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THEORETICAL VIEW ON HEAVY FLAVOUR SCHEMES

9TH LARGE HADRON COLLIDER PHYSICS CONFERENCE (LHCP2021)

7TH - 12TH JUNE 2021

OUTLINE

- Introduction: heavy flavour schemes in QCD calculations

- Matched calculations for inclusive observables

  bb~ > Z [Forte, Napoletano, MU arXiv: 1803.10248] bb~ > H [Duhr, Dulat, Mistlberger, arXiv: 1904.09990]

- Matched calculations for exclusive observables

  Multi-jet merging [Höche et al, arXiv:1904.09382] FONLL differential [Gauld, Gehrmann-De Ridder, Glover, Huss, Majer arXiv:2005.03016]

- Heavy flavour splittings in final states

  tt~bb~ [Jezo et al, arXiv:1802.00426] Ridolfi, MU, Zaro [arXiv: 1911.01975]

- Conclusions

INTRODUCTION

HEAVY FLAVOUR SCHEMES

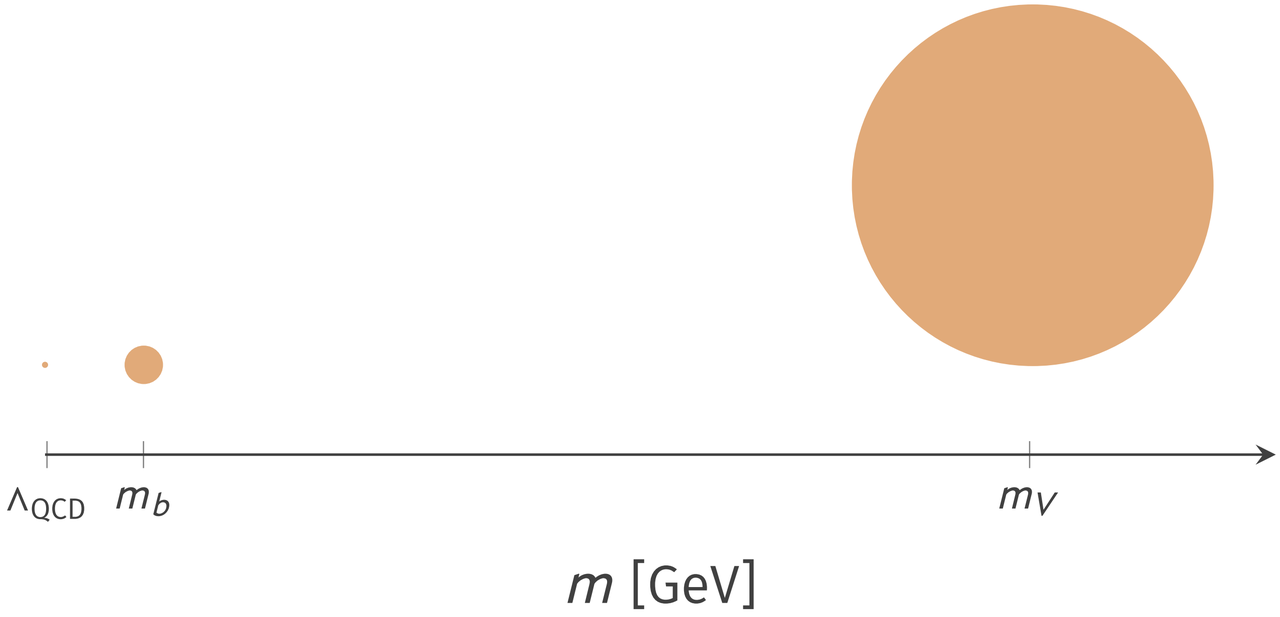
$$\frac{d\sigma_H^{pp\to ab}}{dX} = \sum_{i,j=-n_f}^{+n_f} \int_{\tau_0}^{1} \frac{dz_1}{z_1}\frac{dz_2}{z_2} f_i(z_1,\mu_F)\, f_j(z_2,\mu_F) \frac{d\hat{\sigma}_i^{ij}}{dX}(zS,\alpha_s(\mu_R),\mu_F) + \mathcal{O}\left(\frac{\Lambda^n}{S^n}\right)$$

5F scheme:
b-quarks belong
to proton & $m_b = 0$

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

- 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)

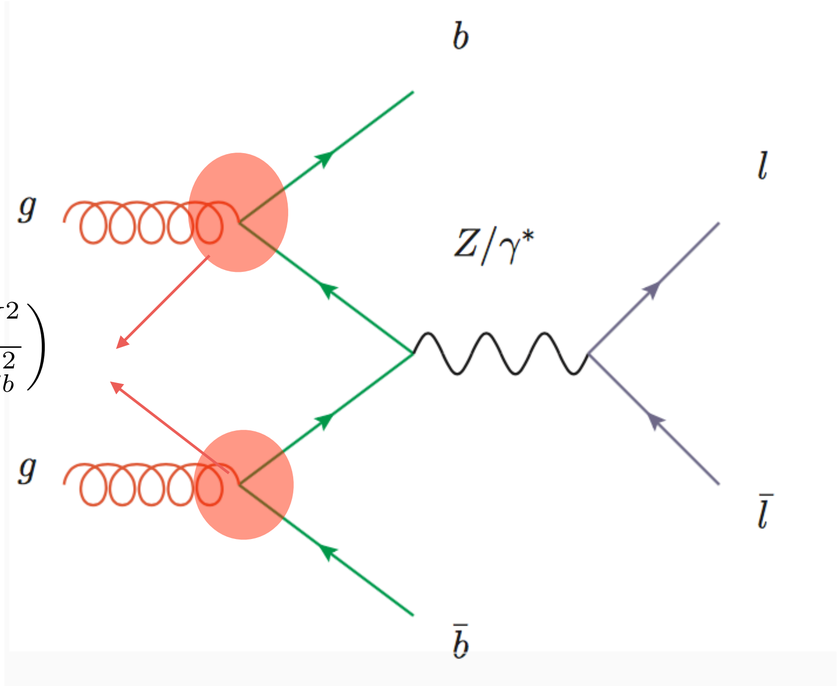


Credit: D. Napoletano

HEAVY FLAVOUR SCHEMES

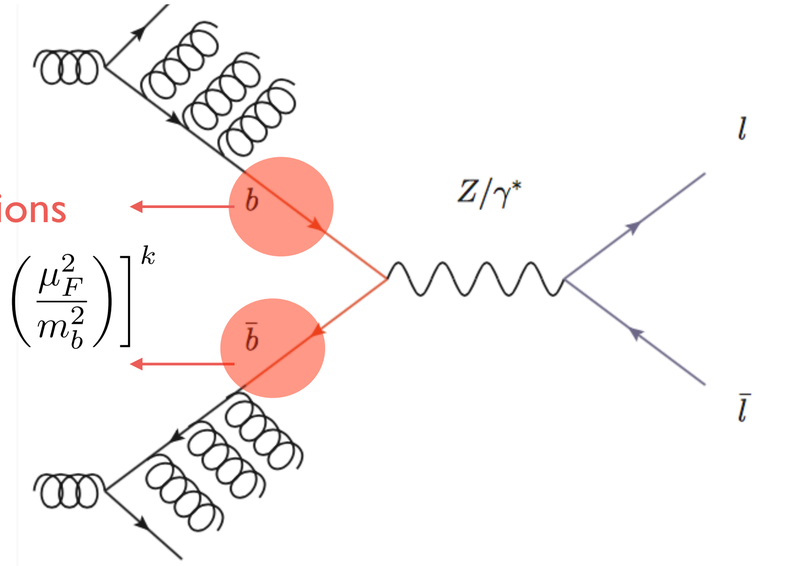
Collinear log

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



DGLAP equations

$$\sum_{k=1}^{\infty}\left[\alpha_s(\mu_F)\,\log\left(\frac{\mu_F^2}{m_b^2}\right)\right]^k$$



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

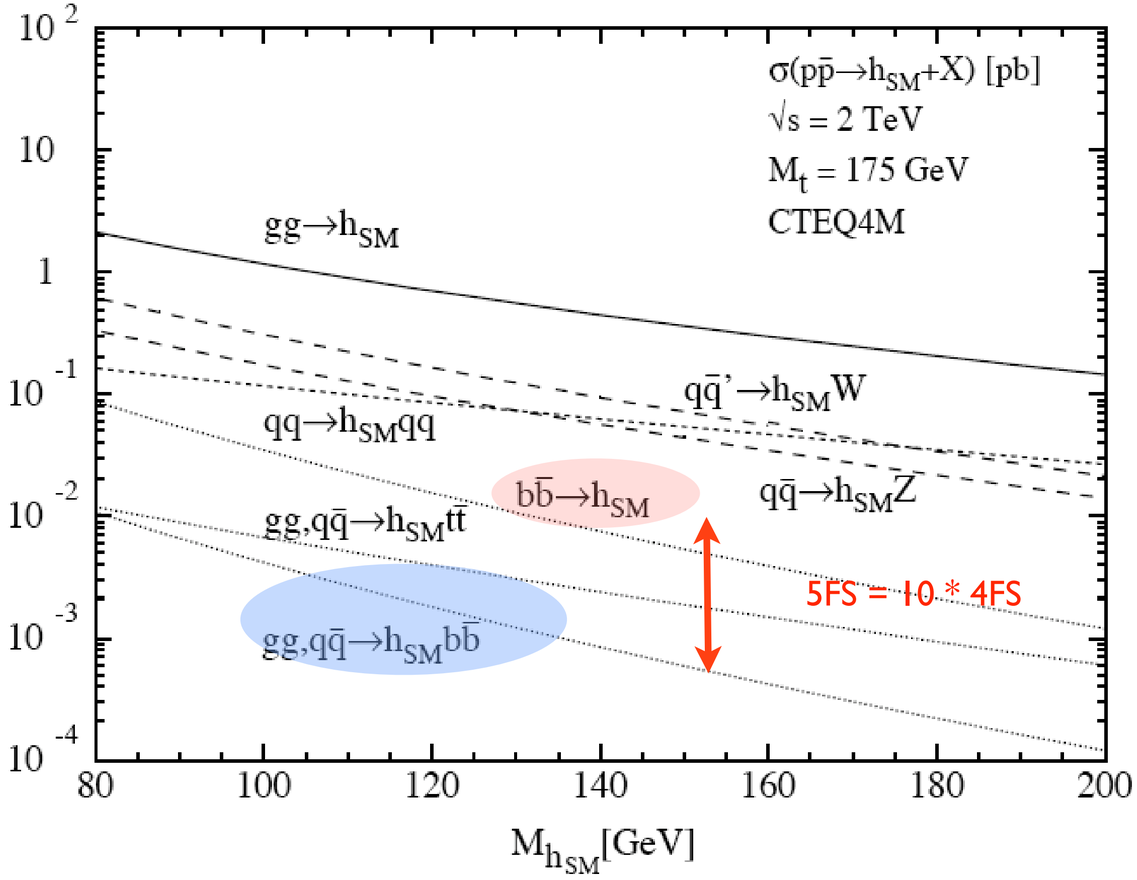
✔ Computing higher orders is easier

✘ Neglects O(m_b/M) and yields less accurate description of bottom quark kinematic distribution

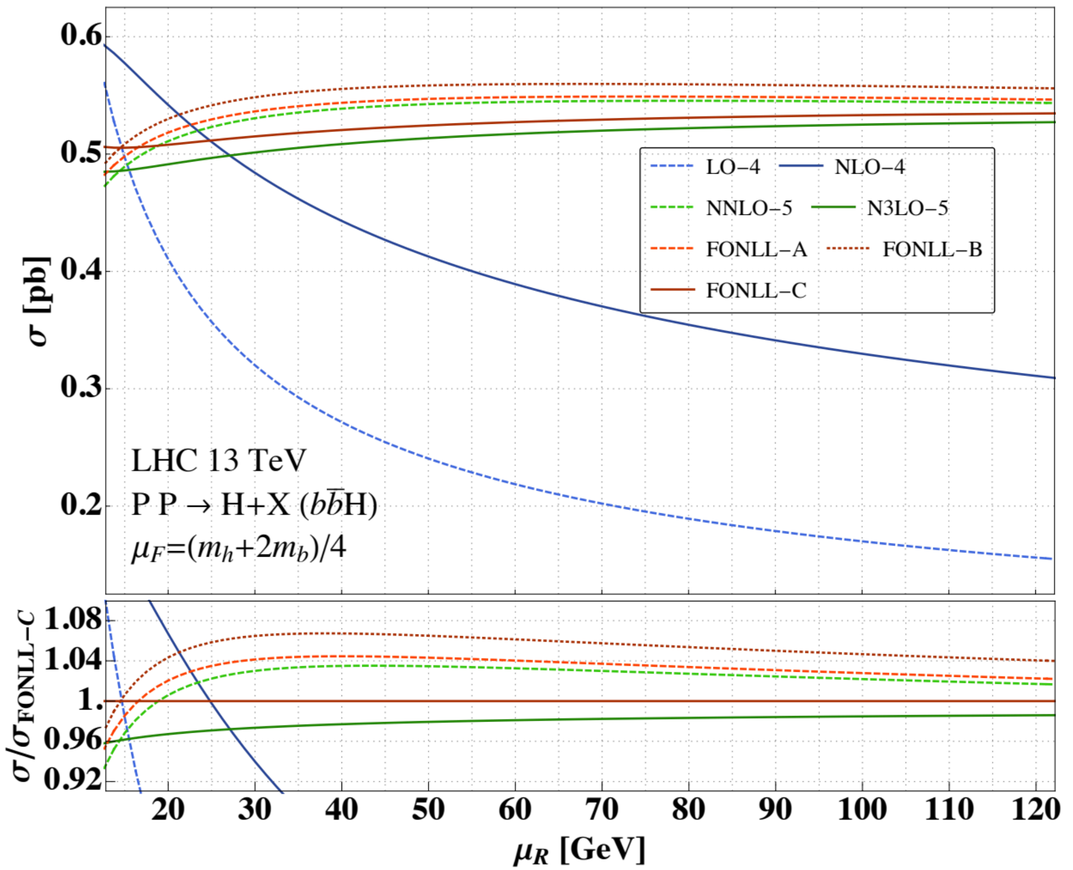
✘ Implementation in MC depends on the gluon splitting model in the PS

