Katharina Voß
on behalf of the ATLAS collaboration

Studies on the improvement of the matching uncertainty definition in top-quark processes simulated with Powheg+Pythia 8 in ATLAS

Open LHC Top WG Meeting

30th November 2023

Outline

New ATLAS matching uncertainty prescription for Powheg+Pythia 8 (Pwg+Py8) top processes based on Pythia 8 p_T^{hard} parameter
[ATL-PHYS-PUB-2023-029]
→ made public on the 21.09.2023
→ summarises studies of matching uncertainty in $t\bar{t}$, t-channel single top and tW processes
In these slides:

- comparison of previous and new prescription in $t\bar{t}$ process
- comparison with p_T^{def} and h_{damp} variation
- introduction of NNLO reweighting and top line shape uncertainty

Uncertainty prescription in Pwg+Py8 $t\bar{t}$ process in ATLAS

- **Status and ongoing studies: nominal samples**
  - top pair production
  - single-top associated production: tW
- **Examples of analyses strongly influenced by modelling systematics**
  - m_{top} measurement (recoil-to-top)
  - entanglement measurement (parton shower uncertainty)

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

Previous matching uncertainty definition for top processes in ATLAS:
compare nominal Pwg+Py8 to MG_aMC@NLO+Py8 sample
→ convolutes multiple modelling differences, not only matching uncertainty!
→ matching uncertainty now updated to use variation of Py8 parameter $p_{\mathrm{T}}^{\mathrm{hard}}$ [SciPost Phys. 12 (2022) 010]

What is $p_{\mathrm{T}}^{\mathrm{hard}}$?

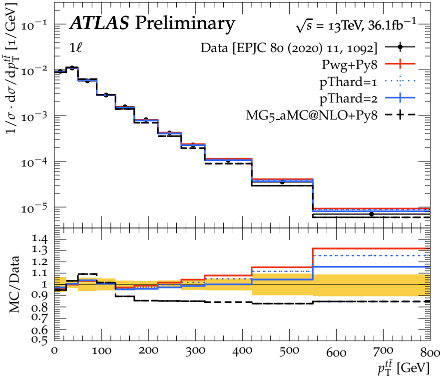
Showering of Pwg LHE files with Py8:
vetoed shower = generate emissions with Py8 in full, unrestricted phase space, but then veto emissions which have hardness scale > Pwg scale

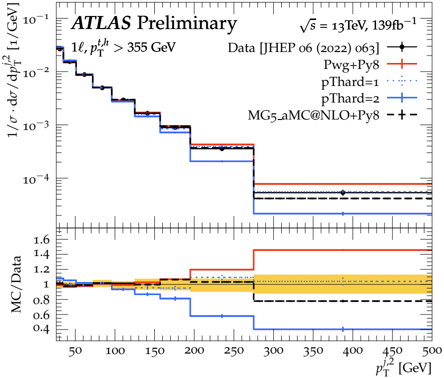
How is the Pwg scale determined?

- Born-like events: SCALUP value of LHE information
- real emission events:
  - $p_{\mathrm{T}}^{\mathrm{hard}} = 0$ (default): SCALUP value of LHE information
  - $p_{\mathrm{T}}^{\mathrm{hard}} = 1$: min(p_{T} of Pwg emission w.r.t. all other final-state particles, p_{T} of Pwg emission w.r.t. the beam axis)
  - $p_{\mathrm{T}}^{\mathrm{hard}} = 2$: min(p_{T} of all final-state particles w.r.t. each-other, p_{T} of all final state particles w.r.t. the beam axis)

Matching uncertainty in $t\bar{t}$ distributions

Distributions sensitive to matching uncertainty = observables which are sensitive to the available radiation phase space
→ $p_T^{t\bar{t}}$, p_T^{j} not from top decay, N_{jets}





→ difference through p_T^{hard} variation, as well as clear difference between MG_aMC@NLO+Py8 and Pwg+Py8 sample

