



Top Quark Modelling and Tuning in ATLAS and CMS

TOP2021 September 14, 2021

Giulia Negro on behalf of the ATLAS and CMS Collaborations

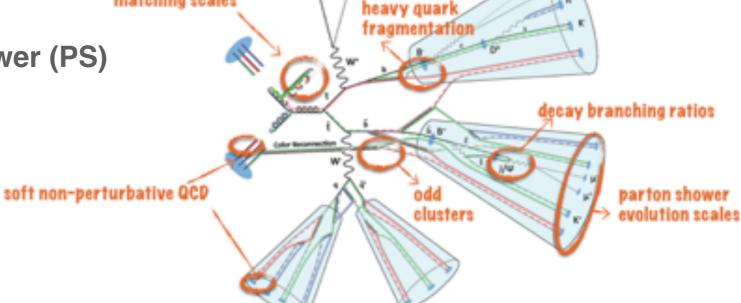
ATLAS helper: Dominic Hirschbühl





Introduction

- MC simulation is a crucial ingredient in top quark analyses:
 - good modelling of data and high accuracy predictions for interpretations
 - well-defined (small!) uncertainties → limiting factor in many precision measurements and searches
- ATLAS and CMS use same generators but have different modelling uncertainty prescriptions:
 - understanding how to combine the differing strategies of ATLAS and CMS is critical
 - <u>LHCtopWG</u> is ideal forum to discuss how to reduce modelling systematics
- TOP groups in both experiments have 'standard' recommendations to assess uncertainties → never to be considered as fixed recipes
 - matrix-elements (ME) scale: μ_R^{ME} and μ_F^{ME} scale variations
 - **PDF**: usually PDF4LHC recommendations
 - top quark p_T modeling and top quark mass: very analysis-dependent
 - uncertainties involving parton shower (PS) generator → next slides



Systematic unc.	CMS	ATLAS
ISR and FSR	Independent μ_{R}^{ISR} , μ_{R}^{FSR} scale	e variations with factor (2,0.5)

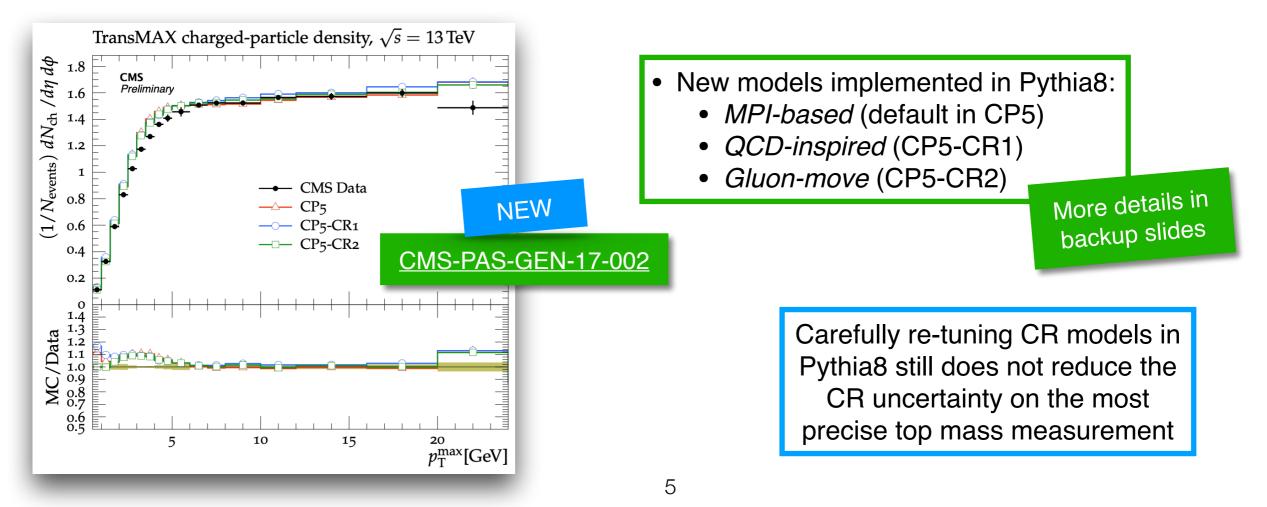
Also studying decorrelated variations for each branching type $(g \rightarrow qq, q \rightarrow qg, ...)$

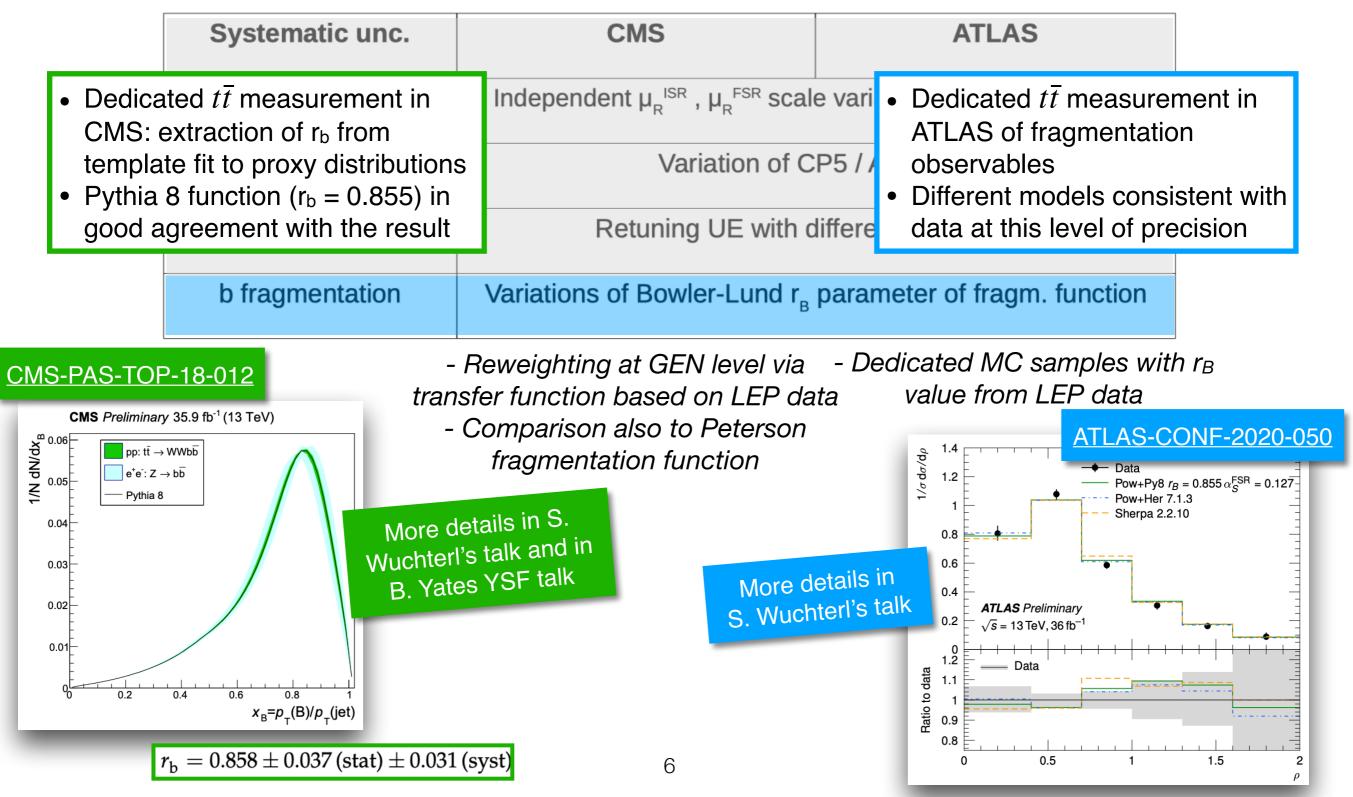
Systematic unc.	CMS	ATLAS		
ISR and FSR	Independent μ_{R}^{ISR} , μ_{R}^{FSR} scale variations with factor (2,0.5)			
UE	Variation of CP5 / A14 tune			
Different neremeter eet end tuning detecte				

