Improved simulations for the production and decay of top quarks with MG5_aMC@NLO

Eps-Hep 2023

Aug 23rd, 2023

Based on:

Simone Amoroso, S. Frixione, S. Mrenna,
arXiv:2308.06389 [hep-ph]

Simone Amoroso, R. Frederix, S.Frixione,
A. Pizzini, in preparation

Simulation of unstable particles at colliders

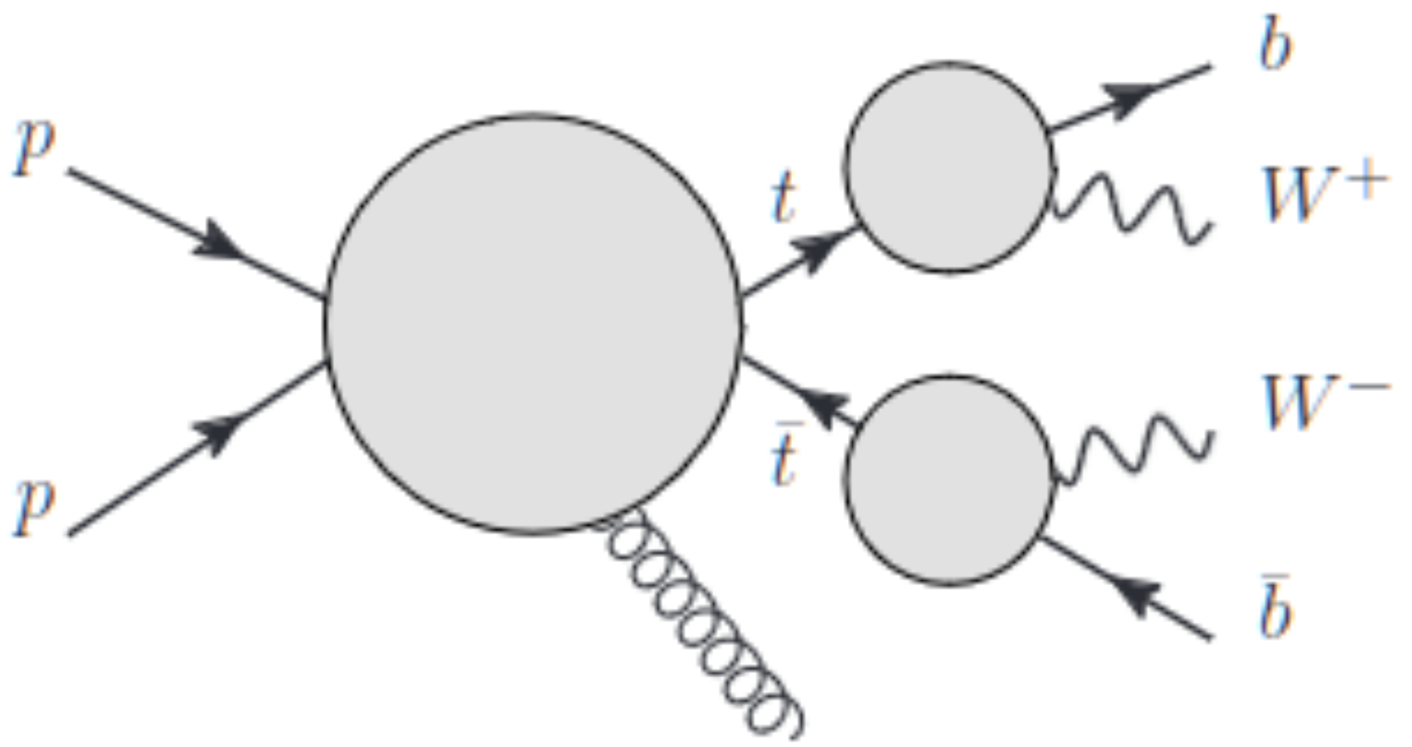
- Simulation of massive unstable particles at colliders
  is of particular phenomenological relevance (W, Z, top, Higgs, BSM, …)
- For the production of stable resonances, NLOPS with
  Powheg and MC@NLO matching available and automated since 10 years

P. Nason, *JHEP* ***0411*** *(2004) 040*
S. Frixione, B. Webber, *JHEP 06 (2002) 029*

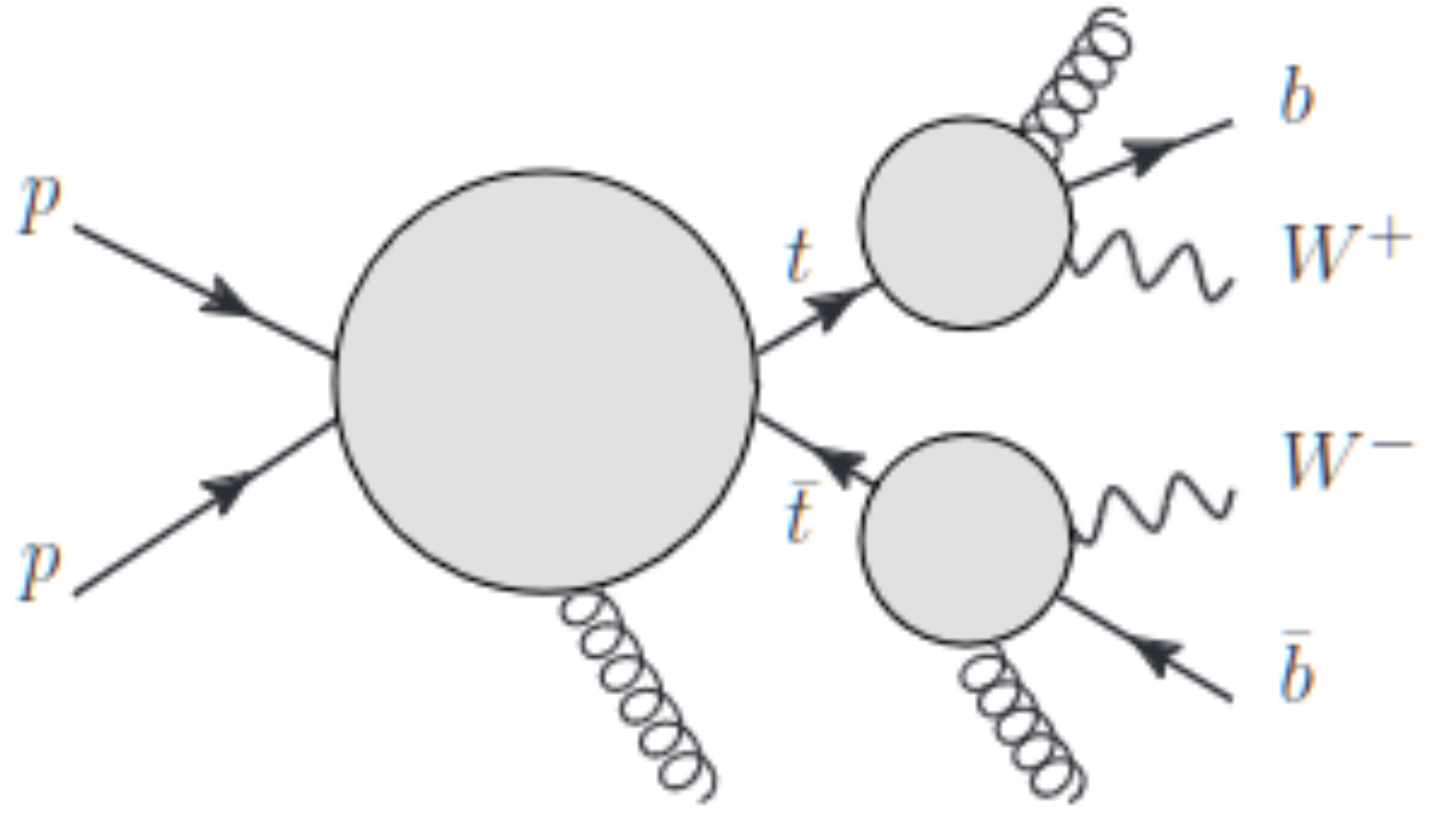
- NNLOPS new frontier: MiNNLOPS for color singlets and top-pair production

P. Monni et al, *JHEP* ***05*** *(2020) 143*

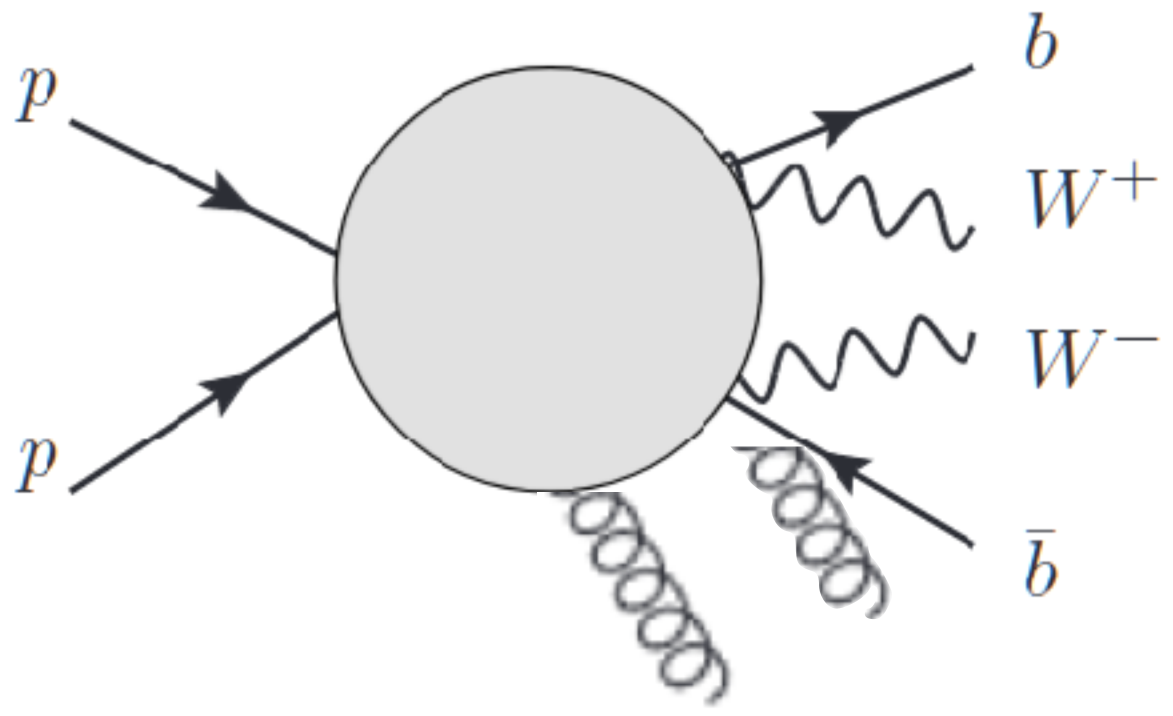
$$pp \to t\bar{t} \otimes t \to Wb$$



$$pp \to t\bar{t} \otimes t \to Wbg$$



$$pp \to b\bar{b}l\bar{l}\nu\bar{\nu}$$



- For resonance decays, situation is less standardized:
  different level of approximations/complexities are possible

