calculation

$$\lim_{m \to 0} \frac{d\sigma(m)}{d\sigma} = d\hat{\sigma}(\overline{\text{MS}}) + \Delta d\sigma$$

⇒ Subtraction terms

$$d\sigma_{\text{SUB}} \equiv \Delta d\sigma = \lim_{m \to 0} d\sigma(m) - d\hat{\sigma}(\overline{\text{MS}})$$

- Subtract $d\sigma_{\text{SUB}}$ from massive partonic cross section while keeping mass terms

$$d\hat{\sigma}(m) = d\sigma(m) - d\sigma_{\text{SUB}}$$

→ $d\hat{\sigma}(m)$ short distance coefficient including $m$

→ allows to use PDFs and FFs with $\overline{\text{MS}}$ factorization ⊕ massive short dist. cross sections

- Treat contributions with charm in the initial state with $m_c = 0$;

   ⇒ scheme choice of practical importance; tiny effect in DIS

GRAPHICAL REPRESENTATION OF SUBTRACTION TERMS FOR $gg \to Q\bar{Q}$

$d\hat{\sigma}^{(0)}(gg \to Q\bar{Q}) \otimes d'_{Q \to Q}(z)$:

$d\hat{\sigma}^{(0)}(gg \to gg) \otimes d'_{g \to Q}(z)$:

$f^{(1)}_{g \to Q}(x_1) \otimes d\hat{\sigma}^{(0)}(Qg \to Qg)$:

$f^{(1)}_{g \to Q}(x_2) \otimes d\hat{\sigma}^{(0)}(gQ \to Qg)$:
Graphical representation of subtraction terms for $q\bar{q} \rightarrow Q\bar{Q}g$ and $gq \rightarrow Q\bar{Q}q$

\[ d\hat{\sigma}^{(0)}(q\bar{q} \rightarrow Q\bar{Q}) \otimes d^{(1)}_{Q \rightarrow Q}(z): \]

\[ d\hat{\sigma}^{(0)}(q\bar{q} \rightarrow gg) \otimes d^{(1)}_{g \rightarrow Q}(z): \]

\[ d\hat{\sigma}^{(0)}(gq \rightarrow gq) \otimes d^{(1)}_{g \rightarrow Q}(z): \]

\[ f^{(1)}_{g \rightarrow Q(x_1)} \otimes d\hat{\sigma}^{(0)}(Qq \rightarrow Qq): \]
$D^0$, $D^+$, $D^{*+}$ FFs with finite-mass corrections [1]

Formalism

- $e^+ + e^- \rightarrow (\gamma, Z) \rightarrow H + X$, $H = D^0, D^+, D^{*+}, \ldots$
- $x = 2(p_H \cdot q)/q^2 = 2E_H/\sqrt{s}$, $\sqrt{\rho_H} \leq x \leq 1$ ($\rho_H = 4m_H^2/s$)

\[
\frac{d\sigma}{dx}(x, s) = \sum_a \int_{y_{\min}}^{y_{\max}} dy \frac{d\sigma_a}{dy}(y, \mu, \mu_f) D_a \left( \frac{x}{y}, \mu_f \right)
\]

$d\sigma_a/dy$ at NLO with $m_q = 0$ [2] and $m_q \neq 0$ [1,3]

- $x_p = p/p_{\max} = \sqrt{x^2 - \rho_H}/(1 - \rho_H)$, $0 \leq x_p \leq 1$

\[
\frac{d\sigma}{dx_p}(x_p) = (1 - \rho_H) \frac{x_p}{x} \frac{d\sigma}{dx}(x)
\]

**Initial-state radiation**

- Use radiator $D_{e\pm}$ [1]

$$\frac{d\sigma_{\text{ISR}}}{dx}(x, s) = \int dx_+ dx_- dx' d\cos \theta' \delta(x - x(x_+, x_-, x', \cos \theta'))$$

$$\times D_{e^+}(x_+, s)D_{e^-}(x_-, s) \frac{d^2\sigma}{dx' d\cos \theta'}(x', \cos \theta', x_+ x_- s)$$