Different parameter set and tuning datasets

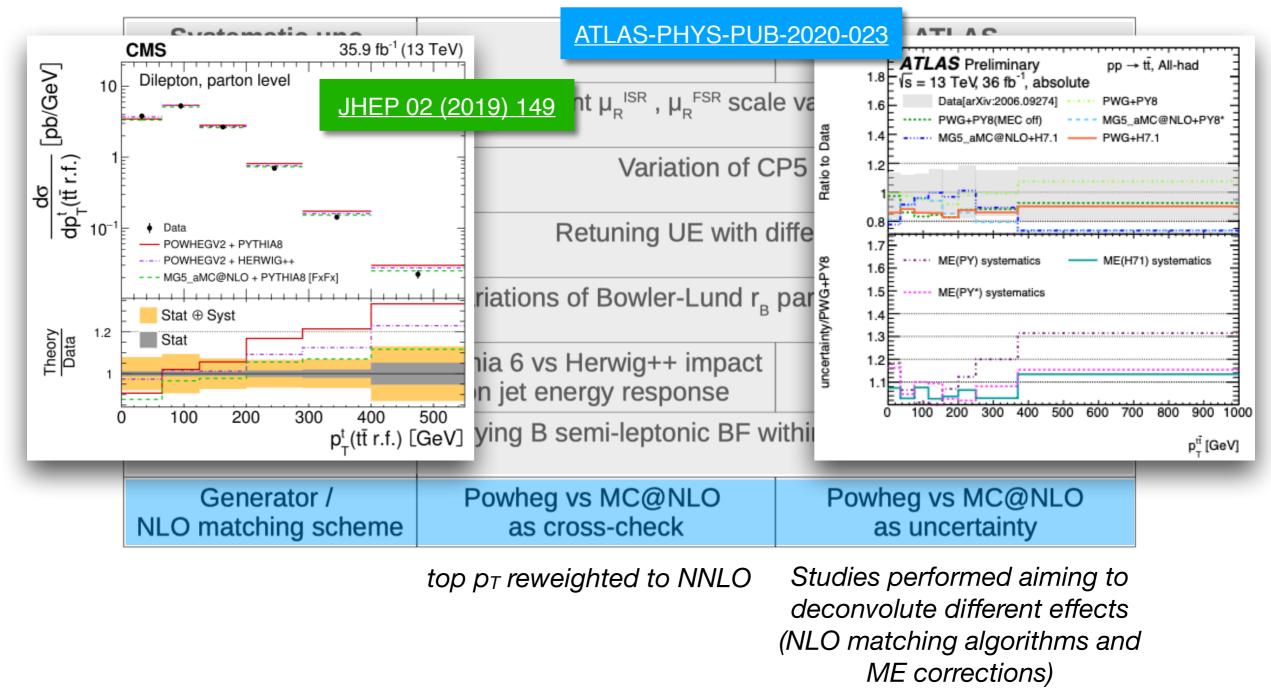
Eur. Phys. J. C 80 (2020) 4 JHEP 03 (2017) 157 • Different tunes in Pythia8: Jet multiplicity in tĒ events, $\sqrt{s} = 13$ TeV • different PS α_s and PDF δη δφ > [GeV] ATLAS Trans-min region $(1/\sigma)d\sigma/dn-jet$ 0.6 1.4 orders (LO, NLO, NNLO) NHEG+PYTHIA8 CUET $p_{-} > 0.5 \text{ GeV}, |\eta| < 2.5$ $\sqrt{s} = 13 \text{ TeV}, 1.6 \text{ nb}^{-1}$ POWHEG+PYTHIA8 CP2 0.5 $p_{-}^{lead} > 1 \text{ GeV}$ • Comparison to $t\bar{t}$ production POWHEG+PYTHIA8 CP4 $\langle \Sigma p_{\gamma} \rangle$ POWHEG+PYTHIA8 CP5 0./ CMS Data measurement at 13 TeV: 0.3 • great agreement when merging additional NLO 0.2 – – PYTHIA 8 Monash Data MEs (FxFx) in CMS ----- PYTHIA 8 A14 --- Herwig7 0.1 – PYTHIA 8 A2 ---- Epos Model / Data 8'0 MC/Data 1.6 1.4 0.8 20 25 5 10 15 30 2 additional jets p_{τ}^{lead} [GeV]

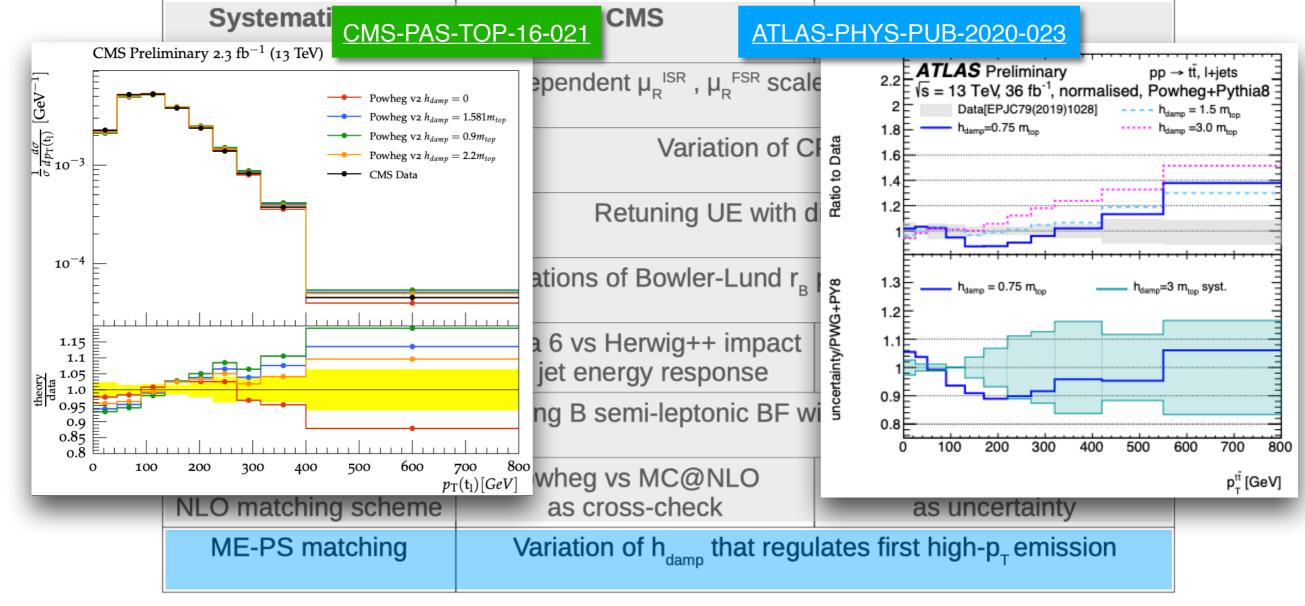
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UE	Variation of CP5 / A14 tune			
CR	Retuning UE with o	lifferent CR models		





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ISR and FSR	Independent μ_{R}^{ISR} , μ_{R}^{FSR} scale variations with factor (2,0.5)				
UE	Variation of CP5 / A14 tune				
CR	Retuning UE with different CR models				
b fragmentation	Variations of Bowler-Lund $r_{_B}$ parameter of fragm. function				
Fragmentation & hadronization	Pythia 6 vs Herwig++ impact Pythia 8 vs Herwig 7 on jet energy response				
Hadron decays	Varying B semi-leptonic BF within PDG value uncertainties				





