

Katharina Voß

# Modelling systematics in ATLAS: Top quark pairs

CPPS Retreat, Meinerzhagen  
16<sup>th</sup> February 2024





# Modelling studies in ATLAS

Goal of modelling studies in ATLAS is the improvement in modelling uncertainties through:

- **Validation of improved nominal samples**  
(e.g. scale uncertainty reduction through higher order accuracy in event generation)
- **Improving modelling uncertainty prescription**  
(e.g. remove overestimation of modelling uncertainty through double-counting)

In the following slides:

An overview of the Powheg+Pythia8 [ $t\bar{t}$  hvq] modelling uncertainty prescription and on-going studies within ATLAS to improve it



# Uncertainty prescription for the $t\bar{t}$ process

## Hard process generation

- **renormalisation and factorisation scale uncertainty**  
varying  $(K_R, K_F) \in \{(1, 0.5), (1, 2), (0.5, 1), (2, 1)\}$  with  $\mu_{R/F} = K_{R/F}\mu_0$
- **PDF uncertainty**  
PDF4LHC variations added in quadrature (nominal NNPDF3.0)
- **NNLO reweighting**  
use NNLO reweighting based on truth  $p_T^{t\bar{t}}$ ,  $m_{t\bar{t}}$ ,  $p_T^t$  and  $p_T^{\bar{t}}$
- **$h_{\text{damp}}$  variation**  
compare nominal  $h_{\text{damp}} = 1.5m_{\text{top}}$  to  $h_{\text{damp}} = 3m_{\text{top}}$
- **top quark mass**  
compare nominal  $m_{\text{top}} = 172.5$  GeV to  $m_{\text{top}} \in \{172.0, 173.0\}$  GeV samples



# NNLO reweighting uncertainty

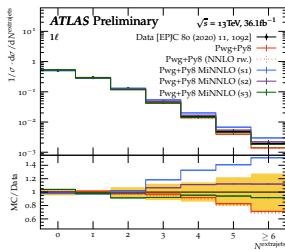
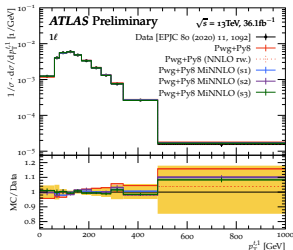
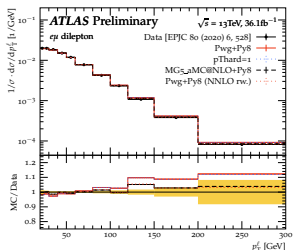
Improving modelling uncertainty prescription: NNLO reweighting  
Validation of improved nominal model:  $t\bar{t}$  MiNNLO

Top  $p_T$  modelled better by aMC@NLO compared to Powheg

→ now introduced NNLO reweighting uncertainty (recursively,  $p_{T\bar{t}}^t, m_{t\bar{t}}, p_T^t, p_T^{\bar{t}}$ )

Moving to  $t\bar{t}$  MiNNLO: studying matching options [ATL-PHYS-PUB-2023-029]

- (s1)  $p_T^{\text{def}} = 1$  (Py8 default),  $p_T^{\text{hard}} = 0$  (Py8 default)
- (s2)  $p_T^{\text{def}} = 2$  (ATLAS  $t\bar{t}$  default),  $p_T^{\text{hard}} = 0$  (Py8 default)
- (s3)  $p_T^{\text{def}} = 1$  (Py8 default),  $p_T^{\text{hard}} = 1$



# u $t\bar{t}/tW$ interference

Validation of improved nominal sample:  $bb4\ell$

Powheg+Pythia8  $t\bar{t}$  hvq (+tW DR)

Separate simulation of  $t\bar{t}$  and  $[tW$  (Powheg+Pythia8)] final state at NLO+PS  
→ afterwards stack simulated events

