Precision calculations for heavy-quark production

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Why are heavy quarks interesting?

- Sensitive to physics covering a broad range of energy scales
  - highest energy scales: tt, ttH, ttW, ttZ, tttt
  - to small scales: bottom + charm
- Unique opportunity to test QCD and the EW/Higgs sector together:
  - Electroweak couplings to fermions
  - Yukawa coupling vs. mass parameters
- Probes of QCD
  - Strong coupling constant
  - PDFs
  - Hadronisation/Fragmentation
  - Jet substructure → jet flavour, dead-cone effects, ...

Heavy-quarks are essential tools
To understand the SM

But: precision theory input needed!

Outline

- Top-quark pair production
- Associated top-quark pair production tt+W/Z/H
- V+heavy flavour (Z/W + charm/bottom)
- Open-bottom

Top-quark pair production

Top-quark pair cross sections at the LHC

NNLO (+NNLL) (+NLO EW)

[Czakon, Fiedler, Mitov '13; Czakon, Heymes, Mitov '16 '17; Czakon, Heymes, Mitov, Pagani, Tsinikos '17; Czakon, Ferroglia, Heymes, Mitov, Pecjak, Scott, Wang, Yang '18; Catani, Devoto, Grazzini, Kallweit, Mazzitelli '19 '20; Kidonakis, Guzzi, Tonero '23]

Best predictions (pp@13 TeV): NNLO QCD: ~5-6%
aN3LO QCD+NLOEW : ~3%

(Estimates of uncertainties from missing higher orders from scale variations)

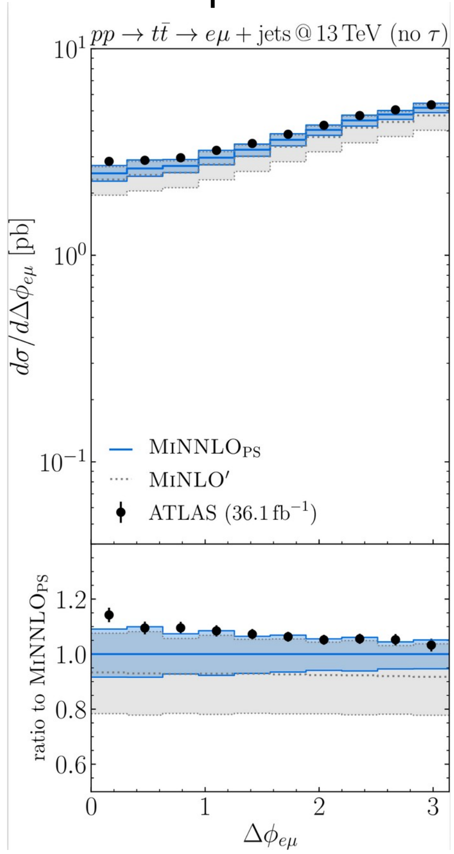
Bringing NNLO QCD to the fiducial phase space

NNLO Prod × Decay
[Behring, Czakon, Mitov, Papanastasiou, Poncelet'19 Czakon, Mitov, Poncelet '21]

NNLO Prod × LO Decay ⊕ PS
[Mazzitelli, Monni, Nason, Re, Wiesemann, Zanderighi '20 '21]

NNLO Prod × LO Decay ⊕ PS

Leptonic



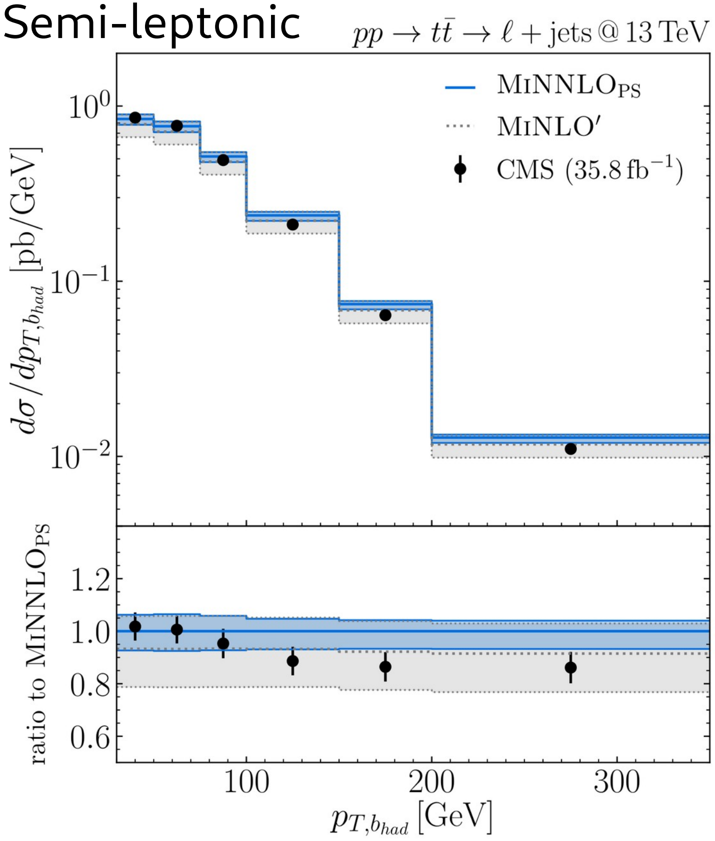
MiNNLOPS
NNLO QCD + PS matched
(here Pythia)

→ comparisons at the fiducial cross section level

→ avoiding unfolding

[Mazzitelli, Monni, Nason, Re, Wiesemann, Zanderighi '20 '21]

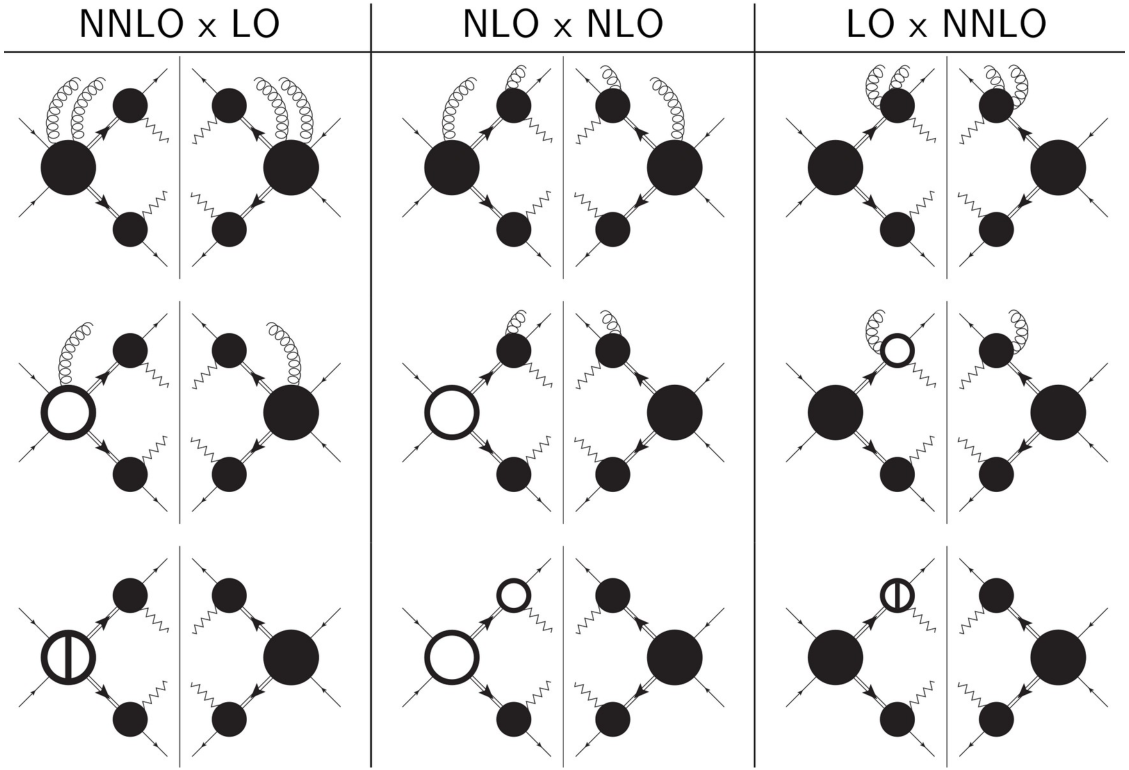
Semi-leptonic



NNLO QCD@NWA in ttbar for leptonic final states

Second-order corrections to production and decay
(all factorizable contributions)

[Behring, Czakon, Mitov, Papanastasiou, Poncelet'19
Czakon, Mitov, Poncelet '21]