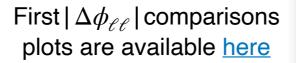
 h_{damp} (1.58 \times m_t) and uncertainties from fit to leading additional jet p_T h_{damp} (1.5 × m_t) based on data but not fitted

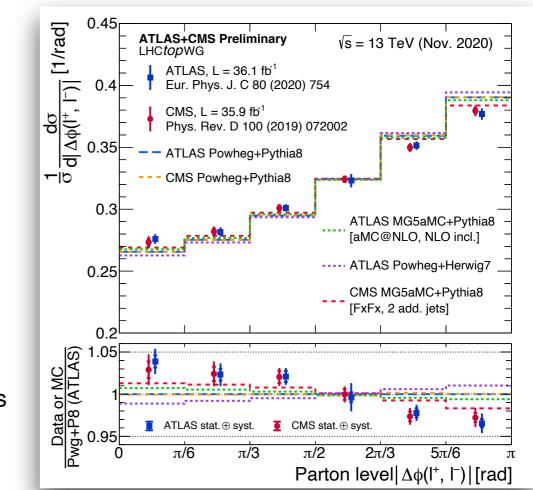
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Fragmentation & hadronization	Pythia 6 vs Herwig++ impact on jet energy response	Pythia 8 vs Herwig 7			
Hadron decays	Varying B semi-leptonic BF w	ithin PDG value uncertainties			
Generator / NLO matching scheme	Powheg vs MC@NLO as cross-checkPowheg vs MC@NL as uncertainty				
ME-PS matching	Variation of h_{damp} that regulates first high-p _T emission				

Common CMS-ATLAS MC samples would help greatly in understanding and comparing many of these uncertainties!

A Top Common sample

- A *tt* sample with common settings would facilitate ATLAS-CMS combinations and comparisons:
 - could help to understand correlations of systematic uncertainties due to MC modelling
 - could remove differences in high-precision measurements (e.g. color reconnection models and parton shower / soft physics settings in top quark mass)
 - could be used as baseline prediction (e.g. for $|\Delta \phi_{\ell\ell}|$ combination @13 TeV)
- First step towards sharing resources, for current and future generators
- Effort carried out within the <u>LHCtopWG</u>: Michael Fenton, Dominic Hirschbühl, Giulia Negro, and Reinhard Schwienhorst





Main settings in ATLAS and CMS

- Both experiments use a similar setup for $t\overline{t}$ simulation, POWHEG-BOX (hvq) + Pythia8, but different nominal samples
 - many parameters are different: Powheg revision & settings, Pythia8 version & settings, usage of EvtGen, etc.

Setting name	Setting description	CMS default	ATLAS default
Powheg			
qmass	top-quark mass [GeV]	172.5	172.5
twidth	top-quark width [GeV]	1.31	1.32
hdamp	first emission damping parameter [GeV]	237.8775	258.75
wmass	W [±] mass [GeV]	80.4	80.3999
wwidth	W^{\pm} width [GeV]	2.141	2.085
bmass	<i>b</i> -quark mass [GeV]	4.8	4.95
Рутніа 8			
	Pythia 8 version	v240	v230
	Tune	CP5	A14
PDF:pSet	LHAPDF6 parton densities to be used for proton beams	NNPDF31_nnlo	NNPDF23_lo
		_as_0118	_as_0130_qed
TimeShower:alphaSvalue	Value of α_s at Z mass scale for Final State Radiation	0.118	0.127
SpaceShower:alphaSvalue	Value of α_s at Z mass scale for Initial State Radiation	0.118	0.127
MPI:alphaSvalue	Value of α_s at Z mass scale for Multi-Parton Interaction	0.118	0.126
MPI:pT0ref	Reference p_T scale for regularizing soft QCD emissions	1.41	2.09
ColourReconnection:range	Parameter controlling colour reconnection probability	5.176	1.71

Common settings

- "Democratic" setup (not optimized to data):
 - same Pythia tune: Monash (basis of both ATLAS and CMS tunes)
 - approximate averages for all physical parameters
 - technical parameters mainly chosen from ATLAS setup

Setting name	Setting description	CMS default	ATLAS default	Common Proposal
Powheg				
qmass	top-quark mass [GeV]	172.5	172.5	172.5
twidth	top-quark width [GeV]	1.31	1.32	1.315
hdamp	first emission damping parameter [GeV]	237.8775	258.75	250
wmass	W [±] mass [GeV]	80.4	80.3999	80.4
wwidth	W^{\pm} width [GeV]	2.141	2.085	2.11
bmass	<i>b</i> -quark mass [GeV]	4.8	4.95	4.875
Рутніа 8				
	Pythia 8 version	v240	v230	v240 (CMS)
				v244 (ATLAS)
	Tune	CP5	A14	Monash
PDF:pSet	LHAPDF6 parton densities to be used for proton beams	NNPDF31_nnlo	NNPDF23_lo	NNPDF23_lo
		_as_0118	_as_0130_qed	_as_0130_qed
TimeShower:alphaSvalue	Value of α_s at Z mass scale for Final State Radiation	0.118	0.127	0.1365
SpaceShower:alphaSvalue	Value of α_s at Z mass scale for Initial State Radiation	0.118	0.127	0.1365
MPI:alphaSvalue	Value of α_s at Z mass scale for Multi-Parton Interaction	0.118	0.126	0.130
MPI:pT0ref	Reference p_T scale for regularizing soft QCD emissions	1.41	2.09	2.28
ColourReconnection:range	Parameter controlling colour reconnection probability	5.176	1.71	1.80

Common sample v0.1

- Production of first sample with common settings (v0.1):
 - exchanged complete set of parameters
 - samples produced independently in the respective frameworks
 - LHE files produced and showered separately by each collaboration
- Focus on generating first ATLAS and CMS samples with same common settings
 - no tuning to data yet
 - no identical events expected, but overall agreement of samples
- barately
 LHCTOP NOTE

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 ATL-PHYS-PUB-2021-016
CMS NOTE-2021/005
31st May 2021

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 Towards Common tł Monte-Carlo Settings for
ATLAS and CMS