**Why is this a problem?**

Real emission correction to  $tW$  Born process includes  $gg/q\bar{q} \rightarrow W^- t\bar{b}$ :

$$\begin{aligned} |\mathcal{M}|^2 &= |\mathcal{M}^{Wt\bar{b}} + \mathcal{M}^{t(\bar{t} \rightarrow W\bar{b})}|^2 \\ &= |\mathcal{M}^{Wt\bar{b}}|^2 + 2\text{Re}\mathcal{M}^{Wt\bar{b}}\mathcal{M}^{t(\bar{t} \rightarrow W\bar{b})} + |\mathcal{M}^{t(\bar{t} \rightarrow W\bar{b})}|^2 \end{aligned}$$



→ huge NLO corrections since  $\sigma_{\text{LO}}(Wt) < \sigma_{\text{LO}}(t\bar{t})$

**Does it makes sense to talk about a  $Wt$  production or only about  $WWb$  and  $WWbb$ ?**

Yes, in phase space regions with small interference (see e.g. [\[arXiv:0908.0631\]](https://arxiv.org/abs/0908.0631)):

- $|\mathcal{M}^{Wt\bar{b}}|^2$  NLO correction to  $Wt$
- LO  $t\bar{t}$  separate process that can be removed

# u $t\bar{t}/tW$ interference

Validation of improved nominal sample:  $bb4\ell$

Powheg+Pythia8  $t\bar{t} \text{ hvq}$  (+ $tW$  DR)

Real emission correction to  $tW$  Born process includes  $gg/q\bar{q} \rightarrow W^- t\bar{b}$ :

$$\begin{aligned} |\mathcal{M}|^2 &= |\mathcal{M}^{Wt\bar{b}} + \mathcal{M}^{t(\bar{t} \rightarrow W\bar{b})}|^2 \\ &= |\mathcal{M}^{Wt\bar{b}}|^2 + 2\text{Re}\mathcal{M}^{Wt\bar{b}}\mathcal{M}^{t(\bar{t} \rightarrow W\bar{b})} + |\mathcal{M}^{t(\bar{t} \rightarrow W\bar{b})}|^2 \end{aligned}$$



**How can we check that applied cuts indeed reduce the sensitivity to the interference terms?**

→ compare two different approximations to remove  $t\bar{t}$  effects in  $Wt$  NLO calculation

- Diagram Removal (DR):  $\mathcal{M}^{\text{DR}} = \mathcal{M}^{Wt\bar{b}} \rightarrow |\mathcal{M}^{\text{DR}}|^2 = |\mathcal{M}^{Wt\bar{b}}|^2$
- Diagram Subtraction (DS):  $|\mathcal{M}^{\text{DS}}|^2 = |\mathcal{M}^{Wt\bar{b}} + \mathcal{M}^{t(\bar{t} \rightarrow W\bar{b})}|^2 - \mathcal{C}^{\text{SUB}}$ , with  $\mathcal{C}^{\text{SUB}} \rightarrow |\mathcal{M}^{t(\bar{t} \rightarrow W\bar{b})}|^2$  for  $m_{Wb} \rightarrow m_t$

$|\mathcal{M}^{\text{DS}}|^2 - |\mathcal{M}^{\text{DR}}|^2 = \text{interference term} = 2\text{Re}\mathcal{M}^{Wt\bar{b}}\mathcal{M}^{t(\bar{t} \rightarrow W\bar{b})}$  (if  $\mathcal{C}^{\text{SUB}} - |\mathcal{M}^{t(\bar{t} \rightarrow W\bar{b})}|^2$  small)

→ if  $|\mathcal{M}^{\text{DS}}|^2 \sim |\mathcal{M}^{\text{DR}}|^2$  (DR/DS uncertainty small), then in phase space region with small interference between  $t\bar{t}$  and  $tW$