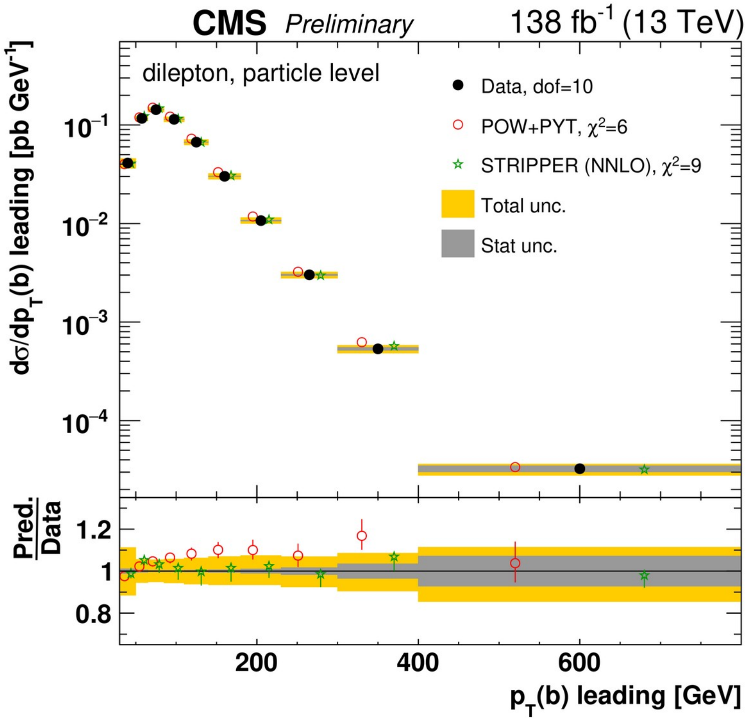


Fiducial phase space predictions in NWA@NNLO

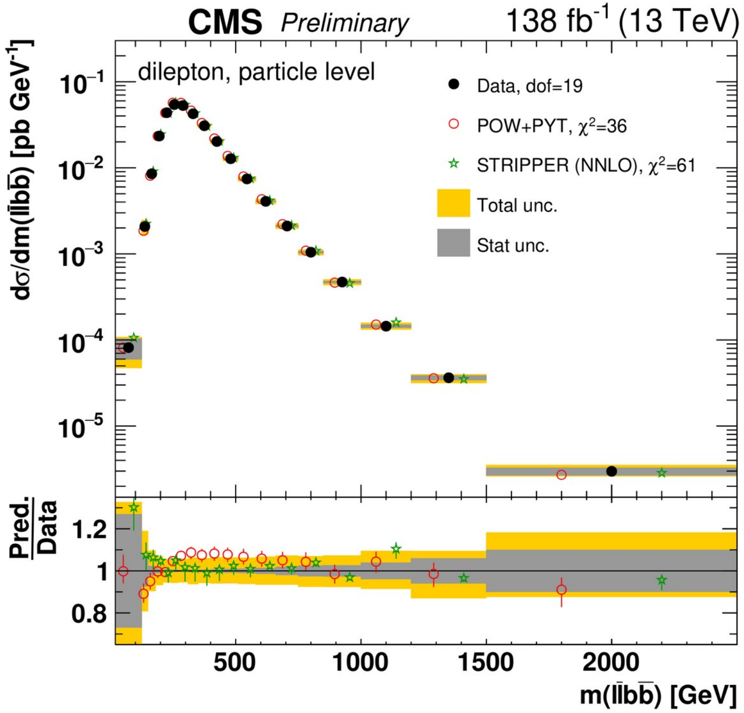
[CMS-PAS-TOP-20-006]

- Good normalization
- Good shape → looks sometimes even better then POW+PYT

Leading b-jet transverse momentum

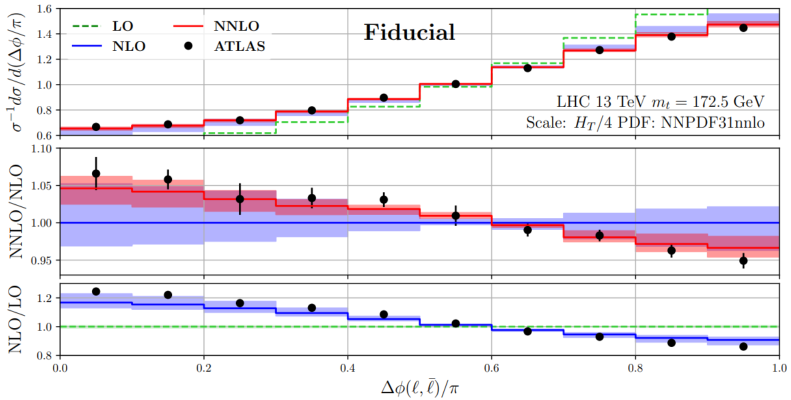


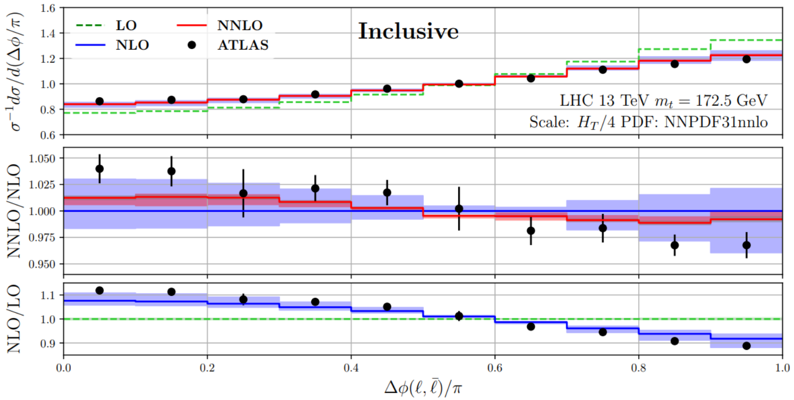
Invariant mass of lepton-pair + b-jet pair



Spin-correlations

Azimuthal correlations for leptons





[Behring, Czakon, Mitov, Papanastasiou, Poncelet'19
Czakon, Mitov, Poncelet '21]

Spin-density-matrix

$$\frac{1}{\sigma}\frac{d\sigma}{d\cos\theta_1^i \, d\cos\theta_2^j} = \frac{1}{4}\left(1 + B_1^i \cos\theta_1^i + B_2^j \cos\theta_2^j - C_{ij}\cos\theta_1^i \cos\theta_2^j\right)$$

Coefficient	LO ($\times 10^3$)	NLO ($\times 10^3$)	NNLO ($\times 10^3$)	CMS ($\times 10^3$)
B_1^k	1^{+0}_{-0} [sc] $\pm$ 1 [mc]	1^{+0}_{-1} [sc] $\pm$ 2 [mc]	-1^{+0}_{-1} [sc] $\pm$ 4 [mc]	5 ± 23
B_1^r	0^{+0}_{-0} [sc] $\pm$ 1 [mc]	0^{+1}_{-0} [sc] $\pm$ 2 [mc]	0^{+1}_{-2} [sc] $\pm$ 2 [mc]	-23 ± 17
B_1^n	0^{+0}_{-0} [sc] $\pm$ 1 [mc]	3^{+1}_{-1} [sc] $\pm$ 1 [mc]	4^{+1}_{-0} [sc] $\pm$ 3 [mc]	6 ± 13
B_2^k	0^{+0}_{-0} [sc] $\pm$ 1 [mc]	0^{+0}_{-1} [sc] $\pm$ 1 [mc]	-5^{+2}_{-3} [sc] $\pm$ 3 [mc]	7 ± 23
B_2^r	0^{+0}_{-0} [sc] $\pm$ 1 [mc]	0^{+2}_{-0} [sc] $\pm$ 1 [mc]	-2^{+0}_{-1} [sc] $\pm$ 2 [mc]	-10 ± 20
B_2^n	0^{+0}_{-0} [sc] $\pm$ 1 [mc]	-2^{+0}_{-1} [sc] $\pm$ 1 [mc]	-3^{+1}_{-0} [sc] $\pm$ 3 [mc]	17 ± 13
C_{kk}	324^{+7}_{-7} [sc] $\pm$ 1 [mc]	330^{+2}_{-2} [sc] $\pm$ 3 [mc]	323^{+2}_{-5} [sc] $\pm$ 6 [mc]	300 ± 38
C_{rr}	6^{+5}_{-5} [sc] $\pm$ 1 [mc]	58^{+18}_{-12} [sc] $\pm$ 2 [mc]	69^{+8}_{-7} [sc] $\pm$ 3 [mc]	81 ± 32
C_{nn}	332^{+1}_{-0} [sc] $\pm$ 1 [mc]	330^{+1}_{-1} [sc] $\pm$ 2 [mc]	326^{+1}_{-1} [sc] $\pm$ 4 [mc]	329 ± 20
$C_{nr}+C_{rn}$	1^{+0}_{-0} [sc] $\pm$ 1 [mc]	-1^{+1}_{-0} [sc] $\pm$ 3 [mc]	-4^{+4}_{-0} [sc] $\pm$ 6 [mc]	-4 ± 37
$C_{nr}-C_{rn}$	0^{+0}_{-1} [sc] $\pm$ 1 [mc]	-1^{+1}_{-0} [sc] $\pm$ 2 [mc]	2^{+4}_{-2} [sc] $\pm$ 8 [mc]	-1 ± 38
$C_{nk}+C_{kn}$	0^{+0}_{-0} [sc] $\pm$ 1 [mc]	2^{+1}_{-0} [sc] $\pm$ 1 [mc]	3^{+4}_{-1} [sc] $\pm$ 3 [mc]	-43 ± 41
$C_{nk}-C_{kn}$	1^{+0}_{-0} [sc] $\pm$ 1 [mc]	1^{+1}_{-1} [sc] $\pm$ 2 [mc]	6^{+0}_{-2} [sc] $\pm$ 7 [mc]	40 ± 29
$C_{rk}+C_{kr}$	-229^{+4}_{-4} [sc] $\pm$ 1 [mc]	-203^{+9}_{-7} [sc] $\pm$ 2 [mc]	-194^{+8}_{-6} [sc] $\pm$ 7 [mc]	-193 ± 64
$C_{rk}-C_{kr}$	1^{+0}_{-0} [sc] $\pm$ 1 [mc]	1^{+0}_{-1} [sc] $\pm$ 4 [mc]	-1^{+1}_{-3} [sc] $\pm$ 5 [mc]	57 ± 46

[CMS 1907.03729]

Higher-order corrections and entanglement measurements?

