THEORETICAL VIEW ON HEAVY FLAVOUR SCHEMES
OUTLINE

➡ Introduction: heavy flavour schemes in QCD calculations

➡ Matched calculations for inclusive observables

➡ Matched calculations for exclusive observables

➡ Heavy flavour splittings in final states
  \[ tt\bar{b}b \] [Jezo et al, arXiv:1802.00426] Ridolfi, MU, Zaro [arXiv: 1911.01975]

➡ Conclusions
INTRODUCTION
HEAVY FLAVOUR SCHEMES

\[
\frac{d\sigma_{pp \rightarrow ab}^{H}}{dX} = \sum_{i,j=-n_f}^{+n_f} \int_{\tau_0}^{1} \frac{dz_1}{z_1} \frac{dz_2}{z_2} f_i(z_1, \mu_F) f_j(z_2, \mu_F) \frac{d\hat{\sigma}_{ij}^{H}}{dX}(zS, \alpha_s(\mu_R), \mu_F) + O \left( \frac{\Lambda^n}{S^n} \right)
\]

- Processes involving HF crucial at the LHC, from flavour physics to Higgs searches and as a window to new physics

- Natural multi-scale problem (mostly focus on bottom quark, so here we compare 4FS versus 5FS unless otherwise specified)

5F scheme: b-quarks belong to proton & \( m_b = 0 \)

4F scheme: b-quarks DO NOT belong to proton & \( m_b \neq 0 \)

Credit: D. Napoletano
HEAVY FLAVOUR SCHEMES

4F scheme

- It does not resum possibly large collinear logs, yet it has them explicitly at each order in perturbative expansion
- Computing higher orders is more difficult due to higher multiplicities
- Mass effects $O(m_b/M)$ are there at any order
- Straightforward implementation in MC event generators at LO and NLO

5F scheme

- DGLAP evolution resums initial state logs into $b$-PDFs leading to more stable predictions
- Computing higher orders is easier
- Neglects $O(m_b/M)$ and yields less accurate description of bottom quark kinematic distribution
- Implementation in MC depends on the gluon splitting model in the PS

Collinear log

$$\alpha_s(M^2) \log \left( \frac{M^2}{m_b^2} \right)$$

DGLAP equations

$$\sum_{k=1}^{\infty} \left[ \alpha_s(\mu_F) \log \left( \frac{\mu_F^2}{m_b^2} \right) \right]^k$$
Lot of progress in understanding the origin of the differences first observed more than 20 years ago

- At that time, calculations in the two schemes were compared and at leading order the effect of collinear resummation is extremely large, now calculations typically known at NNLO (even N3LO in case of bbH) in 5FS and NLO in 4FS
- Calculations were compared at hard scale of the process, while now lower values of fact. and ren. scales are set
At NLO, the resummation effects of the initial state collinear logs into the b-PDFs important only at large \( x \)!

Lot of progress in understanding the origin of the differences first observed more than 20 years ago.

Larger effects at large-\( x \):
\[
x \approx \frac{M^2}{S_{\text{had}}}
\]
DIFFERENCES BETWEEN SCHEMES

Lot of progress in understanding the origin of the differences first observed more than 20 years ago

\[ \frac{b^{\mathcal{O}(\alpha_s^2)}(x, \mu)}{b(x, \mu)} \]

\[ DGLAP @ NLO \]

The possibly large ratios \( \frac{M^2}{m_b^2} \) are always accompanied by universal phase space factors

\[ \log \left( \frac{M^2}{m_b^2} h(z) \right), \quad z = \frac{M^2}{\hat{s}} \]

\[ = \log \left( \frac{\tilde{\mu}^2}{m_b^2} \right), \quad \tilde{\mu}^2 = M^2 \langle h(z) \rangle \approx 0.2 - 0.4 \]
Differences Between Schemes

- Lower $\mu$ scale suggested by kinematics decreases the differences between 5FS b-only contribution to the 4FS description.
- Lower shower scale improves matching between fixed-order (FO) and FO+PS at large $p_T$.