Simulation of unstable particles at colliders

- ***Madspin***: resonance decays and spin correlations at LO

  S. Frixione, E. Laenen, P. Motylinski, B.R. Webber, JHEP 04, 081 (2007)

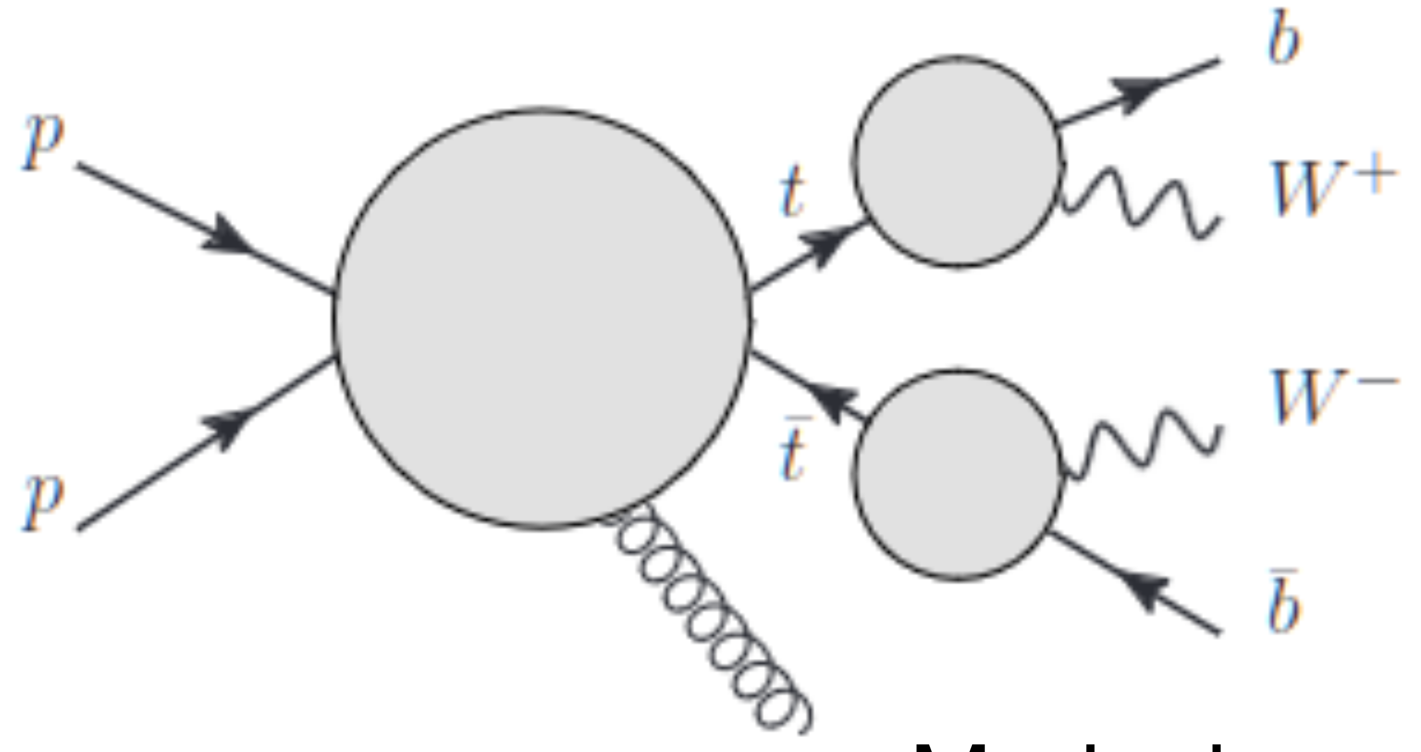
- ***Matrix-element corrections (MEC)***: reweight shower emission to tree-level ME

  E. Norrbin, T. Sjöstrand, Phys. Lett. B 449, 313 (1999)

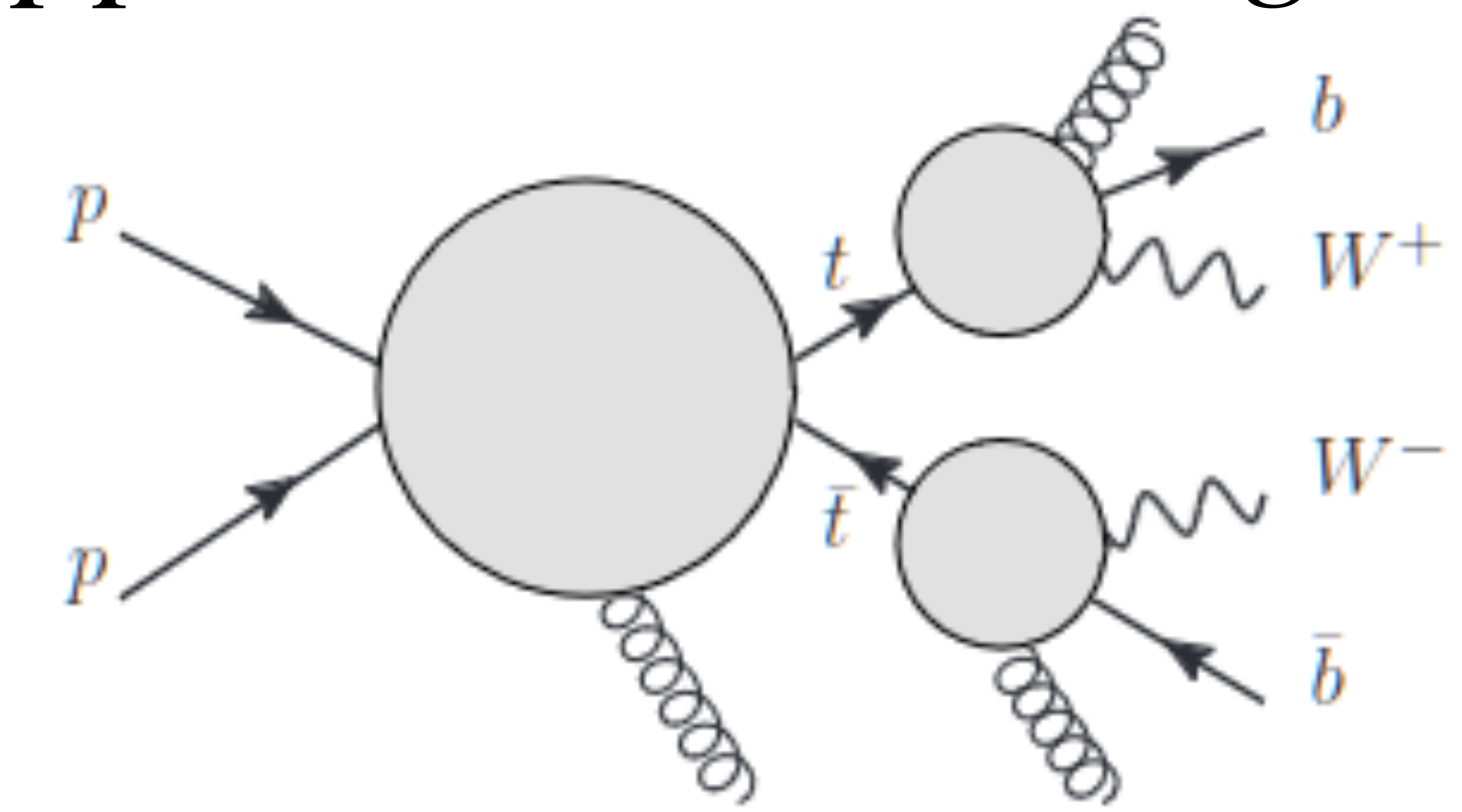
- ***Exact matrix-elements:*** NLO corrections to decay and full off-shell effects

  T. Jezo et al, Eur.Phys.J.C 76 (2016) 12, 691

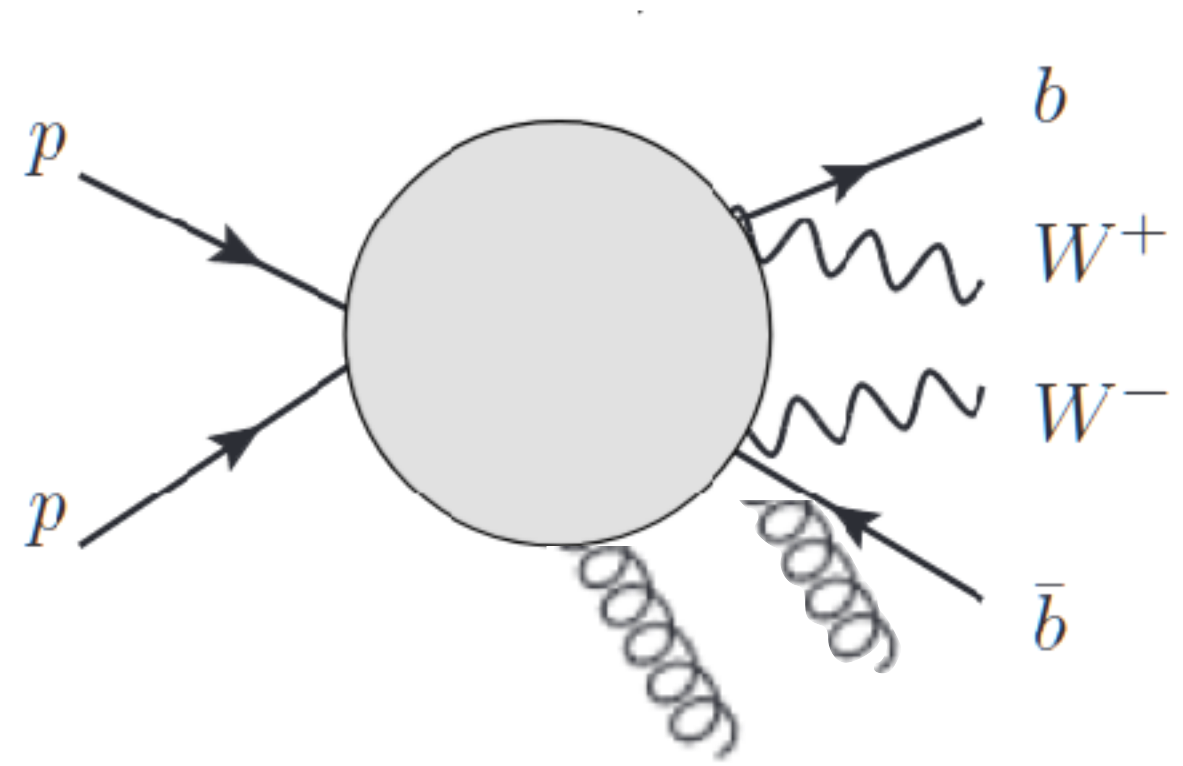
$$pp \to t\bar{t} \otimes t \to Wb \qquad pp \to t\bar{t} \otimes t \to Wbg \qquad pp \to b\bar{b}l\bar{l}\nu\bar{\nu}$$