Matching uncertainty in $t\bar{t}$ distributions

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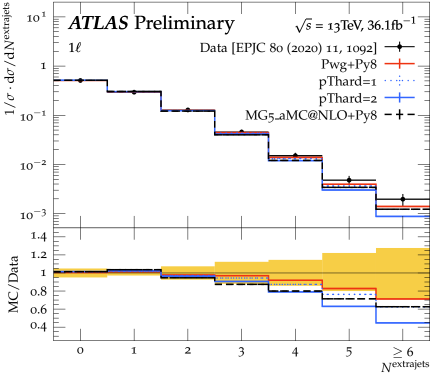
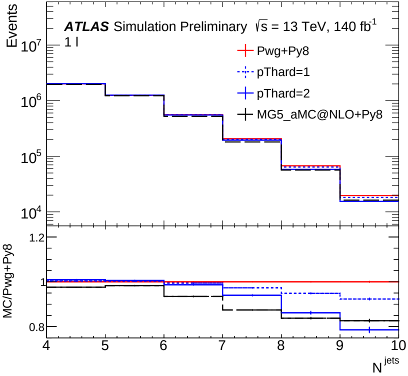


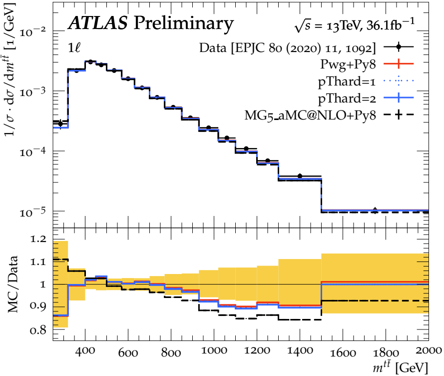


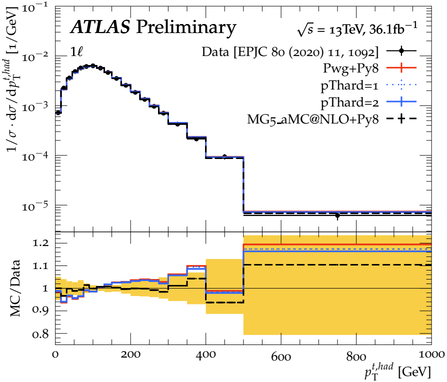
→ again clear difference through p_T^{hard} variation, both on particle and reconstructed level

Matching uncertainty in $t\bar{t}$ distributions

Distributions not sensitive to matching uncertainty = observables which are not strongly sensitive available radiation phase space

→ $m_{t\bar{t}}$, p_T of the top-quark, p_T of top-quark decay products





→ not sensitive to p_T^{hard} variation, but difference between MG_MC@NLO+Py8 and Pwg+Py8!

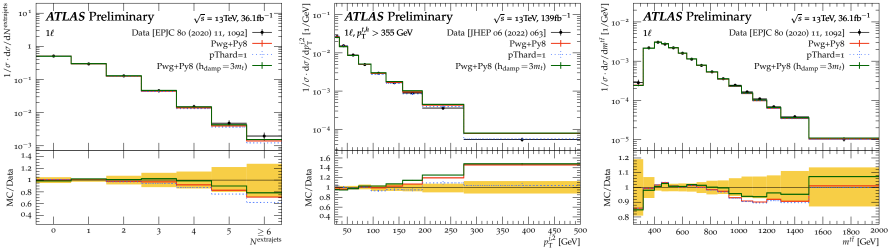
→ p_T^{hard} variation offers targeted matching uncertainty definition

→ $p_T^{hard} = 1$ variation in uncertainty definition due to better agreement with unfolded data

Comparison with h_{damp} variation

Question: How does the h_{damp} variation compare with the $p_{\text{T}}^{\text{hard}}$ variation, since h_{damp} influences the generation of the hardest emission?
Comparison of

