Heavy-flavor production with high-precision: NNLO QCD lessons from top production at hadron colliders

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Motivation:
What can the LHC do for EIC?

- ✓ HF production in DIS: historically, DIS has been all about inclusive hadron production
- ✓ State of the art for HF is:
  - ✓ Full mass dependence at NLO — Kretzer, Schienbein (1998)
  - ✓ Asymptotic behavior for small masses at NNLO and beyond

    Buza, Matiounine, Smith, Migneron, van Neerven (1996 -)
    Blumlein et al
  - ✓ Massive calculation for CC DIS at NNLO

    Berger, Gao, Li, Liu, Zhu (2016)
    Gao (2017)
- ✓ Differential hadron description is also important. It gives much more detailed insight into the structure of the final state.
  - ✓ Ex: NuTev: they measured the s-sbar asymmetry thanks to their charm final state tagging
- ✓ Modern MC generators are capable and can produce – maybe not out of the box for all processes – fully differential predictions for HF at NLO in QCD.

Motivation:
Heavy Flavor Production in DIS

- ✓ Historically, the main focus was on *inclusive* HF production (due to low statistics and large systematics).

  - Differential measurements (b- and c-fragmentation, etc) were also performed at HERA

See talk by Achim Geiser

- ✓ However, future machines will demand more and will be able to push in the direction of high-precision physics.

- ✓ How to deal with this challenge?

  - ✓ No need to reinvent the wheel – turn to the LHC, plenty of lessons!

- ✓ The LHC has already dealt with this problem in an environment that is at least as problematic as DIS and has been able to achieve great physics results with high precision.

- ✓ Most of these results translate directly to DIS. I’ll explain this in the following.

(Stable) Top quark production at the LHC

- ✓ Why top?
    - ✓ Definitely not many tops expected at EIC…
- ✓ Will use it as the blueprint for HF production at hadron colliders. In fact, this is precisely how modern HF production developed at the LHC.

(Stable) Top quark production at the LHC

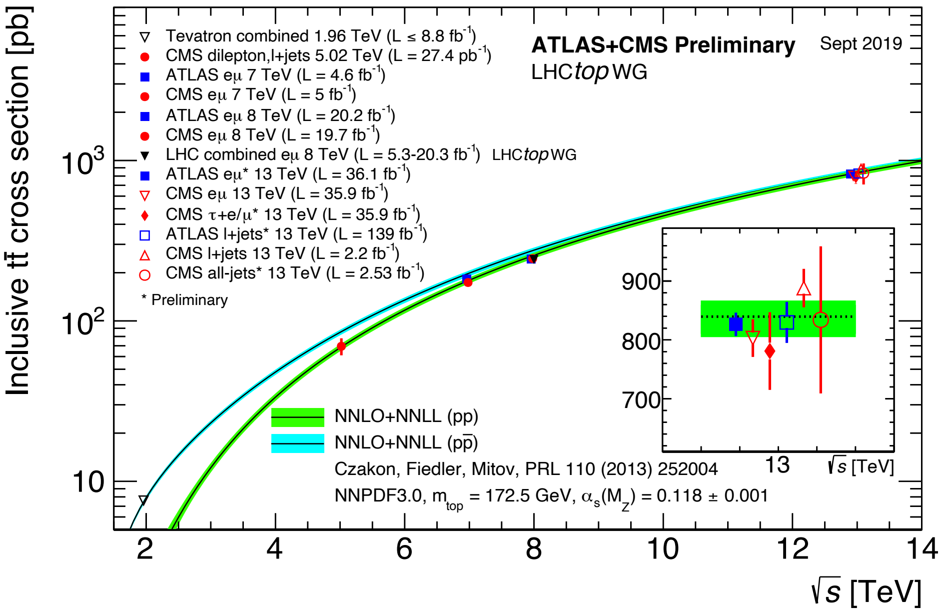
- ✓ Current state-of-the-art for tt_{bar} production is NNLO in QCD + NLO EW
  - ✓ Total cross section known for a long time Czakon, Fiedler, Mitov (2013)
  - ✓ This is the equivalent of inclusive production in DIS. However, there are differences: it is not directly measurable at hadron colliders – fiducial corrections are important
  - ✓ It is not directly measurable experimentally but the effects of fiducial phase space are relatively small and can be modelled easily.
  - ✓ Same result also predicts the total bb_{bar} and cc_{bar} cross-sections in (the 4- and 3-flavor schemes). Fiducial corrections are very large.

- ✓ How well is the total cross-section known?

Quite well. Main uncertainties:

- scales ~ 3%
- pdf (at 68%cl) ~ 2-3%
- alpha$_S$ (parametric) ~ 1.5%
- m$_{top}$ (parametric) ~ 3%

→ All are of similar size!