Madspin



MEC in decay



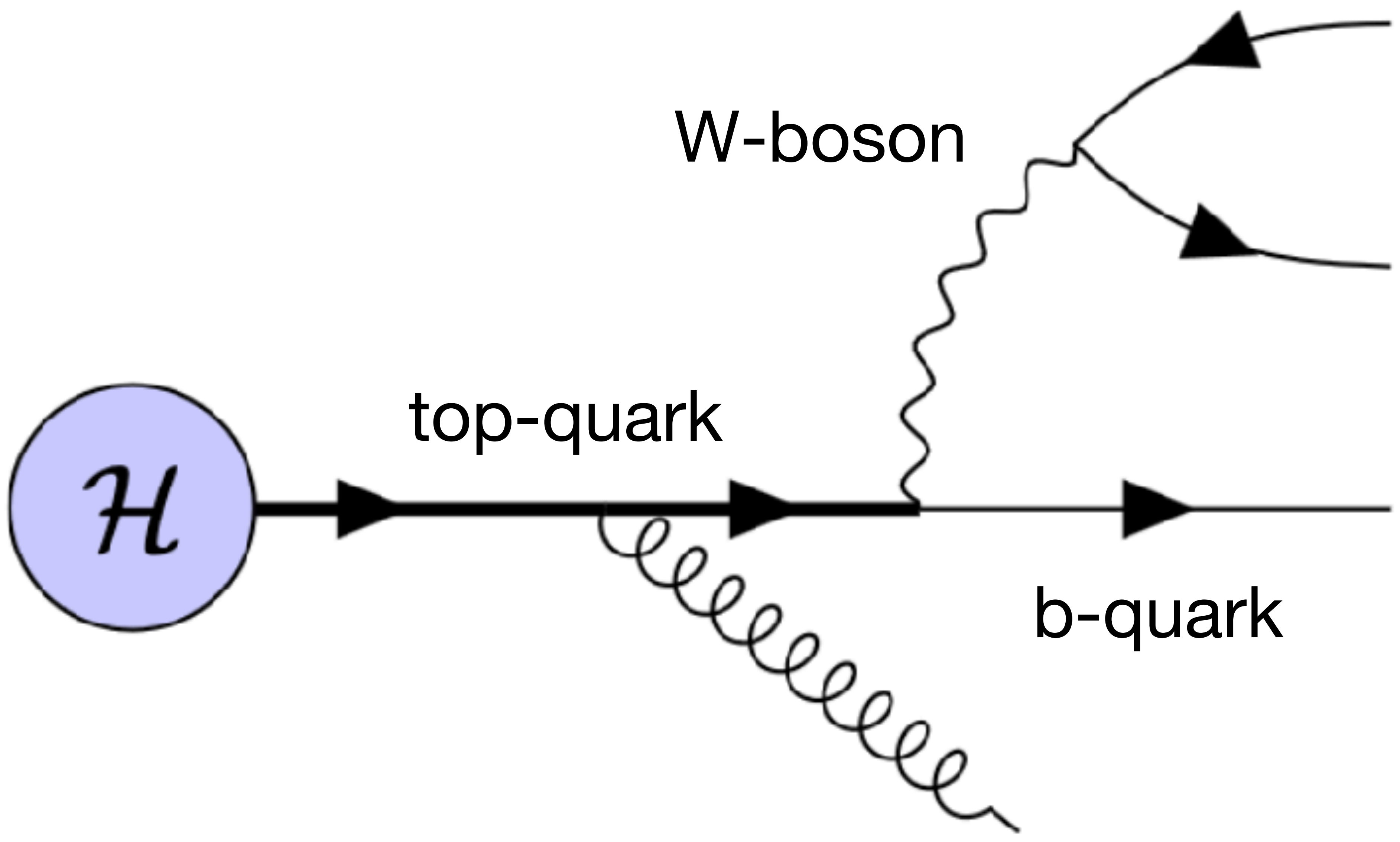
Exact ME

- Will present results for the latter two approaches in the context of MC@NLO matched simulations with the mg5_aMC@NLO+Pythia8 code

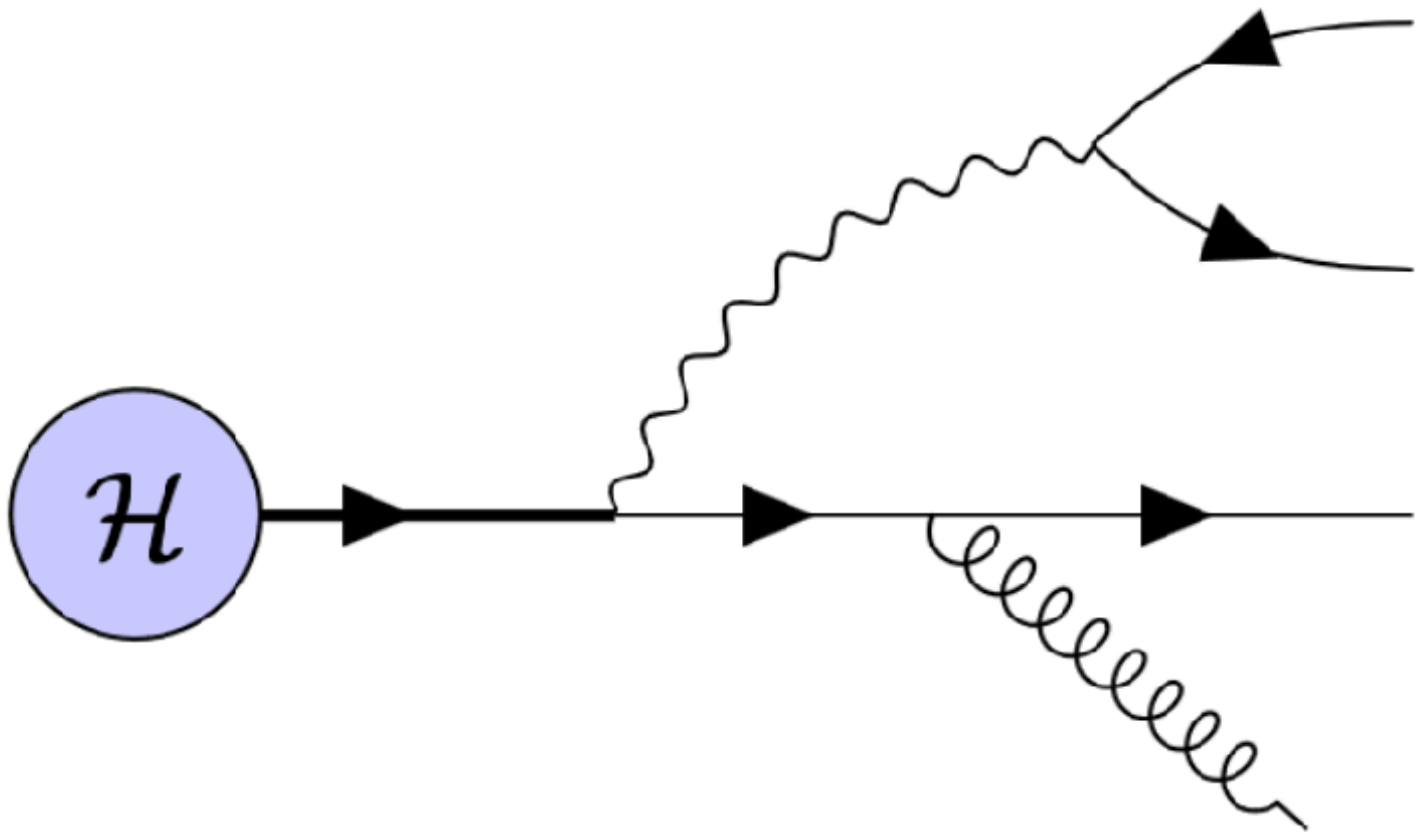
J. Alwall et al, JHEP 07, 079 (2014) C. Bierlich et al. *SciPost Phys. Codebases 8 (2022)*

MEC and MC@NLO matching

- MC@NLO MC subtraction term determined for a shower without any MEC
  - *MEC for production* certain to spoil MC@NLO simulation accuracy
  - *MEC for decays* can instead be included without double counting
- Shower however separates MEC into initial- and final-state emissions
  - ***Needs to distinguish production and decay MEC*** in the final-state shower



Part of the MC@NLO MC subtraction



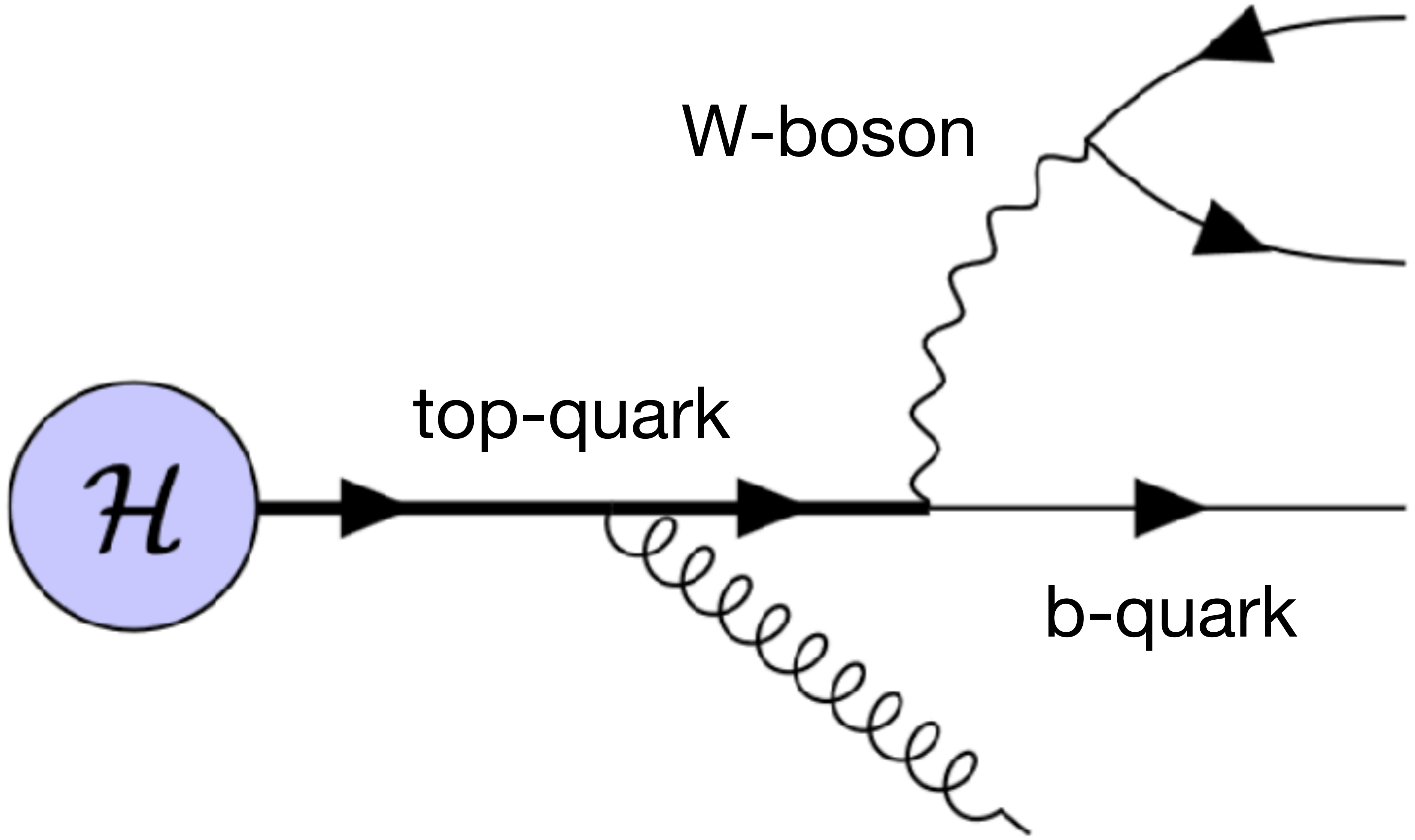
Not included in the MC@NLO MC subtraction