DIFFERENCES BETWEEN SCHEMES

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



Duhr, Dulat, Hirschi, Mistlberger, arXiv: 2004.04752

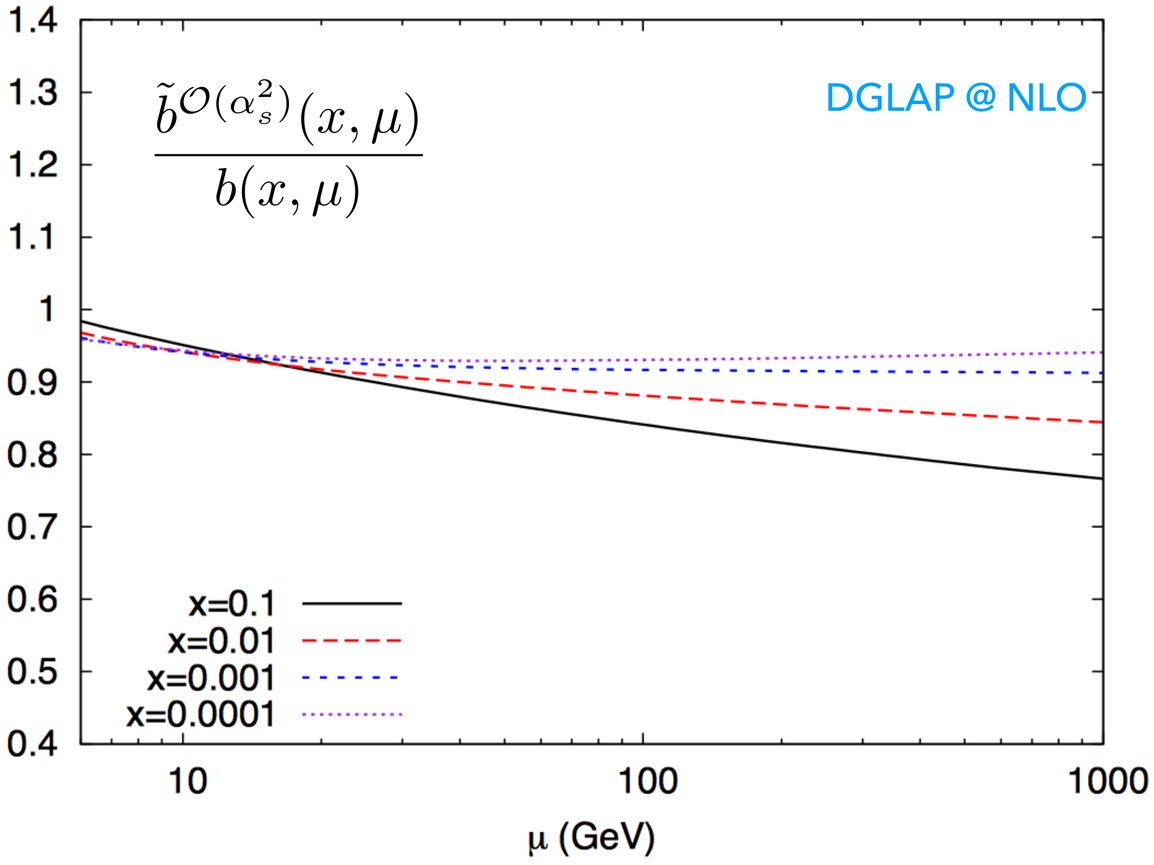


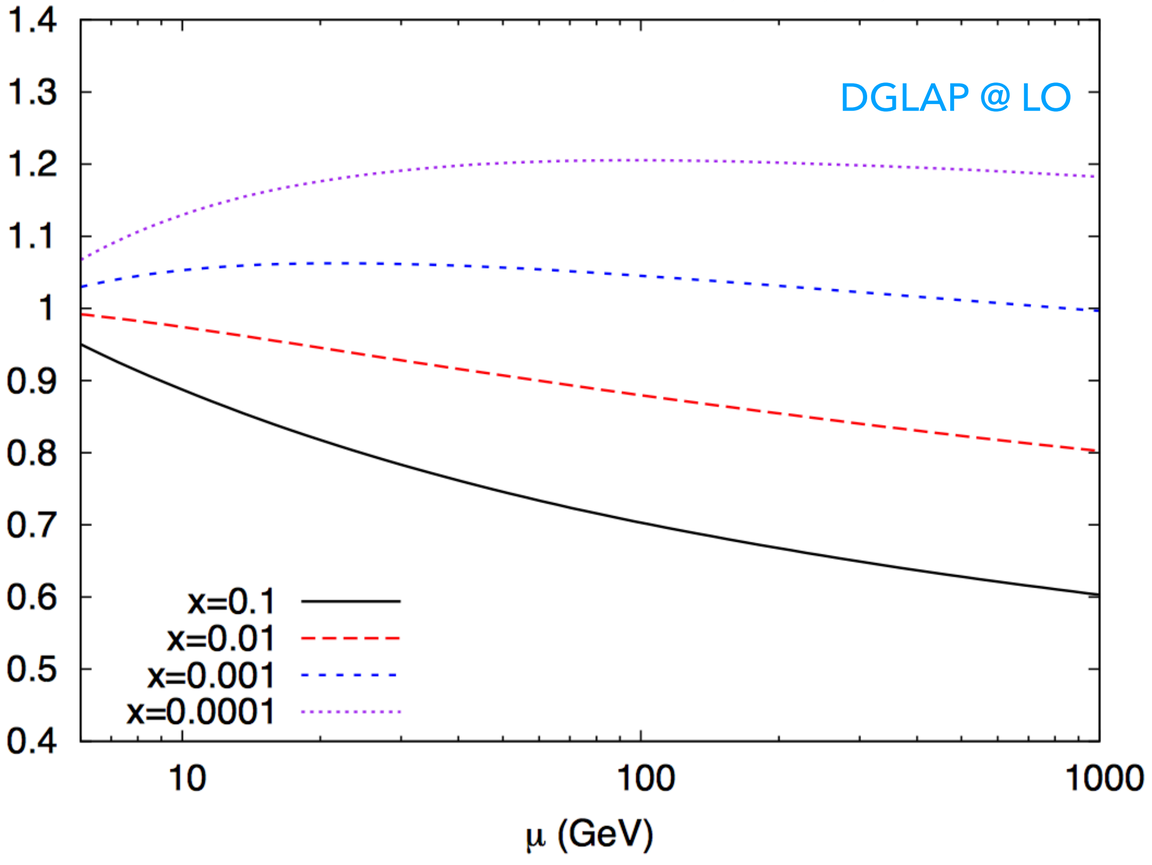
- At that time, calculations in the two schemes were compared and at leading order the effect of collinear resummation is extremely large, now calculations typically known at NNLO (even N3LO in case of bbH) in 5FS and NLO in 4FS
- Calculations were compared at hard scale of the process, while now lower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

DIFFERENCES BETWEEN SCHEMES

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

Maltoni, Ridolfi, MU, arXiv: 1203.6393





At NLO, the resummation effects of the initial state collinear logs into the b-PDFs important only at large x!

Larger effects at large-x:
$x \approx M^2 / S_{had}$

DIFFERENCES BETWEEN SCHEMES

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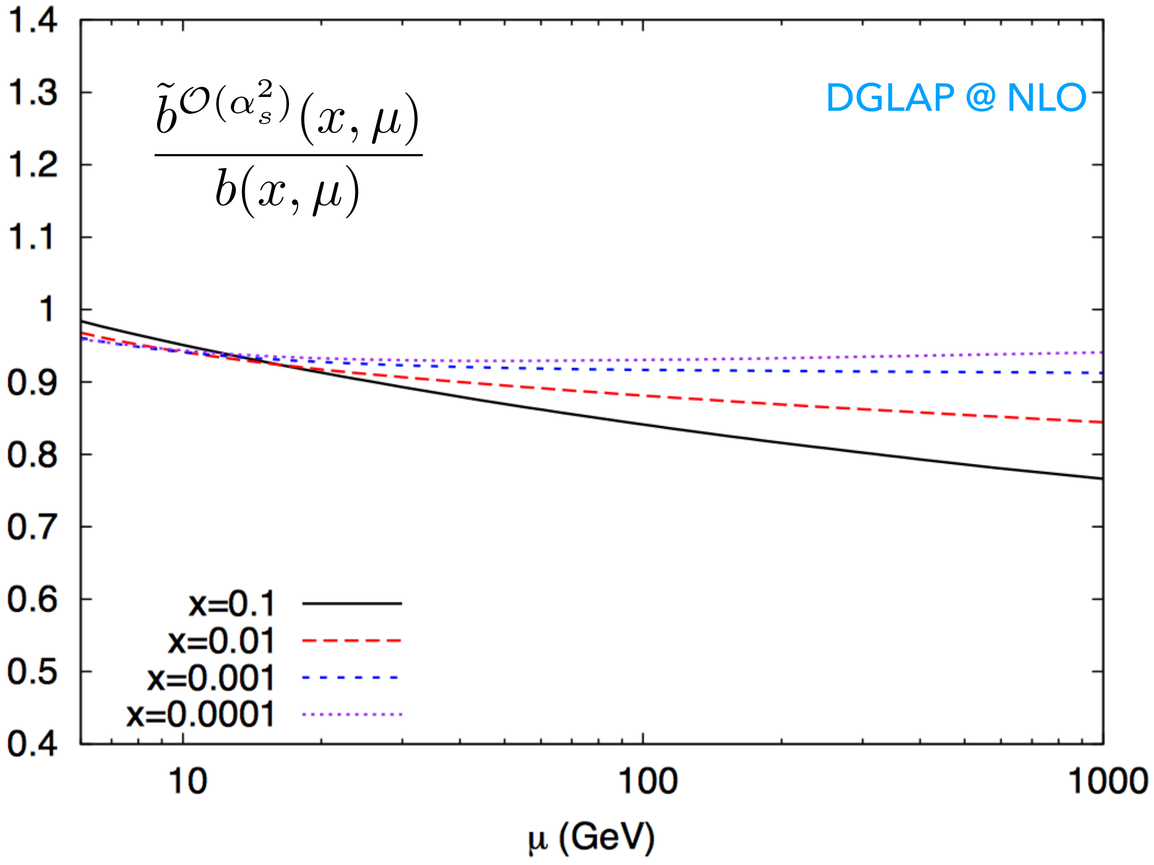
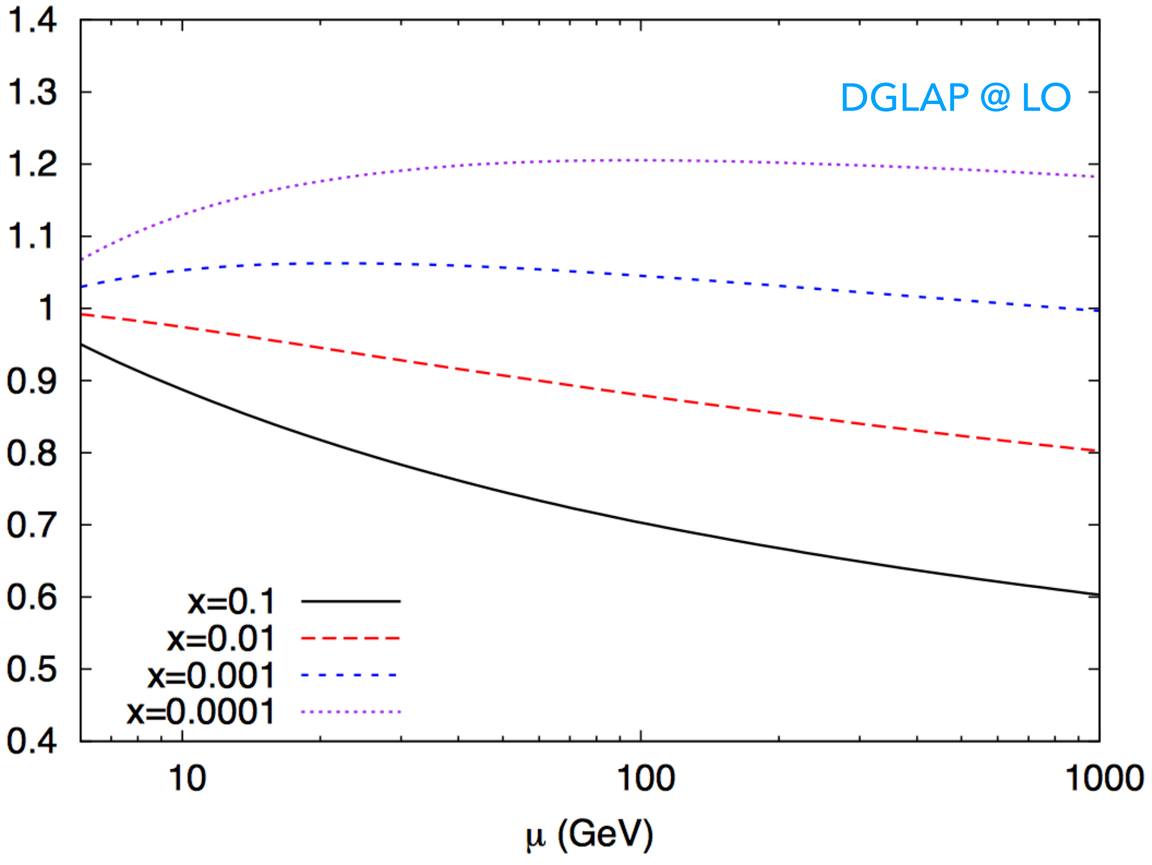