 ATLAS and CMS

 ATLAS and CMS Collaborations

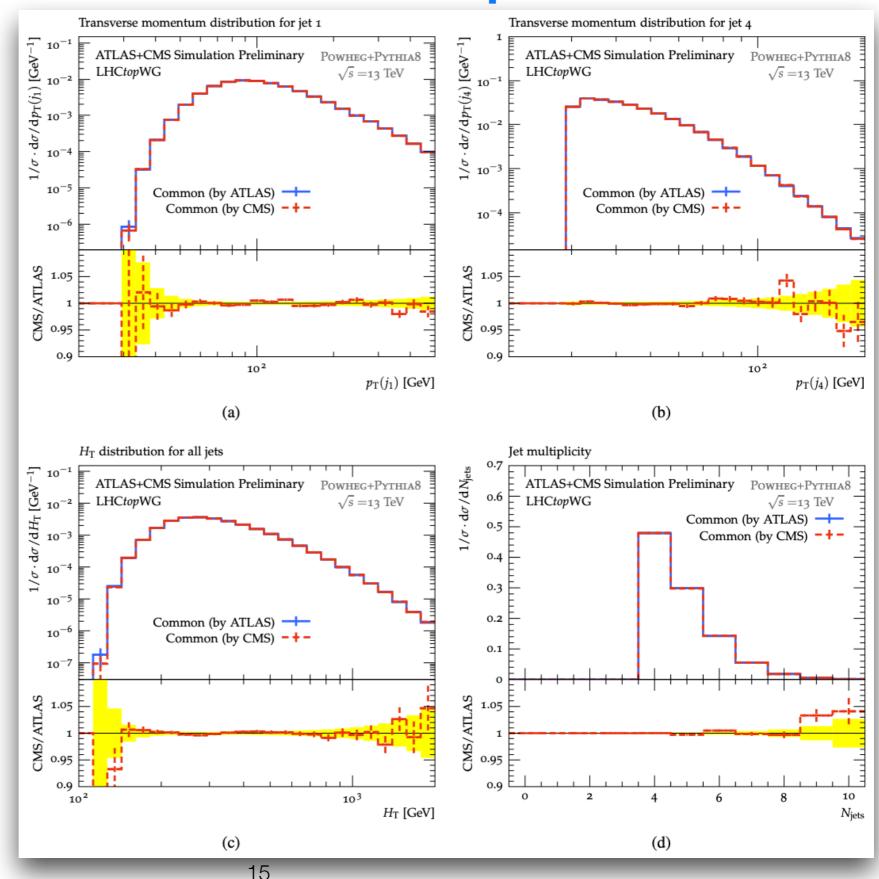
- Technical setup:
 - 10M inclusive events produced in each experiment
 - different Powheg revision but same HVQ program
 - different Pythia version (not all available in respective frameworks) → checked that results are identical
 - no usage of EvtGen
 - comparisons performed at particle level with Rivet v3.1.2 and the "MC_TTBAR" routine ("ONELEP" mode)
- Common settings and results documented in public note

Both ATLAS and CMS use POWHEG+PYTHIA8 Monte-Carlo simulations to model the $t\bar{t}$ process. A commonly agreed upon set of POWHEG and PYTHIA8 parameters is presented and compared to the nominal ATLAS and CMS settings. Samples generated with the different settings are compared using a publicly available Rivet routine. Comparisons are presented to demonstrate that samples produced with the Common Settings by both collaborations are in agreement with each other. Samples generated with the Common Settings can be used to compare ATLAS and CMS analyses.

Validation of samples

 Comparison of samples produced by both experiments using same common settings

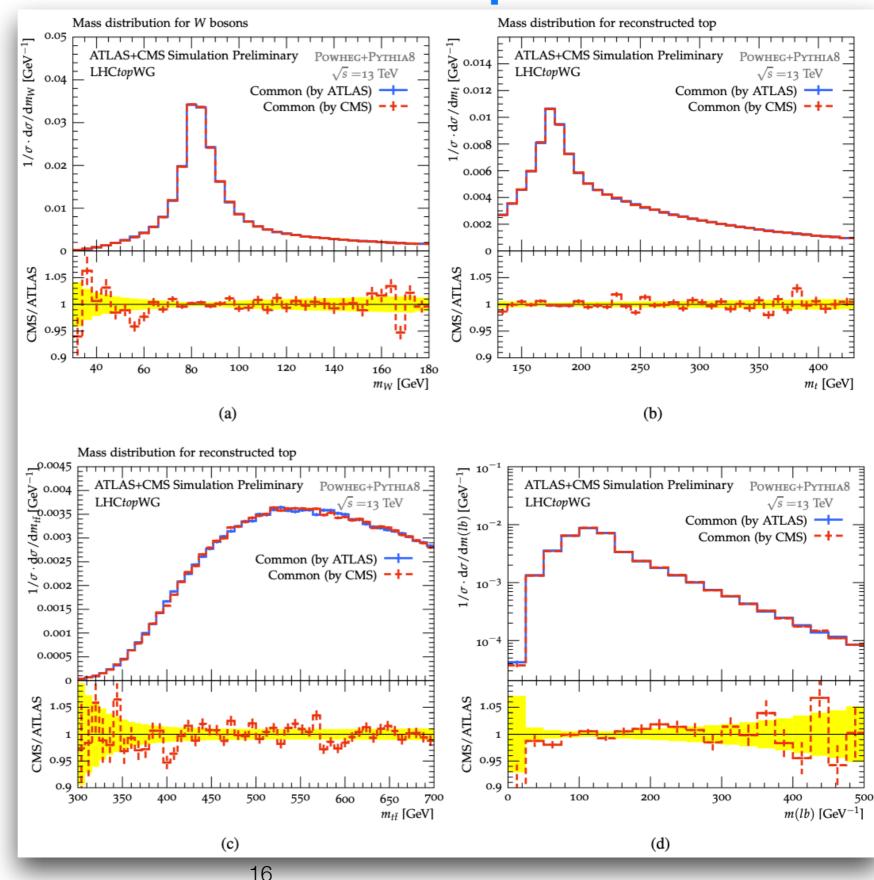
Distributions are in perfect agreement within statistical uncertainties



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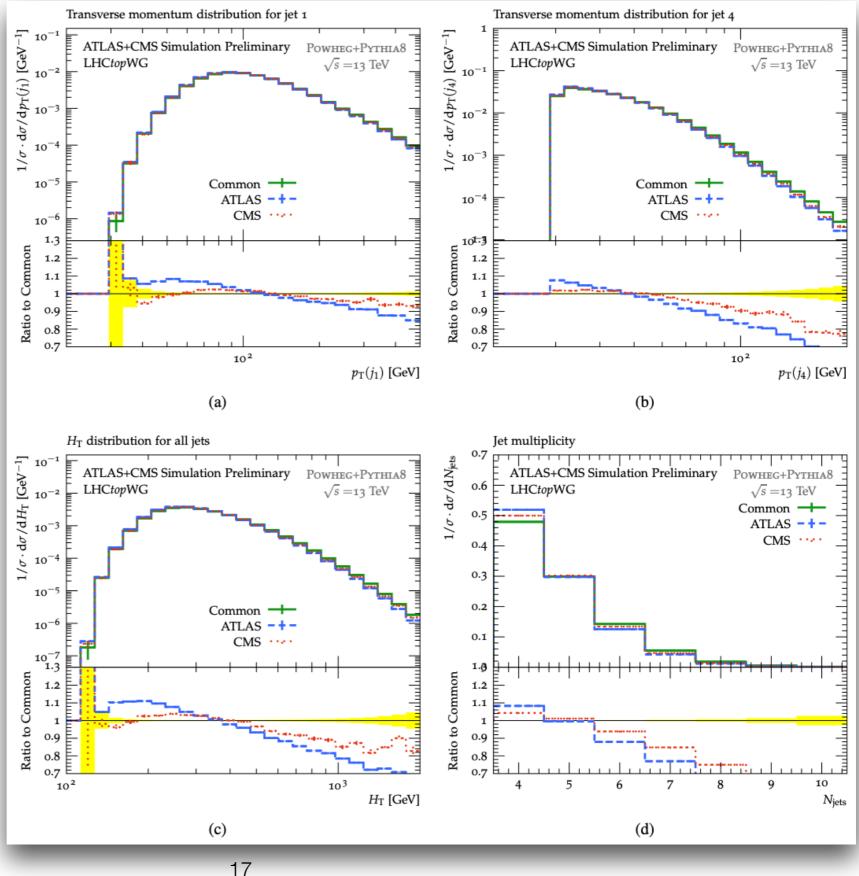
Distributions are in perfect agreement within statistical uncertainties



Common vs ATLAS/CMS

- Comparisons of common settings to nominal settings of each experiment
- Difference between Common sample and ATLAS/CMS ones mainly due to different α_s of the tune