MEC and MC@NLO matching

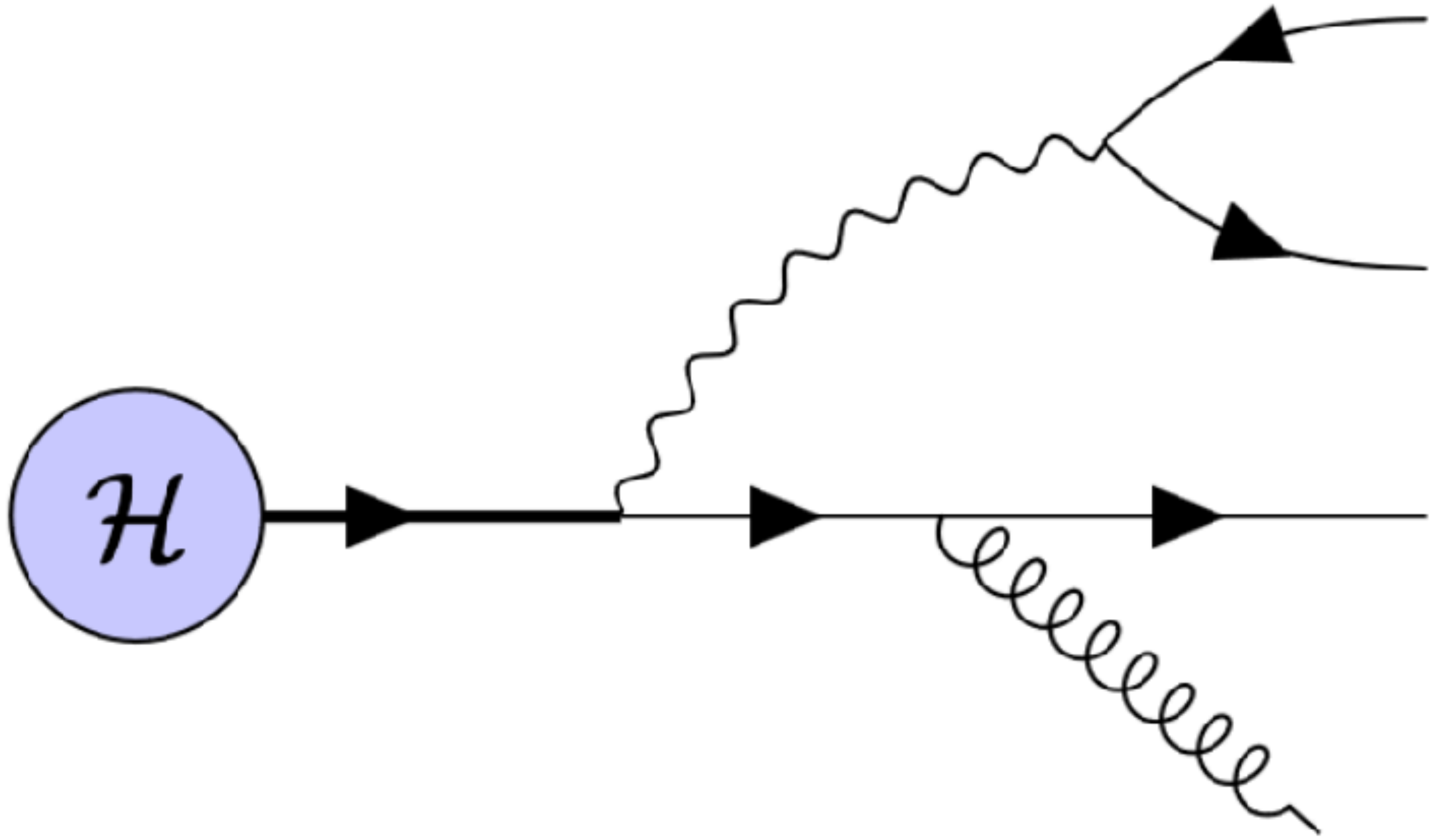
- Due to these subtleties, MEC in decay have so far been switched off in MC@NLO matched simulations, while they are included in Powheg
- It is however possible in Pythia8.3 to separate MEC coming from top-quark production and from top-quark decay

NB, syntax works for most processes, but not all! Future Pythia version to include switches for finer control over MEC

```
Timeshower:MECorrections=on
TimeShower:MEextended=off
```



Part of the MC@NLO MC subtraction



Not included in the MC@NLO MC subtraction

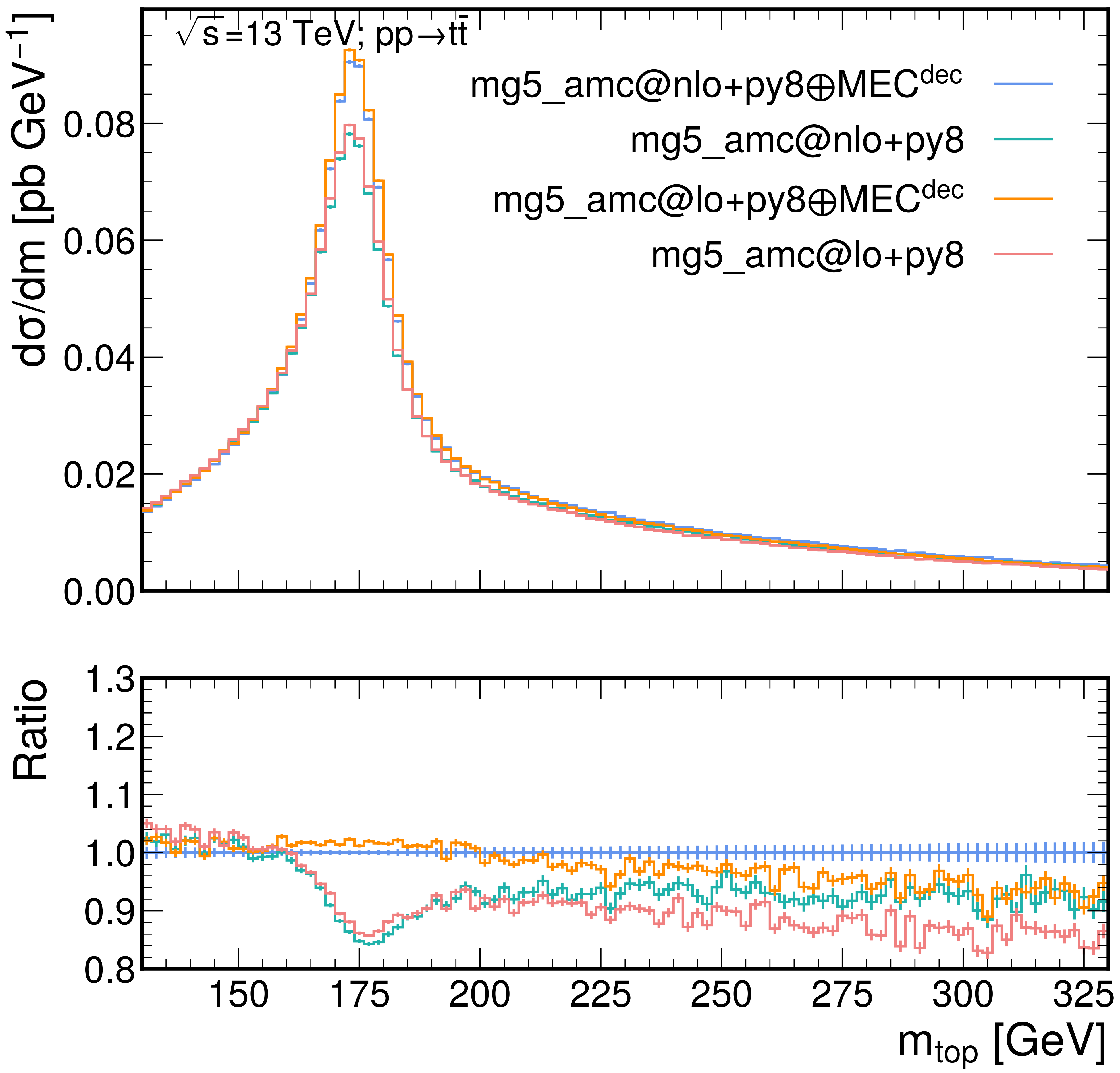
Phenomenological study

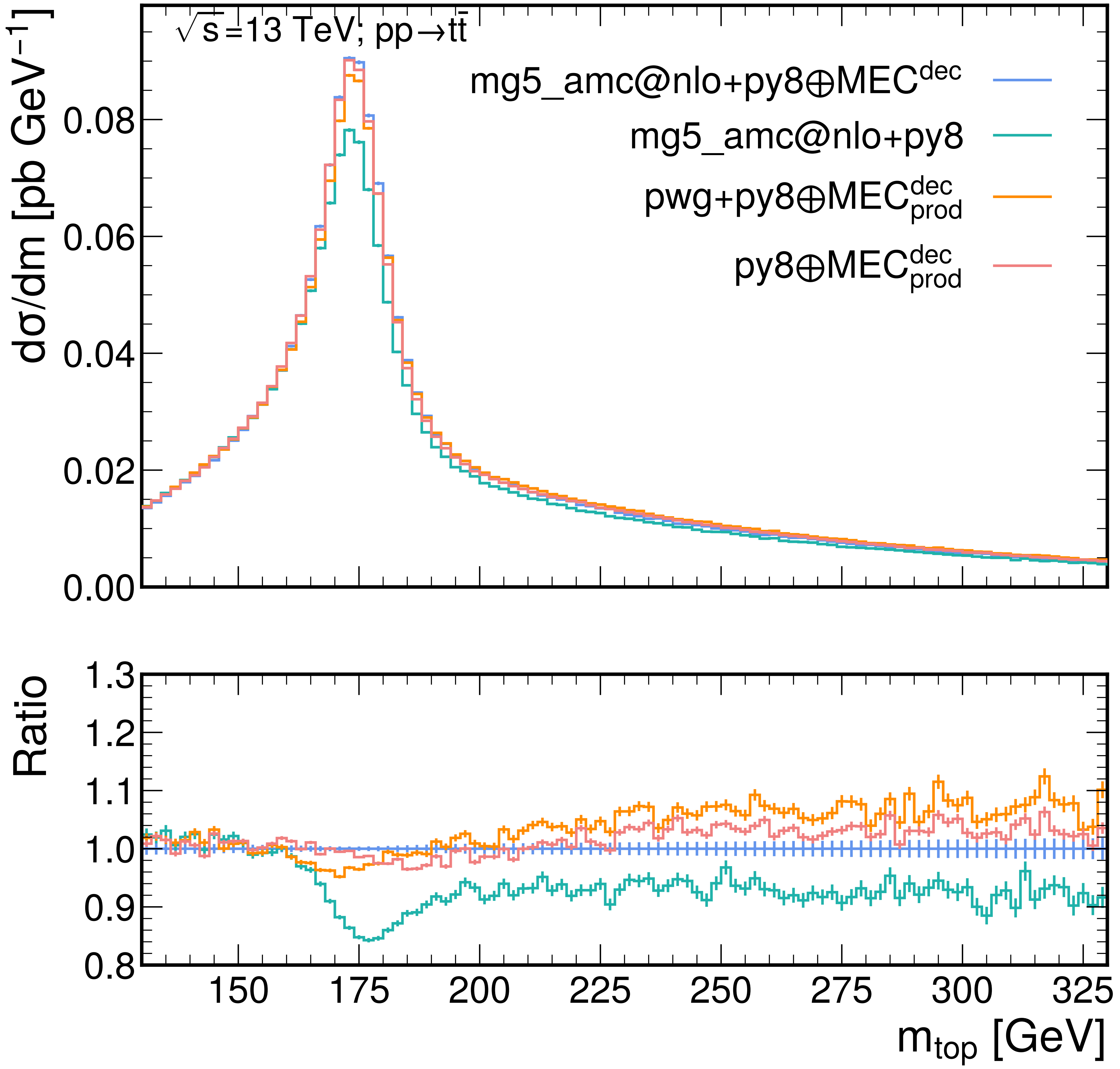
- To evaluate the impact of MEC in decay we performed a phenomenological study comparing the following simulations:
  - **mg5_aMC@NLO + Pythia8** — J. Alwall et al, JHEP 07, 079 (2014)
    LO and NLO QCD events showered with and without MEC in decay
  - **Powheg HVQ + Pythia8 (with MEC)** — S. Frixione, P. Nason, G. Ridolfi, *JHEP **0709** (2007) 126*
  - **Standalone Pythia8 (with MEC)** — C. Bierlich et al. *SciPost Phys. Codebases 8 (2022)*