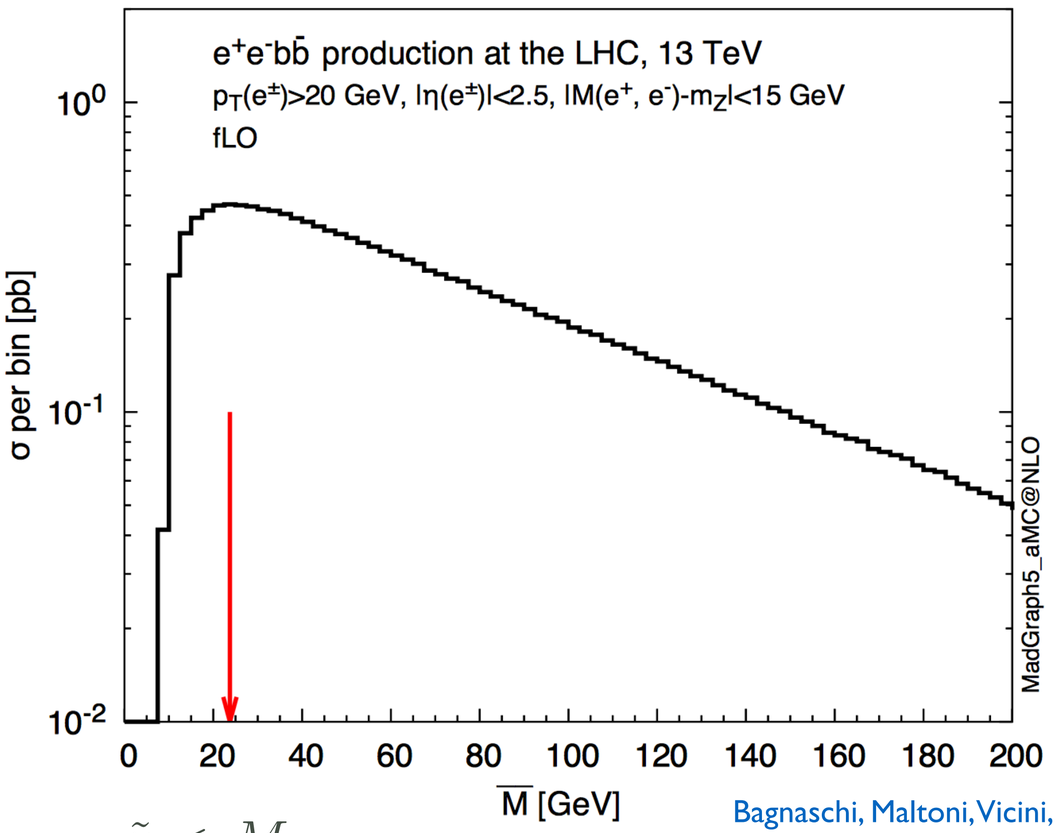
The possibly large ratios M^2/m_b^2 are always accompanied by universal phase space factors

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

$$= \log\left(\frac{\tilde{\mu}^2}{m_b^2}\right), \quad \tilde{\mu}^2 = M^2 < h(z) >$$

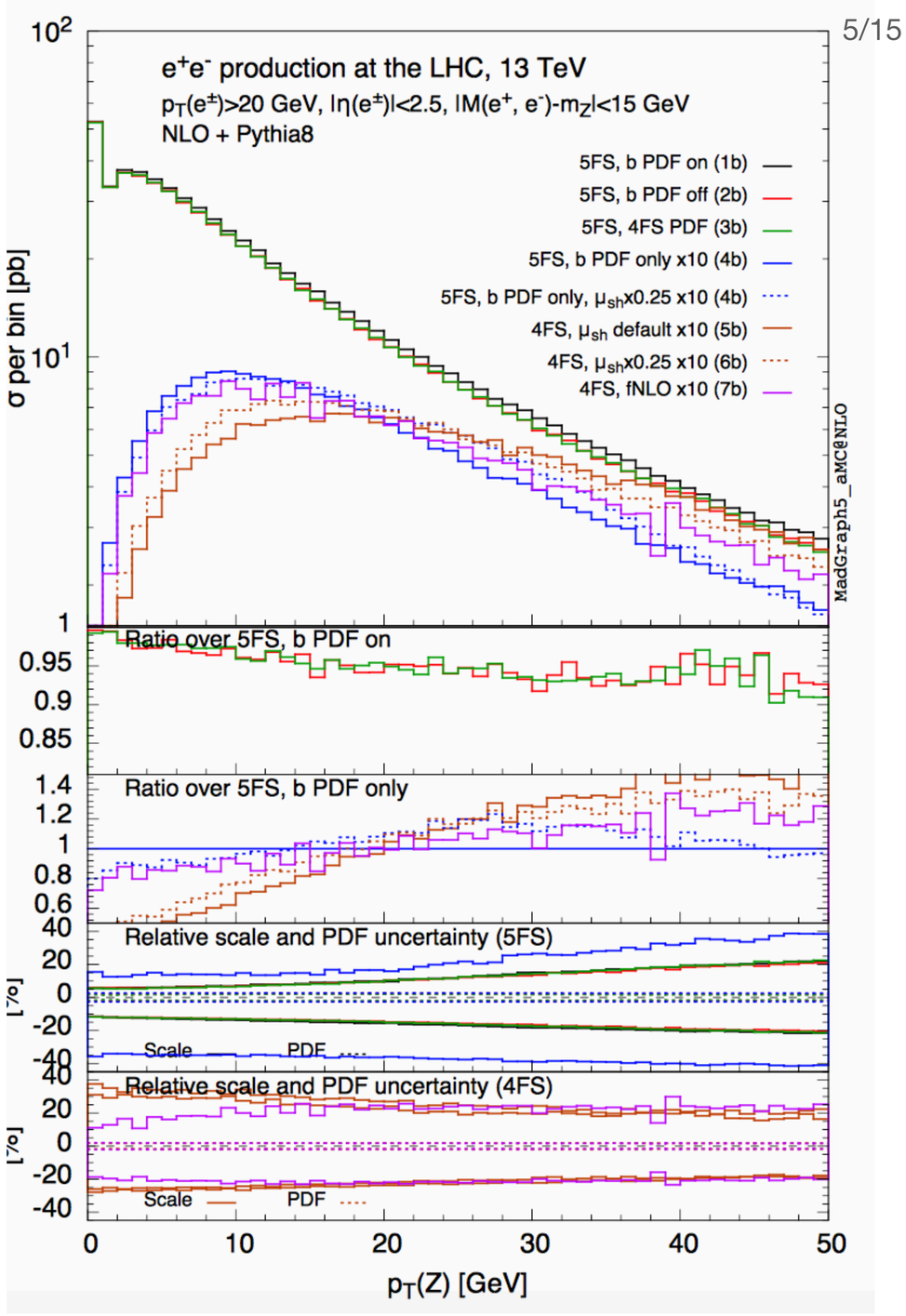
~ 0.2 - 0.4

DIFFERENCES BETWEEN SCHEMES



$\tilde{\mu} < M$

Bagnaschi, Maltoni, Vicini, Zaro, arXiv: 1803.04336



- Lower **μ** 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

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^pLO with DGLAP resummed N^qLL

- Other approaches possible based on EFT

[Bonvini, Papanastasious, Tackmann 2015]

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

[Cacciari, Greco, Nason 1998]

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

[Forte, Laenen, Nason, Rojo 2006 + Ball et al 2016 + Forte, Giani, Napoletano 2019]

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

[Forte, Napoletano, MU 2015 + Forte, Napoletano, MU 2016]

- Matching performed at N3LO

[Duhr, Dulat, Hirschi, Mistlberger, 2020]