- nominal $t\bar{t}$ Pwg+Py8 ($h_{\text{damp}} = 1.5\, m_{\text{top}},\ p_{\text{T}}^{\text{hard}} = 0$)
- $p_{\text{T}}^{\text{hard}}$ varied $t\bar{t}$ Pwg+Py8 ($h_{\text{damp}} = 1.5\, m_{\text{top}},\ p_{\text{T}}^{\text{hard}} = 1$)
- h_{damp} varied $t\bar{t}$ Pwg+Py8 ($h_{\text{damp}} = 3\, m_{\text{top}},\ p_{\text{T}}^{\text{hard}} = 0$)



→ no strong connection between the h_{damp} and $p_{\text{T}}^{\text{hard}}$ variations found, some distributions only influenced by one of the two, some influenced in different ways

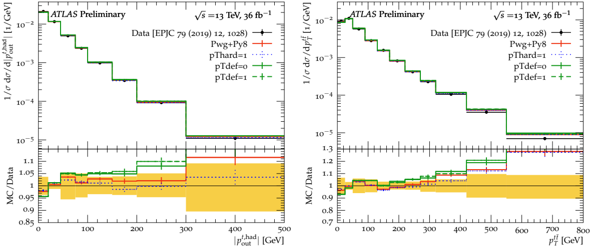
Comparison with p_T^{def} variation

What is p_T^{def}?

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

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

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

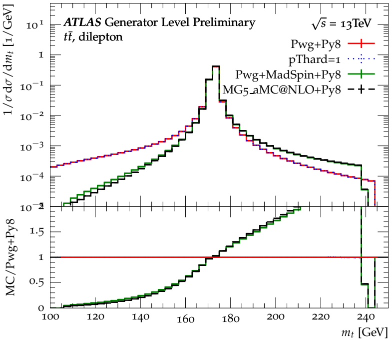


→ p_T^{def} variation has large effect on presented variables, mostly worsening data-MC agreement

New uncertainty definition: top line shape

Previous Pwg+Py8 and MG_aMC@NLO+Py8 comparison also covered difference in the top quark decay modelling and in the approximation of off-shell effects

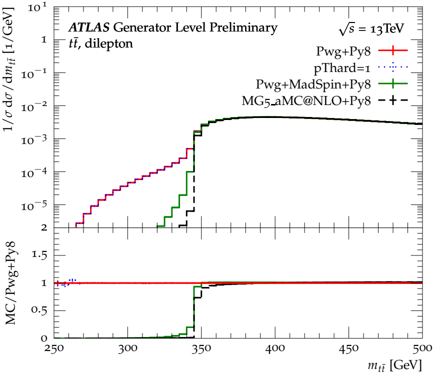
→ introduce new Pwg+MadSpin+Py8 sample, which follows closely the top quark line shape from MG_aMC@NLO+Py8 sample at parton level

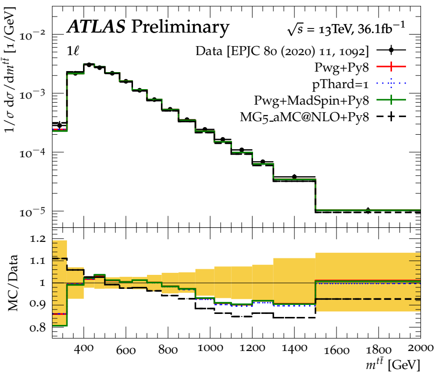


Caveat: mis-match between treatment of MadSpin and Pythia 8 of *b*-quarks leads to non-conservation of invariant mass after the top decay $m(t) \neq m(Wb)$ and increase of the top line shape uncertainty at particle level

Solution: special MadGraph model with massive and massless *b*-quarks and relabelling of particle IDs in LHE files