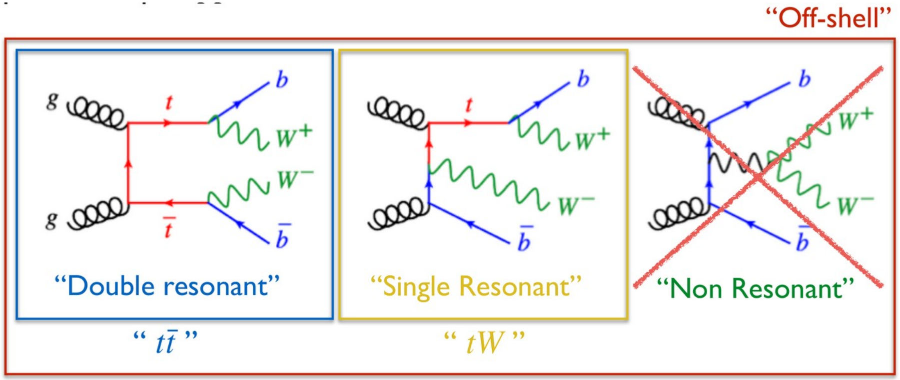
Off-shell top-quark pairs

NLO off-shell

[Bevilacqua, Czakon, Van Hameren, Papadopoulos, Worek '11; Denner, Dittmaier, Kallweit, Pozzorini '11,'12; Cascioli, Kallweit, Maierhöfer, Pozzorini '14 Denner, Pellen '18]

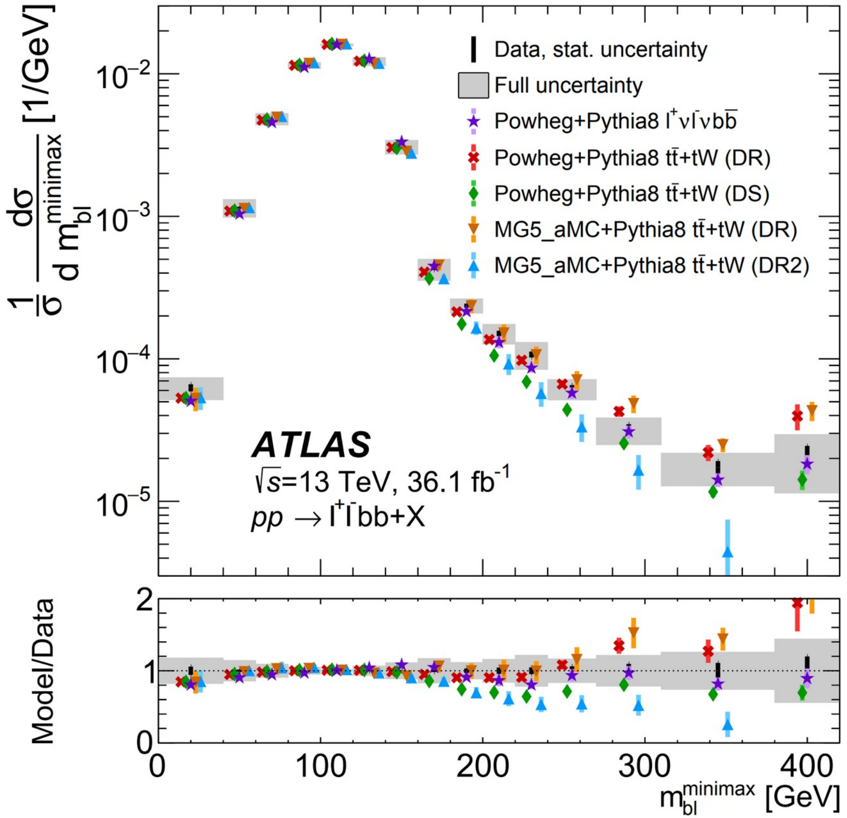
NLO off-shell ⊕ PS

[Jezo, Lindert, Nason, Oleari, Pozzorini '16; Jezo, Lindert, Pozzorini '23]



$\Gamma_t/m_t \to 0$

Credit: Bevilacqua



Associated top-quark pair production

Associated top-quark pairs

Complete NLO → $t\bar{t}\gamma$, $t\bar{t}\gamma\gamma$, $t\bar{t}W$, $t\bar{t}Z$

[Denner, Pellicciolі '21 Pagani, Shao, Tsinikos, Zaro '21 Denner, Lombardi, Pellicciolі '23 Stremmer, Worek '24]

NNLL resummation → $t\bar{t}H$, $t\bar{t}Z$, $t\bar{t}W$, $t\bar{t}t\bar{t}$

[Kulesza, van Beekveld, Motyka, Stebel, Theeuwes, Moreno Valero; Broggio, Ferroglia, Frederix, Pagani, Pecjak, Tsinikos, Yang '17-'22]

First NNLO results (2-loops approx.) → $t\bar{t}H$, $t\bar{t}W$

[Catani, Devoto, Grazzini, Kallweit, Mazzitelli, Savoini '23 Buonocore, Devoto, Grazzini, Kallweit, Mazzitelli, Rottoli, Savoini '23]

The challenge for the higher-order QCD community

2→3 @ 2-loops with masses

(real subtraction is 'simple')

State-of-the-art massive two-loop amplitudes:

- 2→3 with on external mass (mostly planar approx.)
- Computation for of 2→3 with internal and massive final-state particles out of reach for now
- → Approximations

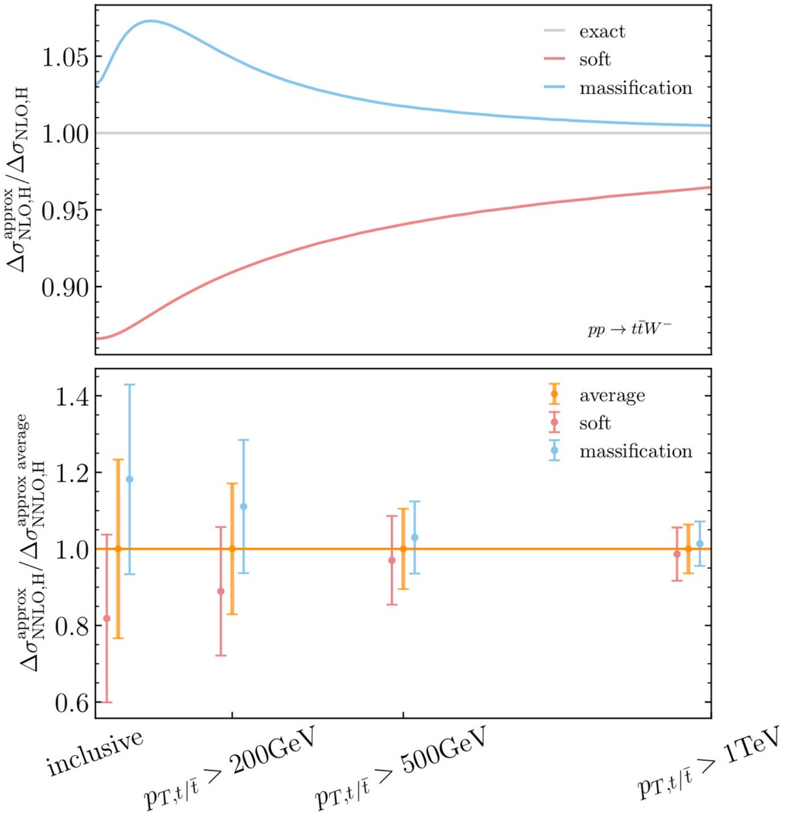
[Abreu, Syrrakos, Canko, Badger, Hartanto, Zoia, Chicherin, Cordero, Ita, Klinkert, Page Tschernow Krys Sotnikov '20-'24]