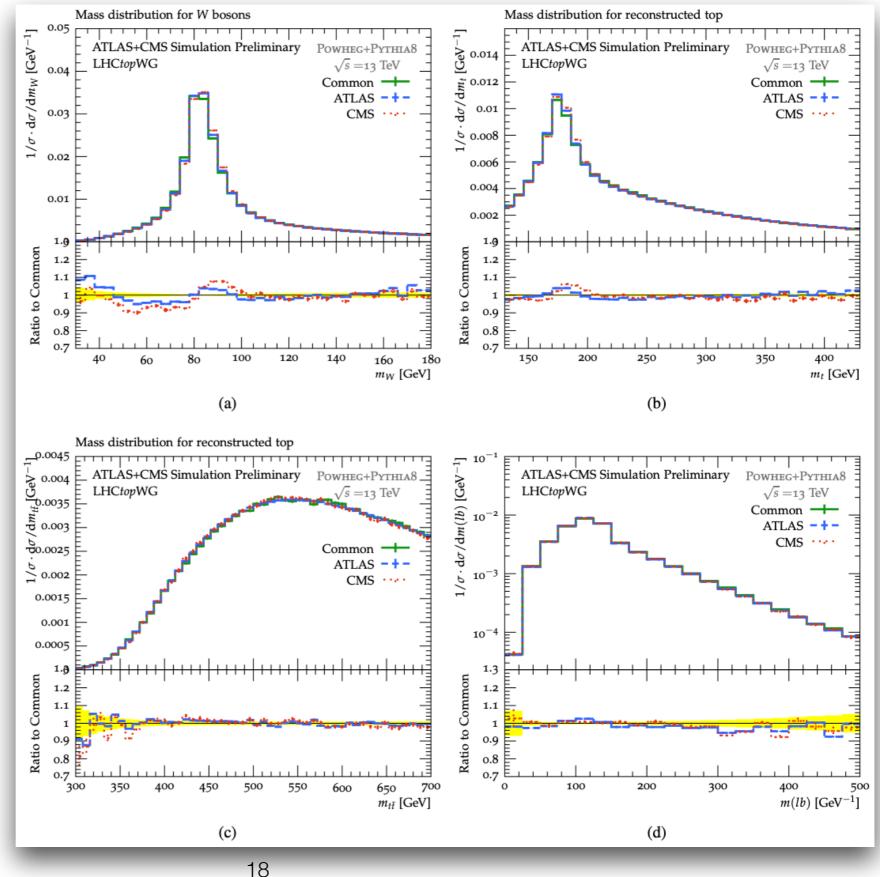
ATLAS and CMS are tuned to their experimental results, while Common settings are not optimized to data



Common vs ATLAS/CMS

- Comparisons of common settings to nominal settings of each experiment
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ATLAS and CMS are tuned to their experimental results, while Common settings are not optimized to data



Common sample v.02

- After first common sample (v0.1), first "physical" common sample (v0.2)
 - set of parameters more tuned on data
- Physics setup for v0.2:
 - Powheg and Pythia settings agreed between ATLAS and CMS experts
 - no usage of Evtgen
- Technical setup for v0.2:
 - LHE files produced by ATLAS (having more technical constraints)
 - use common LHE files, showered separately by CMS and ATLAS

Powheg settings

• Values in v0.1 mainly averaged between ATLAS and CMS

				v0.1	v0.2
Setting name	Setting description	CMS default	ATLAS default	Common Proposal	Common Proposal
	Powneg-Box V2 svn revision	3728	3026	3728 (CMS)	
				3026 (ATLAS)	
topdecaymode	Allowed decays of the top quark	22222	22222	22222	
qmass	top-quark mass [GeV]	172.5	172.5	172.5	
twidth	top-quark width [GeV]	1.31	1.32	1.315	1.311 (PDG, $\alpha_s = 0.118$)
hdamp	first emission damping parameter [GeV]	237.8775	258.75	250	-
wmass	W [±] mass [GeV]	80.4	80.3999	80.4	
wwidth	W^{\pm} width [GeV]	2.141	2.085	2.11	2.085 (PDG, EW fit)
bmass	<i>b</i> -quark mass [GeV]	4.8	4.95	4.875	5.06 (4-loop calculation)
cmass	<i>c</i> -quark mass [GeV]	1.5	1.55	1.525	
smass	s-quark mass [GeV]	0.2	0.5	0.35	
dmass	d-quark mass [GeV]	0.1	0.32	0.21	
umass	u-quark mass [GeV]	0.1	0.32	0.21	
taumass	au mass [GeV]	1.777	1.777	1.777	
mumass	μ mass [GeV]	0.1057	0.1057	0.1057	
emass	e mass [GeV]	0.00051	0.00051	0.00051	
elbranching	W-boson electronic branching fraction	0.108	0.1082	0.1081	0.1083 (PDG, theory)
sin2cabibbo	quark mixing angle	0.051	0.051	0.051	
					A

Setting name	Setting description	CMS default	ATLAS default	Common Proposal	
bmass_lhe	b-quark mass in GeV (for momentum reshuffling)	(5.0)	4.95	4.875	5
cmass_lhe	c-quark mass in GeV (for momentum reshuffling)	(1.5)	1.55	1.525	

5.06 (4-loop calculation)

Powheg-Pythia matching

• Matching done using main31 routine

				v0.1	v0.2
Setting name	Setting description	CMS default	ATLAS default	Common proposal	Common Proposal
	Pythia 8 version	v240	v230	v240 (CMS)	
				v244 (ATLAS)	
Powheg	Interface parameters in PYTHIA8 for matching to POWHEG				
pTdef	Flag for hardness criterion (Powheg vs Pythia8)	1	2	1	
emitted	Flag for defining emissions	0	0	0	
pTemt	Flag for which partons are used to define POWHEG hardness criteria	0	0	0	
pThard	Flag for how to calculate POWHEG hardness criteria	0	0	0	
vetoCount	How many emissions vetoed showers checks after first allowed emission	100	3	50	100
nFinal	Number of outgoing particles for born level process	2	2	2	
veto	Flag for vetoed or unvetoed showers	1	1	1	
MPIveto	Flag for applying veto to Multi Parton Interactions	(0)	0	0	

- Common proposal for v0.2:
 - decided to use CMS values (default settings from Pythia)
- Further Powheg details
 - Main PDF:
 - NNPDF3.1 (NNPDF31_nlo_as_0118)
 - Systematic weights:
 - replicas of NNPDF3.1
 - central PDF for NNPDF3.0
 - independent scale variations with 0.5 / 2.0

Pythia settings

- Settings from Monash tune used in v0.1:
 - no good agreement between common sample and nominal ATLAS and CMS samples
- Common proposal for v0.2:
 - Monash tune + shower settings consistent with the Powheg Sudakov (Monash-CMW)
 - keep default values for other settings
 - use Pythia8 default decay tables