- Consider **stable top-quark production** in pp collisions at 13 TeV
- We set m_{top}=172.5 GeV and use the NNPDF31nnlo PDF for all three cases. Settings related to the production (scales, h_{damp}, μ_{sh}) left to their default values
- For all events, we decay the tops using Madspin, which we then shower in Pythia8.309 with the Monash tune and using the appropriate settings and vetoes

Reconstructed top-quark mass distribution

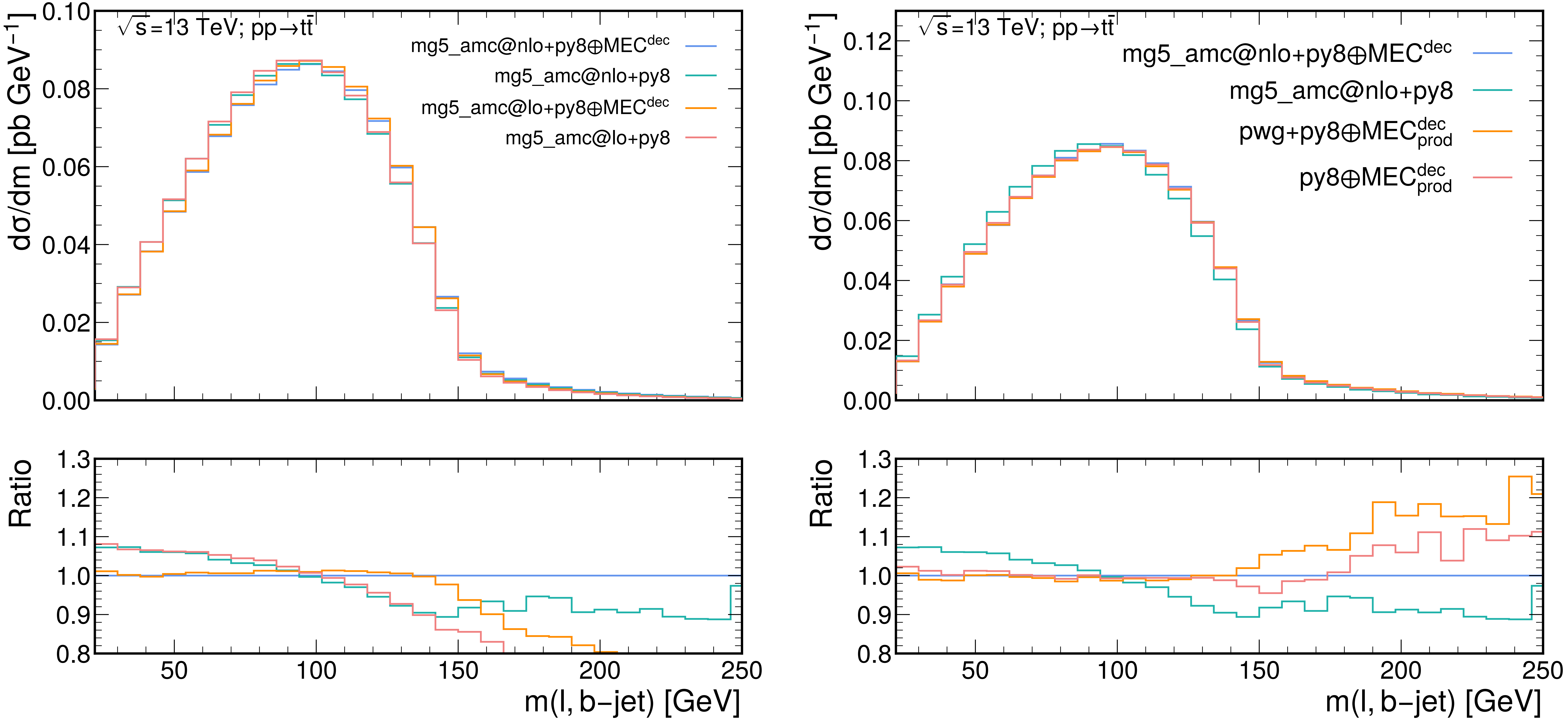
- The peak of the top quark mass reconstructed from its decay products shows large differences between mg5_aMC@NLO and Powheg, Pythia8
- They are significantly reduced after including MEC to decays in mg5_aMC@NLO