Approximations to tackle the 2-loop complexity

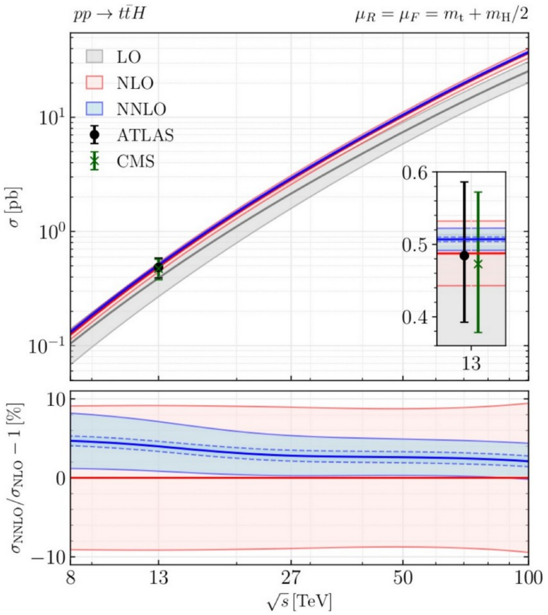
Two strategies have been explored:

- Eikonal approximations: “Soft-Higgs”/”Soft-W”
  - $$\mathcal{M}(\{p_i\},k;\mu_R,\epsilon) \sim \frac{g}{\sqrt{2}}\left(\frac{p_2\cdot\varepsilon^*(k)}{p_2\cdot k}-\frac{p_1\cdot\varepsilon^*(k)}{p_1\cdot k}\right) \times \mathcal{M}_L(\{p_i\};\mu_R,\epsilon)\,,$$ <= qq→tt amps
- ‘Massification’ of V+4j amplitudes
  [Penin’06, Moch Mitov’07, Becher, Melnikov’07]
  - $$|\mathcal{M}^{[p],(m)}> = \prod_i\left[Z_{[i]}\left(\frac{m^2}{\mu^2},\alpha_s(\mu^2),\epsilon\right)\right]^{1/2} \times |\mathcal{M}^{[p]}> + \mathcal{O}\left(\frac{m^2}{Q^2}\right)$$

Comparison of approx. cross-sections

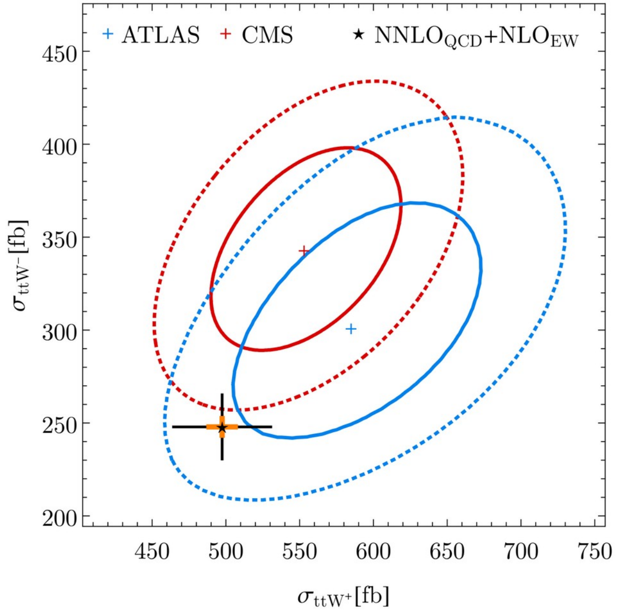


ttH and ttW cross sections / phenomenology



Impact of 2-loop contributions to cross section

- ttH: ~1%
- ttW: ~6-7%



	$\sigma_{t\bar{t}W^+}$ [fb]	$\sigma_{t\bar{t}W^-}$ [fb]	$\sigma_{t\bar{t}W}$ [fb]	
LO_{QCD}	$283.4^{+25.3\%}_{-18.8\%}$	$136.8^{+25.2\%}_{-18.8\%}$	$420.2^{+25.3\%}_{-18.8\%}$	$2.071^{+3.2\%}_{-3.2\%}$
NLO_{QCD}	$416.9^{+12.5\%}_{-11.4\%}$	$205.1^{+13.2\%}_{-11.7\%}$	$622.0^{+12.7\%}_{-11.5\%}$	$2.033^{+3.0\%}_{-3.4\%}$
$NNLO_{QCD}$	$475.2^{+4.8\%}_{-6.4\%} \pm 1.9\%$	$235.5^{+5.1\%}_{-6.6\%} \pm 1.9\%$	$710.7^{+4.9\%}_{-6.5\%} \pm 1.9\%$	$2.018^{+1.6\%}_{-1.2\%}$
$NNLO_{QCD}+NLO_{EW}$	$497.5^{+6.6\%}_{-6.6\%} \pm 1.8\%$	$247.9^{+7.0\%}_{-7.0\%} \pm 1.8\%$	$745.3^{+6.7\%}_{-6.7\%} \pm 1.8\%$	$2.007^{+2.1\%}_{-2.1\%}$
ATLAS [11]	$585^{+6.0\%+8.0\%}_{-5.8\%-7.5\%}$	$301^{+9.3\%+11.6\%}_{-9.0\%-10.3\%}$	$890^{+5.6\%+7.9\%}_{-5.6\%-7.9\%}$	$1.95^{+10.8\%+8.2\%}_{-9.2\%\ -6.7\%}$
CMS [10]	$553^{+5.4\%+5.4\%}_{-5.4\%-5.4\%}$	$343^{+7.6\%+7.3\%}_{-7.6\%-7.3\%}$	$868^{+4.6\%+5.9\%}_{-4.6\%-5.9\%}$	$1.61^{+9.3\%+4.3\%}_{-9.3\%-3.1\%}$

[10] = [CMS 2208.06485]
[11] = [ATLAS-CONF-2023-019]

Adding NNLL resummation

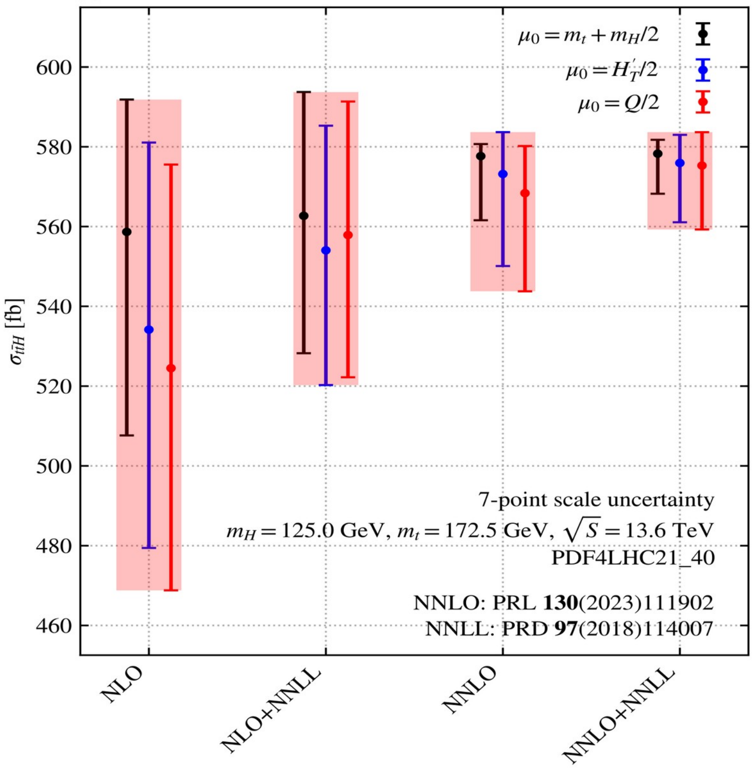
Adding NNLL soft gluon resummation
[Kulesza, Motyka, Stebel, Theeuwes'17]

$$\alpha_s^n \left(\frac{\log^m(1-\rho)}{1-\rho} \right)_+ \qquad \rho = Q^2/\hat{s}$$

$$d\sigma^{\mathrm{N(N)LO+NNLL}} = d\sigma^{\mathrm{N(N)LO}} + d\sigma^{\mathrm{NNLL}} - d\sigma^{\mathrm{NNLL}}|_{\mathrm{N(N)LO}}$$

Further stabilizing the scale dependence

[Balsach, Kulesza, Motyka, Stebel, presented at SM@LHC24]