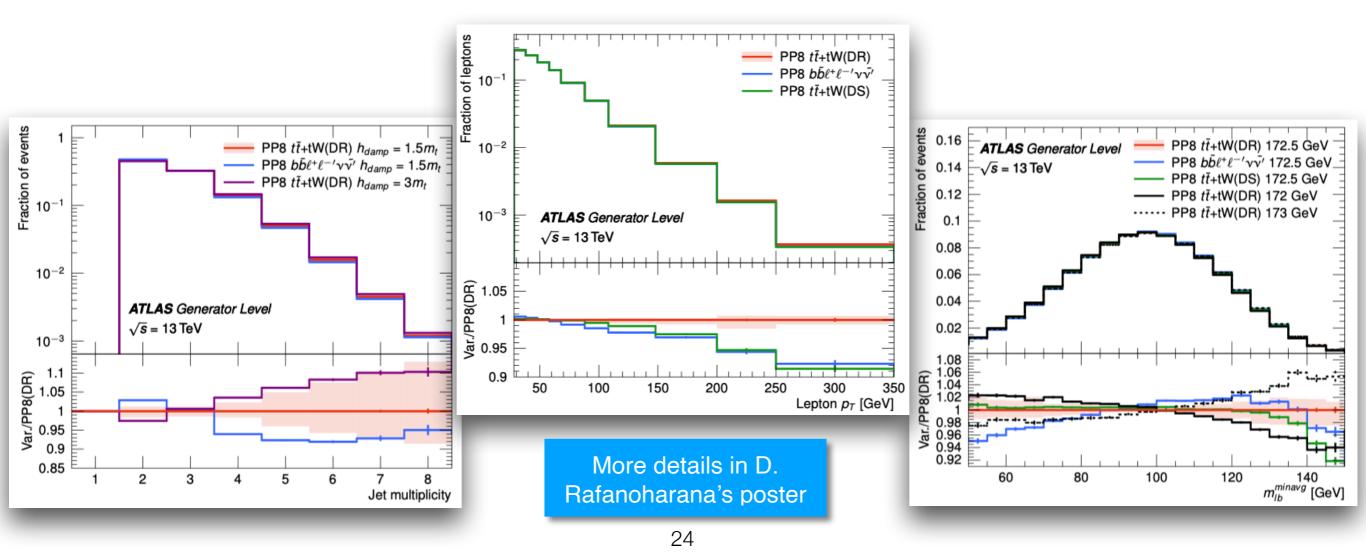
```
"Tune:ee = 7",
"Tune:pp = 14",
"PDF:pSet = LHAPDF6:NNPDF23_lo_as_0130_qed",
"SpaceShower:alphaSvalue = 0.118",
"SpaceShower:alphaSorder = 2",
"SpaceShower:alphaSuseCMW = on",
"TimeShower:alphaSvalue = 0.118",
"TimeShower:alphaSorder = 2",
```

- List of all settings:
 - http://www.atlas.uni-wuppertal.de/~hirsch/Pythia8_MonashCMW.txt

Status and next steps

- First comparisons with v0.2 settings done:
 - much better agreement between common sample and nominal samples from ATLAS and CMS
- First comparisons of LHE files done:
 - tested that both experiments can read LHE files from the other experiment
 - LHE files with 20k events produced in both experiments
 - comparisons of weights distributions seem promising
- Production of common sample v0.2 ongoing:
 - use common LHE files produced by ATLAS
 - showering done independently in both experiments
- Comparisons at parton and particle level:
 - additional Rivet routines (MC_PARTONICTOPS, MC_TTBAR, MC_FSPARTICLES)
- Comparisons to data:
 - select few Rivet routines like all-had, lepton+jets, dilepton
 - differential analyses, angular correlations, event kinematics, ISR and FSR
- Documentation of settings and results in a new PUB note
 - similar to v0.1 one but with more comparisons

- A *tt* sample including all off-shell effects (i.e. double, single and non-resonant contributions):
 - improves description of the off-shell phase space (currently modelled by tt+tW) for searches
 - provides a theoretically more solid definition of the top quark mass
 - one of the best MC setups for $t\bar{t}$ but currently implemented only for different flavour leptons processes \rightarrow difficult to use directly in comparisons with data



Summary

- ATLAS and CMS have different modelling uncertainty prescriptions → a common sample would be useful to:
 - reduce modeling uncertainties
 - facilitate ATLAS + CMS combinations
- First successfully produced MC sample with common settings (v0.1)
 - exchanged full list of Powheg and Pythia8 parameters, not optimised for agreement with data
 - produced consistent samples in separate frameworks
- Production of first "physical" common sample (v0.2) ongoing:
 - agreed on v0.2 settings, more tuned to data
 - common LHE files will be showered separately in both experiments
 - documentation of settings and results in new PUB note:
 - also comparisons to data at parton and particle level
- Ultimate goal:
 - real common sample using identical events
 - common Pythia8 tuning using ATLAS and CMS data
 - sharing of resources and of prescriptions for nominal and systematic uncertainties

Stay tuned.. new results coming soon!



Powheg settings

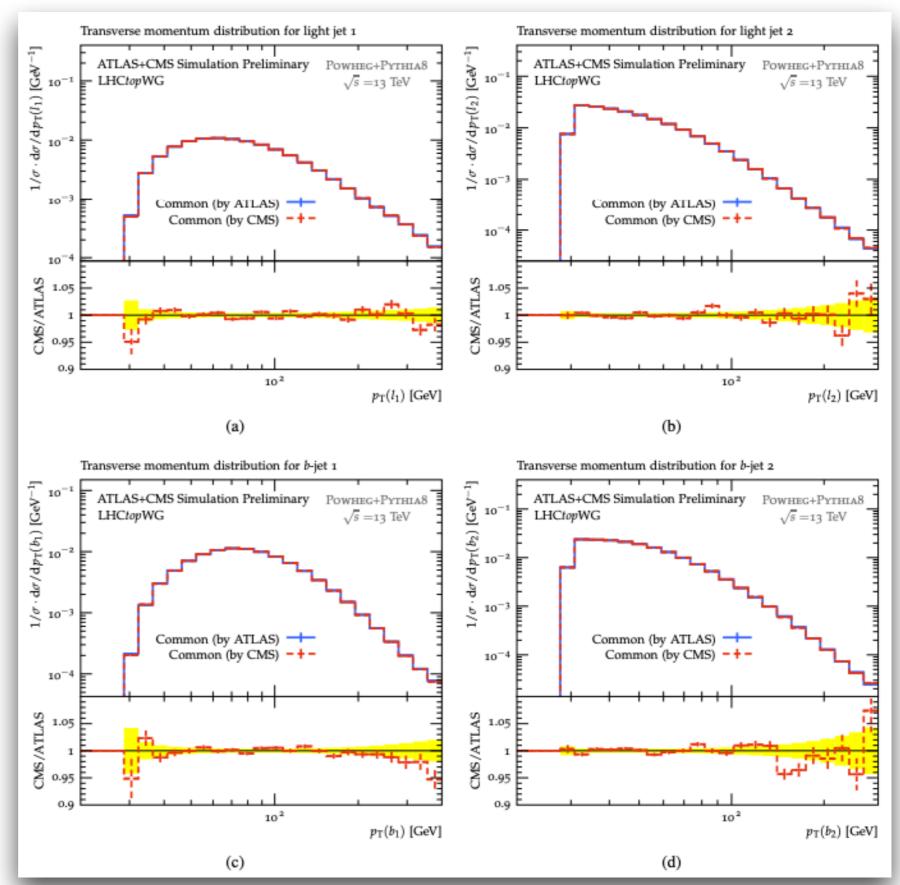
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vetoCount	How many emissions vetoed showers checks after first allowed emission	100	3	50
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veto	Flag for vetoed or unvetoed showers	1	1	1
MPIveto	Flag for applying veto to Multi Parton Interactions	(0)	0	0
TimeShower	Final State Radiation Parameters			
mMaxGamma	Maximum invariant mass for $\gamma \rightarrow f\bar{f}$	1.0	(10)	10
alphaSorder	Order of running for α_s	2	(1)	1
alphaSvalue	Value of α_s at Z mass scale	0.118	0.127	0.13650
pTmaxMatch	Flag for setting maximum shower scale algorithm	2	2	2
SpaceShower	Initial State Radiation Parameters			
alphaSorder	Order of running for α_s	2	(1)	1
alphaSvalue	Value of α_s at Z mass scale	0.118	0.127	0.1365
pTmaxMatch	Flag for setting maximum shower scale algorithm	2	2	2
rapidityOrder	Force emissions to be ordered in rapidity	on	on	on
rapidityOrderMPI	Force emissions in secondary scatterings to be ordered in rapidity	(on)	on	on
pT0Ref	Reference p_T scale for regularizing soft QCD emissions	(2)	1.56	2
MPI	Multi-Parton Interaction Parameters			
alphaSorder	Order of running for α_s	2	(1)	1
alphaSvalue	Value of α_s at Z mass scale	0.118	0.126	0.130
ecmPow	Exponent control kinematic dependence of pT0	0.03344	(0.215)	0.215
bprofile	impact parameter profile choice flag for hadron beams	2	(3)	3
coreRadius	Inner radius of core when using $bprofile = 2$	0.7634	(0.4)	0.4
coreFraction	Matter content fraction of core when using $bprofile = 2$	0.63	(0.5)	0.5
pT0ref	Reference p_T scale for regularizing soft QCD emissions	1.41	2.09	2.28
BeamRemnants	Parameters for all partons extracted from a beam			
primordialKThard	Parameter controlling k_T of beam remnant initiators in hard-interations	(1.8)	1.88	1.8
ColourReconnection	Colour Reconnection Parameters			
range	Parameter controlling colour reconnection probability	5.176	1.71	1.80
ParticleDecays	Particle Decay Settings			
allowPhotonRadiation	Allow photon radiation in decays to lepton pairs	on	(off)	off

