NLO Monte Carlo predictions for heavy-quark production
(pp collisions @ ALICE)

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based on JHEP 1408 (2014) 109
Outline

1. Heavy quark production pp-baseline @ ALICE

2. GM-VFNS, FONLL, POWHEG methods

3. Results and comparison of the methods with ALICE data
Motivation

- **Goal:**
  - Heavy quarks sensitive to nuclear medium - used @ ALICE to study the suppression factor in PbPb collisions
  - For isolation of nuclear medium effects - understanding of pp baseline needed

\[ R_{AA}(p_t) = \frac{1}{\langle T_{AA} \rangle} \cdot \frac{dN_{AA}/dp_t}{d\sigma_{pp}/dp_t} \]

**arXiv:1205.6443 [hep-ex]**
2. GM-VFNS, FONLL, POWEHG methods
GM-VFNS

Main goal

- Construct single inclusive cross-section valid in a wide $p_T$ range
- Combine the massive calculation valid for small $p_T$ with massless calculation valid for large $p_T$

- $\text{GM-VFNS} \rightarrow \text{ZM-VFNS for } p_T \gg m$
  (this is the case by construction)

- $\text{GM-VFNS} \rightarrow \text{FFNS for } p_T \sim m$
  (formally this can be shown; numerically problematic in the S-ACOT scheme)
### List of subprocesses

| Only light lines | Heavy quark initiated ($m_Q = 0$) | Mass effects: $m_Q \neq 0$ |
|------------------|----------------------------------|-----------------------------|
| 1. $gg \to qX$   | 1. -                             | 1. $gg \to QX$              |
| 2. $gg \to gX$   | 2. -                             | 2. -                        |
| 3. $qg \to gX$   | 3. $Qg \to gX$                   | 3. -                        |
| 4. $qg \to qX$   | 4. $Qg \to QX$                   | 4. -                        |
| 5. $q\bar{q} \to gX$ | 5. $Q\bar{Q} \to gX$ | 5. -                        |
| 6. $q\bar{q} \to qX$ | 6. $Q\bar{Q} \to QX$ | 6. -                        |
| 7. $qg \to \bar{q}X$ | 7. $Qg \to \bar{Q}X$ | 7. -                        |
| 8. $qg \to \bar{q}'X$ | 8. $Qg \to \bar{q}X$ | 8. $qg \to \bar{Q}X$        |
| 9. $qg \to q'X$  | 9. $Qg \to qX$                   | 9. $qg \to QX$              |
| 10. $qq \to gX$  | 10. $QQ \to gX$                  | 10. -                       |
| 11. $qq \to qX$  | 11. $QQ \to qX$                  | 11. -                       |
| 12. $q\bar{q} \to q'X$ | 12. $Q\bar{Q} \to qX$ | 12. $q\bar{q} \to QX$       |
| 13. $q\bar{q}' \to gX$ | 13. $Q\bar{q} \to gX, q\bar{Q} \to gX$ | 13. -                       |
| 14. $q\bar{q}' \to qX$ | 14. $Q\bar{q} \to QX, q\bar{Q} \to qX$ | 14. -                       |
| 15. $qq' \to gX$ | 15. $Qq \to gX, qQ \to gX$       | 15. -                       |
| 16. $qq' \to qX$ | 16. $Qq \to QX, qQ \to qX$       | 16. -                       |

⊕ charge conjugated processes

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hep-ph/0502194
GM-VFNS

**Fragmentation functions**

- Fragmentation approach in GM-VFNS - treat heavy quark fragmentation as any other FF
- Scale dependent FF determined from a fit to LEP data

**FF ansatz for charmed mesons**

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

**FF ansatz for B-mesons**

\[
D_h(z, \mu_0^2) = N z^\alpha (1 - z)^\beta
\]

[arXiv:0712.0481 [hep-ph]]

\[
\chi^2 / \text{d.o.f.} = 1.495
\]
FONLL approach to combination of massive & massless

- Master formula

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

fixed order massive calculation with 4 massless quarks

resummed massless result with massless HQ

- Suppression factor to regulate a divergence in \( \sigma_{\text{RS}} \) for small \( p_T \)

\[ G(m, p_T) = \frac{p_T^2}{p_T^2 + a^2m^2} \]