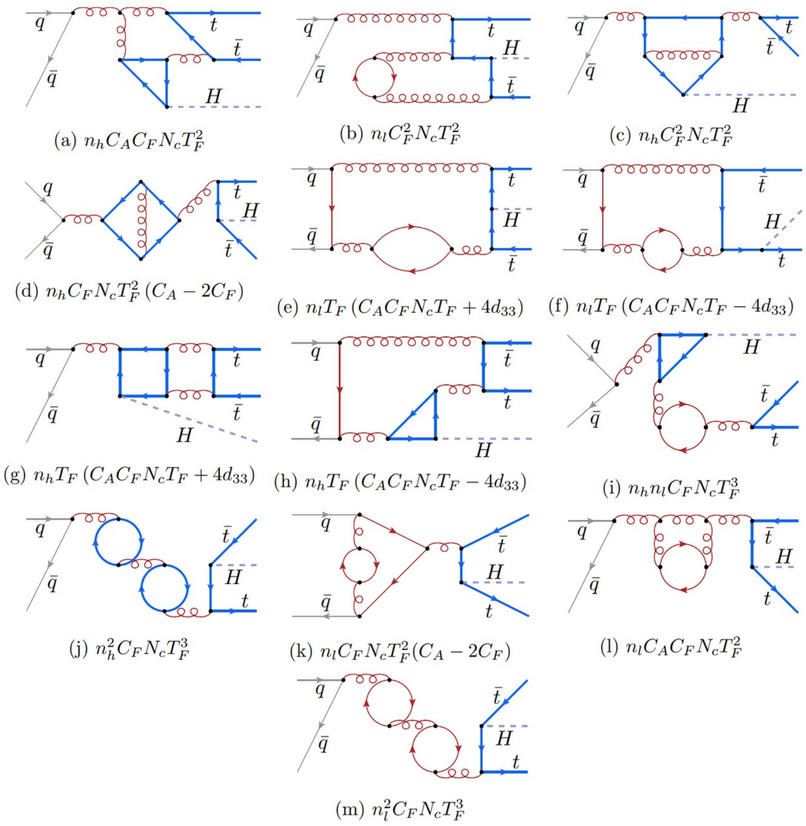


More on resummation and aNNLO → Nikolaos' talk

Beyond soft approximations/massification

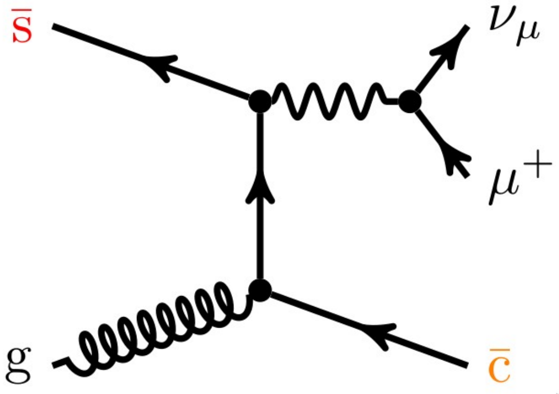
- Analytic results for two-loop master integrals with a light-quark loop in the leading colour approximation [Febres Cordero, Figueiredo, Kraus, Page, Reina ’23]
- Semi-numerical calculation of the gg → ttH one-loop amplitude to to O(ε2) [Buccioni, Kreer, Liu, Tancredi ’23]
- Two-loop amplitudes in the high-energy (boosted) limit, |sij| ≫ mt2 [Wang, Xia, Yang,Ye’24]
- Numerical results for the Nf part of the two-loop qqbar → ttH virtual amplitude [Agarwal,Heinrich, Jones, Kerner, Klein, Lang, Magerya, Olsson’24]

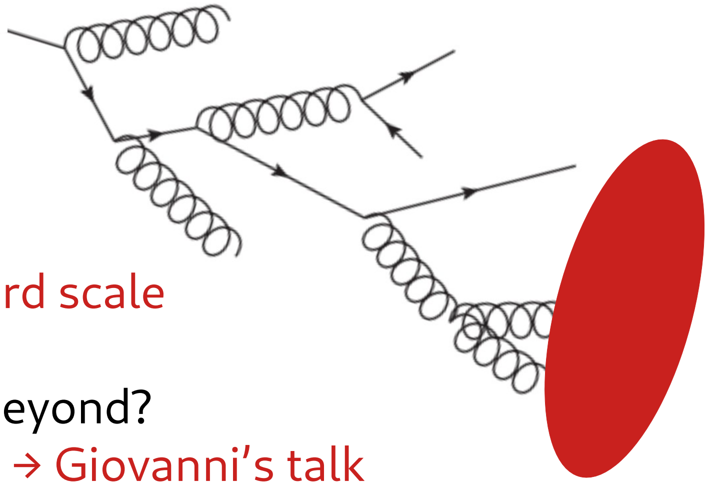
→ see Vitaly’s talk



V+heavy flavour

V+heavy flavour



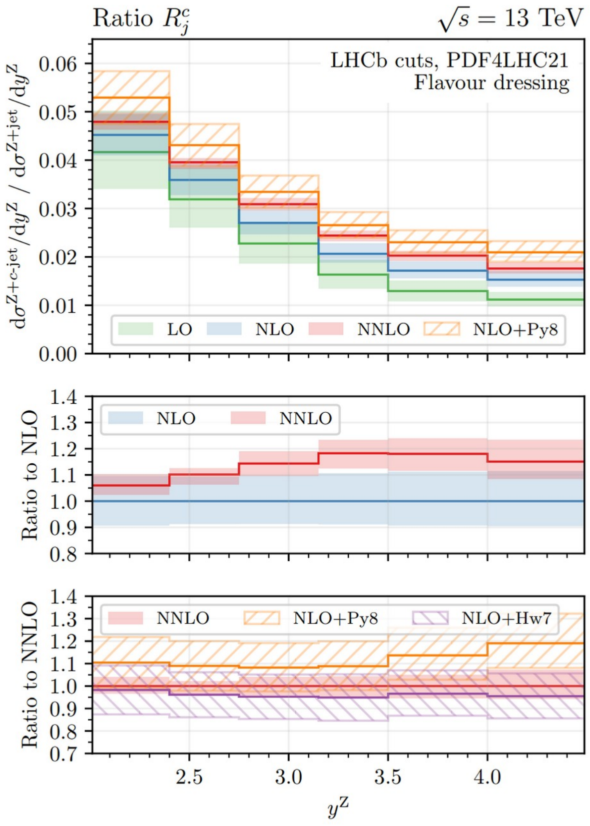


b/c quarks light w.r.t. to hard scale
→ flavoured-jets
→ IR-safety @ NNLO and beyond?
→ flavoured jet-algorithms → Giovanni's talk

- Basis for LHC phenomenology: NLO+PS simulations
  [Sherpa, Madgraph]
  [Campbell,Ellis,Maltoni,Willenbrock, Febres Cordero, Maltoni,Reina,Wackeroth,Caola '06-'18]
  [Bevilacqua,Garzelli,Kardos,Toth'21]
  [Ferrario Ravasio,Oleari'23]
- New NNLO QCD calculations:
  - Single flavoured jets
    - W/Z + charm
      [Gehrmann-De Ridder, Gehrmann, Glover, Huss, Garcia, Stagnitto '23]
      [Czakon,Mitov,Pellen,Poncelet '21'22]
  - Two flavoured jets
    - W + bb~ (5FS & 4 FS)
      [Hartanto, Poncelet, Popescu, Zoia '22]
      [Buonocore,Devoto,Kallweit,Mazzitelli, Rottoli,Savoini '22]
    - Z + bb~ → Javier's talk
      [Mazzitelli, Sotnikov, Wiesemann'24]

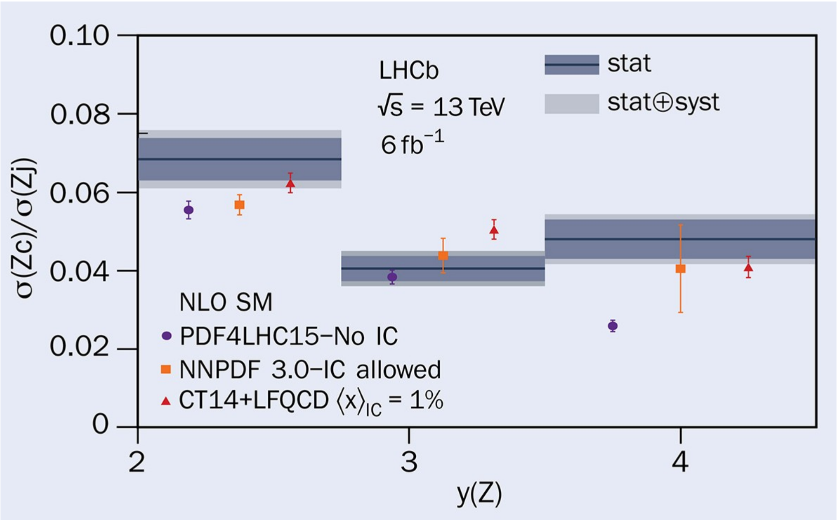
Z+charm in LHCb

Using “Flavour dressing” algorithm [Gauld, Huss, Stagnitto’22]



[Gehrmann-De Ridder, Gehrmann, Glover, Huss, Garcia, Stagnitto ‘23]

“Intrinsic charm”