# u $t\bar{t}/tW$ interference

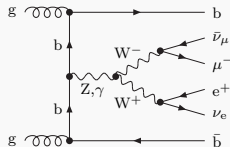
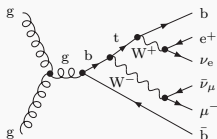
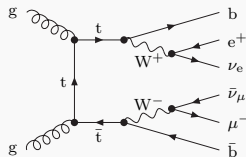
Validation of improved nominal sample:  $bb4\ell$

$bb4\ell$  [arXiv:1607.04538] [arXiv:2307.15653]

Matrix element calculation includes double-, single- and non-resonant diagrams

→ interference terms fully included without approximation at NLO

→ no additional  $tW$  sample to describe  $WWbb$  final state



Currently developing modelling uncertainty prescription for the  $bb4\ell$  process

**Strategy:** Compare systematic uncertainties in Powheg+Pythia8  $t\bar{t}$  and  $bb4\ell$  using the same prescription



# Uncertainty prescription for the $t\bar{t}$ process

Improving modelling uncertainty prescription: targeted matching uncertainty

## Matching uncertainty [ATL-PHYS-PUB-2023-029]

- Pythia 8  $p_T^{\text{hard}}$  variation  
compare nominal  $p_T^{\text{hard}} = 0$  to  $p_T^{\text{hard}} = 1$  sample

Previous matching uncertainty definition in ATLAS: Pwg+Py8 vs. MG\_aMC@NLO+Py8

→ convolutes multiple modelling differences, not only matching uncertainty!

→ updated matching uncertainty: variation of Py8 parameter  $p_T^{\text{hard}}$  [SciPostPhys.12(2022)010]

## What is $p_T^{\text{hard}}$ ?

Showering of Pwg LHE files with Py8: vetoed shower = generate emissions with Py8 in full, unrestricted phase space, but then veto emissions which have hardness scale  $>$  Pwg scale

How is the Pwg scale determined?

- Born-like events: SCALUP value of LHE information
- real emission events:
  - $p_T^{\text{hard}} = 0$  (default): SCALUP value of LHE information
  - $p_T^{\text{hard}} = 1$ :  $\min(p_T$  of Pwg emission w.r.t. all other FS particles or beam axis )
  - $p_T^{\text{hard}} = 2$ :  $\min(p_T$  of all FS particles w.r.t. each-other and w.r.t. the beam axis )



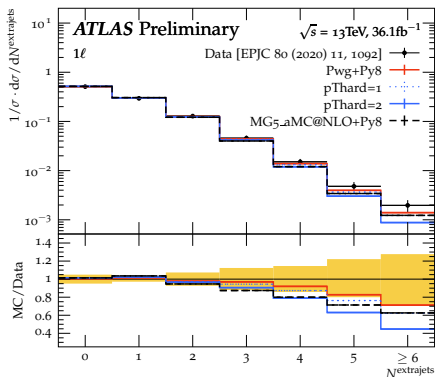
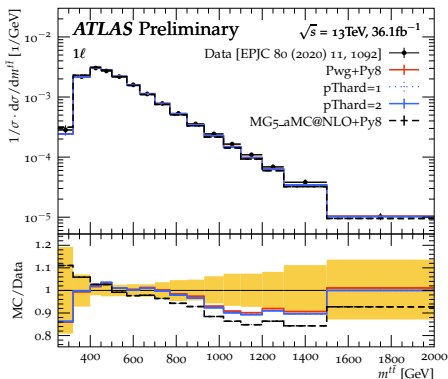


# Uncertainty prescription for the $t\bar{t}$ process

Improving modelling uncertainty prescription: targeted matching uncertainty

Matching uncertainty [ATL-PHYS-PUB-2023-029]

- Pythia 8  $\rho_T^{\text{hard}}$  variation  
compare nominal  $\rho_T^{\text{hard}} = 0$  to  $\rho_T^{\text{hard}} = 1$  sample





# Uncertainty prescription for the $t\bar{t}$ process

## Parton shower uncertainties

- **initial state radiation**

Pythia 8 Var3c variations, vary ISR  $\alpha_S(M_Z) = \{0.115, 0.140\}$ , nominal  $\alpha_S(M_Z) = 0.127$  [ATL-PHYS-PUB-2014-021]