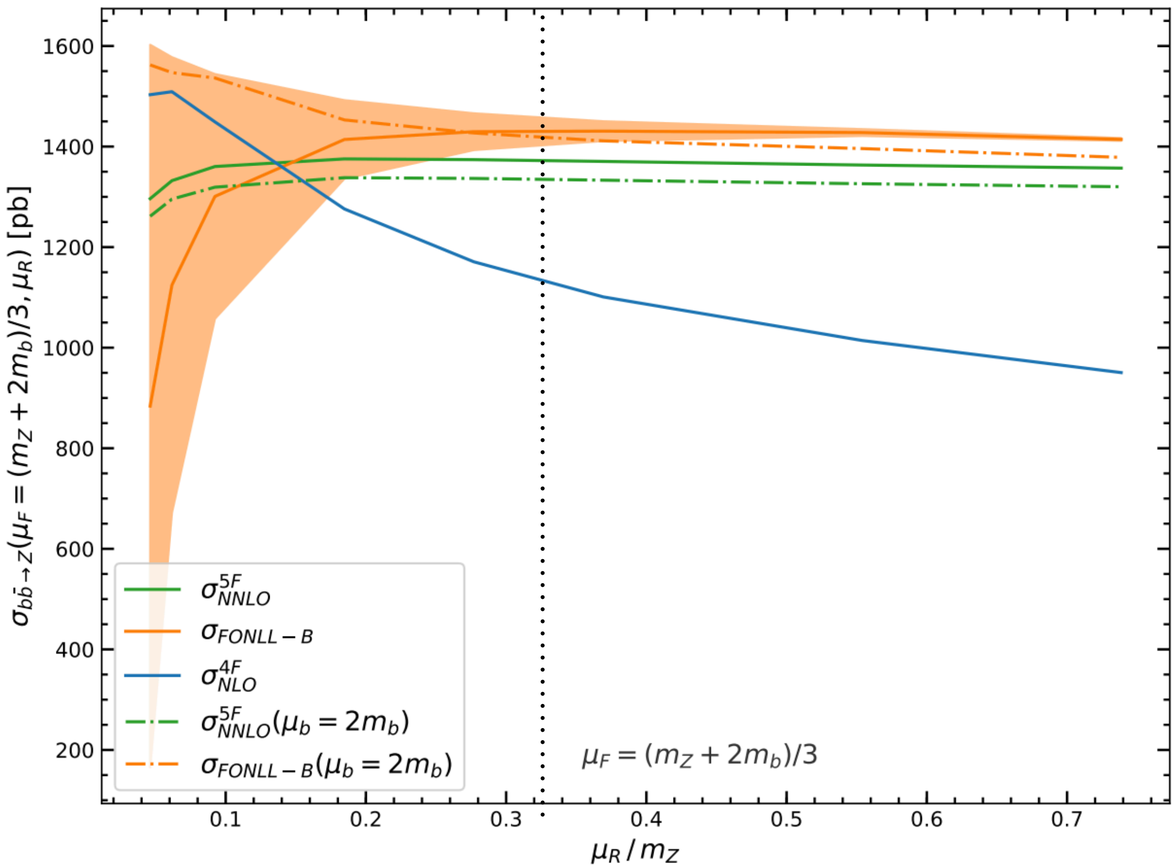
$$L = \log \frac{\mu_F^2}{m_b^2}$$

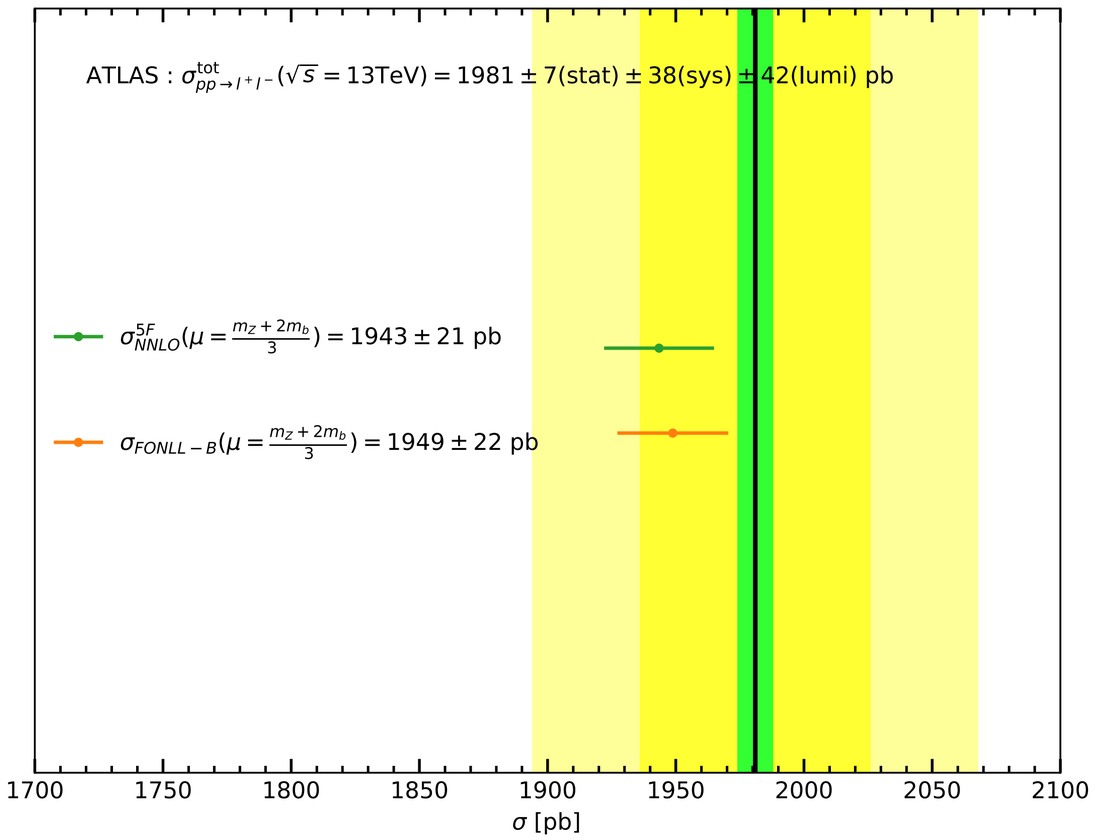
$$\begin{aligned}\sigma^{(FONLL)} &= \sigma^{(4)} + \sigma^{(5)} - \text{double counting} \\ &= \mathcal{L}_{ij}(x_1, x_2, \mu^2) \otimes \sum_p^N \left(\alpha_S^{(5)}(\mu^2)\right)^p \\ &\times \left\{ \mathcal{B}_{ij}^{(p)}\left(x_1, x_2, \frac{\mu^2}{m_b^2}\right) + \sum_{k=0}^{\infty} \mathcal{A}_{ij}^{(p),(k)}(x_1, x_2)\left(\alpha_S^{(5)}(\mu^2) L\right)^k \right\} \\ &- \text{double counting}\end{aligned}$$

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 α_S and PDFs

BB~ → Z FONLL @ N2LO (5FS) + NLO (4FS)

Forte, Napoletano, MU arXiv: 1803.10248

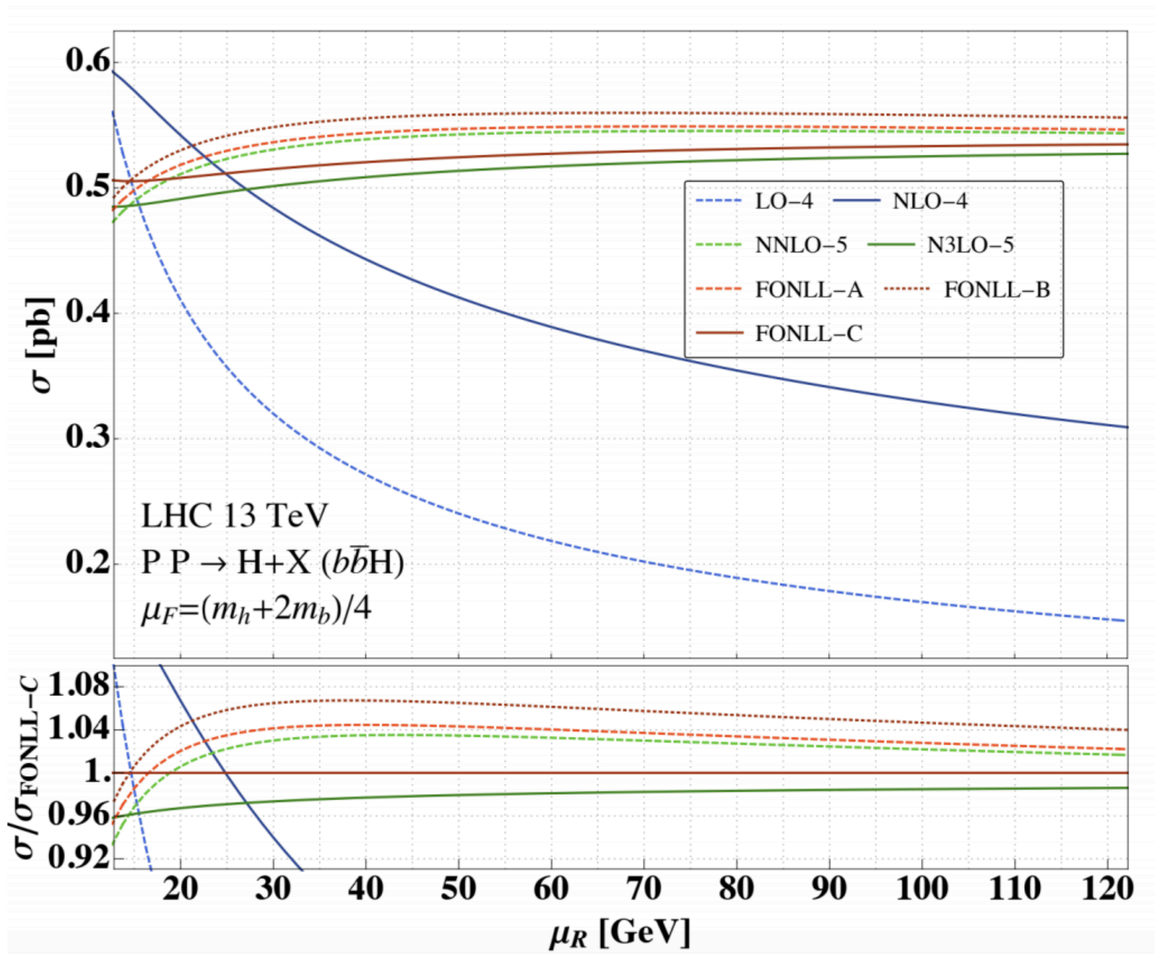


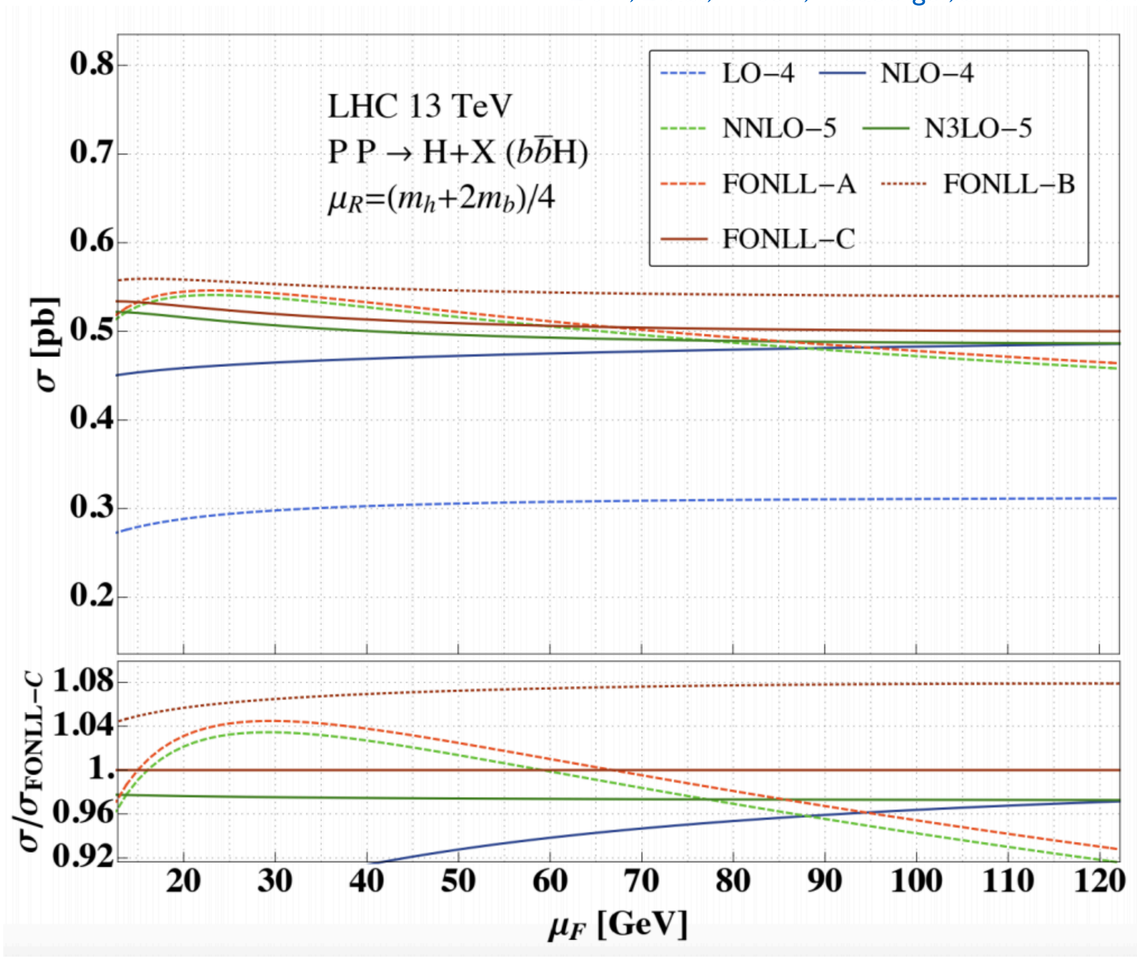


- Factorisation scale dependence very slight, renormalisation scale dependence stronger
- Lower choose of factorisation scale improves perturbative stability and takes 4F and 5F predictions closer to each other
- The perturbative expansion is unstable in 4FS, FONLL stable when going from FONLL-A to B
- FONLL results close to the 5FS and closer to experimental data

BB~ → H FONLL @ N3LO (5FS) + NLO (4FS)