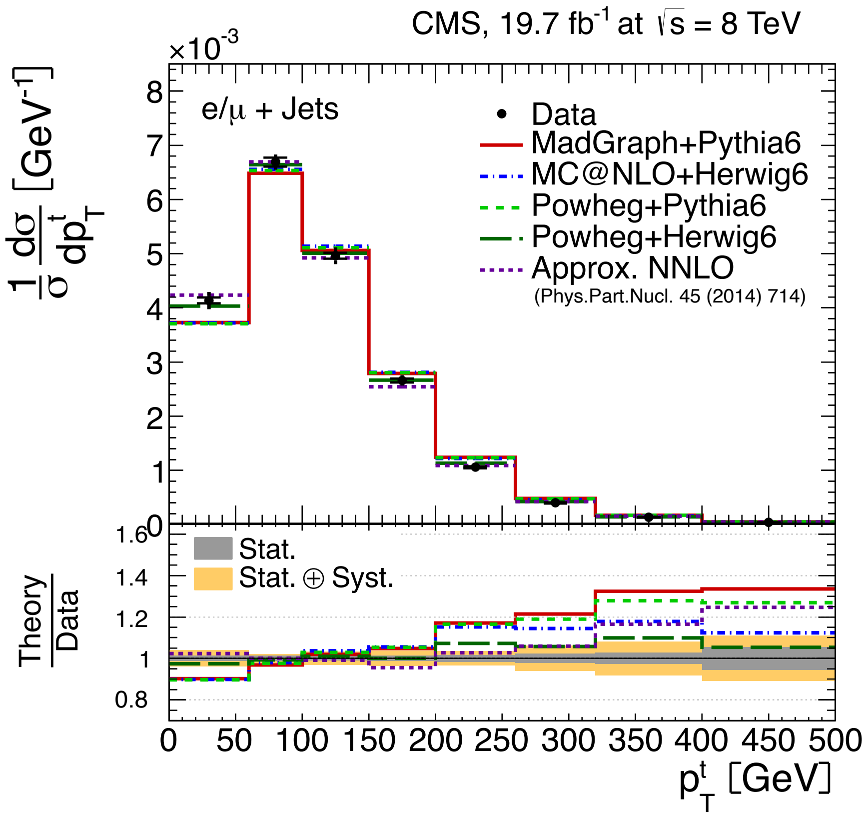


(Stable) Differential top quark production at the LHC

- ✓ Kinematics matters, too!

- ✓ A famous issue: the top P_T problem

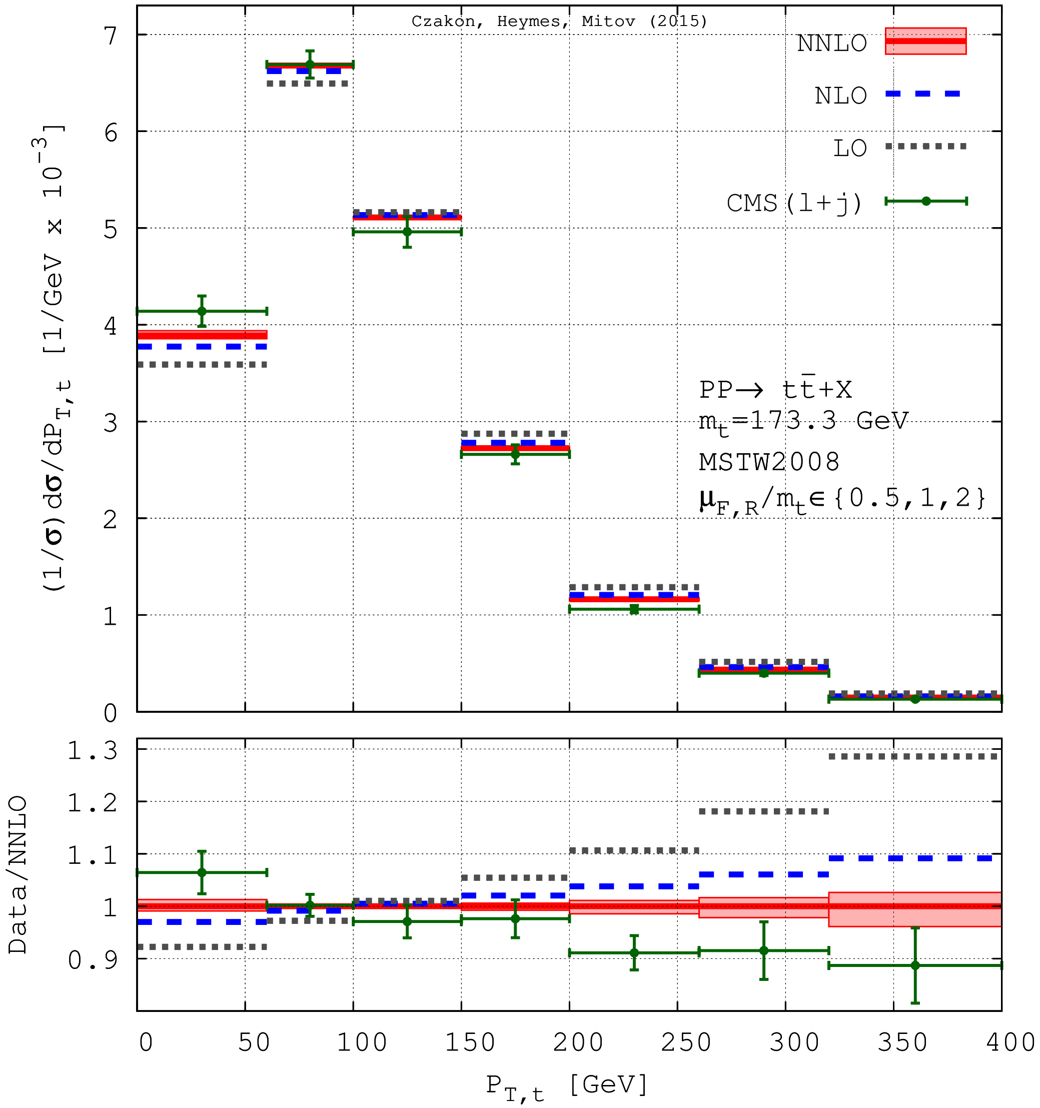
  - NLO MC generators cannot describe the top P_T spectrum well.
  - Description of tails is very important in top physics.
  - The top P_T problem’s impact extends beyond top physics (P_T rescaling of generators)



(Stable) Differential top quark production at the LHC

- ✓ Understanding the top quark P_T spectrum:

Czakon, Heymes, Mitov (2015)