New uncertainty definition: top line shape

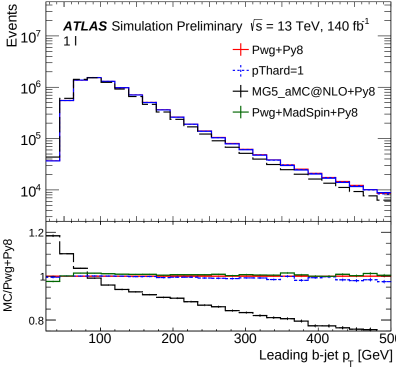


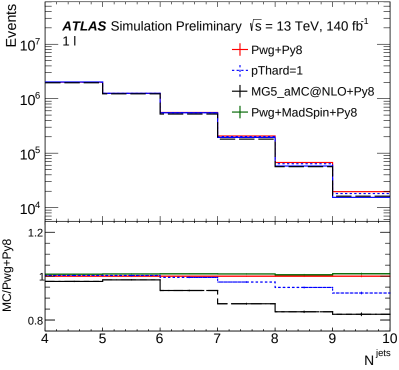


→ difference in parton level in low $m_{t\bar{t}}$ region between Pwg+Py8 and Pwg+MadSpin+Py8 also seen in low $m_{t\bar{t}}$ reconstructed distribution

→ no large deviation of the Pwg+Py8 and MG_aMC@NLO+Py8 parton level high $m_{t\bar{t}}$ distribution, but difference seen in reconstructed $m_{t\bar{t}}$ = not just top line shape effect

New uncertainty definition: top line shape



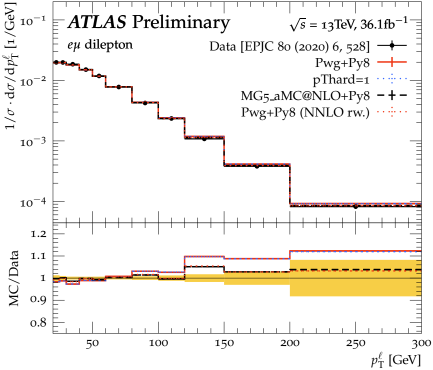


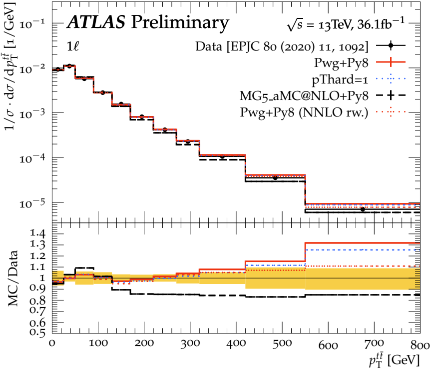
→ clear difference between Pwg+Py8 and MG_aMC@NLO+Py8 in leading b-jet p_T (influences selection efficiency) and N_{jets}

→ observables, which should not depend on line shape, do not show large difference between Pwg+Py8 and Pwg+MadSpin+Py8

New uncertainty definition: NNLO reweighting

Comparison of Pwg+Py8 and MG_aMC@NLO+Py8 also covered accidentally the mismodelling of the top p_{T}:
$t\bar{t}$ MG_aMC@NLO+Py8 was found to model the top p_{T} shape better than Pwg+Py8
→ now added a dedicated uncertainty:
reweighting recursively the truth $p_{\mathrm{T}}^{t\bar{t}}$, $m_{t\bar{t}}$, p_{T}^{t} and $p_{\mathrm{T}}^{\bar{t}}$ to NNLO

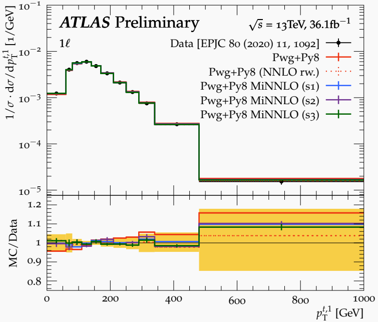




Studies on nominal $t\bar{t}$ sample

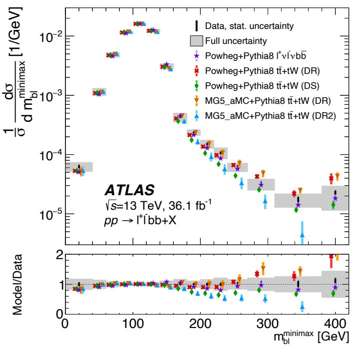
Nominal ATLAS $t\bar{t}$ samples is modelled with Pwg+Py8 (hvq)
→ studies on alternative nominal samples on-going (recipe for systematic uncertainties is needed for a new nominal sample)