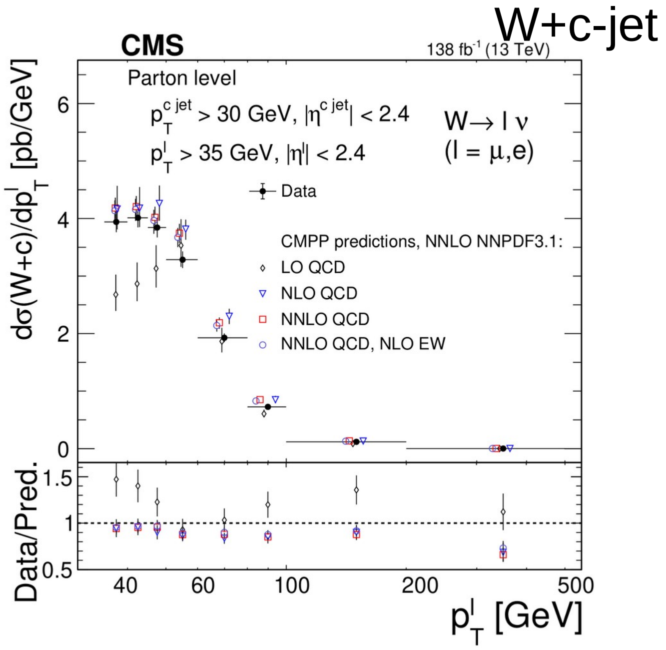


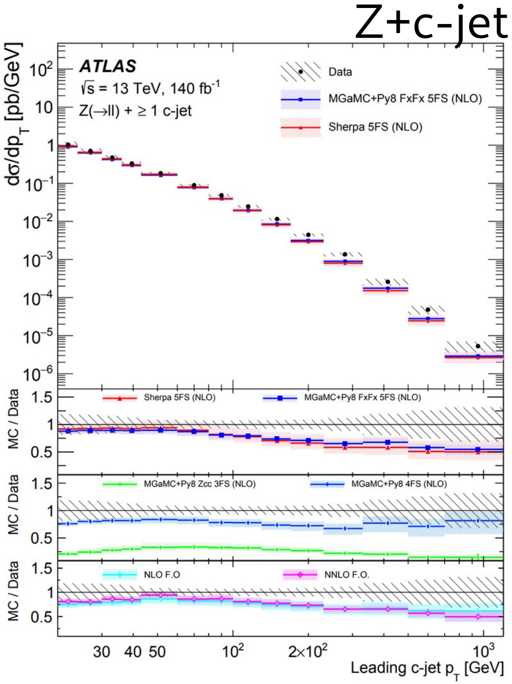
[CERN/LHCb 2109.08084]

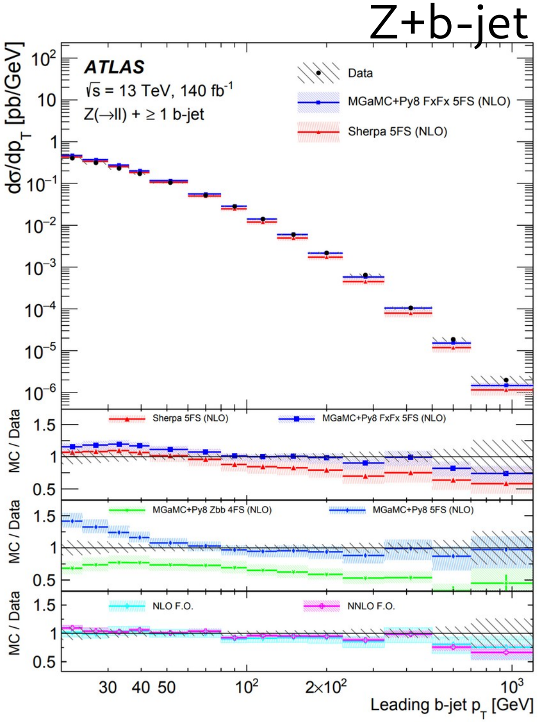
High-pT behaviour of flavoured jet cross section

[CMS 2302.00336]

[ATLAS 2403.15093]







At high pTs shapes between predictions and data

→ region were flavoured quarks are quasi massless

→ region were flavoured jet-algorithms differ → needs to be better understood

Wbb @ NNLO QCD

[Hartanto, Poncelet, Popescu, Zoia ‘22]

- LHC @ 8 TeV in 5 FS, NNPDF31, scale: $H_T = E_T(lv) + pT(b1) + pT(b2)$
- Phasespace definition to model **[CMS, 1608.07561]:** pT(l) ≥ 30 GeV |y(l)| < 2.1 pT(j) ≥ 25 GeV, |y(j)| < 2.4
- Inclusive (at least 2 b-jets) and exclusive (exactly 2 b-jets, no other jets) jet phase spaces (defined by the flavour-kT jet algorithm [Banfi’06])

- Inclusive :
  ~ +20% corrections
  ~ 7% scale dependence
- Exclusive:
  ~ + 6% corrections
  ~ 2.5% scale dependence (7-pt)
  Compare decorrelated model: [Steward’12]
  ~ 11% scale dependence

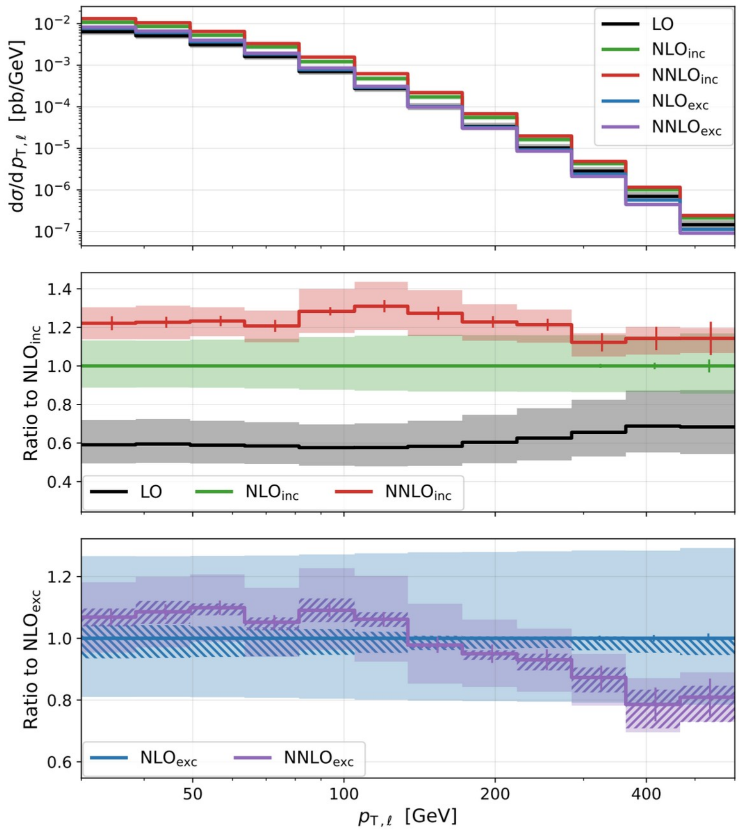
	inclusive [fb]	$\mathcal{K}_{\rm inc}$	exclusive [fb]	$\mathcal{K}_{\rm exc}$
$\sigma_{\rm LO}$	$213.2(1)^{+21.4\%}_{-16.1\%}$	-	$213.2(1)^{+21.4\%}_{-16.1\%}$	-
$\sigma_{\rm NLO}$	$362.0(6)^{+13.7\%}_{-11.4\%}$	1.7	$249.8(4)^{+3.9(+27)\%}_{-6.0(-19)\%}$	1.17
$\sigma_{\rm NNLO}$	$445(5)^{+6.7\%}_{-7.0\%}$	1.23	$267(3)^{+1.8(+11)\%}_{-2.5(-11)\%}$	1.067

$$\sigma_{Wb\bar{b},{\rm excl.}} = \sigma_{Wb\bar{b},{\rm incl.}} - \sigma_{Wb\bar{b}j,{\rm incl.}}$$