- Small modification to fixed-order result so that PDFs and strong coupling constant with \( n_f = 5 \) can be used

Add to \( q\bar{q} \) - channel

\[ -\alpha_s \frac{2T_F}{3\pi} \log \frac{\mu^2}{m^2} \sigma^{(0)}_{q\bar{q}} \]

Add to \( gg \) - channel

\[ -\alpha_s \frac{2T_F}{3\pi} \log \frac{\mu^2}{\mu_f^2} \sigma^{(0)}_{gg} \]
FONLL

- **FONLL approach to combination of massive & massless**
- Fragmentation approach in FONLL

\[
D^H_i(z, \mu'_F) = D^Q_i(z, \mu'_F) \otimes D^H_Q(z)
\]

perturbative FF satisfying
DGLAP evolution in the scale

- Non-perturbative fragmentation fitted using moments

\[
D_N \equiv \int D^H_Q(z) z^N \frac{dz}{z}
\]

\[
\frac{d\sigma}{dp_T} = \int dz \bar{p}_T D^H_Q(z) \frac{A}{\bar{p}_T^N} \delta(p_T - z\bar{p}_T) = \frac{A}{\bar{p}_T^N} D_N
\]

non-perturbative part describes hadronisation of heavy quark into heavy hadron (fitted from LEP data)
### GM-VFNS & FONLL

#### NLO and NLL
- which order is included in GM-VFNS or FONLL

\[ L = \ln \left( \frac{m}{p_T} \right) \]

\[ a = \frac{\alpha_s}{2\pi} \]

| Order | LL | NLL | NNLL | ... |
|-------|----|-----|------|-----|
| LO    | 1  |     |      |     |
| NLO   | \(aL\) | \(a\) |     |     |
| NNLO  | \((aL)^2\) | \(a(aL)\) | \(a^2\) |     |
| ...   | ... | ... | ... | ... |

Fixed Order → Resummed
### GM-VFNS & FONLL

#### NLO and NLL
- Which order is included in GM-VFNS or FONLL

#### Fixed Order

\[ L = \ln \left( \frac{m}{p_T} \right) \]
\[ a = \frac{\alpha_s}{2\pi} \]

| Order | LL | NLL | NNLL | ...
|-------|----|-----|------|----
| LO    | 1  |     |      |    |
| NLO   | aL | a   |      |    |
| NNLO  | (aL)^2 | a(aL) | a^2 |    |
| ...
|     |     |     |      |    |

Resummed
### GM-VFNS & FONLL

#### NLO and NLL

- which order is included in GM-VFNS or FONLL

![Diagram]

|        | LL | NLL | NNLL | ... |
|--------|----|-----|------|-----|
| LO     |    |     |      |     |
| NLO    | aL | a   |      |     |
| NNLO   | (aL)^2 | a(aL) | a^2  |     |
| ...    | ... | ... | ...  | ... |

**Fixed Order**

\[ L = \ln \left( \frac{m}{p_T} \right) \]

\[ a = \frac{\alpha_s}{2\pi} \]
## GM-VFNS & FONLL

### NLO and NLL

- Which order is included in GM-VFNS or FONLL

### L = \ln \left( \frac{m}{p_T} \right)

### a = \alpha_s / (2\pi)

| Order  | LL  | NLL | NNLL | ...
|--------|-----|-----|------|-----
| LO     | 1   |     |      |     
|        | m\neq 0 |     |      |     
| NLO    | aL  | a   |      |     
|        | m\neq 0 | m\neq 0 |     |     
| NNLO   | (aL)^2 | a(aL) | a^2 |     
|        | m=0 | m=0 |      |     
| ...    |     |     |      |     

### Resummed

### Fixed Order
POWHEG

POWHEG & MC generators

- Complicated machinery needed to go from QFT to simulating real exclusive events
- A lot of moving parts
  - **hard matrix element**
    - QFT calculations using Feynman diagrams
    - most rigorous part of MC
  - **parton showers**
    - generating soft & collinear radiation
    - makes ME more realistic
  - **hadronisation**
    - using color information to turn partons into hadrons
    - very model dependent
  - **underlying event**
POWHEG