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Experimental data

<table>
<thead>
<tr>
<th>Type</th>
<th>$\sqrt{s}$ [GeV]</th>
<th>H</th>
<th>Collaboration</th>
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<tbody>
<tr>
<td>$d\sigma/dx_p$</td>
<td>10.52</td>
<td>$D^0, D^+, D^{*+}$</td>
<td>Belle 06</td>
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<tr>
<td>$d\sigma/dx_p$</td>
<td>10.52</td>
<td>$D^0, D^+, D^{*+}$</td>
<td>CLEO 04</td>
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<tr>
<td>$(1/\sigma_{tot})d\sigma/dx$</td>
<td>91.2</td>
<td>$D^{*+}$</td>
<td>ALEPH 00</td>
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<tr>
<td>$(1/\sigma_{tot})d\sigma/dx$</td>
<td>91.2</td>
<td>$D^0, D^+, D^{*+}$</td>
<td>OPAL 96,98</td>
</tr>
</tbody>
</table>

Theoretical input

- $m_c = 1.5$ GeV, $m_b = 5.0$ GeV, $\alpha(m_{\Upsilon}) = 1/132$,
  $\alpha_s(m_Z) = 0.1176 \sim \Lambda_{\text{QCD}}^{(5)} = 221$ MeV
- Bowler ansatz [1]

\[
D_Q^{H_c}(z, \mu_0) = Nz^{-(1+\gamma^2)}(1 - z)^a e^{-\gamma^2/z}
\]

RESULTS: GOODNESS

- $\chi^2$/d.o.f.

<table>
<thead>
<tr>
<th>$H$</th>
<th>VFNS</th>
<th>Belle/CLEO</th>
<th>ALEPH/OPAL</th>
<th>Global</th>
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<tr>
<td>$D^0$</td>
<td>GM</td>
<td>3.15</td>
<td>0.794</td>
<td>4.03</td>
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<tr>
<td></td>
<td>ZM</td>
<td>3.25</td>
<td>0.789</td>
<td>4.66</td>
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<td>$D^+$</td>
<td>GM</td>
<td>1.30</td>
<td>0.509</td>
<td>1.99</td>
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<td></td>
<td>ZM</td>
<td>1.37</td>
<td>0.507</td>
<td>2.21</td>
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<tr>
<td>$D^{*+}$</td>
<td>GM</td>
<td>3.74</td>
<td>2.06</td>
<td>6.90</td>
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<tr>
<td></td>
<td>ZM</td>
<td>3.69</td>
<td>2.04</td>
<td>7.64</td>
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</table>

- Quark mass effects improve global fits and Belle/CLEO fits for $D^0$, $D^+$, but have no impact on ALEPH/OPAL fits.
- Belle and CLEO data on $D^0$, $D^{*+}$ moderately compatible.
- OPAL fits for $D^0$, $D^+$ excellent; ALEPH and OPAL data on $D^{*+}$ moderately compatible.
- Tension between Belle/CLEO and ALEPH/OPAL data.
RESULTS: GLOBAL FITS

- Belle/CLEO data push $\langle z \rangle_c(m_Z)$ up by 0.03–0.04
**HADROPRODUCTION OF** $D^0, D^+, D^{*+}, D^+_s$

**GM-VFNS RESULTS w/ KKKSc FFs [1]**

1. $d\sigma/dp_T$ [nb/GeV] $|y| \leq 1$ prompt charm
2. Uncertainty band: $1/2 \leq \mu_R/m_T, \mu_F/m_T \leq 2$ ($m_T = \sqrt{p_T^2 + m_c^2}$)
3. CDF data from run II [2]
4. GM-VFNS describes data within errors

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New KKKSc FFs improve agreement w/ CDF data.

NLO GM-VFNS predictions for $D$'s at the LHC

Predictions for ALICE

- $pp$ collisions, $\sqrt{S} = 7$ TeV
- CTEQ6.5 PDF, KKKSc FF, $m_c = 1.5$ GeV
- Results for $D^0 + \bar{D}^0$, $D^{*+} + D^{*-}$, $D^+ + D^-$
- Error bands: Varying $\mu_R$ by factors 2 up and down
  (Except for very small $p_T$ this gives maximal variation in the cross section)
PRELIMINARY ALICE RESULTS FOR $D^0$ AND $D^+$


- pQCD predictions (GM-VFNS, FONLL) compatible with data
GM-VFNS predictions for $D^0$, $D^{*\pm}$, $D^\pm$ production at ATLAS

- **pp collisions**, $\sqrt{S} = 7$ TeV
- CTEQ6.6 PDF, KKKS06 FF, $m_c = 1.5$ GeV
- Rapidity bins (top to bottom):
  - $|\eta| < 0.2$, $0.2 < |\eta| < 0.5$, $0.5 < |\eta| < 0.8$, $0.8 < |\eta| < 1.3$, $1.3 < |\eta| < 2.1$
- Results for average $(D^0 + \bar{D}^0)/2$, $(D^{*+} + D^{*-})/2$, $(D^+ + D^-)/2$
LHCb: $D^0$ cross section (talk by P. Urquijo at LPCC, Dec. 2010)