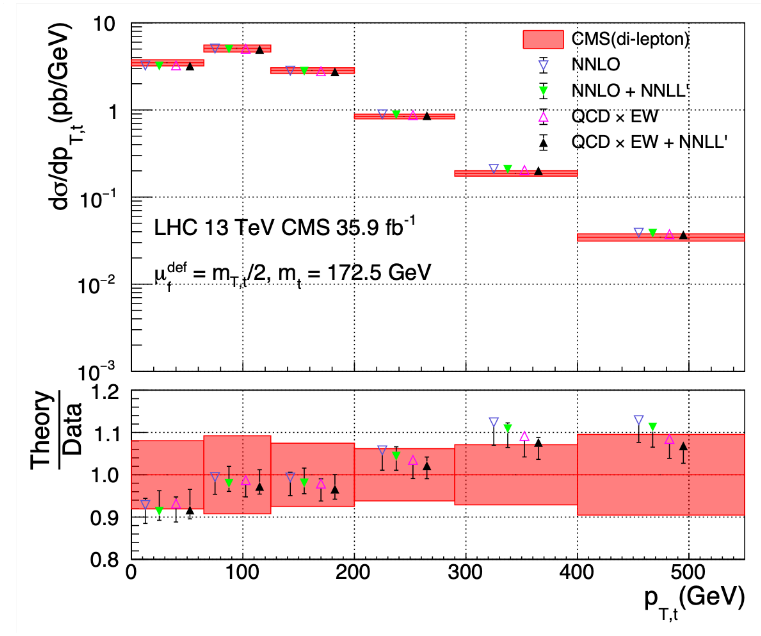
- ✓ NNLO QCD corrections systematically improve the agreement with CMS data.
- ✓ Agreement with ATLAS (not shown) even better.
- ✓ NNLO does what one normally expects:
  - Convergence
  - Decrease of scale error
  - Pdf error not included

(Stable) Differential top quark production at the LHC

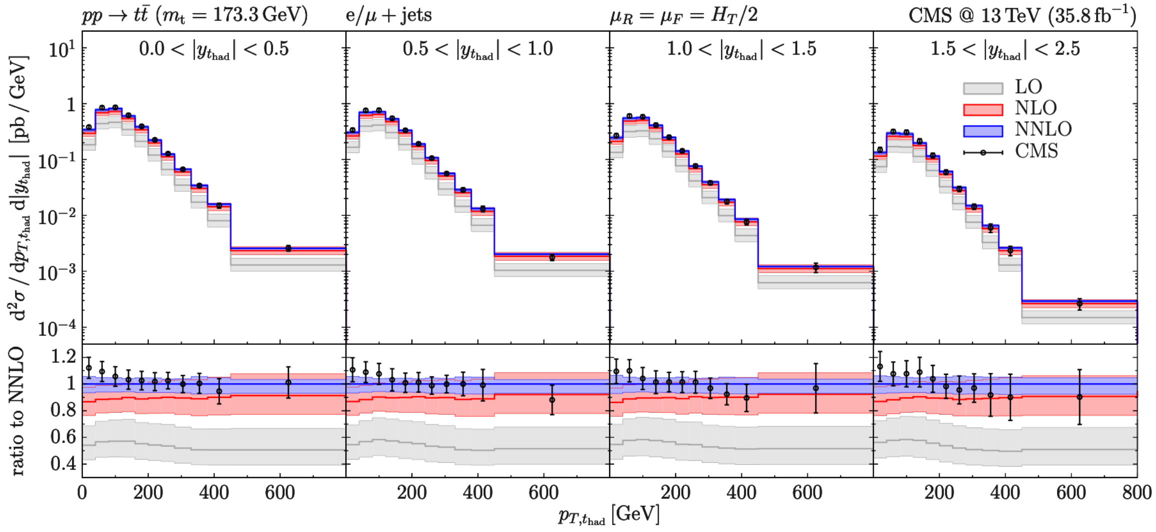
✓ The theoretical description of top production is much more advanced than that:

- Multidimensional distributions are computed with flexible Monte Carlo programs
- Fixed order QCD combined with EW and with soft/collinear resummation
  - Some examples:

Czakon, Ferroglia, Mitov, Pagani, Papanastasiou, Pecjak, Scott, Tsinikos, Wang, Yangl, Zaro (2020)



Catani, Devoto, Grazzini, Kallweit, Mazzitelli (2019)

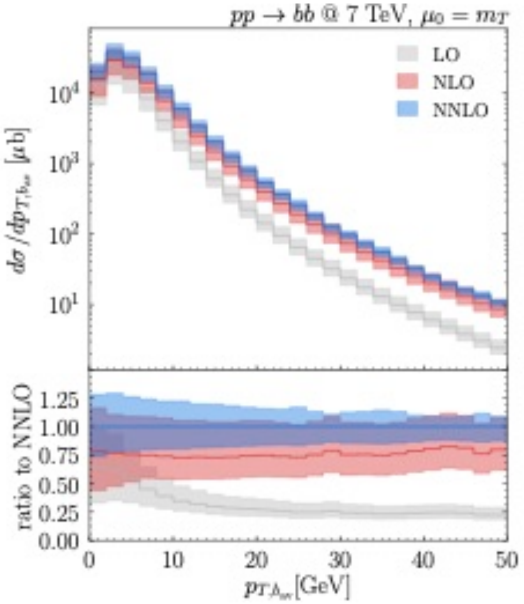


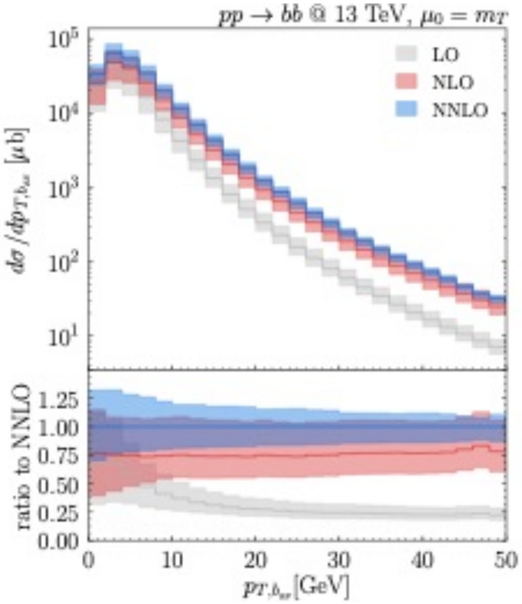
- Many other observables and studies performed specific to top quarks
- Finally, decays of tops are also included at NNLO (although this is specific to the top quark and not of direct interest to b- and c- production)