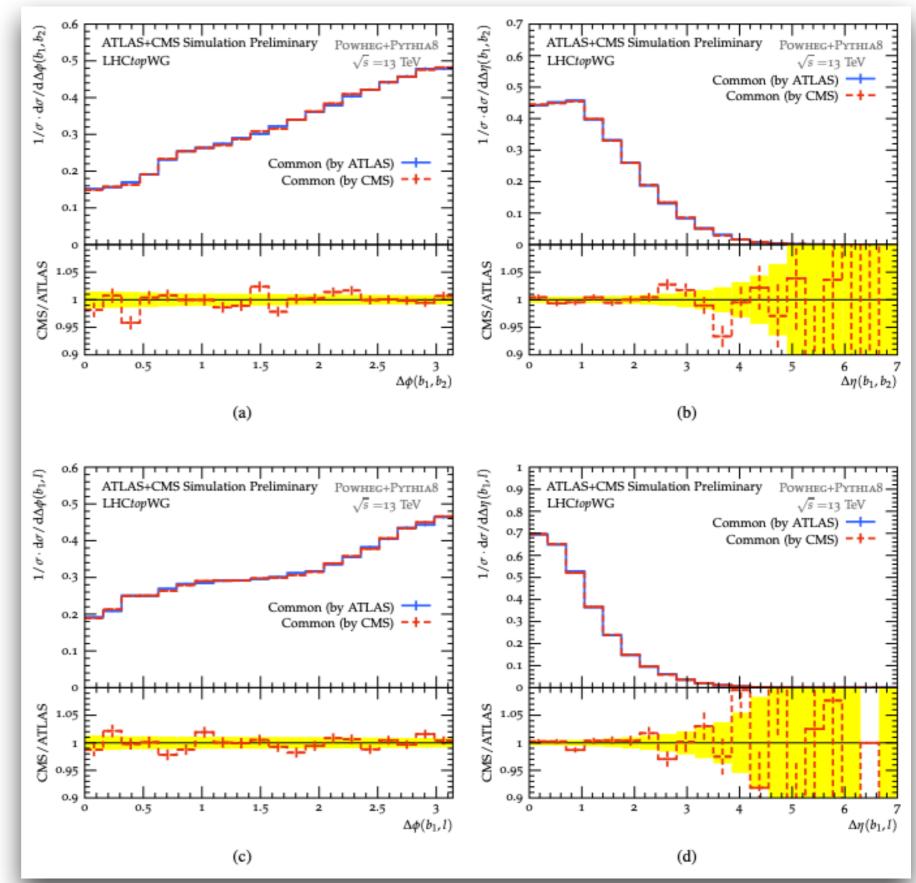
Validation of samples

- Comparison of samples produced by both experiments using same common settings
- Distributions are in perfect agreement within statistical uncertainties



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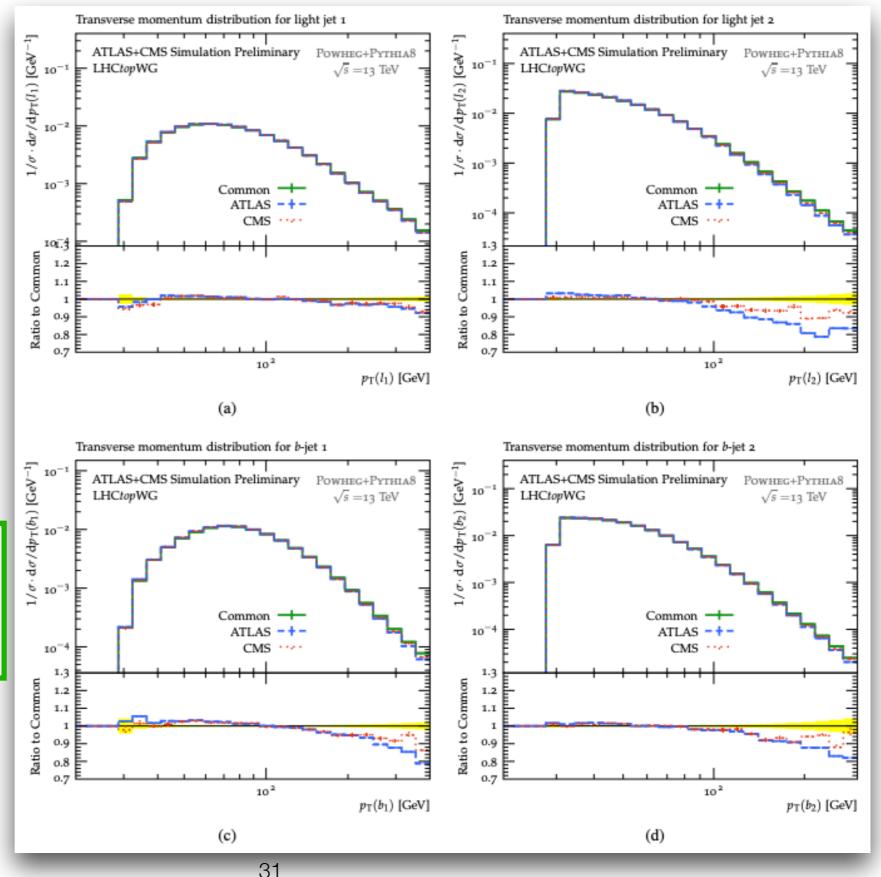
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Common vs ATLAS/CMS

- Comparisons of common settings to nominal settings of each experiment
- Difference between Common sample and ATLAS/CMS ones mainly due to different α_s of the tune