Bagnaschi, Maltoni, Vicini, Zaro, arXiv: 1803.04336
Degrande, MU, Wiesemann, Zaro, arXiv: 1507.02549
MATCHING BETWEEN SCHEMES - INCLUSIVE OBSERVABLES
HEAVY FLAVOUR SCHEME MATCHING FOR INCLUSIVE OBSERVABLES

- FONLL widely used method based on standard QCD to match 4FS and 5FS calculations at all orders and for all processes, matching fixed order calculation at $N_{\text{pLO}}$ with DGLAP resummed $N_{\text{qLL}}$

- Other approaches possible based on EFT

- FONLL first applied to b-quark hadro-production (final state b production)

- Then applied to DIS for initial charm and then initial bottom

- Generalised to two initial bottom quark (bbH, bbZ) at NNLO

- Matching performed at N3LO

For a consistent subtraction of double counting one needs to re-express both the 5FS cross section and the 4FS one in terms of the same $\alpha_s$ and PDFs
Factorisation scale dependence very slight, renormalisation scale dependence stronger
Lower choose of factorisation scale improves perturbative stability and takes 4F and 5F predictions closer to each other
The perturbative expansion is unstable in 4FS, FONLL stable when going from FONLL-A to B
FONLL results close to the 5FS and closer to experimental data
The difference between FONLL-C and the 5FS is not large in absolute value, however when compared to the very small 1% scale variation of the 5FS N3LO calculation [Duhr, Dulat, Mistlberger, arXiv: 1904.09990] it is significant.
MATCHING BETWEEN SCHEMES - EXCLUSIVE OBSERVABLES
EXCLUSIVE OBSERVABLES

- So far, considered inclusive observables. What about exclusive obs? [See S. Hoeche’s talk]
- In absence of matched calculations for exclusive observables, a practical recipe is to use 4FS for prediction of the shapes of distributions sensitive to the bottom quark kinematics, and 5FS for the total cross section (normalisation)
- Strong dependence on PS model often observed in 5FS calculations

Hbt production at the 13 TeV LHC

NLO+Pythia8/Herwig++, F=4
mH = 200 GeV, tanβ = 8

4FS yb^2, PY8
5FS yb^2, PY8
4FS yt^2 (x0.1), PY8
5FS yt^2, HW++
4FS yt^2 (x0.1), HW++
5FS yb^2 (x0.1), HW++
4FS yb^2, HW++
5FS yb^2, HW++
4FS yb^2 (x0.1), HW++

Wiesemann et al, arXiv: 1409.5301
Degrande, MU, Wiesemann, Zaro arXiv: 1507.02549
EXPLOITING THE B-QUARK MATCHING SCALE

- Simplest possible option: switch from 4FS to 5FS at a b-quark matching scale $\mu_b$ higher than $m_b$, so that switching between 4FS and 5FS happen in a region where mass effects nor collinear logs resummation are crucial [Bertone et al, arXiv: 1711.03355]
- $\mu_b$ usually = $m_b$. No reason why it has to be $m_b$, it could be up to 10*$m_b$.
- In practice, choose a factorisation scale $\mu_F$
  - Events with kinematics for which $\mu_F \leq \mu_b$ computed in 4FS and full $m_b$ dependence retained
  - Events with kinematics for which $\mu_F > \mu_b$ are to be evaluated in 5F scheme where the $m$ set to zero.
- Discontinuity in the predictions within experimental error
• Very recently several new frameworks have been developed to match 4FS and 5FS at the level of exclusive observables.
• Here focus on two of those
• No time to discuss method based on B-hadron veto [Bagnaschi et al, arXiv:1803.04335] nor the massive 5FS (5FMS) [Krauss, Napoletano, arXiv:1712.06832] [Figueroa et al 1805.01353] [Forte, Giani 1905.0227]

MATCHING 4FS AND 5FS IN FULLY DIFFERENTIAL CALCULATIONS

‣ #1: multi-jet merging of simulations in 5FS with calculations for the production of b-quark associated final states in 4FS
[Höche et al, arXiv:1904.09382]