Differential bottom quark production at the LHC

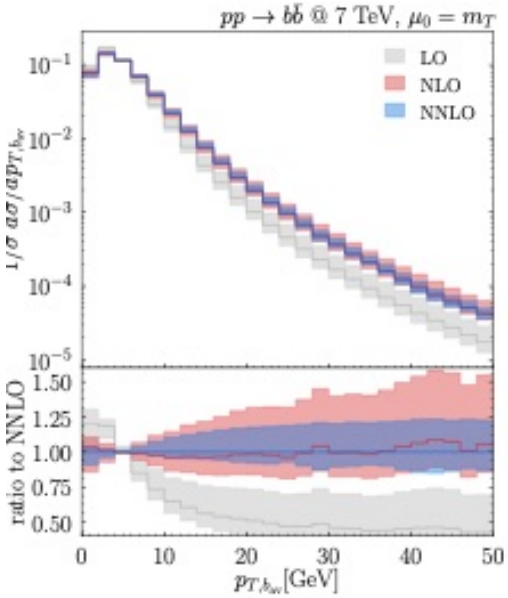
✓ The calculation of $t\bar{t}_{\mathrm{bar}}$ production can be directly extended (in 4-flavor scheme) to bb_{bar}:

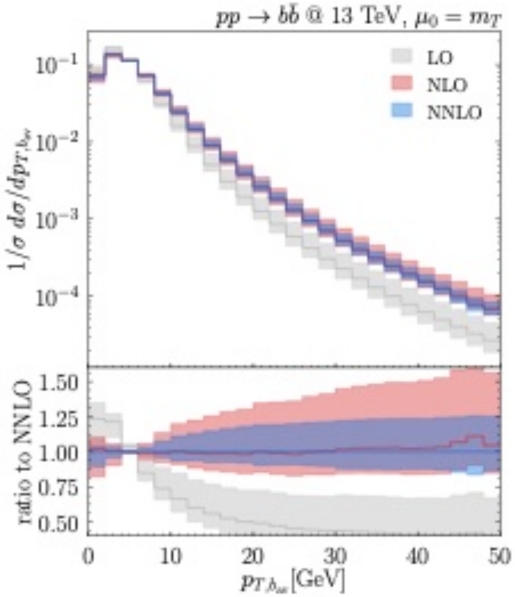
Catani, Devoto, Grazzini, Kallweit, Mazzitelli (2020)





- Important step towards understanding HF production at hadron colliders
- Scale uncertainty at NNLO does not appear to be as reduced as for top





From quarks to observables

- ✓ Both calculations shown: tt_{bar} and bb_{bar} are in some sense incomplete
  - Predictions are at the level of bare quarks. These are not observable
- ✓ This is OK for top quarks because they never hadronize; one needs to account for their weak decay (at quark level) to W+b. The top quark is basically on-shell when decays and this description works very well for top. tt_{bar} production + decay fully known through NNLO in QCD

Behring, Czakon, Mitov, Papanastasiou, Poncelet (2019-)

- ✓ However: for HF (b- and c-) production one needs predictions for either b/c jets or B/D mesons.
  - This is one essential difference between top and b-/c-production.
- ✓ Luckily, there is a lot of progress on precision (NNLO) predictions for HF jets and mesons at the LHC.
  - Top quark production physics is again among the main drivers: top decays to b-quarks ~100% of the time so adequate description of b-final states is needed:
    - ➢ B-mesons (discussed next)
    - ➢ B-jets
  - Progress in other LHC processes, too

See also talks by:

- Achim Geiser
- Ingo Schienbein

B-meson production in top quark decays and other processes

What is b-fragmentation?

- ✓ What is b-fragmentation?
  - The non-perturbative process of formation of B-flavored hadrons (most of the time mesons) from QCD partons.

- ✓ It is process independent as long as QCD factorization applies, i.e. there is a hard scale. Examples:
  - For open B production: P_T of the B
  - B production in top decay: m_{top}
  - B production at LEP (Z-pole): m_Z

- ✓ How do we describe b-fragmentation? Two approaches:
  - Fragmentation as used in MC event generators: uses a model that is tuned to data which 'decides' how at low scales the partons resulting from the shower are organized into hadrons. This is the case for heavy as well as light hadrons.

  - Analytic approach (used in this work): the transition b → B at low energy is described in terms of an explicit non-perturbative function "Fragmentation function". This function is the exact equivalent of pdfs in the description of collider processes. It is also:
    - ➢ Non-perturbative
    - ➢ Process independent
    - ➢ Extracted from experiment (typically e^+e^-; will discuss LHC later on)

What is b-fragmentation?

✓ The essence of the non-perturbative aspect was understood long ago (late 1970's)

Kartvelishvili, Likhoded, Petrov (1978)
Peterson, Schlatter, Schmitt, Zerwas (1983
…

✓ The heavy-flavored hadron B is produced at a scale $\mu \sim m_B$ by the non-perturbative fragmentation of the b-quark $D_{b\text{->}B}(z)$.

- Here z is the fraction of b's momentum carried by B: $p_B = z\, p_b$.

✓ The description of b-quark production down to scales $\mu \sim m_B$ can be described in perturbation theory. The modern framework was laid down 30 years ago as is known as the ***Perturbative Fragmentation Function*** approach

Mele, Nason (1991)

✓ The idea is based on factorization and properly accounts for the separation of process-independent and process-dependent corrections as well as short- from long-distance physics.