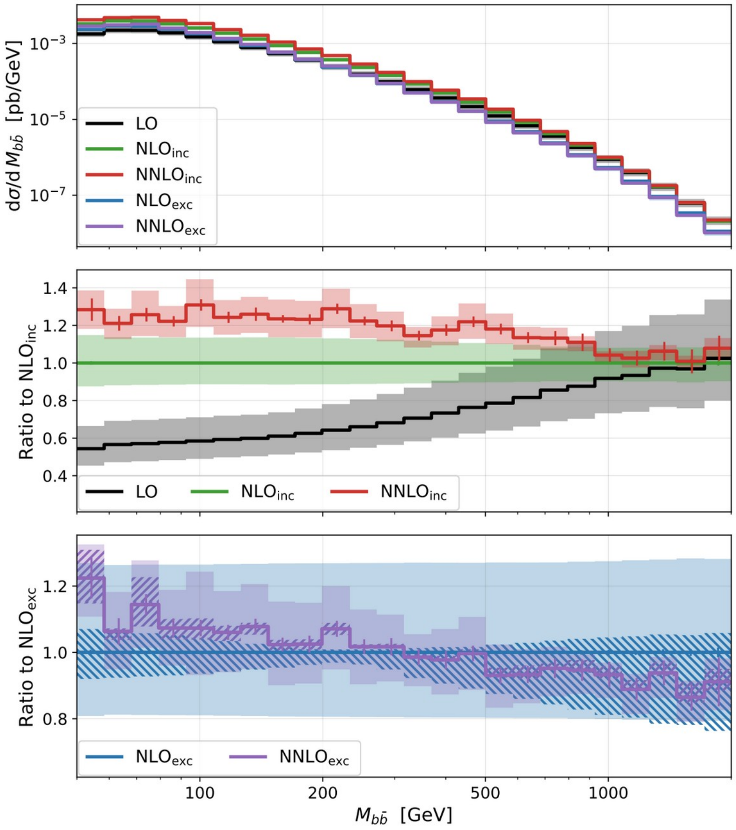
$$\Delta\sigma_{Wb\bar{b},excl.} = \sqrt{(\Delta\sigma_{Wb\bar{b},incl.})^2 + (\Delta\sigma_{Wb\bar{b}j,incl.})^2}$$

Differential cross sections

Transverse momentum of lepton

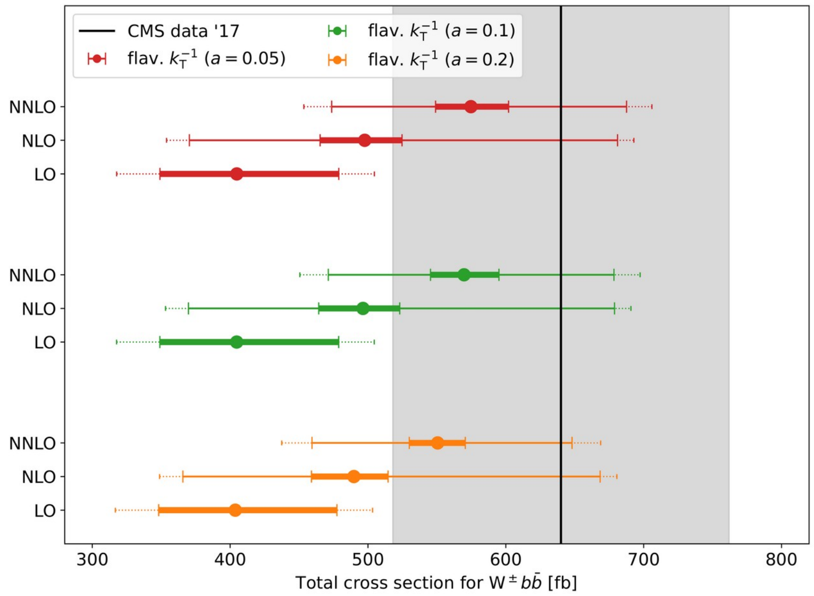


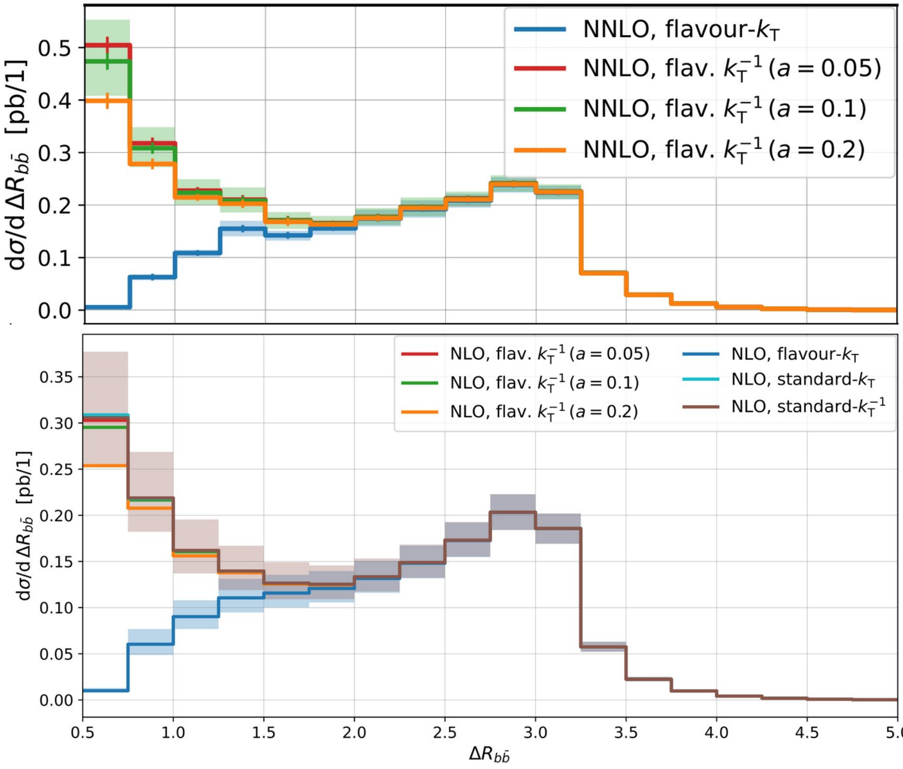
Invariant mass b-jet pair



W+2 bjets: flavour anti-kT

[Hartanto, Poncelet, Popescu, Zoia ‘22]





Comparison to data
[CMS 1608.07561]

(assumes small unfolding corrections → wip)

Significant differences between kT and anti-kT
In small DeltaR(bb) region.

Computation in 4FS

[Buonocore, Devoto, Kallweit, Mazzitelli, Rottoli, Savoini ‘22]

Credit: Luca Buonocore RadCor23

	2209.03280	2212.04954
α_s and PDF scheme	5FS	4FS
Jet clustering algorithm	flavour k_T and flavour anti-k_T algorithm (R=0.5)	k_T and anti-k_T algorithm (R=0.5)
pdf sets	`NNPDF31_as_0118` (LO, NLO, NNLO)	`NNPDF30_as_0118_nf_4` (LO) `NNPDF31_as_0118_nf_4` (NLO, NNLO)

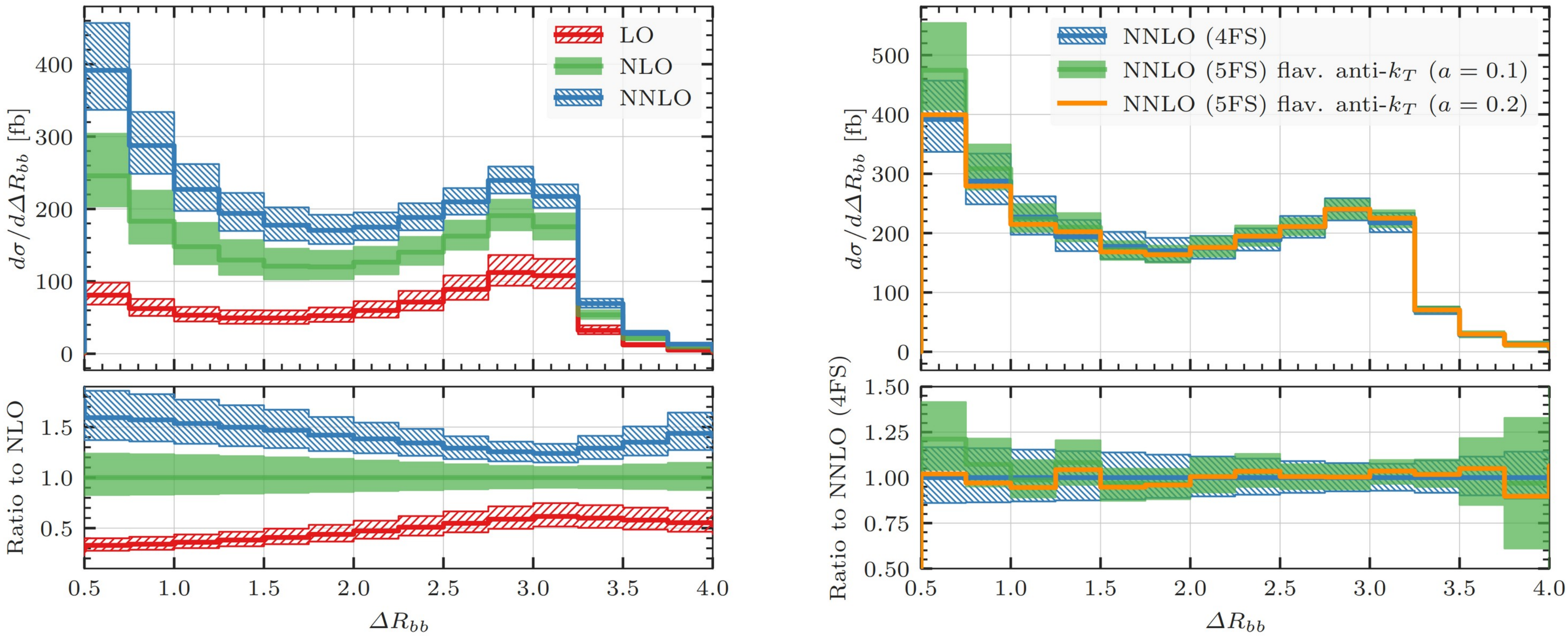
↓

Massification of 2-loop amplitude [Penin’06, Moch Mitov’07, Becher, Melnikov’07]

$$|\mathcal{M}^{[p],(m)}> = \prod_i \left[Z_{[i]}\left(\frac{m^2}{\mu^2}, \alpha_s(\mu^2), \epsilon\right)\right]^{1/2} \times |\mathcal{M}^{[p]}> + \mathcal{O}\left(\frac{m^2}{Q^2}\right)$$