- **final state radiation**

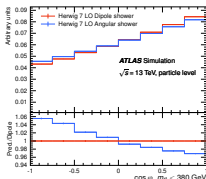
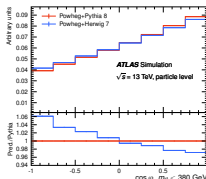
vary  $\mu_R$  FSR splitting kernels by factor 0.5 and 2

- **parton shower**

comparison of nominal Pwg+Py8 with Pwg+Herwig 7 (H7)

**Improving modelling uncertainty prescription:** factorised parton shower uncertainty

Example entanglement in  $t\bar{t}$  [2311.07288]:



→ dipole vs angular ordered shower has the largest influence on the Py8 vs H7 difference in the entanglement measurement

**Goal:** factorised parton shower uncertainty to understand which part of the parton shower modelling (e.g. shower ordering or hadronisation) influences measurement the most



# Uncertainty prescription for the $t\bar{t}$ process

## Specialised uncertainty definitions

- **top line shape** (only for analysis in off-shell region)  
comparison of nominal Pwg+Py8 to Pwg+MadSpin+Py8  $t\bar{t}$  sample
- **recoil-to-top**  
compare nominal (recoil-to-colour) to alternative recoil-to-top sample
- **underlying event**  
Py8 A14 Var1 variations (MPI and UE tuning parameters) [\[ATL-PHYS-PUB-2014-021\]](#)
- **colour reconnection**  
comparison of nominal to tuned results with different CR models CR1 and CR2  
[\[ATL-PHYS-PUB-2017-008\]](#)

# u Top lineshape uncertainty

**Improving modelling uncertainty prescription:** dedicated line shape uncertainty

**Validation of improved nominal sample:**  $bb4\ell$

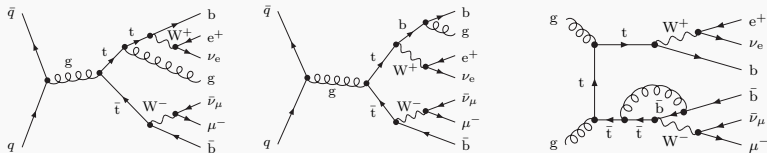
$P_{\text{whg}}+P_{\text{y8}}$   $t\bar{t}$   $h\nu q$ : narrow width approximation + LO top decay

Narrow width approximation: simulate  $t\bar{t}$  with on-shell final state particles and subsequent top decay at LO with Breit-Wigner smearing of the top quark invariant masses

[Frixione,Laenen,Motylinski,Webber-method arXiv:0702198]

$bb4\ell$ : complete offshell effects and top decay at NLO

Description of top decay at NLO:



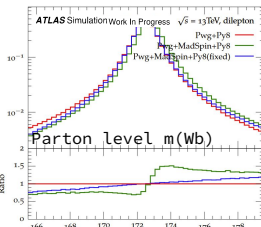
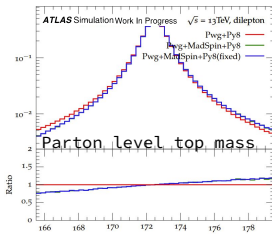
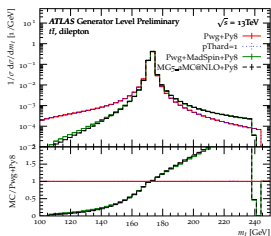
& top off-shell effects are included without approximation since full top quark propagator is used in NLO matrix element calculation

# Top lineshape uncertainty

**Improving modelling uncertainty prescription:** dedicated line shape uncertainty

**Validation of improved nominal sample:**  $bb4\ell$

Recently introduced top line shape uncertainty in the Powheg+Pythia8  $h\nu q t\bar{t}$  uncertainty prescription to quantify the discrepancy between  $h\nu q$  internal and external MadSpin implementations of Breit-Wigner smearing of top quark mass [ATL-PHYS-PUB-2023-029]