- Prelim. results ($\mathcal{L} = 1.8 \text{ nb}^{-1}$), $D^0 \rightarrow K^- \pi^+$, Data: 12% correlated error not shown

- BAK et al. = GM-VFNS: B. Kniehl, G. Kramer, I. Schienbein, H. Spiesberger
- MC et al. = FONLL: M. Cacciari, S. Frixione, M. Mangano, P. Nason, G. Ridolfi
Prelim. results ($\mathcal{L} = 1.8 \text{ nb}^{-1}$), $D^+ \rightarrow K^- \pi^+ \pi^+$, Data: 14 % correlated error not shown

- BAK et al.= GM-VFNS: B. Kniehl, G. Kramer, I. Schienbein, H. Spiesberger
- MC et al.= FONLL: M. Cacciari, S. Frixione, M. Mangano, P. Nason, G. Ridolfi
Preliminary ($\mathcal{L} = 1.8 \text{ nb}^{-1}$), $D^{*+} \rightarrow (D^0 \rightarrow K^- \pi^+)\pi^+$, Data: 14 % corr. error not shown

- BAK et al. = GM-VFNS: B. Kniehl, G. Kramer, I. Schienbein, H. Spiesberger
- MC et al. = FONLL: M. Cacciari, S. Frixione, M. Mangano, P. Nason, G. Ridolfi
Preliminary ($\mathcal{L} = 1.8 \text{ nb}^{-1}$), $D_s \to K^- K^+ \pi^+$, Data: 16% corr. error not shown

- BAK et al. = GM-VFNS: B. Kniehl, G. Kramer, I. Schienbein, H. Spiesberger
- MC et al. = FONLL: M. Cacciari, S. Frixione, M. Mangano, P. Nason, G. Ridolfi
NLO GM-VFNS predictions for $B'$s at the LHC
Comparison with CMS [PRL106(2011)112001]

$$\mu_{F,R} = \xi_{F,R} \sqrt{m_b^2 + p_T^2}$$

$$\mu_{F,R} = \sqrt{m_b^2 + \xi_{F,R} p_T^2}$$

- Inputs: CTEQ6.5 PDFs, KKSS FFs (LEP1+SLC fit) [1]
- Uncertainty band: $1/2 \leq \xi_F, \xi_R \leq 2$

**Summary**

- **GM-VFNS** (cf. ACOT scheme) with non-perturbative FFs provides rigorous theoretical framework for global analysis of inclusive heavy-hadron production:
  - full mass dependence
  - scaling violations and universality of FFs
  - no spurious $x \to 1$ problems to be fixed
  - no ad-hoc weight functions, no hidden theoretical errors

- Processes available at NLO:
  - $e^+ e^- \to H + X$
  - $\gamma\gamma \to H + X$ direct, singly and doubly resolved
  - $\gamma p \to H + X$ direct and resolved
  - $p\bar{p}, pp \to H + X$

- New $D^0, D^+, D^{*+}$ FFs w/ mass effects from Belle, CLEO, ALEPH, and OPAL data

- $D$ (and $B$) hadroproduction predictions in good agreement w/ CDF data
  - Mass effects **positive and moderate**
Up-to-date NLO GM-VFNS predictions for $D^0$, $D^\pm$, $D^{\ast\pm}$, $D_s^\pm$ and $B$ hadroproduction at LHC available

First comparisons promising

In the long run, LHC data will provide tight constraints on $D$ and $B$ FFs and allow for nontrivial tests of QCD factorization with heavy quarks
**HADROPRODUCTION OF $B^0$, $B^+$** [1]

**NEW FFs from LEP1/SLC data** [2]

**Petersen**

$$D(x, \mu_0^2) = N \frac{x(1-x)^2}{[(1-x)^2 + \epsilon x]^2}$$

**Kartvelishvili-Likhoded**

$$D(x, \mu_0^2) = Nx^\alpha (1-x)^\beta$$

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GM-VFNS PREDICTION VS. CDF II [1,2]

CDF (1.96 TeV):
- open squares $J/\psi X$ [1]
- solid squares $J/\psi K^+$ [2]

CTEQ6.1M PDFs
- $m_b = 4.5$ GeV
- $\Lambda^{(5)}_{\text{MS}} = 227$ MeV $\sim \alpha_s^{(5)} = 0.1181$
- $1/2 \leq \mu_R/m_T, \mu_F/m_T, \mu_R/\mu_F \leq 2$
  ($m_T = \sqrt{p_T^2 + m_b^2}$)

GM-VFNS PREDICTION VS. CDF II [1]

CDF II (preliminary) [1]

\[ \mu_R = \mu_F = m_T \]

for \( p_T \gg m_b \):

- GM-VFN merges w/ ZM-VFN
- FFN breaks down

data point in bin [29,40] favors GM-VFN

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**Historical Remark:** First consistent NLO analysis [1] of $B$ data from LEP1 (OPAL [2]) and Tevatron Run I (CDF [3]).