Fixed order accuracy: MiNNLO



→ studying different matching options for $t\bar{t}$ MiNNLO [ATL-PHYS-PUB-2023-029]

$t\bar{t}/tW$ interference: $bb4\ell$

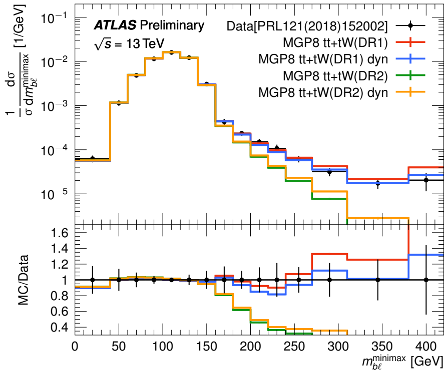


[PhysRevLett.121.152002]

Preliminary studies looking also at: $t\bar{t}$ Sherpa for high E_T^{miss} region, $t\bar{t}$ POWHEG+VINCIA

Studies on nominal tW

Studies on $t\bar{t}/tW$ interference presented in [ATL-PHYS-PUB-2021-042]
→ some improvement in data-MC agreement found using dynamical scale in aMC@NLO+Py8 and reduced difference between different subtraction schemes
→ tW with dynamical scales new ATLAS default for Pwg+Py8



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

Hard process generation

- **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)
- **new prescription: 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_{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

Matching uncertainty

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

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

Parton shower uncertainties

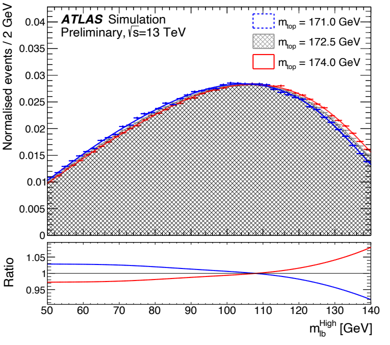
- **initial state radiation**
  Pythia 8 Var3c variations, vary ISR $\alpha_S(M_Z) = \{0.115, 0.140\}$, nominal $\alpha_S(M_Z) = 0.127$ [ATL-PHYS-PUB-2014-021]
- **final state radiation**
  vary FSR α_S by factor 0.5 and 2
- **parton shower**
  comparison of nominal Pwg+Py8 with Pwg+Herwig 7 (H7)

Specialised uncertainty definitions

- **new prescription: 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]

$t\bar{t}$ modelling uncertainties: m_{top} measurement

m_{top} in $t\bar{t} \to$ dilepton with template method at $\sqrt{s} = 13$ TeV [ATLAS-CONF-2022-058]



- Recoil-to-top: large impact
- Matrix-element matching: comparison of Pwg+Py8 and aMC@NLO+Py8
  $\to$ now new prescription to avoid double-counting of modelling systematics

	m_{top} [GeV]
Result	172.21
Statistics	0.20
Method	0.05 ± 0.04
Matrix-element matching	0.40 ± 0.06
Parton shower and hadronisation	0.05 ± 0.05
Initial- and final-state QCD radiation	0.17 ± 0.02
Underlying event	0.02 ± 0.10
Colour reconnection	0.27 ± 0.07
Parton distribution function	0.03 ± 0.00
Single top modelling	0.01 ± 0.01
Background normalisation	0.03 ± 0.02
Jet energy scale	0.37 ± 0.02
b-jet energy scale	0.12 ± 0.02
Jet energy resolution	0.13 ± 0.02
Jet vertex tagging	0.01 ± 0.01
b-tagging	0.04 ± 0.01
Leptons	0.11 ± 0.02
Pile-up	0.06 ± 0.01
Recoil effect	0.39 ± 0.09
Total systematic uncertainty (without recoil)	0.67 ± 0.05
Total systematic uncertainty (with recoil)	0.77 ± 0.06
Total uncertainty (without recoil)	0.70 ± 0.05
Total uncertainty (with recoil)	0.80 ± 0.06

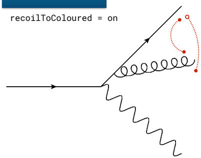
What is recoil-to-top?