Duhr, Dulat, Hirschi, Mistlberger, arXiv: 2004.04752



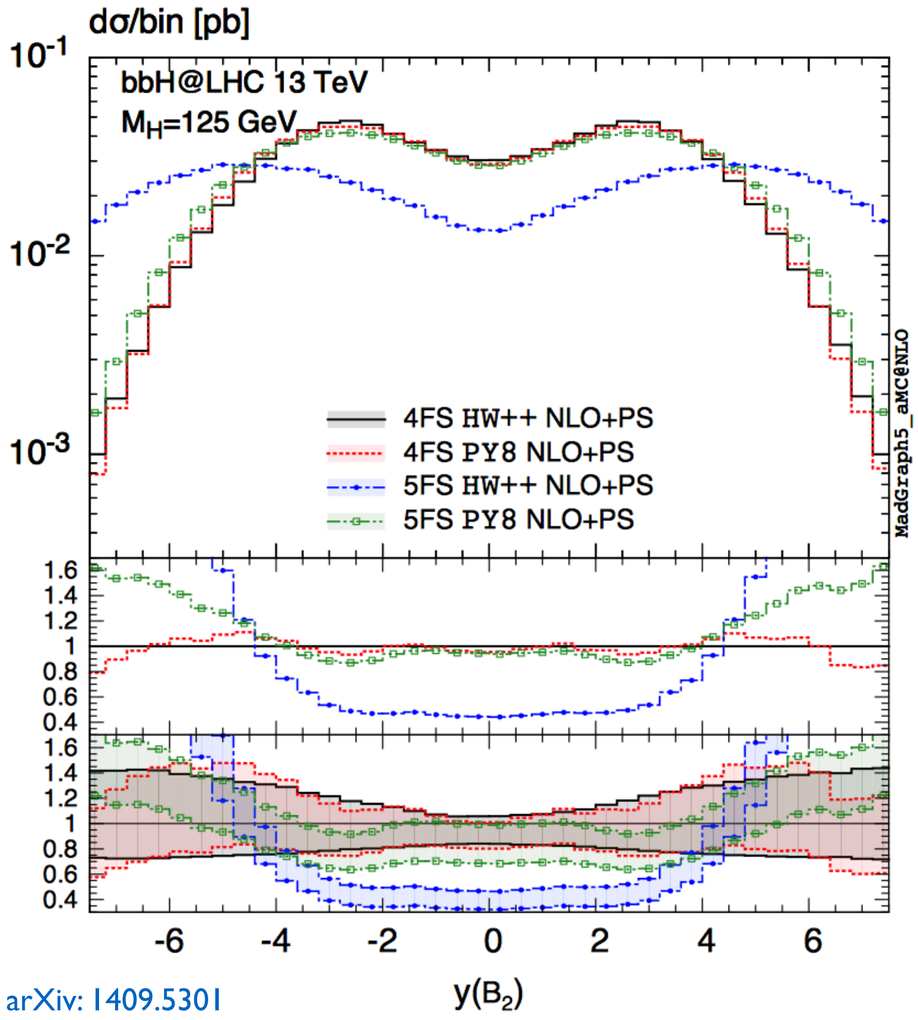


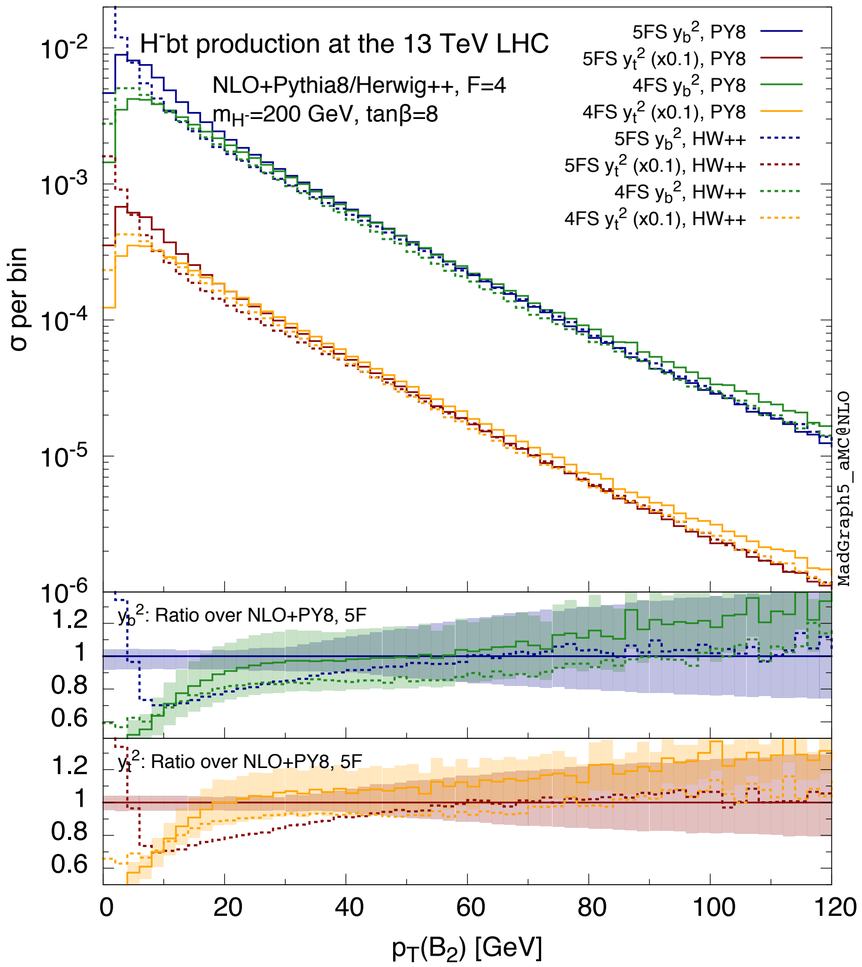
- The difference between FONLL-C and the 5FS is not large in absolute value, however when compared to the very small 1% scale variation of the 5FS N3LO calculation [Duhr, Dulat, Mistlberger, arXiv: 1904.09990] it is significant

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



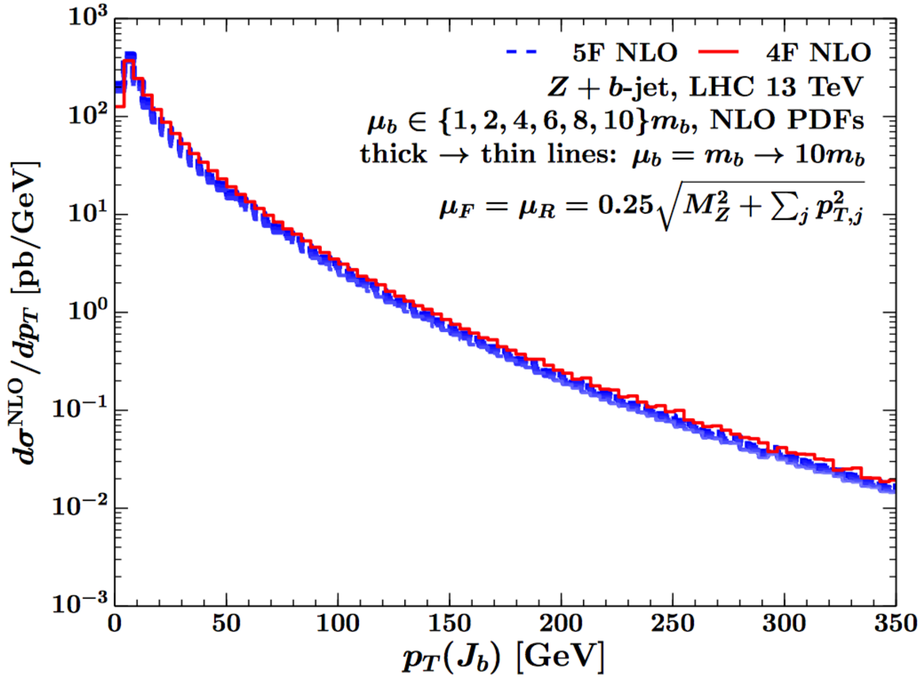


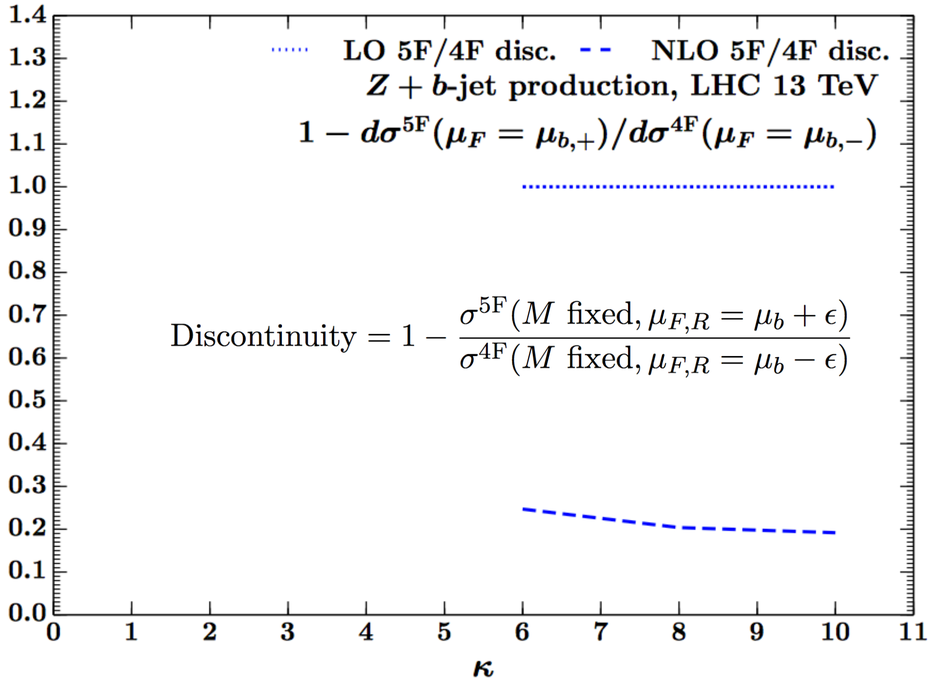
Wiesemann et al, arXiv: 1409.5301

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 μ_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]
- μ_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 μ_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





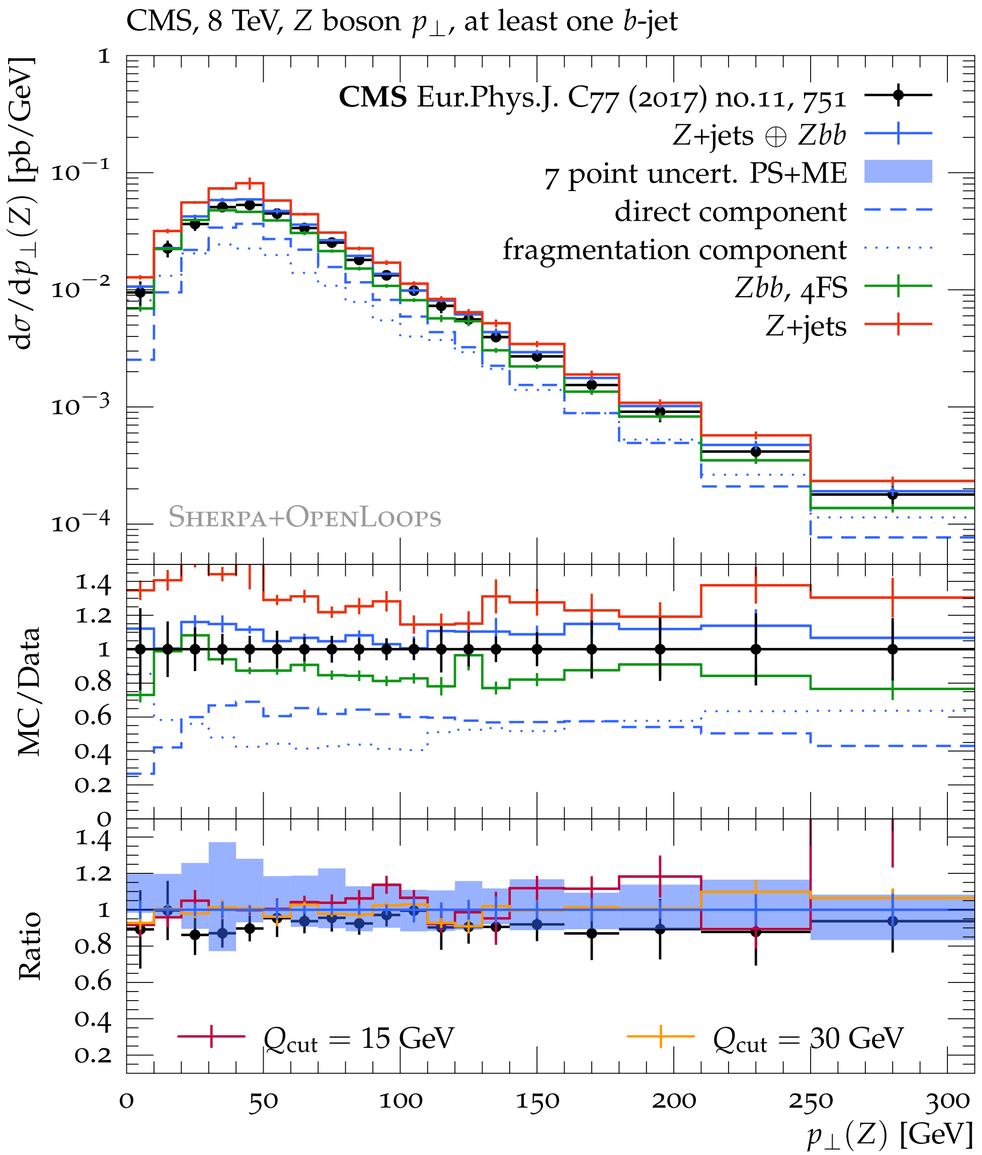
Bertone, Glazov, Mitov, Papanastasiou, MU arXiv: 1711.03355

MATCHING 4FS AND 5FS IN FULLY DIFFERENTIAL CALCULATIONS

- 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]

- **#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



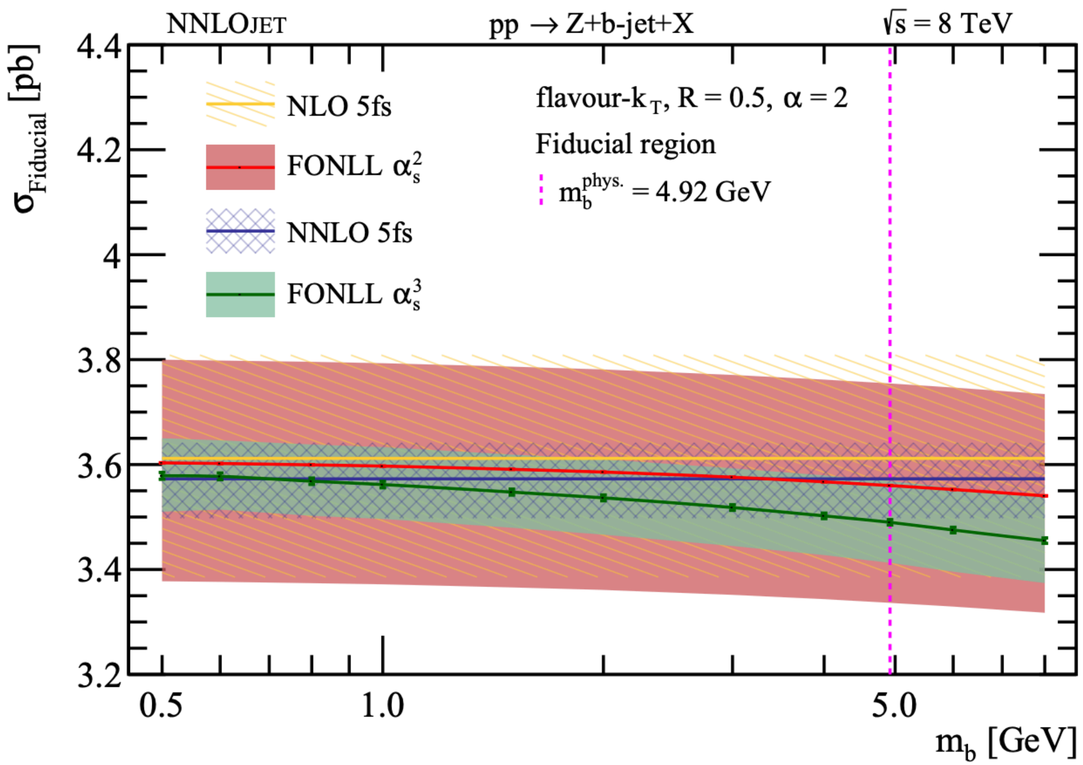
Höche, Krause, Siegert, arXiv: 1904.09382