- **Statement [4]:** *This stands in contrast with the approach of [1] where large logarithmic corrections in the function $D(x, m^2)$ are simply discarded.* Misleading because Sudakov logs fully included at NLO (in coefficient functions and evolution kernels), but not resummed because unnecessary in our scheme.

- **Statement [5]:** *... due to the large size of mass corrections up to $p_T \sim 20$ GeV.* Lack of mass effects [1] will therefore erroneously overestimate the production rate at small $p_T$.
  Incorrect because mass corrections yield moderate enhancement, by about 20%, 10% at $p_T = 2m, 4m$.

**Digression: FONLL scheme [1]**

\[ \text{FONLL} = \text{FO} + (\text{RS} - \text{FOM0}) \times G(m, p_T) \]

- **FO**: *fixed order*
- **FOM0**: *massless limit* thereof
- **RS**: *resummed*
- shift $p_T \to m_T$ in $(\text{RS} - \text{FOM0})$
- $G(m, p_T) = \frac{p_T^2}{p_T^2 + c^2 m^2}$ with $c = 5$ to suppress $(\text{RS} - \text{FOM0})$ being *abnormally large* for $m_T < 5m$
- **NB**: $G(m, p_T) = 4\%, 14\%, 26\%$ for $p_T/m = 1, 2, 3$

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POSSIBLE MISUNDERSTANDINGS CONCERNING FONLL

- from CDF, PRD71(2005)032001
- large scale uncertainty of RS for $p_T \to 0$
- why not in FONLL?
- $G(m, p_T)$ not varied?

- from CDF, PRD75(2007)012010
- NLO = FO
- why FONLL $\not\rightarrow$ NLO for $p_T \to 0$?
- NLO evaluated with
  - MRSD0 ('93): unacceptably weak $g$, revoked!
  - $\alpha_s^{(5)}(m_z) = 0.111$: $3.3\sigma$ below world average!
- obsolete NLOQCD still used as benchmark, e.g. Happacher, Giromini, Ptohos, PRD73(2006)014026
 obsolete FFN as above
 up-to-date FFN evaluated with

- CTEQ6.1M PDFs
- \( m_b = 4.5 \text{ GeV} \)
- \( \Lambda_{\text{MS}}^{(5)} = 227 \text{ MeV} \sim \alpha_s^{(5)} = 0.1181 \)
- \( D(x) = B(b \rightarrow B) \delta(1 - x) \) with
  \( B(b \rightarrow B) = 39.8\% \)

LOW-$p_T$ IMPROVEMENT OF GM-VFNS [1]

\[ \frac{d\sigma}{dp_T} [\text{nb/GeV}] \]

\[ pp \to B^+ X \]

\[ \sqrt{s} = 1.96 \text{ TeV} \]

\[-1 \leq y \leq 1 \]

- evaluate \( d\hat{\sigma}_{ZM}^{(1)}(Q + g/q \to Q + X) \)
  @ LO to match
  \( f_{g\to Q} \otimes d\hat{\sigma}^{(0)}(Q + g/q \to Q + g/q) \)

- evaluate
  \( d\hat{\sigma}^{(0)}(gg/q\bar{q} \to Q\bar{Q}) \otimes d_{Q\to Q}^{(1)} \)
  w/ \( m_Q \neq 0 \) to match
  \( d\hat{\sigma}_{GM}^{(1)}(gg/q\bar{q} \to Q/\bar{Q} + X) \)

- impose \( \theta(\hat{s} - 4m_Q^2) \) on massless kinematics

- choose \( \mu_F^2 = m_Q^2 + \xi p_T^2 \) so that
  \( \mu_F \xrightarrow{p_T\to 0} m_Q = \mu_0 \)

- \( G(m, p_T) \equiv 1 \) in contrast to FONLL

\[ \mu = \sqrt{m_b^2 + \xi p_T^2} \]

\[ m_b = 4.5 \text{ GeV} \]

- black: \( \xi = 1/4 \), red: \( \xi = 1/2, 1/8 \)