PFF formalism

✓ In the Perturbative Fragmentation Function approach an observable for a meson B can schematically be written as:

Mele, Nason (1991)

$$O_B\left(\frac{Q^2}{m^2},\alpha_S\right) = O_b\left(\frac{Q^2}{m^2},\alpha_S\right) \otimes D^{\mathrm{np}}_{b\to B}(z)$$

Non-perturbative.
Fit from data

- m: mass of the b-quark
- Q >> m: a hard scale that depends on the process

$$O_b\left(\frac{Q^2}{m^2},\alpha_S\right) = \sum_{i,j=\text{all massless partons}} C_i\left(\frac{Q^2}{\mu_F^2},\alpha_S\right) \otimes E_{i\to j}\left(\frac{\mu_F^2}{\mu_0^2},\alpha_S\right) \otimes D_{i\to b}\left(\frac{\mu_0^2}{m^2},\alpha_S\right)$$

Perturbative cross-section for producing any parton ‘i’

DGLAP evolution: for a parton ‘i’ produced at a high scale μ_F to evolve via radiation to a parton ‘j’ at to low scale μ_0~m

PFF: perturbative splitting of the parton ‘j’ into a heavy quark b. This happens at a low (perturbative) scale μ_0~m

PFF formalism: main features

- ✓ The formalism applies to the small-mass limit m<<Q.
  - ✓ Power corrections $(m/Q)^n$ are neglected
  - ✓ All logarithmic terms $\mathrm{Log}^n(m/Q)$ are included correctly, as well as mass independent terms
  - ✓ At large Q (example: large P_T) the formalism correctly resums all collinear logs
  - ✓ It is not applicable at small Q (i.e. small P_T) where missing corrections m/Q~1 become sizable
    - ➢ For this regime one needs to supplement the PFF predictions with dedicated fixed order calculations that contain all mass dependence (but no resummation).
  - ✓ This matching is the basis for the so called FONLL approach at NLO

Cacciari, Greco, Nason, Oleari,… (1990's)

Heavy flavor production: past work

- ✓ Many FONLL applications exist:
  - e^+e^-
  - Hadron colliders (remember the b-saga at the Tevatron?)
  - DIS
  - Top decay
- Works on heavy flavor production by many groups

Cacciari, Mangano, Nason (1990's -)
Binnewies, Kniehl, Kramer (1997 -)
Kniehl, Kramer, Schienbein, Spiesberger (2004 -)
Kniehl, Kramer, Moosavi Nejad (2012)

- A lot of work in the context of Nuclear Collisions:

- The only existing NNLO application is in QED: electron spectrum in muon decay

Anastasiou, Melnikov, Petriello (2005)

PFF formalism: "new" developments (i.e. beyond NLO)

✓ How to go beyond NLO?

✓ A number of ingredients are needed at NNLO (all already known):

- PFF @ NNLO

  Melnikov, Mitov (2004)

- Time-like NNLO splitting functions

  Mitov, Moch, Vogt (2006)
  Almasy, Moch, Vogt (2012)

- e^+e^- coefficient functions (for fits of the non-perturbative FF)

  Rijken, van Neerven (1996)
  Mitov, Moch (2006)

- Fits of FF at NNLO (no applications yet!)

  Fickinger, Fleming, Kim, Mereghetti (2016)
  Salajegheh, Nejad, Khanpour, Kniehl, Soleymaninia (2019)

✓ The only missing piece [by far the most complicated one!] for a complete NNLO application are the coefficient functions at NNLO

- In this talk: First NNLO application: b-production in tt_{bar} production at the LHC

NNLO corrections to B production in $t t_{bar}$ production

- ✓ $t t_{bar}$ is the natural first application in view of top mass applications (mainly using $m_{B\ell}$)

  Kharchilava (1999)
  ATLAS CERN-THESIS-2020-105 (2020)

- ✓ Past work at NLO
  - Top decay

    Cacciari, Corcella, Mitov (2001)
    Corcella, Drollinger (2005)
    Corcella, Mescia (2009)
    Moosavi Nejad, Soleymaninia, Khorramian, Maktoubian, Balali, Abbaspour (2012 -)
    Kniehl, Kramer, Moosavi Nejad (2012)

  - Top production and decay in the NWA

    Biswas, Melnikov, Schulze (2010)

- ✓ In this work we:
  1. Produce NNLO fragmentation functions using previous NP FF extractions

     Cacciari, Nason, Oleari (2005)
     Fickinger, Fleming, Kim, Mereghetti (2016)

  2. Calculate NNLO corrections to massless parton production in $t t_{bar}$ production and decay
     - ➢ Use the STRIPPER framework Czakon (2010) with additional subtraction in final state
     - ➢ Upon convoluting (2.) with our FF (1.) we have a fully differential MC calculation for one B-hadron + anything else. Extension to other processes is straightforward.

A note on the fragmentation function

✓ As a basis for our study we take the fragmentation function from

Fickinger, Fleming, Kim, Mereghetti (2016)

- In principle it is ideal for us since it is:

    1. Extracted at NNLO (from e+e-)
    2. Soft gluon resummation (using SCET) at NNLL
    3. LHAPDF grids available from authors upon request

- In practice there are some differences which do not allow us to reuse them directly:

    1. Only b-initiated contribution included (specifically, the Non-Singlet b-b_{bar})
    2. DGLAP evolution is affected by soft-gluon resummation/matching. Does not match the factorization scale dependence of our partonic calculation.

✓ Our resolution: some ambiguity remains; we build two “variants” of it and compare them

1. Construct FF set with “correct” DGLAP evolution: take their b->B FF, evaluate it at low scale (this maintains soft-gluon resummation for PFF), then evolve it upwards ourselves with standard DGLAP. Include all other partonic contributions i -> B.

2. Reuse their resummed NS component at all scales and supplement it with the other partonic components evolved with ”correct” DGLAP evolution.