ATLAS default $t\bar{t}$ Pwg+Py8 setting: `recoilToColoured = on` $\rightarrow$ out of cone radiation is supressed

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

PYTHIA

`recoilToColoured = on`



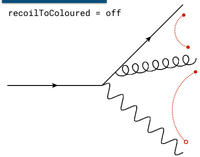
$g - t$ dipole treated as $g - b$:

Phase space & recoils set by b

Affects b fragmentation

PYTHIA

`recoilToColoured = off`



$g - t$ dipole treated as $g - W$:

Phase space & recoils set by W

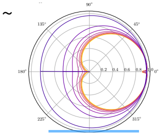
b fragmentation more "normal"?

recoilToTop UserHook

Suppresses radiation in W hemisphere

$\otimes$ Correction factor

~



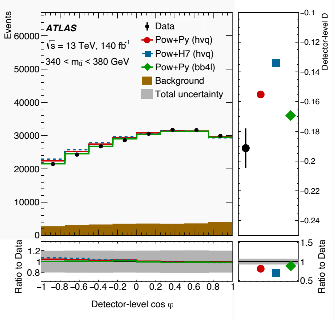
(graphic taken from [Peter Skands])

Uncertainty prescription: comparison of nominal $t\bar{t}$ Pwg+Py8 sample to $t\bar{t}$ Pwg+Py8 produced with the [TopRecoil UserHook]

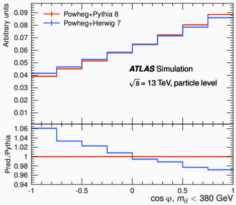
$\rightarrow$ number of analyses including this systematic uncertainty is increasing

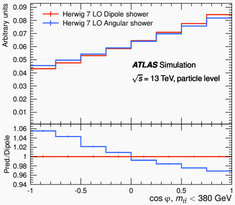
$t\bar{t}$ modelling uncertainties: entanglement

Entanglement in top pair production (dilepton) at $\sqrt{s} = 13$ TeV [arXiv:2311.07288]



Measured observable: average angle $\cos\phi$ between the two charged leptons in top and anti-top restframe





studied different hadronisation models
$\rightarrow$ negligible effect on $\cos\phi$

$\rightarrow$ PS uncertainty defined by comparison of Pwg+Py8 (nominal) and Pwg+H7 can lead to large uncertainty covering different uncertainty sources, completely factorised uncertainty definition would be desirable

Conclusions and Outlook

Nominal samples

- **top quark pair production**: working on improved description with MiNNLO and *bb*4ℓ
  → [*bb*4ℓ CMS talk in this session by Laurids Jeppe]
  → waiting for public release of `bb4l-sl` code
- tW **DR/DS**: recommendation to use dynamical scales
- **in general**: moving toward more recent generator versions and considering recent matrix element correction recommendations for MG_aMC@NLO+Py8 samples [arXiv:2308.06389]
  → [Talk in this session by Stefano Frixione]

Modelling uncertainties

- new prescription for **matching uncertainty** of varying Pythia 8 $p_{\mathrm{T}}^{\mathrm{hard}}$ parameter for $t\bar{t}$ and single top processes
  → targeted matching uncertainty, avoiding double-counting of systematic effects present in the previous comparison of Pwg+Py8 and MG_aMC@NLO+Py8 samples
- number of analyses using the **recoil-to-top uncertainty** prescription is increasing
- **factorised parton shower uncertainty** desirable to better identify and understand uncertainty sources