→ top line shape uncertainty can be sizeable e.g. in top mass measurements → uncertainty removed when moving to  $bb4\ell$



# Conclusions and Outlook

Goal of modelling studies in ATLAS is the improvement in modelling uncertainties through:

- **Validation of improved nominal samples**
  - $bb4\ell$
  - $t\bar{t}$  MiNNLO
  - $t\bar{t}$  Powheg+VINCIA
- **Improving modelling uncertainty prescription**
  - recently finished:  $p_T^{\text{hard}}$ , lineshape, NNLO reweighting
  - factorised parton shower uncertainty study



# Conclusions and Outlook

Goal of modelling studies in ATLAS is the improvement in modelling uncertainties through:

- **Validation of improved nominal samples**
  - $bb4\ell$
  - $t\bar{t}$  MiNNLO
  - $t\bar{t}$  Powheg+VINCIA
- **Improving modelling uncertainty prescription**
  - recently finished:  $p_T^{\text{hard}}$ , lineshape, NNLO reweighting
  - factorised parton shower uncertainty study

**Thank you for your attention!**



**Back Up**

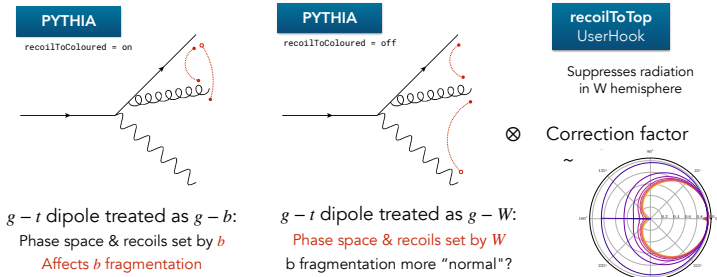


# u Recoil uncertainty

Validation of improved nominal sample: Powheg+VINCIA

**ATLAS default**  $t\bar{t}$  Powg+Py8 setting:  
`recoilToColoured = on` → out of cone radiation is suppressed

**Recoil-to-top:**  $W$ -boson as a recoiler (more out of cone radiation), but multiply with correction factor → in principle the better description!



( graphic taken from [Peter Skands] )

**Uncertainty prescription:**  $t\bar{t}$  Powg+Py8 vs.  $t\bar{t}$  Powg+Py8 with [TopRecoil UserHook]

→ especially top mass measurement found to be sensitive to this uncertainty

→  $t\bar{t}$  Powheg+VINCIA sample would provide correct emission pattern, matching options currently studied in ATLAS



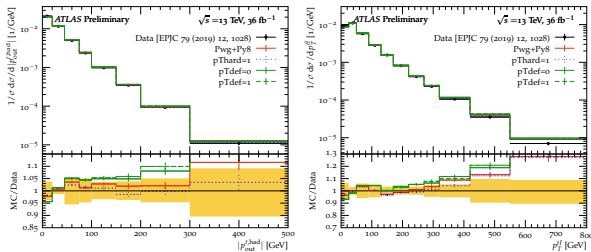
# Comparison with $p_T^{\text{def}}$ variation

## What is $p_T^{\text{def}}$ ?

Which  $p_T$  definition is used when calculating the hardness in the matching?

- $p_T^{\text{def}} = 0$ : Pwg ISR  $p_T$  definition for ISR and FSR
- $p_T^{\text{def}} = 1$  (Pythia 8 default): Pwg ISR  $p_T$  and FSR  $d_{ij}$  definition
- $p_T^{\text{def}} = 2$  (ATLAS default): Pythia 8  $p_T$  definition

→ ATLAS default  $p_T^{\text{def}} = 2$  chosen due to better data-MC agreement



→  $p_T^{\text{def}}$  variation has large effect on presented variables, mostly worsening data-MC agreement