The idea
➡ Generate showered events for Z+j
➡ Use clustering to determine whether core hard process is Z+bb~ or Z+j
➡ Throw away events if core process belongs to first type
➡ Generate Z + bb~ in the 4FS
➡ Sum the two samples with no overlap: fully differential 4FS and 4FS results can be combined automatically

‣ Results in good agreement with CMS measurement for the whole $p_T$ spectrum
MATCHING 4FS AND 5FS IN FULLY DIFFERENTIAL CALCULATIONS


\[ d\sigma^{\text{FONLL}} = d\sigma^{5\text{fs}} + (d\sigma^{4\text{fs}}_{m_b} - d\sigma^{4\text{fs}}_{m_b \to 0}) \]

- Applied to Z+ b-jet production (NNLO massless calculation for Z+b-jet in the NNLOJET framework matched with NLO massive calculation from aMC@NLO)
FINAL STATE SPLITTINGS

- Quarks’ case well understood

\[ M \sim \frac{\alpha_s(k^2)}{2\pi k^2} |M|^2 \otimes P_{qq}(x) \]

- Gluon case more delicate

\[ M \sim \frac{\alpha_s(k^2)}{2\pi k^2} |M|^2 \otimes P_{qg}(x) \]

In principle no soft terms to resum...

Resums to all orders soft dominant terms

Quite large differences in a region where all PS model should be equal (to the LO Matrix Element!)

b-jets multiplicity in e+e- scattering

• Processes relevant for precision physics and Higgs physics receive large contributions from topologies with final state $g > b\bar{b}$ splittings.
• $t\bar{t} > b\bar{b}$ is one example: 4FS calculation at NLO shows that FS splittings dominant in most phase space
• Is it appropriate to simulate these splittings at the matrix element level?

Collinear approximation keeping FS splittings surprisingly close to full ME

Jezo et al, arXiv:1802.00426
Extra radiation off parent gluon missing if b-quark generated at ME level, even at NLO+PS. How important is it?
- Importance can be assessed using fragmentation functions approach [Ridolfi, MU, Zaro, arXiv: 1911.01975]

- For most exclusive observables (such as fragmentation functions) dominant effect from radiation off parent gluon
- For most inclusive observables (such as jet multiplicities) effects are much smaller
- What happens in between? Can this have effects on relevant observables?
CONCLUSIONS

- In past ten years there has been lot of progress in understanding differences and comparing predictions in different heavy flavour schemes for HFs in the initial state.

- For inclusive observables there exist general and well-tested frameworks to match predictions in different schemes, although not yet available for all processes.
- Mass effects typically small but relevant at the current level of precision!

- For exclusive observables many new exciting developments (including first FONLL-B computation for Z+b) & work in progress to compare them for relevant observables.

- As far as final states are concerned, need to understand interplay between PS and collinear resummation in final states. FF-based studies highlight possible pathologies in the simulation of final-state $g\to b\bar{b}$ splittings at the ME-level, for exclusive observables (regardless of $m_b=0$ or $m_b\neq 0$ in the ME).

THANK YOU FOR YOUR ATTENTION
EXTRA MATERIAL
Z+B-JET AT 8 TEV

CMS 19.8 fb⁻¹ (8 TeV)

Z/γ*(→ ll) + at least 1 b jet
anti-k_t (R = 0.5) jets
p_T^{jet} > 30 GeV, |η^{jet}| < 2.4

CMS 19.8 fb⁻¹ (8 TeV)

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anti-k_t (R = 0.5) jets
p_T^{jet} > 30 GeV, |η^{jet}| < 2.4
THE FONLL METHOD

For a consistent subtraction of double counting one needs to re-express both the 5FS cross section and the 4FS one in terms of the same $\alpha_s$ and PDFs.