Comparison 4FS(+PS) vs 5FS

[Buonocore, Devoto, Kallweit, Mazzitelli, Rottoli, Savoini ‘22]



Open-bottom

Open-bottom production at NNLO+NNLL QCD

Not just ttbar with a small mass:

→ overall scale much smaller O(100GeV) vs O(10GeV) → slower perturbative convergence

→ large logarithms log(pT/m) are more prominent → resummation, 4 vs 5 flavour scheme

State-of-the-art for open-flavour

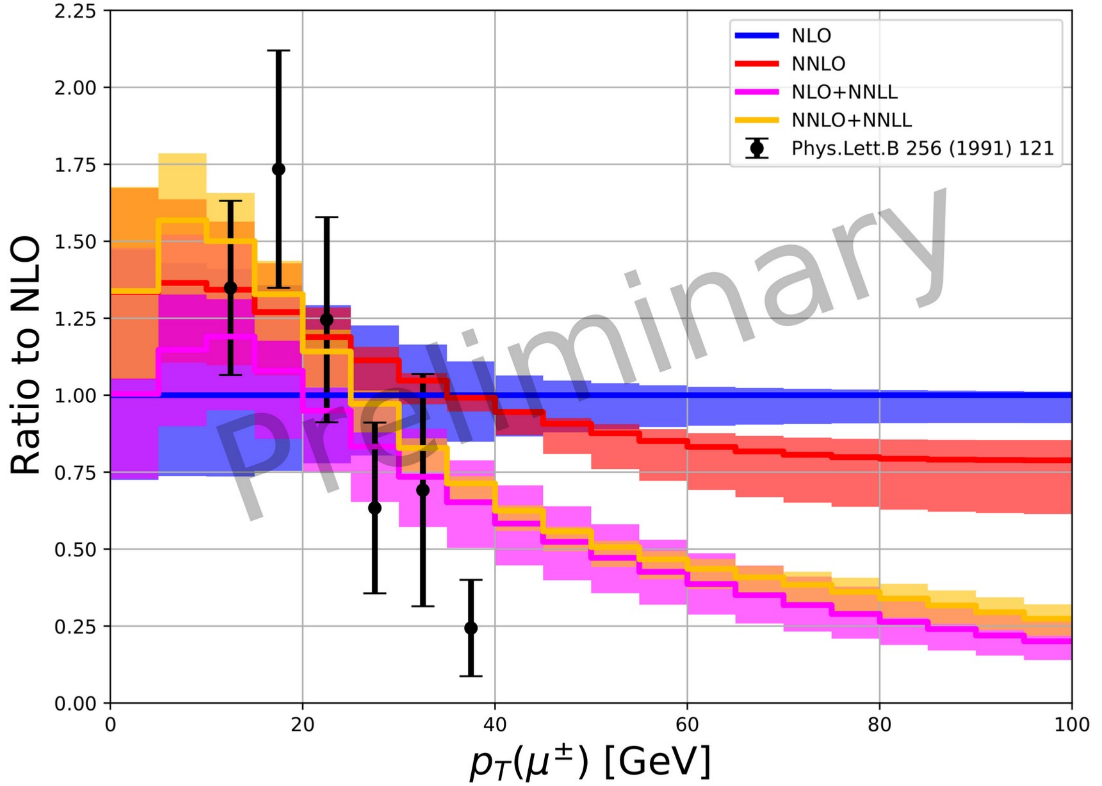
- NLO+NLL in variable flavour number schemes ('FONLL'[Cacciari, Greco, Nason'98])
- B-hadron in NNLO+PS [Mazzitelli, Ratti, Wiesemann, Zanderighi'23]
  → LL resummation by shower
- New: FONLL @ NNLO [Czakon, Generet, Mitov, Poncelet in preparation, presented at Moriond QCD]
  Based on perturbative fragmentation implementation used for
  pp → tt~ → B-hadrons (and other identified particles like muons, J/Psi, …)
  [Czakon, Generet, Mitov, Poncelet'22'23]

→ also see Kay's talk

Example: open-bottom @ SppS

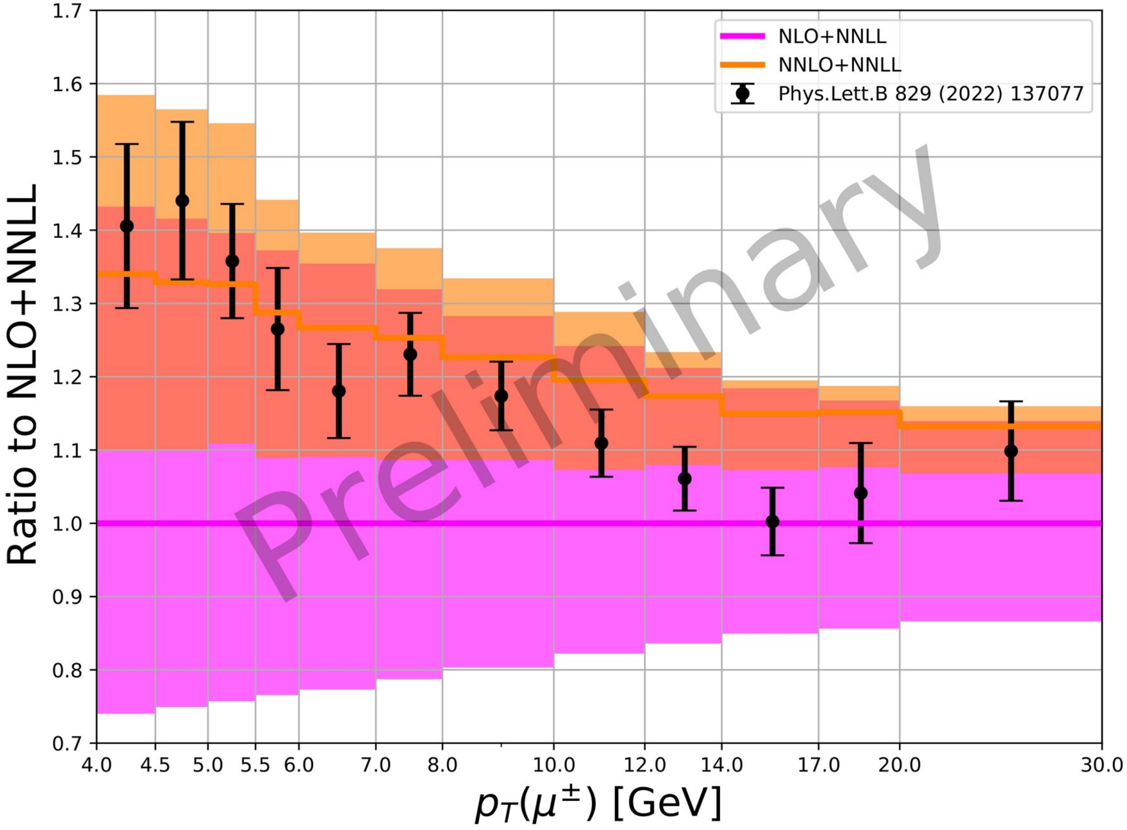
[thanks to Terry!]

- pT distribution of muons originating from B-hadrons <=> proxy for B-hadron pT
- Fixed-order inconsistent at high pT
- Resummed results consistent
- Resummation needed for pT(mu+) > 30 GeV
  <=>
  pT(B) > 60 GeV



Example: open-bottom @ ATLAS 5.02 TeV

- Reduction of scale dependence
- Better agreement with data
  → normalization & shape



Many results to come…

Summary

Summary

- NNLO QCD is the name of the game in heavy flavour production:
  tt, ttW, ttH, W+c, Z+c, Z+b, W+bb, Z+bb
- + resummation: soft-gluon, or mass-logs (FONLL)
- Beyond 'inclusive' partonic computations
  → predictions for fiducial phase spaces
  → matched to parton-showers
- Precision computations for heavy flavour jets (bottom/charm)
  → often in massless quark approximation
  → require flavoured jet-algorithms
- Biggest challenge for fixed-order: 2-loop amplitudes
  - simplification through massification or eikonal approximations
  - First steps for ttH