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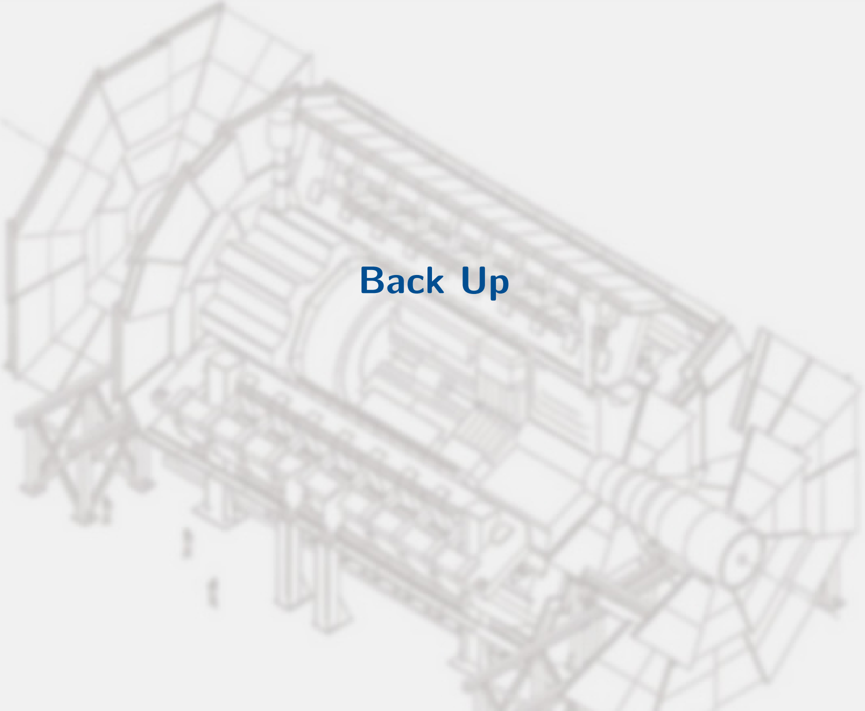
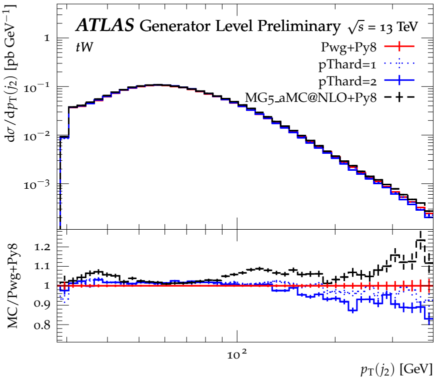
Thank you for your attention!

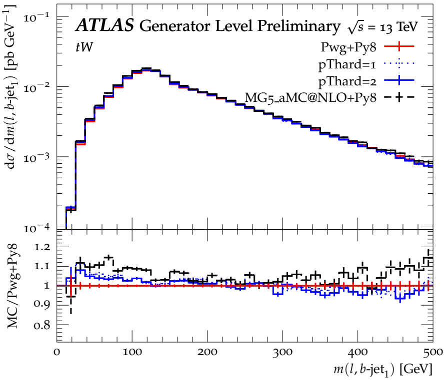
Back Up



Matching uncertainty in tW distributions

→ p_T^{hard} variation also tested in single top t-channel production and tW associated production





→ shape variation through p_T^{hard} variation in $p_T(j_2)$ distribution, which is sensitive to matching
→ smaller variation through p_T^{hard} variation in less matching-sensitive observable $m_{\ell b}$ than with MG_aMC@NLO+Py8

$t\bar{t}$ modelling uncertainties: $\sigma_{t\bar{t}}$ measurement

→ inclusive $\sigma_{t\bar{t}}$ measurement could profit strongly from $t\bar{t}$ NNLO+PS sample

Inclusive and differential $t\bar{t} \to$ dilepton cross section at $\sqrt{s} = 13$ TeV [JHEP 07 (2023) 141]

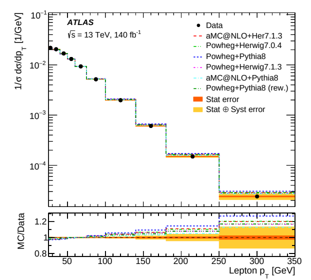
NNLO p_T^t rwgt. largest syst. uncertainty for inclusive measurement due to influence on preselection efficiency (top $p_T \to$ lepton p_T)