- **NLO cross-sections**
  - NLO cross-sections complicated objects - combining 2 types of processes
    - virtual (loop) corrections - containing UV & IR divergence
      - same phase-space as tree-level $\Phi_B$
    - real emission corrections - containing IR divergence
      - phase-space with $n+1$ particles $\Phi_R$
    
    $$d\sigma = \left( B(\Phi_B) + \hat{V}(\Phi_B) \right) d\Phi_B + R(\Phi_R) d\Phi_R$$
  
  - Cancellation of UV divergence ‘simple’ through renormalization of couplings constants etc.
  - Cancellation of IR divergence only in sufficiently inclusive quantities (!)
  
  - To cancel IR singularities in each part separately, one introduces auxiliary subtraction terms & one has to factorize the phase-space $\Phi_R(\Phi_B, \Phi_{rad})$
    
    $$\sigma = \int d\Phi_B \left[ B(\Phi_B) + \hat{V}(\Phi_B) + \int d\Phi_{rad} C(\Phi_R(\Phi_B, \Phi_{rad})) \right] + \int d\Phi_R \left[ R(\Phi_R) - C(\Phi_R) \right]$$
  
  - Imperfect cancellation of singularities for exclusive quantities e.g. in a Monte Carlo
**NLO cross-sections & parton shower**

- How to use NLO cross-sections in parton showers?
- In parton shower language an equivalent of a NLO cross-section is a cross-section with one emission:

\[
\frac{d\sigma}{dt} = \frac{d\Phi_B B(\Phi_B)}{2\pi} \left( \Delta_i(t_I, t_0) + \sum_{(j,k)} \Delta_i(t_I, t) \frac{\alpha_s(t)}{2\pi} P_{i,jk}(z) \frac{dt}{t} d\phi \right)
\]

- Expanding in \(\alpha_s\) we get:

\[
\frac{d\sigma}{dt} = \frac{d\Phi_B B(\Phi_B)}{2\pi} \left( 1 - \sum_{(j,k)} \int \frac{dt'}{t'} \int d\phi \frac{\alpha_s(t')}{2\pi} P_{i,jk}(z) + \sum_{(j,k)} \frac{\alpha_s(t)}{2\pi} P_{i,jk}(z) \frac{dt}{t} d\phi \right)
\]

- Shower cross-section contains approximate virtual & real corrections in the collinear limit.

**NOTE:** Sudakov form-factor resums universal part of the virtual(!) correction.

- Goal of NLO Monte Carlos is to recover exact NLO cross-sections when we expand the parton shower cross-section in \(\alpha_s\).
**POWHEG**

**POWHEG method**

- Main idea - replace the parton shower approximation for no radiation and the first (hardest) emission by the full NLO calculation
- Separate the real emission into singular and regular part
  \[ R = R^S + R^F \]
- POWHEG cross-section with the hardest emission
  \[
  d\sigma = d\Phi_B \tilde{B}^S(\Phi_B) \left( \Delta^S_{t_0} + \Delta^S_t \frac{R^S(\Phi)}{B(\Phi_B)} d\Phi_{\text{rad}} \right) + R^F d\Phi_R
  \]
  where the modified Born contains also the virtual corrections
  \[
  \tilde{B}^S = B + V + \int R^S d\Phi_{\text{rad}}
  \]
- Modified Sudakov form-factor & modified shower generating emission only with lower $p_T$ than the first emission
  \[
  \Delta^S_t = \exp \left[ - \int \theta(t_r - t) \frac{R^S(\Phi_B, \Phi_{\text{rad}})}{B(\Phi_B)} d\Phi_{\text{rad}} \right]
  \]
POWHEG

- POWHEG with heavy flavor

- NLO matrix element based on FFNS massive calculation
  (with 4 active flavors for bottom production)

- Parton shower in the initial state resums only LL via the
  splittings in the Sudakov form-factor as opposed to NLL
  provided by NLO PDFs

- Parton shower in the final state together with the
  hadronisation model provides a different (exclusive) information
  equivalent to the fragmentation function approach (inclusive)

arXiv:0707.3088 [hep-ph]
3. Results and comparison of the methods with ALICE data
Results