A note on the fragmentation function

✓ We have also produced LHAPDF grids based on the NLO NP FF from

Cacciari, Nason, Oleari (2005)

1. Implemented our own NLL soft-gluon resummation on top
2. Added NNLO DGLAP
3. Added all partonic channels

   - In principle the perturbative part is equivalent to the one constructed recently in

Ridolfi, Ubiali, Zaro (2019)

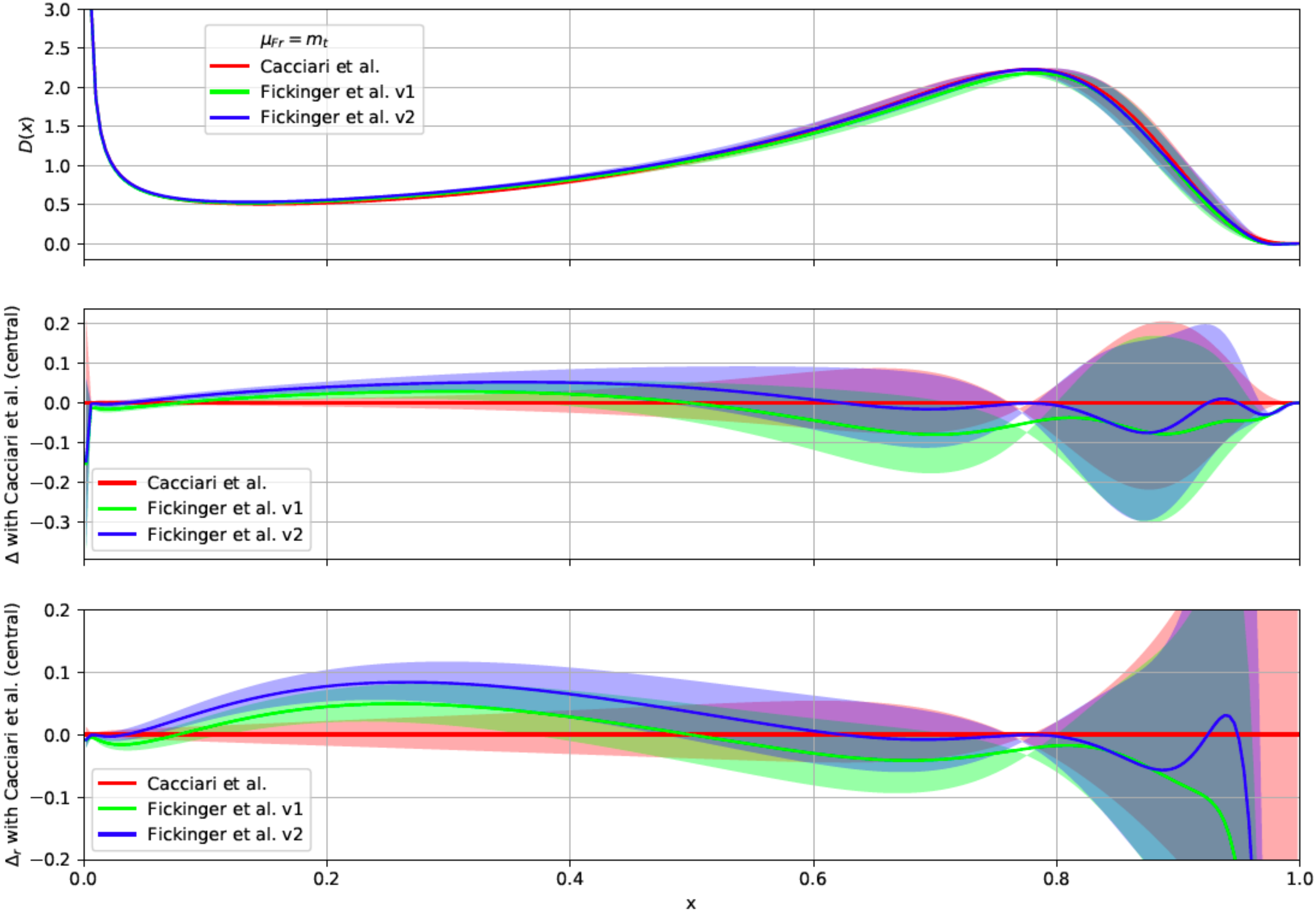
✓ We have not utilized the NNLO Non-Perturbative FF extracted in

Salajegheh, Nejad, Khanpour, Kniehl, Soleymaninia (2019)

- it does not utilize the Perturbative Fragmentation Function framework and is therefore not directly compatible with our calculation

Comparison of the fragmentation functions

✓ NNLO comparison of our 3 fragmentation functions (bands: FF uncertainty)



A note on the fragmentation function

✓ Few comments on the extracted FF's:

- Our predictions are for B+B_{bar}
- Besides the differences in their definitions, the 3 FF's are compatible
- The low-x region is not very relevant, especially here, since we do not include power corrections in m_b
- The end-result strongly depends on its consistent implementation. In particular soft-gluon resummation at large x:
  - ➢ An application of a FF should match its extraction!

- Heavy-flavor FF's is a great place for practicing all the bells and whistles of soft-gluon resummation.
- An old issue: the available LEP data used for b-FF's is not separated into different hadron species, i.e. the predictions are for averaged B-production.
  - ➢ Can we use the LHC data to start producing new fits on b-fragmentation? More later.

B-production in top decay at NNLO

- ✓ First application: B-production in the decay of unpolarized top quark

- ✓ Some defaults:

  - $\mu_{Fr} = m_t$
  - $\alpha_S(m_Z)=0.118$
  - Scale uncertainty: standard 7-point variation
  - m_t=172.5 GeV

  - For applications in top-pair production we will use:

  - $\mu_F = \mu_R = m_t/2$
  - NNPDF3.1 pdf set
  - P_T and rapidity cut on the B
  - B mesons inside b-jets:

    - ○ all jets are defined as light flavorless jets <u>(Important!)</u>

      - We plot the distribution of the jet in which the B is found.

      - This makes sense since in the perturbative calculation b-quark (and b_{bar}) enter on equal footing with all other partons.