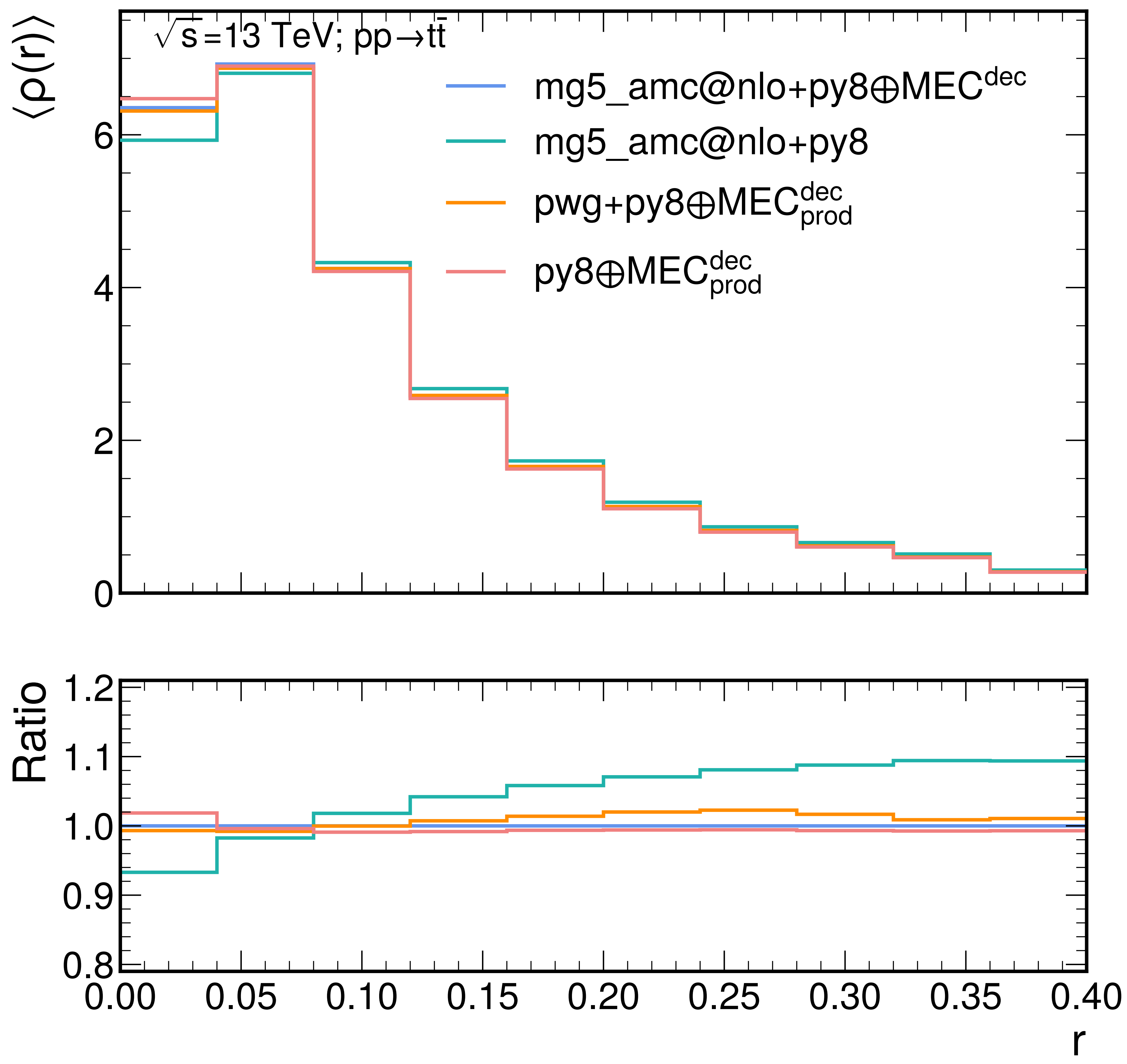
M_{BL} DISTRIBUTION

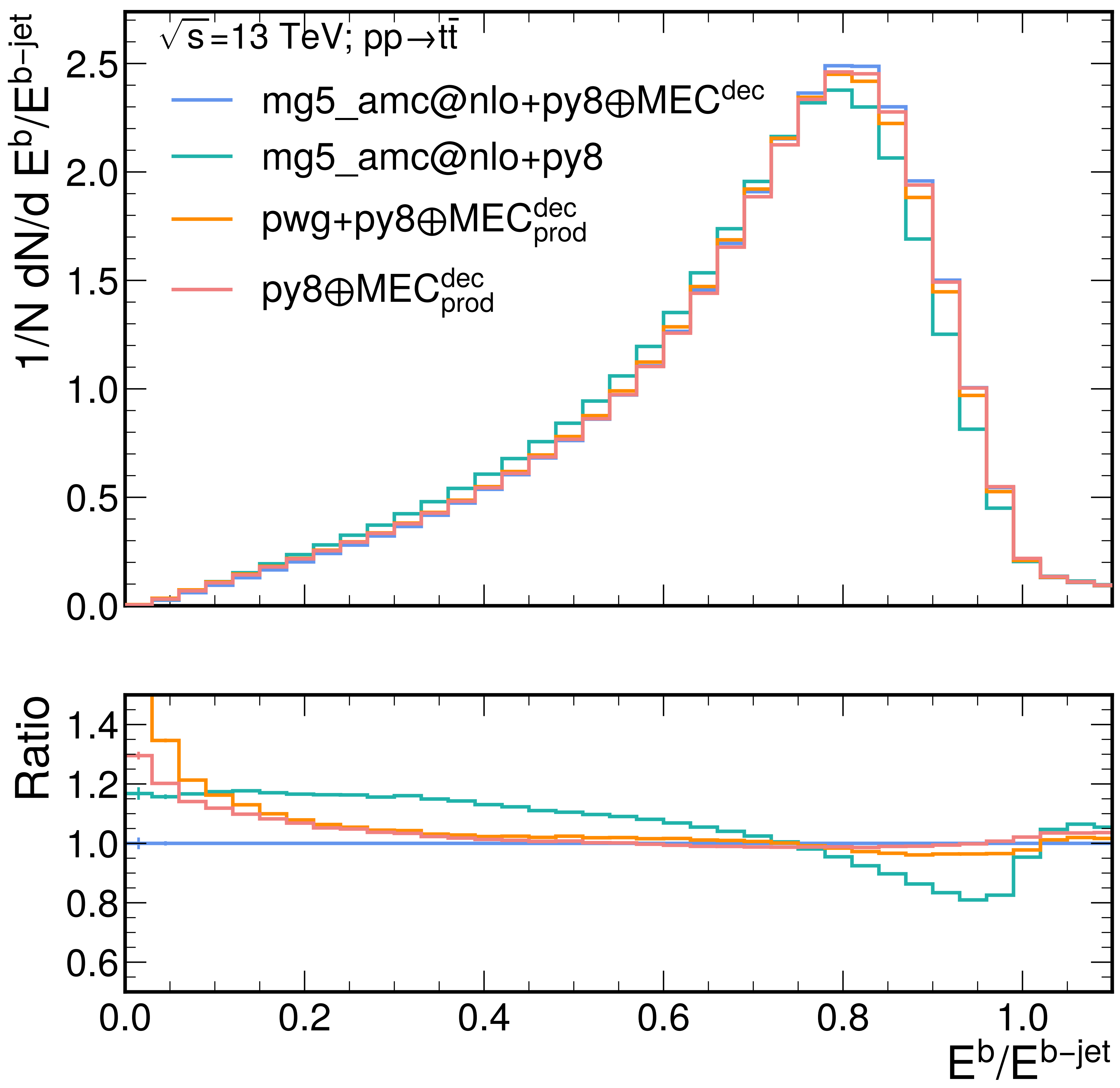
- The m_{bl} distribution has a kinematic edge at ~150 GeV sensitive to the top mass. In this region MEC to decay brings the three codes in agreement
- Above 150 GeV differences in the production give residual ~20% differences



Properties of b-quark jets

- The b-jet shape and b-fragmentation function are sensitive to the pattern of emission inside the b-jet, modified by higher order corrections
- Differences of up to 20% visible when including MEC in decay

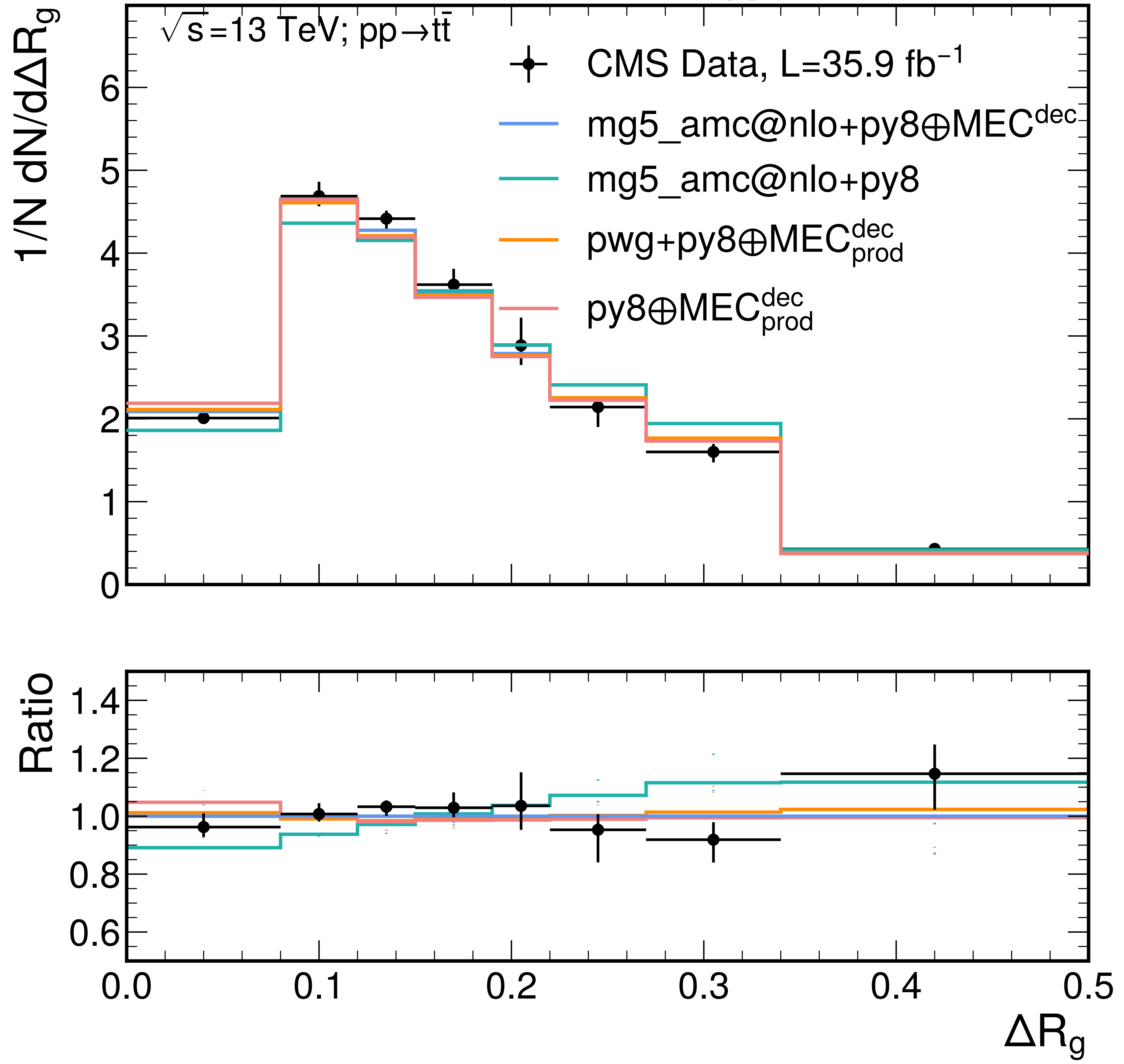




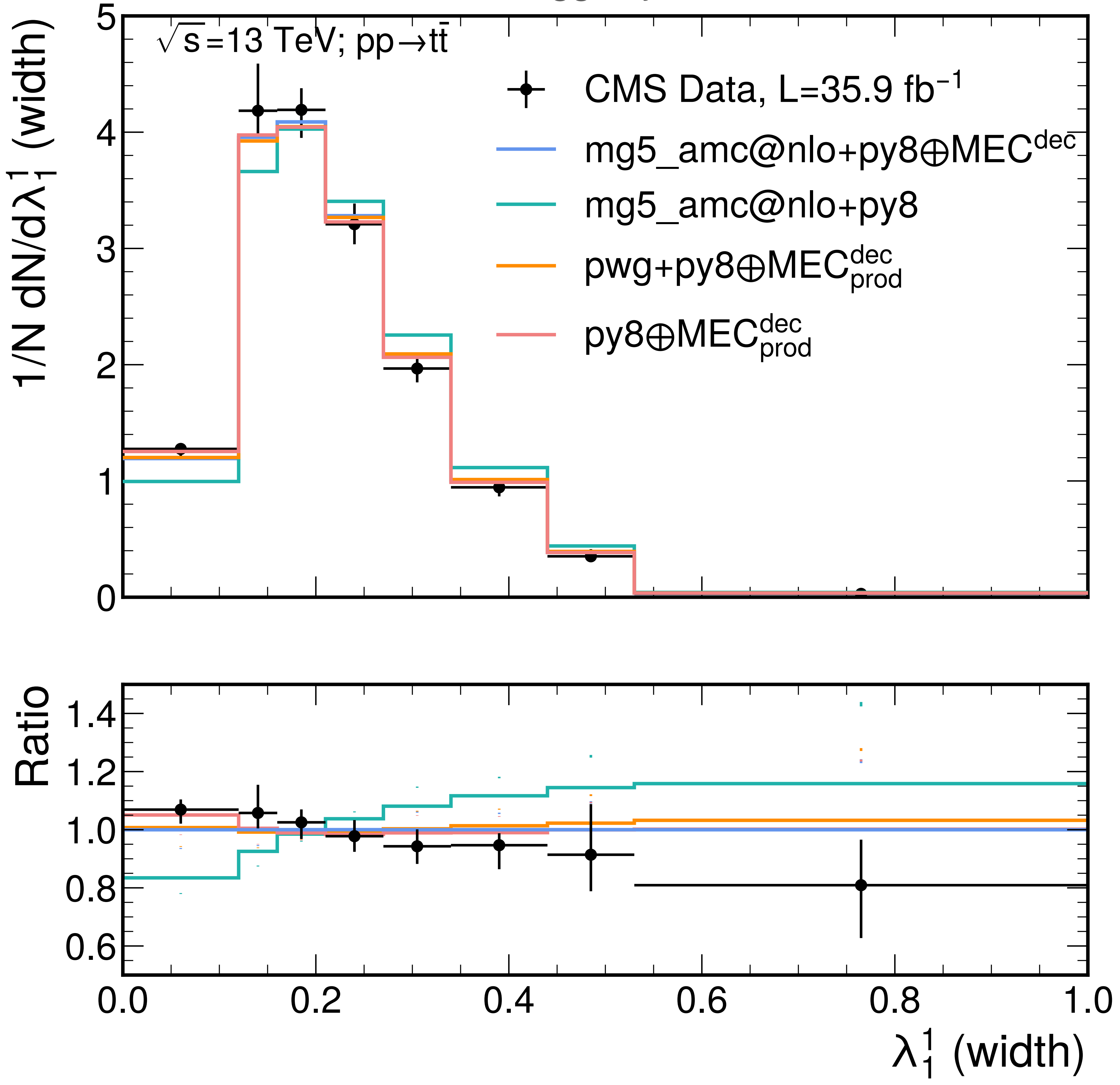
B-jet substructure in data

- Comparing to CMS 13 TeV jet substructure observables in ttbar
- Reduction in spread among generators, and improved description of the data