Source of uncertainty	$\Delta\sigma^{\text{fid}}_{t\bar{t}}/\sigma^{\text{fid}}_{t\bar{t}}$ [%]	$\Delta\sigma_{t\bar{t}}/\sigma_{t\bar{t}}$ [%]
Data statistics	0.15	0.15
MC statistics	0.04	0.04
Matrix element	0.12	0.16
h_{damp} variation	0.01	0.01
Parton shower	0.08	0.22
$t\bar{t}$ + heavy flavour	0.34	0.34
Top p_T reweighting	0.19	0.58
Parton distribution functions	0.04	0.43
Initial-state radiation	0.11	0.37
Final-state radiation	0.29	0.35
Electron energy scale	0.10	0.10
Electron efficiency	0.37	0.37
Electron isolation (in situ)	0.51	0.51
Muon momentum scale	0.13	0.13
Muon reconstruction efficiency	0.35	0.35
Muon isolation (in situ)	0.33	0.33
Lepton trigger efficiency	0.05	0.05
Vertex association efficiency	0.03	0.03
Jet energy scale & resolution	0.10	0.10
b-tagging efficiency	0.07	0.07
$t\bar{t}/Wt$ interference	0.37	0.37
Wt cross-section	0.52	0.52
Diboson background	0.34	0.34
$t\bar{t}V$ and $t\bar{t}H$	0.03	0.03
Z+jets background	0.05	0.05
Misidentified leptons	0.32	0.32
Beam energy	0.23	0.23
Luminosity	0.93	0.93
Total uncertainty	1.6	1.8

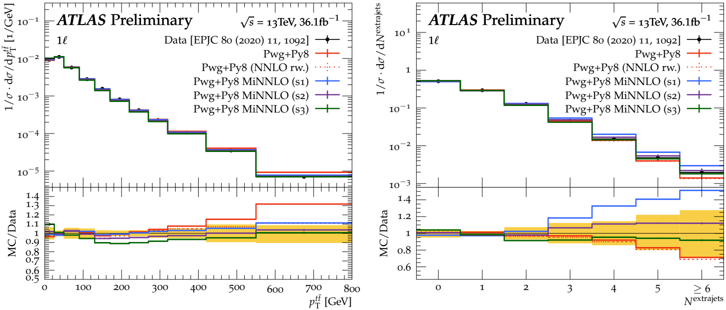
$G_{e\mu}$ ($e\mu$ reco. eff.),

$E_{e\mu} = A_{e\mu} \cdot G_{e\mu}, A_{e\mu} = N^{t\bar{t},\text{fiducial}}_{e\mu} / N^{t\bar{t}}$

Systematic uncertainty name	$\Delta C_b/C_b$ [%]	$\Delta G_{e\mu}/G_{e\mu}$ [%]	$\Delta E_{e\mu}/E_{e\mu}$ [%]
Matrix element	−0.10 ± 0.22	0.25 ± 0.11	0.29 ± 0.12
h_{damp}	−0.06 ± 0.08	−0.05 ± 0.04	−0.05 ± 0.05
Parton shower and hadronisation	0.16 ± 0.08	−0.26 ± 0.04	0.04 ± 0.05
Top p_T reweighting	0.03 ± 0.08	0.22 ± 0.04	0.61 ± 0.05
$t\bar{t}$ + heavy flavour	−0.33 ± 0.08	0.01 ± 0.04	0.01 ± 0.05
ISR (high)	−0.01 ± 0.08	0.06 ± 0.04	0.35 ± 0.05
ISR (low)	0.04 ± 0.08	−0.13 ± 0.04	−0.35 ± 0.05
FSR (high)	0.05 ± 0.09	−0.07 ± 0.04	−0.12 ± 0.05
FSR (low)	−0.09 ± 0.15	0.10 ± 0.07	0.16 ± 0.09
PDF	0.02 ± 0.08	0.04 ± 0.04	0.42 ± 0.05



Studies on nominal $t\bar{t}$ sample: MiNNLO



→ studying different matching options for $t\bar{t}$ MiNNLO [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), $p_T^{\text{hard}} = 1$