Take the 5FS cross section

$$\sigma^{(5)} = \int dx_1 dx_2 \sum_{i,j=g,q,b} f^{(5)}_i(x_1, \mu^2) f^{(5)}_j(x_2, \mu^2) \hat{\sigma}^{(5)}_{ij}(x_1, x_2, \alpha_s^{(5)}(\mu^2))$$

If no intrinsic bottom component, then $b$-PDF is determined in terms of gluon and light quarks $q$ by DGLAP evolution:

$$f^{(5)}_b(x, \mu^2) = \sum_{i=q,g} \int_x^1 \frac{dy}{y} f^{(5)}_i(y, \mu^2) C_{bi} \left( \frac{x}{y}, \alpha_s^{(5)}(\mu^2), L \right)$$

$$\sigma^{(5)} = \int \int dx_1 dx_2 \sum_{ij=q,g} f^{(5)}_i(x_1, \mu^2) f^{(5)}_j(x_2, \mu^2) A^{(5)}_{ij}(x_1, x_2, L, \alpha_s^{(5)}(\mu^2))$$

with $A^{(5)}_{ij} = C_{bi} \otimes C_{bj} \otimes \hat{\sigma}^{(5)}_{ij}$.
THE FONLL METHOD

- For a consistent subtraction of double counting one needs to re-express both the 5FS cross section and the 4FS one in terms of the same $\alpha_s$ and PDFs.
- Take the 4FS cross section

$$\sigma^{(4)} = \int dx_1 dx_2 \sum_{i,j=g,q} f_i^{(4)}(x_1, \mu^2) f_j^{(4)}(x_2, \mu^2) \, \hat{\sigma}^{(4)}_{ij}(x_1, x_2, \frac{\mu^2}{m_b}, \alpha^{(4)}_s(\mu^2))$$

- Both $\alpha_s$ and PDFs can be re-expressed in terms of their 5F counterparts [Buza et al hep-ph/9612398]
- $K_{ij}$ polynomial in $L$
- Invert Eqns and obtain

$$\alpha^{(5)}_s(\mu^2) = \alpha^{(4)}_s(\mu^2) + \sum_{i=2}^{\infty} c_i(L) \times (\alpha^{(4)}_s(m_b^2))^i,$$

$$f_i^{(5)}(x, \mu^2) = \int x \, \frac{dy}{y} \sum_j K_{ij}(y, L, \alpha^{(4)}_s(\mu^2)) f_j^{(4)}\left(\frac{x}{y}, \mu^2\right)$$

$$\sigma^{(4)} = \iint dx_1 dx_2 \sum_{ij=q,g} f_i^{(5)}(x_1, \mu^2) f_j^{(5)}(x_2, \mu^2) B_{ij}^{(4)}\left(x_1, x_2, \frac{\mu^2}{m_b}, \alpha^{(5)}_s(\mu^2)\right)$$
For a consistent subtraction of double counting one needs to re-express both the 5FS cross section and the 4FS one in terms of the same $\alpha_s$ and PDFs.

\[
\sigma^{(5)} = \int \int dx_1 dx_2 \sum_{ij=q,g} f_i^{(5)}(x_1, \mu^2) f_j^{(5)}(x_2, \mu^2) A_{ij}^{(5)}(x_1, x_2, L, \alpha_s^{(5)}(\mu^2))
\]

\[
\sigma^{(4)} = \int \int dx_1 dx_2 \sum_{ij=q,g} f_i^{(5)}(x_1, \mu^2) f_j^{(5)}(x_2, \mu^2) B_{ij}^{(4)}\left(x_1, x_2, \frac{\mu^2}{m_b^2}, \alpha_s^{(5)}(\mu^2)\right)
\]

To identify the double-counting, expand the cross sections at the order $N$.

\[
A_{ij}^{(5)}(x_1, x_2, L, \alpha_s^{(5)}(\mu^2)) = \sum_{p=0}^{N} (\alpha_s^{(5)}(\mu^2))^p \sum_{k=0}^{\infty} A_{ij}^{(p), (k)}(x_1, x_2) (\alpha_s^{(5)}(\mu^2)L)^k
\]

\[
B_{ij}^{(4)}\left(x_1, x_2, \frac{\mu^2}{m_b^2}, \alpha_s^{(5)}(\mu^2)\right) = \sum_{p=0}^{N} (\alpha_s^{(5)}(\mu^2))^p B_{ij}^{(p)}\left(x_1, x_2, \frac{\mu^2}{m_b^2}\right)
\]
THE FONLL METHOD