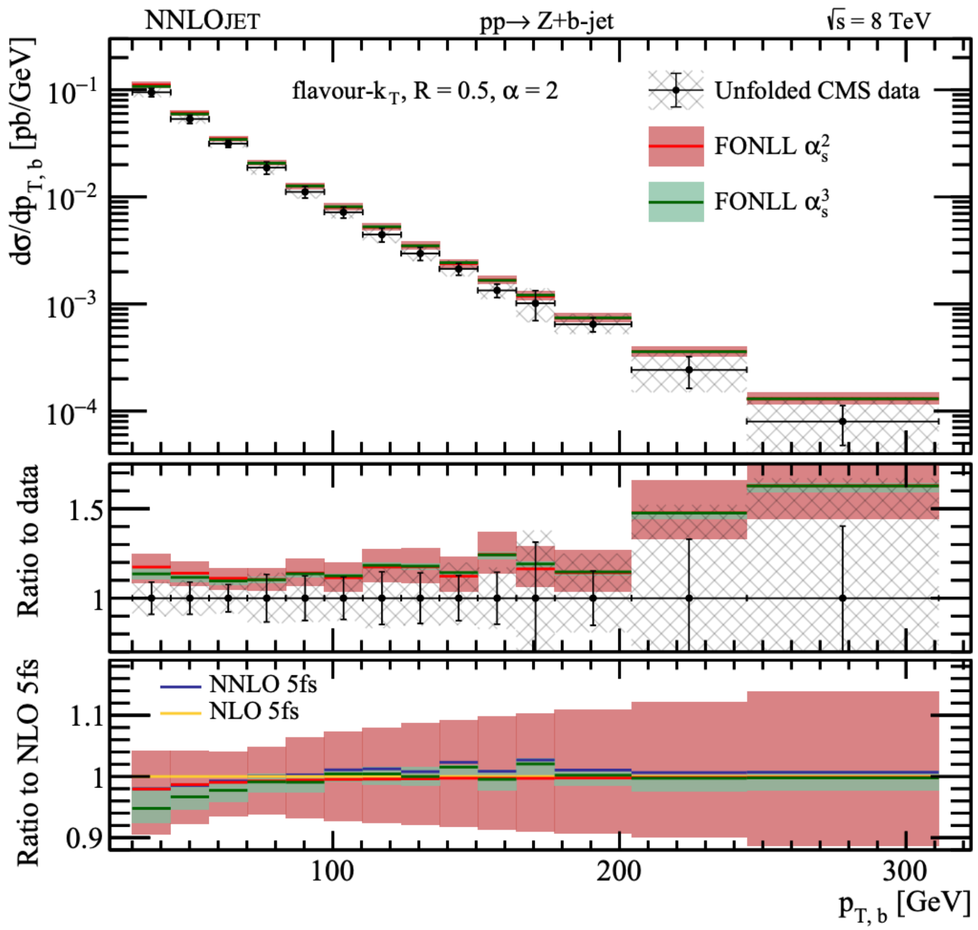
MATCHING 4FS AND 5FS IN FULLY DIFFERENTIAL CALCULATIONS

- **#2:** Differential FONLL at high order [Gauld, Gehrmann-De Ridder, Glover, Huss, Majer arXiv:2005.03016]

$$d\sigma^{\mathrm{FONLL}} = d\sigma^{5\mathrm{fs}} + \left(d\sigma^{4\mathrm{fs}}_{m_b} - d\sigma^{4\mathrm{fs}}_{m_b\to 0}\right)$$

- 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)



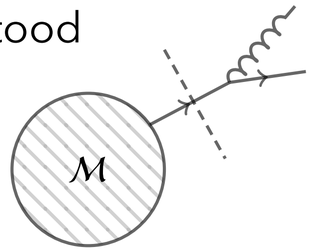


Gauld, Gehrmann-De Ridder, Glover, Huss, Majer arXiv:2005.03016

FINAL STATE SPLITTING

FINAL STATE SPLITTINGS

- Quarks' case well understood

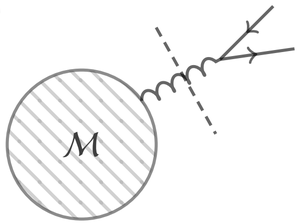


$$\sim \frac{\alpha_s(k_\perp^2)}{2\pi k_\perp^2} |\mathcal{M}|^2 \otimes P_{qq}(x)$$

$$\left(\frac{\log^k(1-x)}{1-x}\right)_+$$

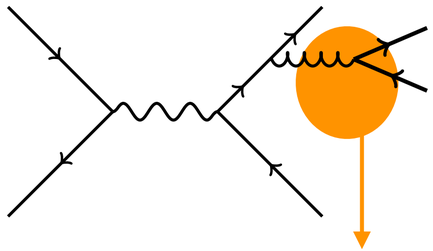
Resums to all orders soft dominant terms

- Gluon case more delicate



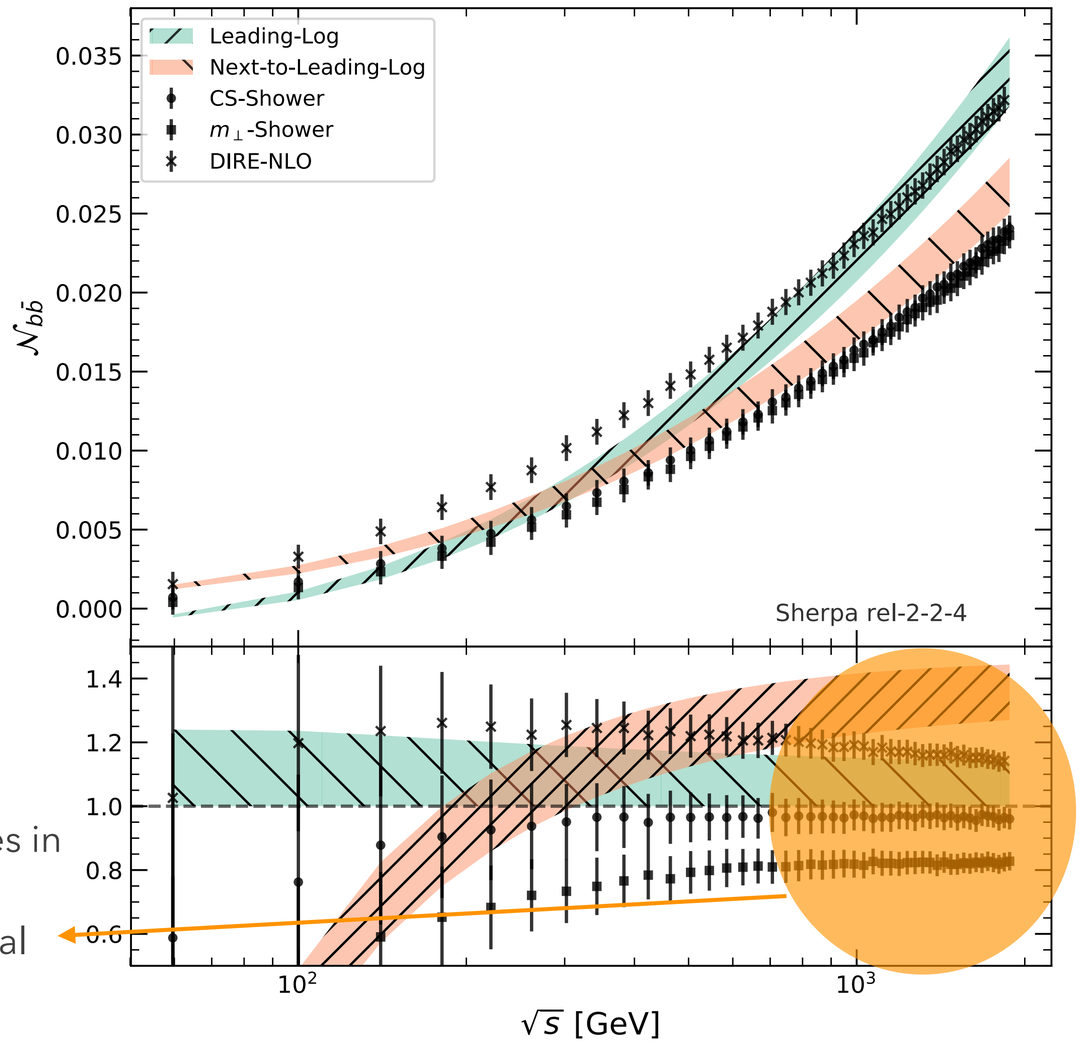
$$\sim \frac{\alpha_s(?^2)}{2\pi k_\perp^2} |\mathcal{M}|^2 \otimes P_{qg}(x)$$

In principle no soft terms to resum…



b-jets multiplicity in e+e- scattering

[M. Seymour, Nucl.Phys.B 436 (1995)]

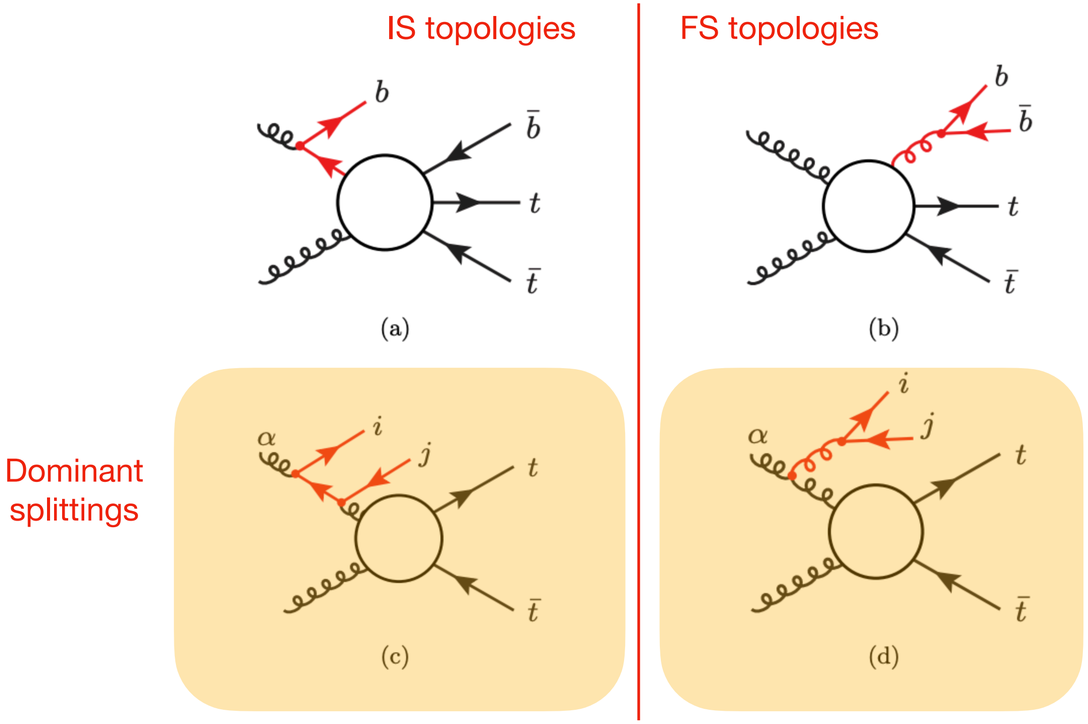


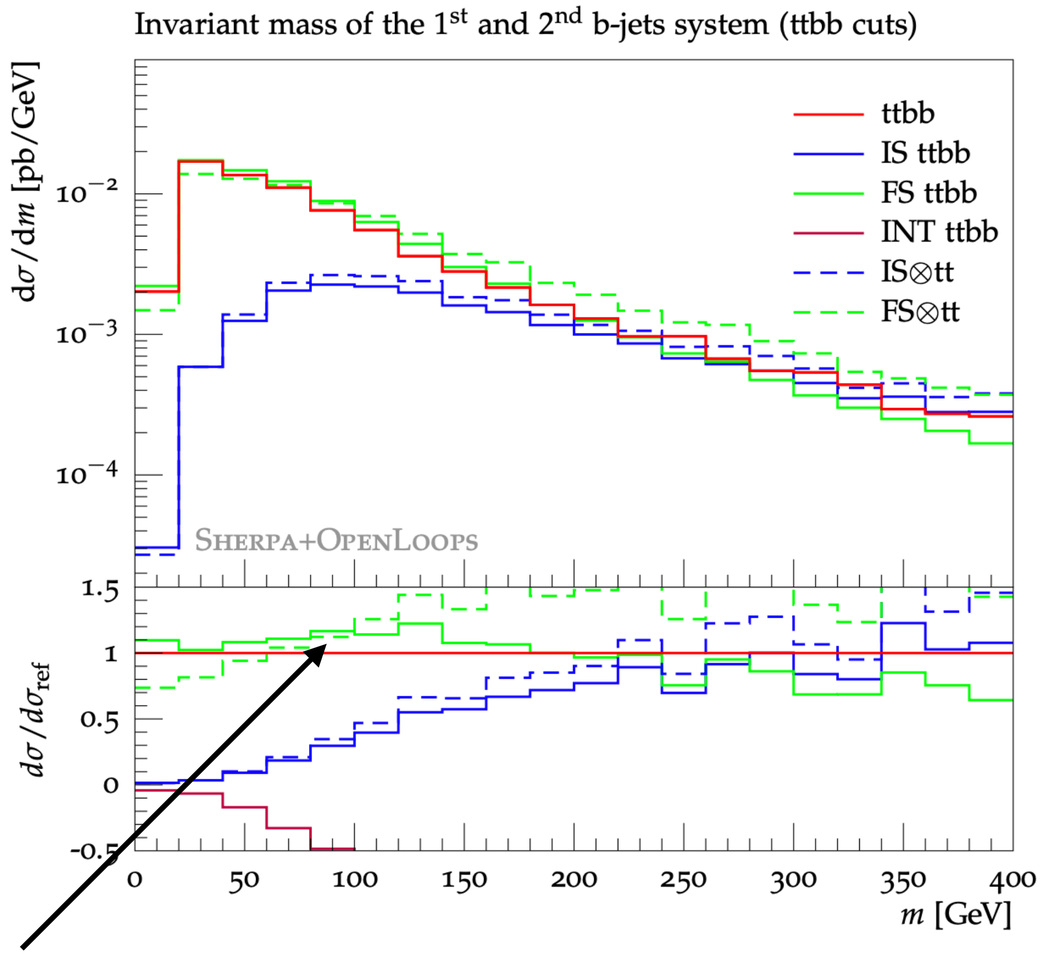
Quite large differences in a region where all PS model should be equal (to the LO Matrix Element!)