**Comparison with ALICE data**

- Single inclusive production @ $\sqrt{s} = 2.76$ TeV and central rapidity $|y| < 0.5$
- Scales are chosen as $\mu = \mu_f = \sqrt{m^2 + p_T^2}$
- Dominant theoretical uncertainty
  - scale uncertainty

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**arXiv:1205.4007 [hep-ex]**
Results

- **Comparison with ALICE data**
  - Heavy flavor decay into muons @ $\sqrt{s} = 2.76$ TeV and forward rapidity $2.5 < y < 4.0$
  - heavy flavor (bottom & charm channels combined) decaying into muons
  - Dominant theoretical uncertainty
    - PDF uncertainty (included in the POWHEG)

\[ \frac{d}{dp_t}(p^0, 0.5 \text{ GeV}) \]

\[ 2.5 < y < 4.0 \]

\[ \text{pp} \rightarrow \text{HF} + X \rightarrow (\mu^+ + \mu^-)/2 \text{ at } \sqrt{s} = 2.76 \text{ TeV} \]

\[ \text{ALICE/POWHEG} \]

\[ \text{FONLL/POWHEG} \]

\[ \text{GM-VFNS/POWHEG} \]

\[ \text{arXiv:1205.6443 [hep-ex]} \]
Results

- **Comparison with ALICE data**
  - Single inclusive production @ $\sqrt{s} = 7$ TeV and central rapidity $|y| < 0.5$
  - Dominant theoretical uncertainty - scale uncertainty

![Graphs comparing ALICE data with theoretical predictions for D^0 production at $\sqrt{s} = 7$ TeV](image)

*arXiv:1111.1553 [hep-ex]*
Results

**Comparison with ALICE data**

- Single inclusive production @ $\sqrt{s} = 7$ TeV and central rapidity $|y| < 0.5$
- Dominant theoretical uncertainty
  - scale uncertainty
- Problem with the PYTHIA hadronization model in the presence of strange quark?

*arXiv:1208.1948 [hep-ex]*
Results

**Comparison with ALICE data**

- Heavy flavor decay into muons @ $\sqrt{s} = 7$ TeV and forward rapidity $2.5 < y < 4.0$

- Heavy flavor (bottom & charm channels combined) decaying into muons

- Dominant theoretical uncertainty
  - PDF uncertainty (included in the POWHEG)

\[ \text{arXiv:1201.3791 [hep-ex]} \]
Results

- **Comparison with ALICE data**
  - Heavy flavor decay into electrons @ $\sqrt{s} = 7$ TeV and central rapidity $|y| < 0.8$
  - In GM-VFNS the decay of a B-hadron into lepton parametrized as a "lepton fragmentation"

\[
D_{i \to l}(x, \mu_F) = \int_x^1 \frac{dz}{z} D_{i \to B} \left( \frac{x}{z}, \mu_F \right) \frac{1}{\Gamma_B} \frac{d\Gamma}{dz}(z, P_B).
\]

**arXiv:1212.4356 [hep-ph]**

**Comparison with ALICE data**

- Heavy flavor decay into electrons @ $\sqrt{s} = 7$ TeV and central rapidity $|y| < 0.8$
- In GM-VFNS the decay of a B-hadron into lepton parametrized as a "lepton fragmentation"

\[
D_{i \to l}(x, \mu_F) = \int_x^1 \frac{dz}{z} D_{i \to B} \left( \frac{x}{z}, \mu_F \right) \frac{1}{\Gamma_B} \frac{d\Gamma}{dz}(z, P_B).
\]

**arXiv:1208.1902 [hep-ex]**
Results

**Comparison with ALICE data**

- Heavy flavor decay into electrons @ $\sqrt{s} = 5.023$ TeV and central rapidity $|y| < 0.8$
- Possible baseline for future heavy quark production measurements in pPb collisions

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**pp → c+X → e+X at $\sqrt{s} = 5.023$ TeV**

![Graph 1](image1)

**pp → b+X (→ c+X) → e+X at $\sqrt{s} = 5.023$ TeV**

![Graph 2](image2)
Conclusions

- All three methods describe the data within experimental and theoretical errors
- Different treatment of fragmentation functions might explain small discrepancies