Subtraction term: take the logarithmic (massless) terms in the B expansion that appear both in the 5FS and in the 4FS expansions.

\[
\sigma^{(4),(0)} = \int \int dx_1 dx_2 \sum_{ij=q,g} f^{(5)}_i(x_1, \mu^2) f^{(5)}_j(x_2, \mu^2) B^{(0)}_{ij} \left( x_1, x_2, \frac{\mu^2}{m_b^2}, \alpha_s^{(5)}(\mu^2) \right)
\]

\[
B^{(0),(p)}_{ij} \left( x_1, x_2, \frac{\mu^2}{m_b^2} \right) = \sum_{k=0}^p A_{ij}^{(p-k),(k)}(x_1, x_2) L^k
\]

To identify the double-counting, expand the cross sections at the order N.

\[
A^{(5)}_{ij} \left( x_1, x_2, L, \alpha_s^{(5)}(\mu^2) \right) = \sum_{p=0}^N (\alpha_s^{(5)}(\mu^2))^p \sum_{k=0}^\infty A_{ij}^{(p),(k)}(x_1, x_2) \left( \alpha_s^{(5)}(\mu^2) L \right)^k
\]

\[
B^{(4)}_{ij} \left( x_1, x_2, \frac{\mu^2}{m_b^2}, \alpha_s^{(5)}(\mu^2) \right) = \sum_{p=0}^N (\alpha_s^{(5)}(\mu^2))^p B^{(p)}_{ij} \left( x_1, x_2, \frac{\mu^2}{m_b^2} \right)
\]
Very recently several new frameworks have been developed to match 4FS and 5FS at the level of exclusive observables.

#3: Build combination of 5FS and 4FS, vetoing B-Hadrons [Bagnaschi et al, arXiv:1803.04335]

In 5FS B-hadrons in PS from bb~ or bg channels (initial state) or g>bb~ splittings. The latter removed by vetoing B-hadrons in final state to avoid double-counting.

\[ d\sigma^{\text{mass}} = d\sigma^{5\text{FS-Bveto}} + d\sigma^{4\text{FS}} \]

- b-contribution: non-trivial shape, the two contributions are of the same order of magnitude at large \( p_T \), while at low \( p_T \) gluon splitting from light-quark induced processes dominates.
- Non-trivial shape distortion.
- Effects after merging about 1% using MG5_aMCatNLO
#3: 5F Massive Scheme (5FMS) [Krauss, Napoletano, arXiv:1712.06832]
Scheme devised to construct an extension of 5FS, allowing for massive partons in the initial state, at NLO accuracy.
Catani-Seymour subtraction of infrared divergences to the case of massive initial states.
A CLOSER LOOK AT G > BB~ SPLITTINGS

- **LO** shape does not change with scale
  - Not reliable prediction
- **Resummed** predictions very close to each other
  - Correct shower description (LL) for gluon fragmentation
- **NLO** prediction harder than resummed ones (+70% for μ=100GeV)
- **NNLO** has decent agreement with resummed predictions
  - Justifies t\(\bar{t}bb\)+jet @NLO as reference for t\(\bar{t}bb\)
- Dominant effect from radiation off the parent gluon
  - Not included when b quarks are generated at the ME level
  - Large effect on *exclusive* observables

Energy fraction of the b quark

\[ \mu_0 = 4.7 \text{ GeV}; \text{ w/o } O(\alpha_s^2) \text{ IC} \]

- \( \mu = 10 \text{ GeV} \)
- \( \mu = 30 \text{ GeV} \)
- \( \mu = 100 \text{ GeV} \)
- \( \mu = 300 \text{ GeV} \)

Ridolfi, MU, Zaro, arXiv: 1911.01975