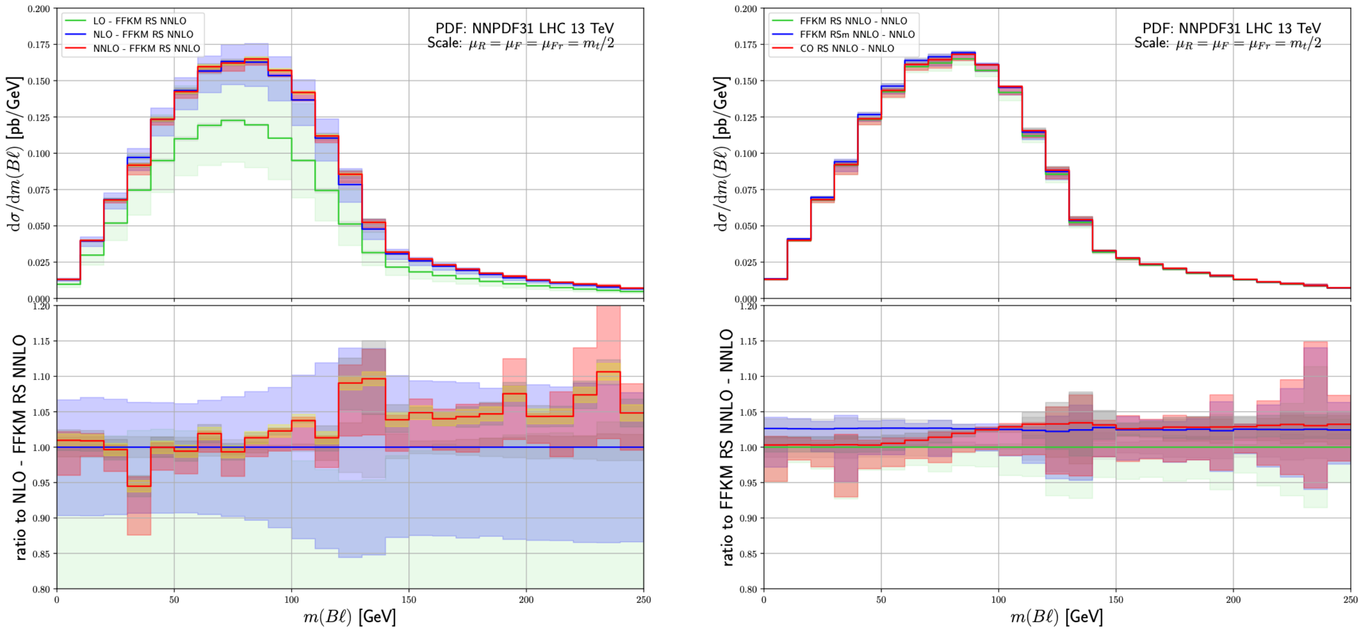
B-production in $t\bar{t}_{bar}$ + decay at NNLO

- ✓ B-μ invariant mass (observable of main interest; extract m_{top} etc)

Czakon, Generet, Mitov, Poncelet; to appear

NNLO variations:

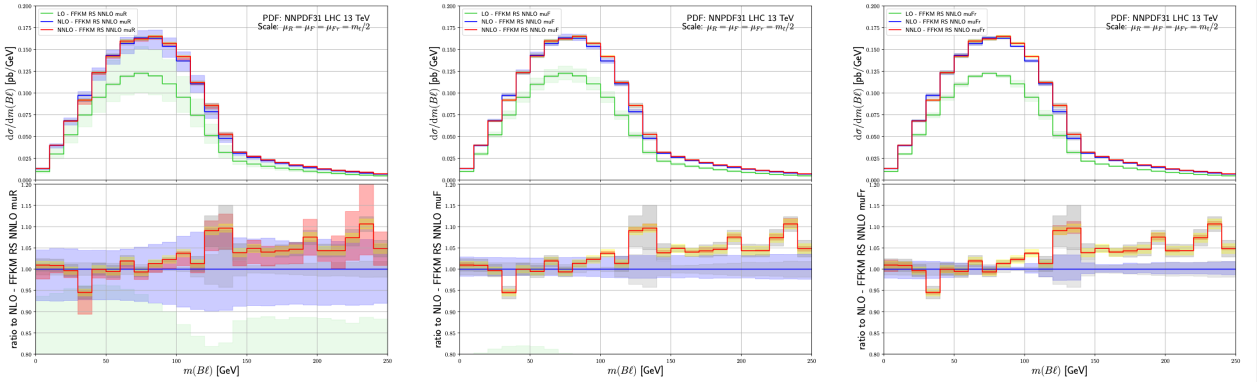
PDF
Scale
FF



Compare 3 NNLO FF:

PRELIMINARY

Variation of 1 scale at a time:



μ_R

μ_F

μ_{Fr}

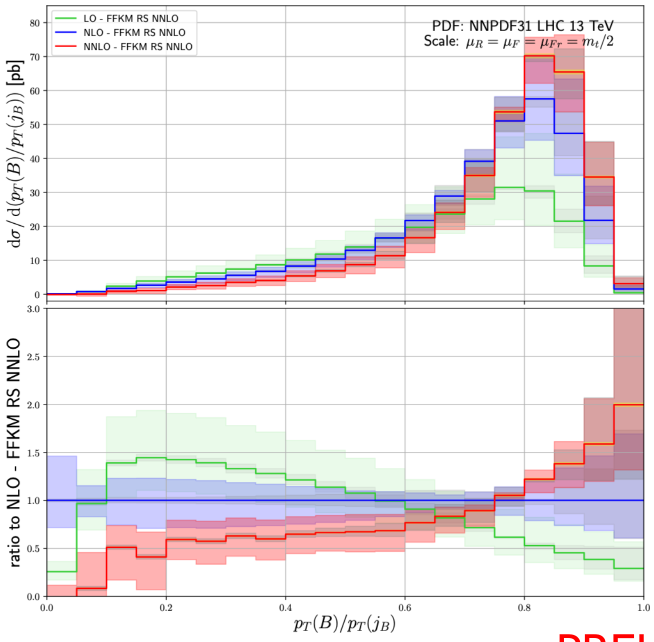
B-production in tt_{bar} + decay at NNLO