Distance between subjects in b-tagged jets



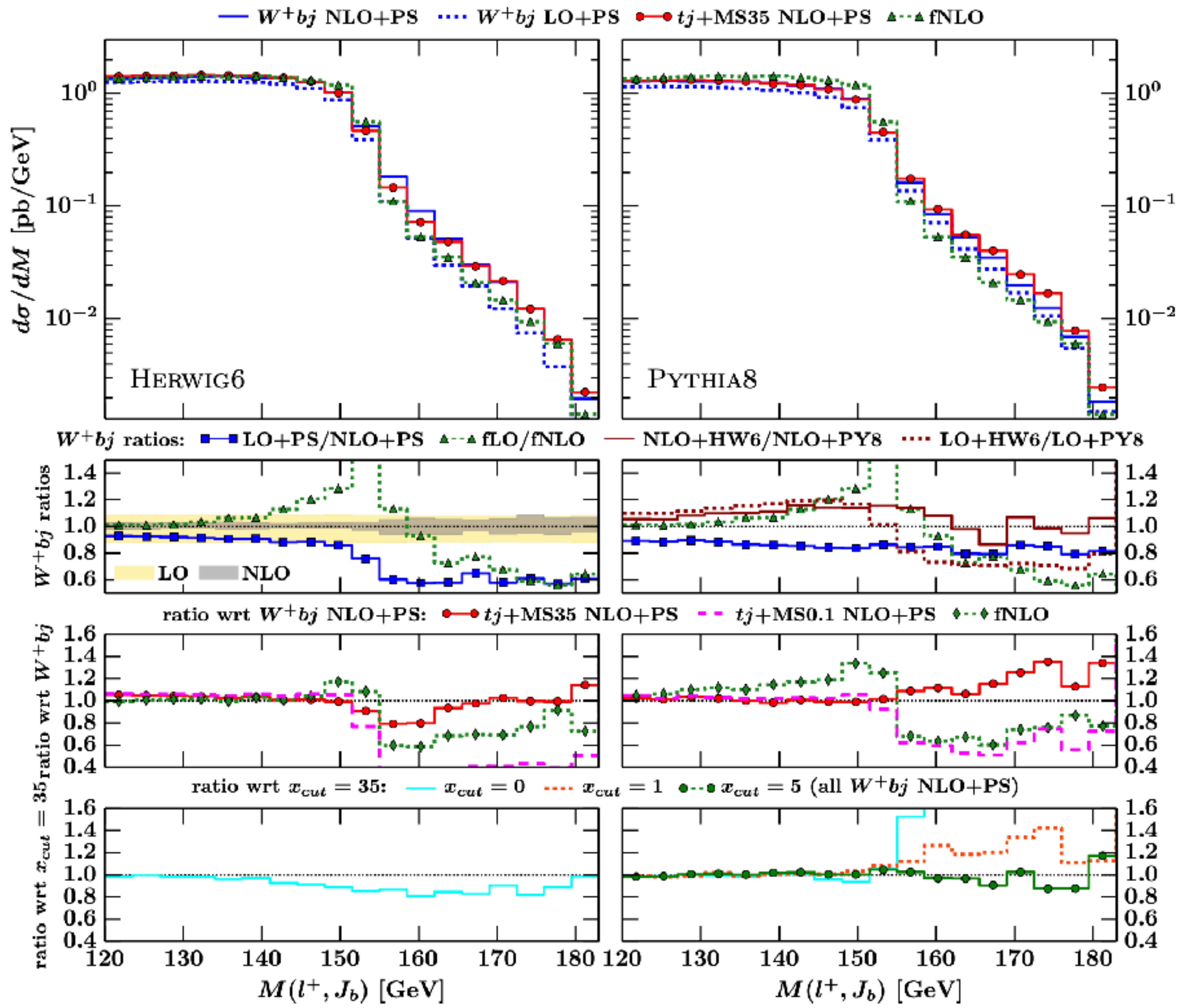
width of b-tagged jets



CMS Collaboration, *Phys.Rev.D 98 (2018) 9*

Resonance-aware matching with MC@NLO

- Consider simulation for the full 6-fermion process at NLOPS with mg5_aMC@NLO
- Requires handling of intermediate resonant states in the matching to the shower



- Formalism exists and first applied to off-shell Wt production in the 4FS

R. Frederix et al, JHEP 06 (2016) 027

- definition of the MC@NLO MC counterterms
- treatment of resolved MC emissions off intermediate resonances
- Writing of resonances information in the LHE record (for correct shower treatment)

Bb4l with mg5_aMC@NLO

- Generation done with mg5_aMC@NLO public code v2.9.13

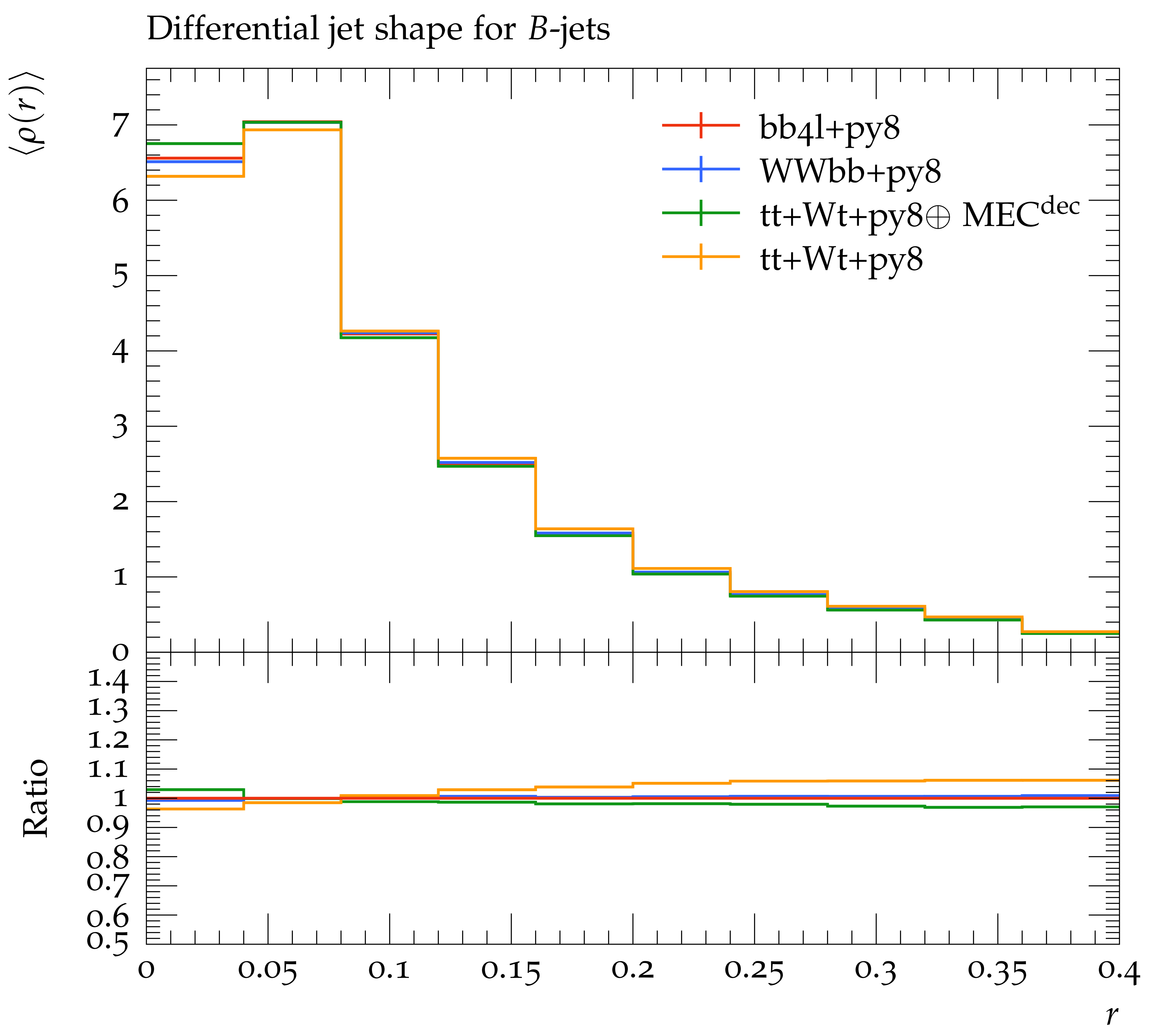
```
import model loop_sm
define  mupm = mu+ mu-
define epm = e+ e-
define vmupm = vm vm~
define vepm = ve ve~
set complex_mass_scheme
generate p p > epm mupm vmupm vepm b b~ [QCD]
```

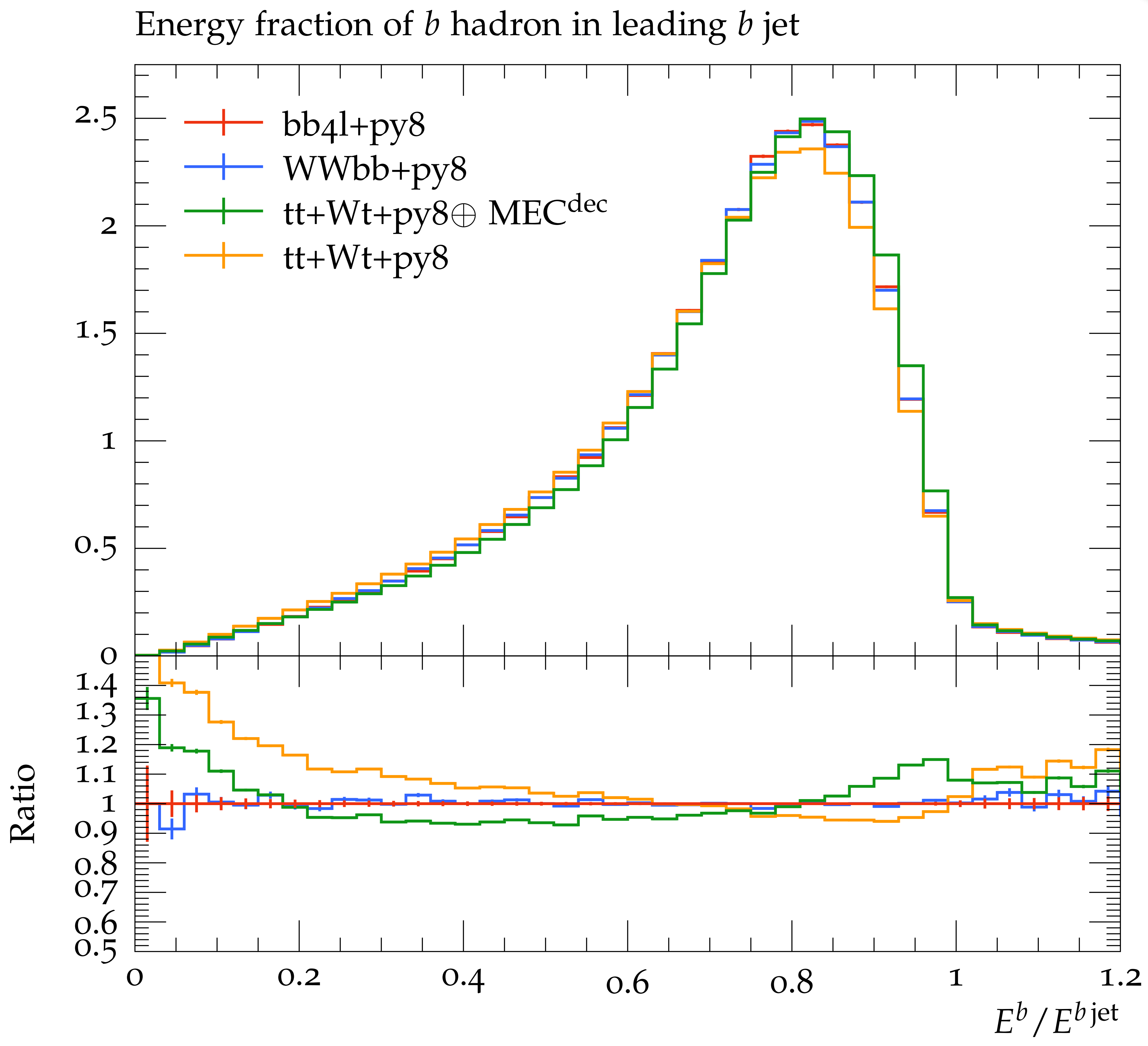
- m_{top} =172.5, Γ_{top}=1.33 GeV, NNPDF31nnlo 4FS PDFs
- Consider both bb4l process and WWbb + Madspin
  - Decaying the Ws with Madspin allows for same-flavor dileptonic decays or semileptonic (*but would be missing some non-resonant diagrams!!*)
- Compare to standard ttbar+Wt production + Madspin (using a LO top-width)