Credit: D. Napoletano

FINAL STATE SPLITTINGS

- Processes relevant for precision physics and Higgs physics receive large contributions from topologies with final state g> bb~ splittings.
- tt~bb~ 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?



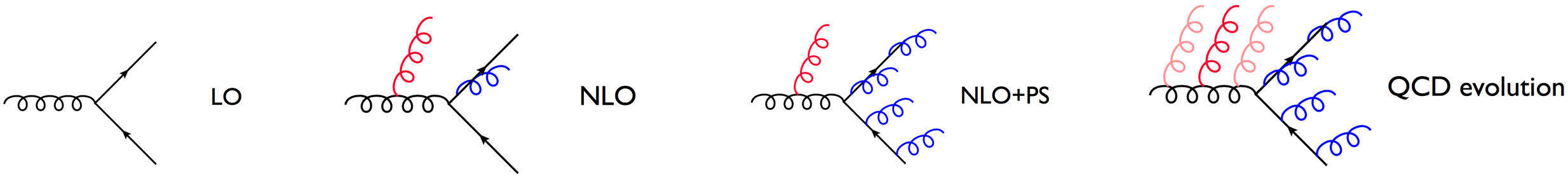


Collinear approximation keeping FS splittings surprisingly close to full ME

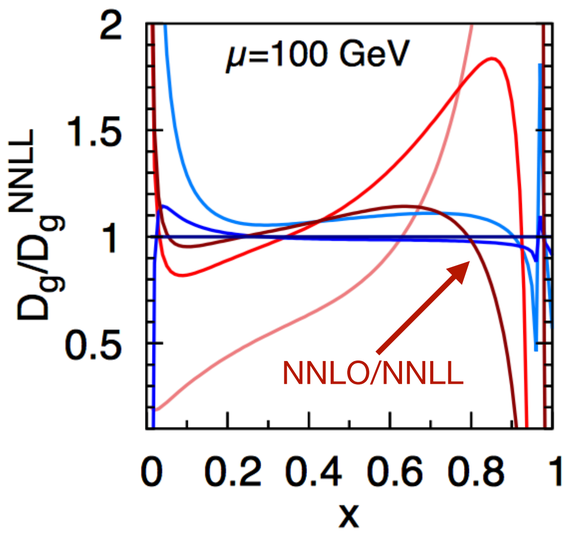
Jezo et al, arXiv:1802.00426

A CLOSER LOOK AT G > BB~ SPLITTINGS

Credit: M. Zaro

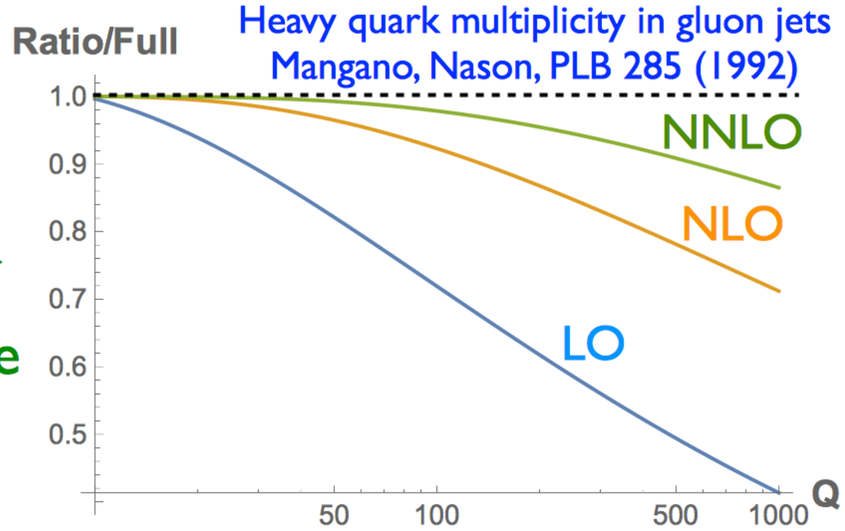


- Extra radiation off parent gluon missing if b-quark generated at ME level, even at NLO+PS. How important is it?
- Importance can be assessed using fragmentation functions approach [Ridolfi, MU, Zaro, arXiv: 1911.01975]



Exclusive

Inclusive



- 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.

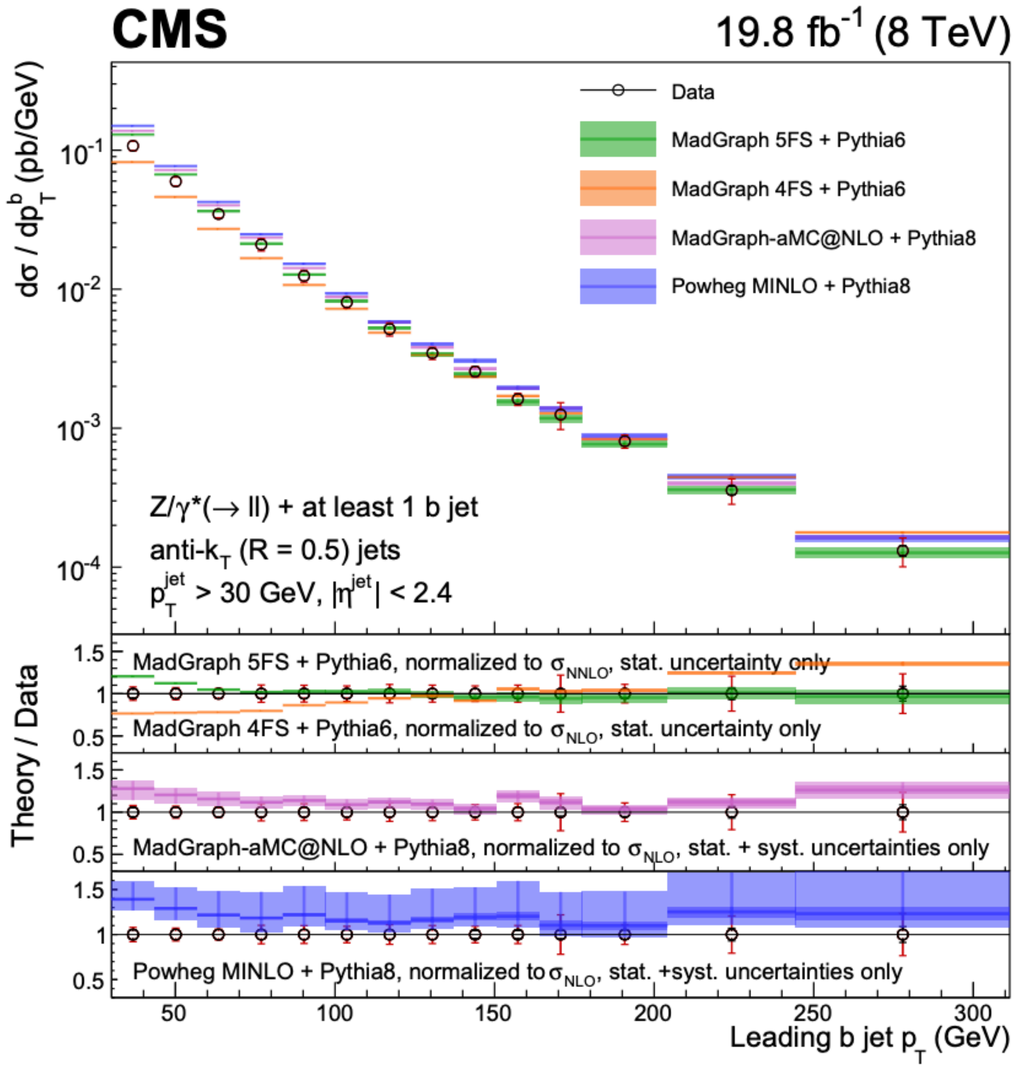
- As far as final states are concerned, need to understand interplay between PS and collinear resummation in final states. FF-based studies highlight possible pathologies in the simulation of final-state $g \to b\bar{b}$ splittings at the ME-level, for exclusive observables (regardless of mb=0 or mb≠0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

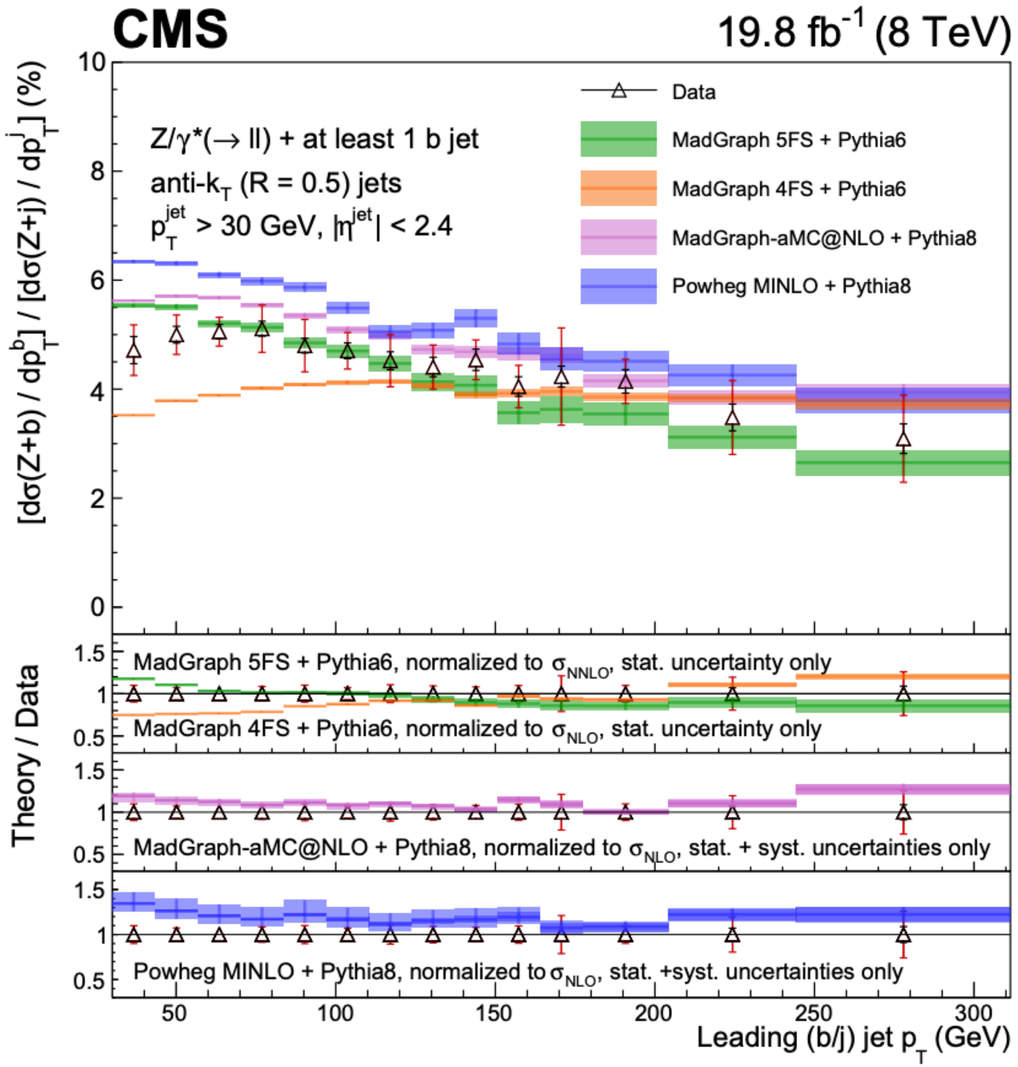
THANK YOU FOR YOUR ATTENTION

EXTRA MATERIAL

Z+B-JET AT 8 TEV

CMS colllab, arXiv:1611.06507





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 α_S and PDFs
- Take the 5FS cross section