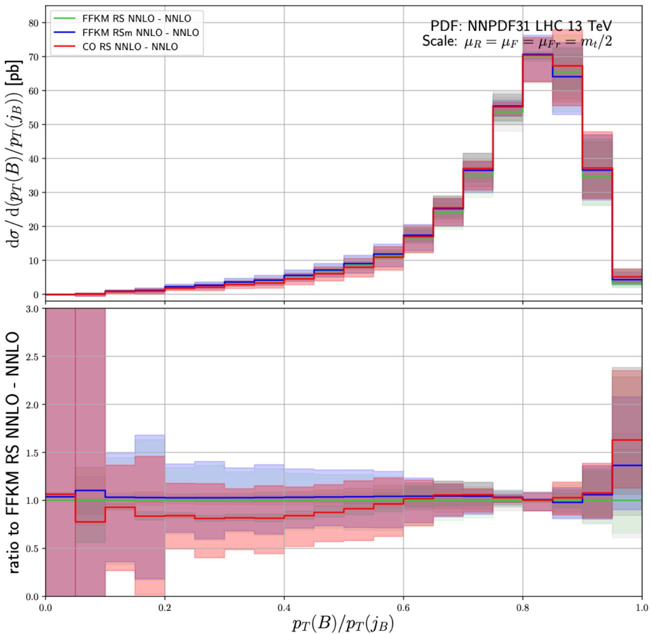
- ✓ Extraction of non-pert B-fragmentation from LEP has its limitations. Use the LHC?
- ✓ Meson-in-jet observable:

Czakon, Generet, Mitov, Poncelet; to appear

NNLO variations:

PDF
Scale
FF





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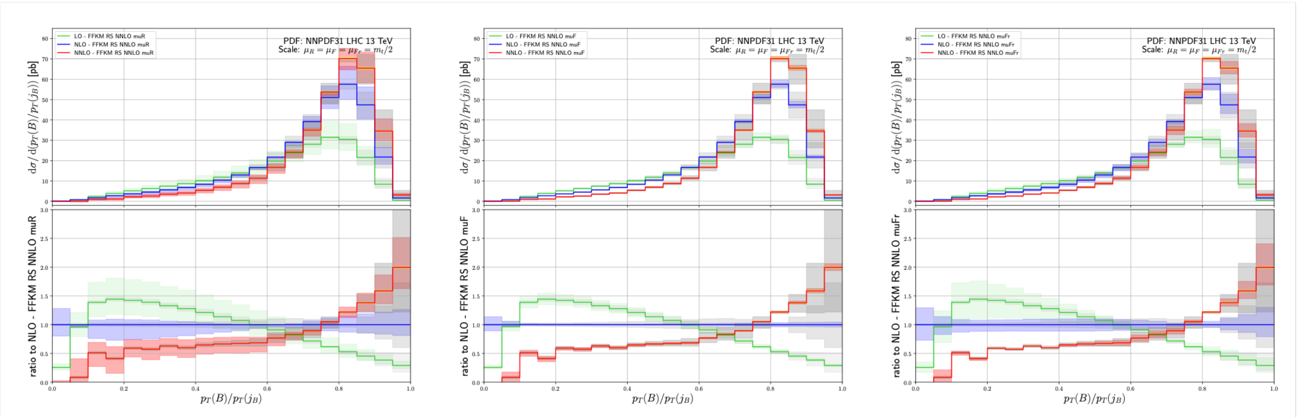

μ_R

μ_F

μ_{Fr}

Flavored jets (b- and c-) at NNLO

Flavored jets

- ✓ HF jets are present in all colliders
  - Nuclear Collisions — Vitev et al (2013 -); Senzel, Uphoff, Xu, Greiner (2016)
  - DIS, LEP, LHC

- ✓ In the following I'll focus on hadron colliders and on NNLO precision. The leads to a new feature:

  - ➢ As was pointed out long ago, flavor-tagging of jets breaks the IR safety of standard flavorless jet algorithms — Banfi, Salam, Zanderighi (2006)

- ✓ A decent theory activity on this; practically no exp measurements have used this

- ✓ An explosion of recent theory developments that are finally face this problem head-on:

  - Higgs decay to bb$_{bar}$ — Gauld, Gehrmann-De Ridder, Glover, Huss, Majer (2019)
  - Z+b — Gauld, Gehrmann-De Ridder, Glover, Huss, Majer (2020)
  - W+c — Czakon, Mitov, Pellen, Poncelet (2020)
  - tt (t→ b+W) — Czakon, Mitov, Poncelet (2020)

- ✓ In each case above the treatment is somewhat different. Numeric differences between algorithms are not small. Many developments are to be expected here soon…

Conclusions

- ✓ There has been tremendous progress in HF production at hadron colliders:
    - ✓ Top quark production is firmly at NNLO in QCD
    - ✓ Bottom and charm were until recently “neglected” but they also start to catch up:
        - ✓ New NNLO results have just appeared for both direct and associated production

- ✓ Still, many things need to be done:
        - Flavored jets at NNLO needs to develop
        - Production of identified HF hadrons at NNLO is only now beginning
    - ✓ However, I have no doubt, these will see tremendous progress in the very near future
- ✓ How can LHC help EIC?
    - ✓ Direct translation of applications: for example, the most advanced NNLO HF calculation at CC DIS is a (simplified) version of single top production at the LHC…
    - ✓ One important aspect not covered here is the interplay between pp methods and Nuclear Collisions. HF is a major probe and it is mandatory to explore synergies between the two