Properties of b-quark jets

- Distributions sensitive to radiation in top decay exhibit differences at the 10% level between LOPS and NLOPS simulations
- MEC in decays improve the agreement with bb4l, but residual differences around the peak of the fragmentation-function

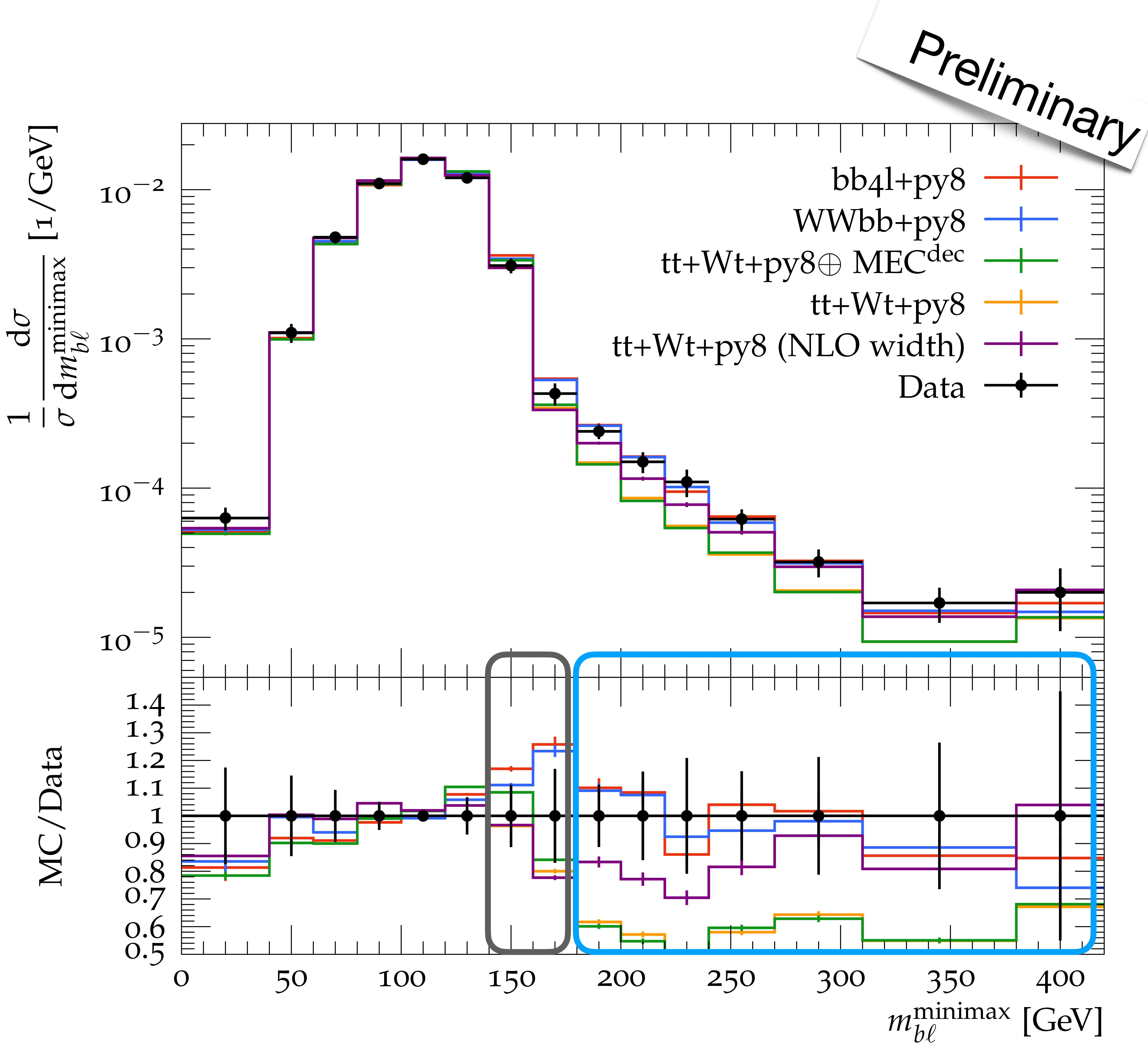
Preliminary





Description of the off-shell region

- ATLAS 13 TeV measurement of $m_{bl}^{minimax}$ used as benchmark
- Good description of the data with both bb4l and WWbb+Madspin
- MEC to top decay brings tt+Wt closer to bb4l around the kinematic edge
- tt+Wt with LO width significantly below the data in the off-shell region
- Better agreement with an NLO width



ATLAS Collaboration, *Phys.Rev.Lett.* 121 (2018) 15

Computational considerations

- MEC to top decays do not impact computing performance
- Improved accuracy of bb4l and WWbb comes with computational cost:
  - Longer integration/event generation time
  - Large fraction of negative weighted events
- Mitigation techniques such as ***folding*** or ***MC@NLO-Δ*** matching* do not change the negative weight fraction significantly *R. Frederix et al, JHEP 07 (2020) 238*
  - Still helpful as one needs to simulate/ntuplise/analyse less events

	MC@NLO			MC@NLO-Δ		
Folding parameters ($n\xi$, ny , $n\varphi$)	111	221	441	111	221	441
Neg. events fraction	43.55 %	42.08 %	41.08 %	40.87 %	37.66 %	36.09 %
Relative cost function c(f)	60.09	39.86	31.42	30.00	16.42	12.92
Elapsed time 10^3 events (min)	16	30	68	24	51	94
Effective time (c(f) $\times$ time) (min)	961	1196	2137	720	837	1215

* New public version of ***MC@NLO-Δ*** expected to perform better

Summary

- Presented two approaches to *improve the simulation of top-quark production* processes with the mg5_aMC@NLO program

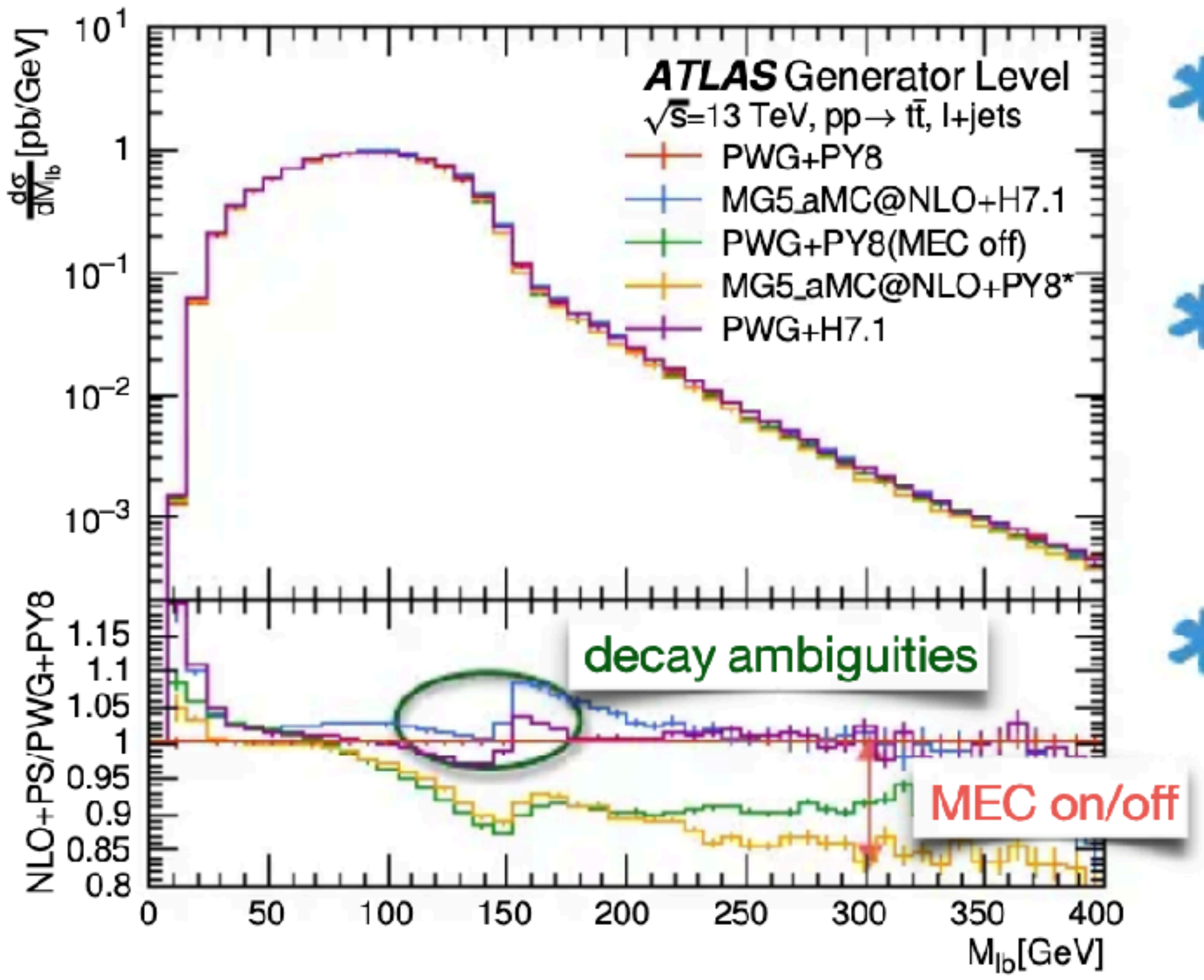
- Inclusion of *Matrix-Element Corrections to resonance decays* https://amcatnlo.web.cern.ch/amcatnlo/list_detailed2.htm
  - Promotes radiation from top decays to NLO accuracy (requires special settings)
  - Reduces differences across generators

- Full *off-shell calculation of the bb4l process* or WWbb+Madspin
  - NLO accuracy for top decays and interference with Wt process
  - Comes at a significant computational burden (CPU cost and negative weights fraction)

- Very *relevant for LHC phenomenology* and precision top-quark measurements

Backup

- Some differences in the Pythia8 settings used to shower mg5_aMC events, to be consistent with the MC subtraction
  - **Matrix-Element corrections** (MEC) to the top decay are used when showering Powheg events, but not in mg5_aMC@NLO
  - An event-wide **global recoil** is used for the Pythia8 FSR emissions



ATL-PHYS-PUB-2020-023

- Huge effect when considering top decay sensitive observables
- Disabling MEC to the decay in Powheg restores agreement with mg5_aMC@NLO
- H7 adds MEC in MC@NLO matching, unclear if this adds some double-counting

18