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

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

$$f_b^{(5)}(x,\mu^2) = \sum_{i=q,g} \int_x^1 \frac{dy}{y} f_i^{(5)}(y,\mu^2) C_{bi}\left(\frac{x}{y}, \alpha_S^5(\mu^2), L\right)$$

$$\sigma^{(5)} = \iint dx_1 dx_2 \sum_{ij=q,g} f_i^{(5)}(x_1,\mu^2) f_j^{(5)}(x_2,\mu^2) A_{ij}^{(5)}\left(x_1,x_2,L,\alpha_s^{(5)}(\mu^2)\right)$$

with $\quad A_{ij}^{(5)} = C_{bi} \otimes C_{bj} \otimes \hat{\sigma}_{ij}^{(5)}$

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 α_S and PDFs
- Take the 4FS cross section

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

- Both α_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

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

$$f_i^{(5)}(x,\mu^2) = \int_x^1 \frac{dy}{y} \sum_j K_{ij}\left(y, L, \alpha_s^{(4)}(\mu^2)\right) f_j^{(4)}\left(\frac{x}{y}, \mu^2\right)$$

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

THE FONLL METHOD

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

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

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

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

$$\sigma^{(4),(0)} = \iint dx_1 dx_2 \sum_{ij=q,g} f_i^{(5)}(x_1,\mu^2) f_j^{(5)}(x_2,\mu^2) B_{ij}^{(0)}\left(x_1, x_2, \frac{\mu^2}{m_b^2}, \alpha_s^{(5)}(\mu^2)\right)$$

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

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

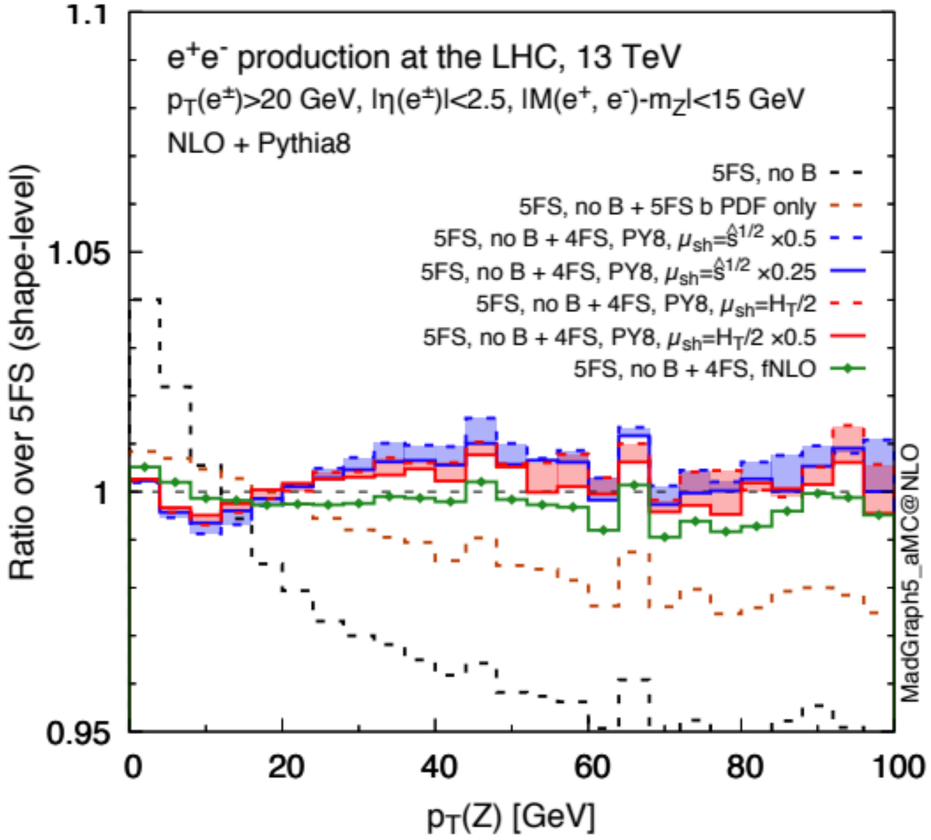
$$A_{ij}^{(5)}\left(x_1, x_2, L, \alpha_s^{(5)}(\mu^2)\right) = \sum_{p=0}^{N} \left(\alpha_s^{(5)}(\mu^2)\right)^p \sum_{k=0}^{\infty} A_{ij}^{(p),(k)}(x_1, x_2) \left(\alpha_s^{(5)}(\mu^2) L\right)^k$$

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

MATCHING 4FS AND 5FS IN FULLY DIFFERENTIAL CALCULATIONS

- 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.



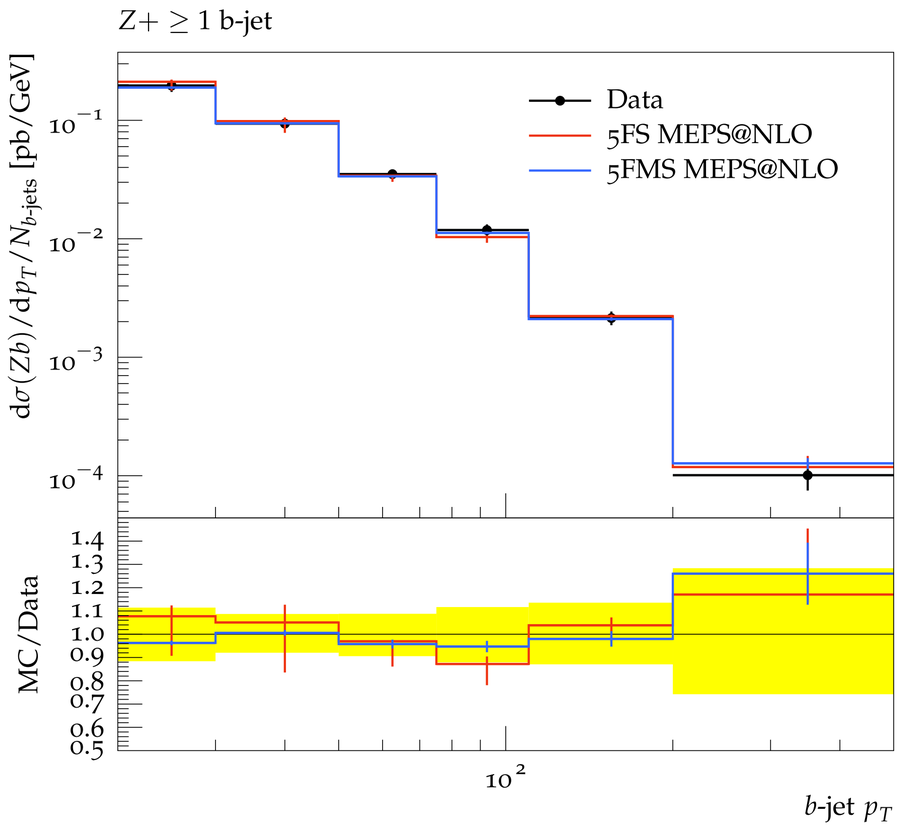
Bagnaschi, Maltoni, Vicini, Zaro, arXiv: 1803.04336

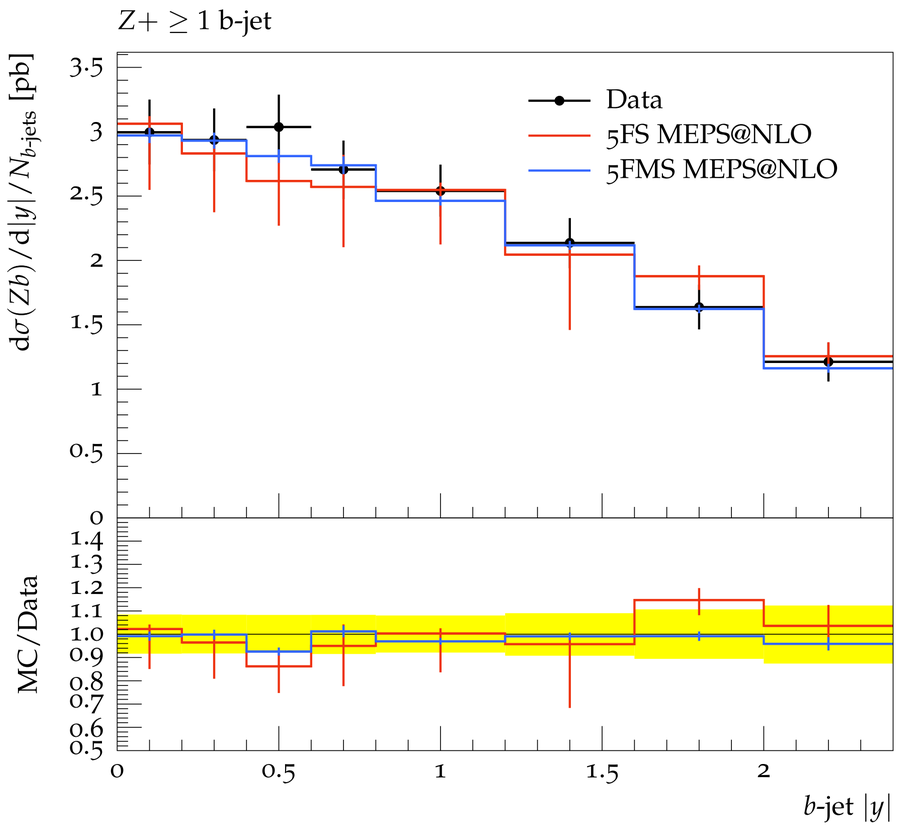
$$d\sigma^{\text{mass}} = d\sigma^{\text{5FS-Bveto}} + d\sigma^{\text{4FS}}$$

- 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

MATCHING 4FS AND 5FS IN FULLY DIFFERENTIAL CALCULATIONS

- **#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.

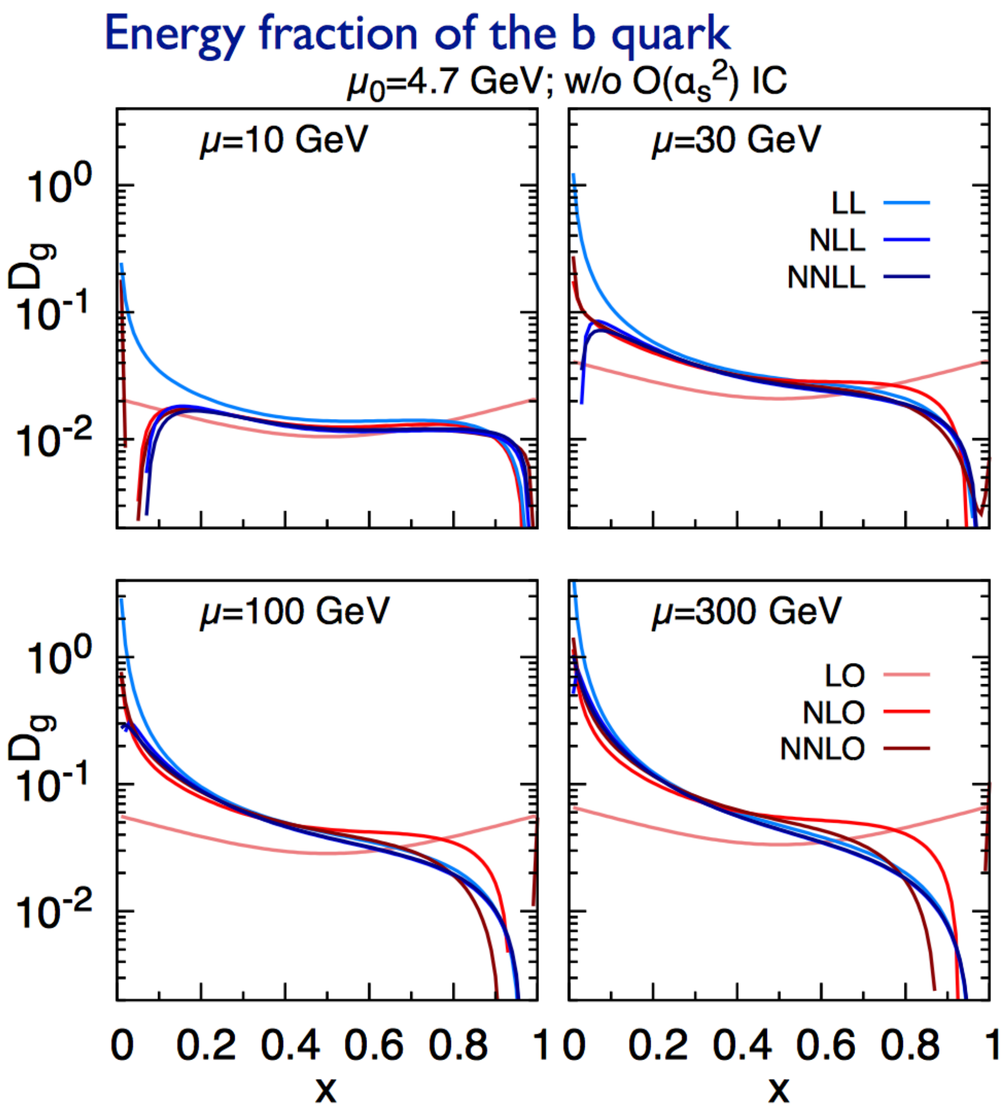




Credit: D. Napoletano

A CLOSER LOOK AT G > BB~ SPLITTINGS

Ridolfi, MU, Zaro, arXiv: 1911.01975



- 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 $t\bar{t}b\bar{b}$+jet @NLO as reference for $t\bar{t}b\bar{b}$
- Dominant effect from radiation off the parent gluon
  - ✦ Not included when b quarks are generated at the ME level
  - ✦ Large effect on *exclusive* observables