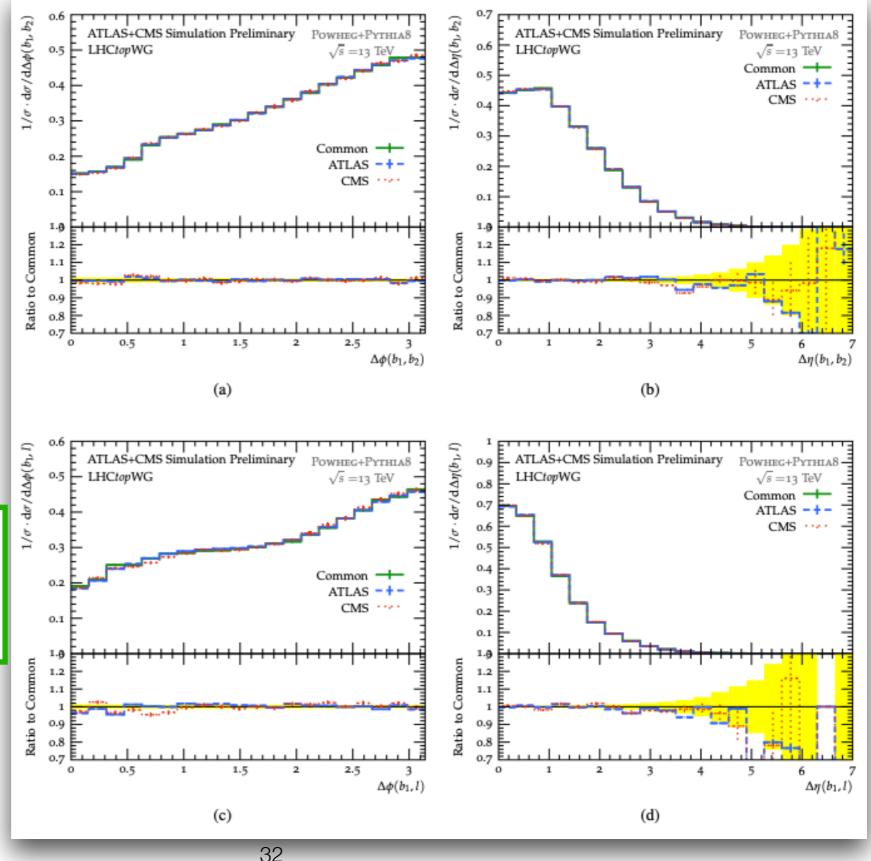
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NEW

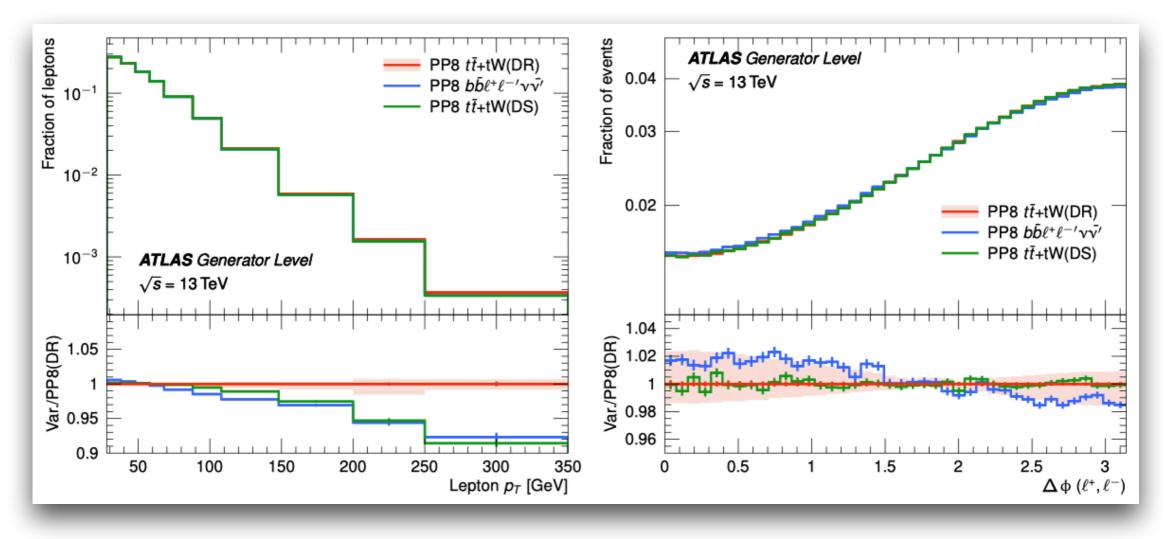


Figure: Shape comparison between the sum of $t\bar{t}$ and tW (diagram removal) distributions generated with POWHEG+PYTHIA 8 hvq (red line) and the $b\bar{b}\ell^+\ell^-'\nu\bar{\nu}'$ sample generated with the POWHEG+PYTHIA 8 *bb*4 ℓ generator (blue line) and distributions generated with POWHEG+PYTHIA 8 hvq using the diagram-subtraction scheme for tW (green) for the p_T of both leptons (left) and the $\Delta\Phi$ distribution (right). Scale variations in the matrix element and the parton shower (ISR and FSR) are combined in the red uncertainty band for the nominal $t\bar{t}+tW$ (DR) setup. All events must have exactly one electron and one muon with opposite sign, at least two jets and exactly two *b*-tagged jets. Since same-flavour channels are not included in the *bb*4 ℓ event generation, the $\tau\tau$ channel is vetoed in all samples. While the nominal $t\bar{t}$ sample includes the spin-correlation only in an approximate way, the *bb*4 ℓ sample is produced with exact spin-correlations at NLO. The comparison is performed at stable particle level with $\tau > 30$ ps. A description of the *bb*4 ℓ generator can be found in Eur. Phys. J. C 76, 691 (2016).

NEW

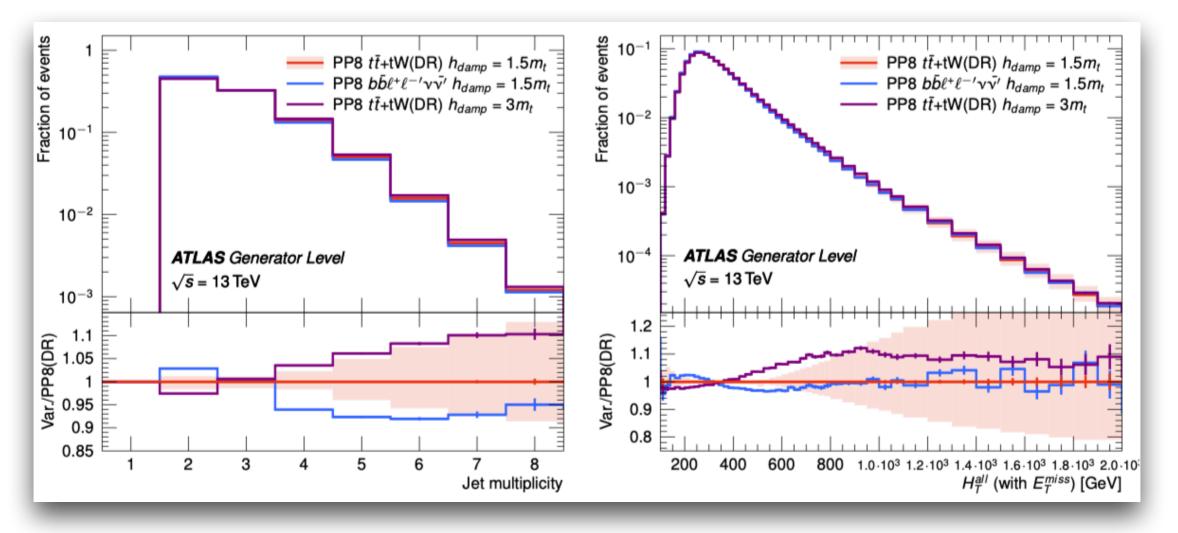


Figure: Shape comparison between the sum of $t\bar{t}$ and tW (diagram removal) distributions generated with POWHEG+PYTHIA 8 hvq (red line) and the $b\bar{b}\ell^+\ell^-'\nu\bar{\nu}'$ sample generated with the POWHEG+PYTHIA 8 $bb4\ell$ generator (blue line) and distributions generated with POWHEG+PYTHIA+8 hvq using a higher h_{damp} value in the $t\bar{t}$ generation (violet) for the jet multiplicity (left) and the H_T distribution (right). Scale variations in the matrix element and the parton shower (ISR and FSR) are combined in the red uncertainty band for the $t\bar{t}+tW(DR)$ setup. All events must have exactly one electron and one muon with opposite sign, at least two jets and exactly two *b*-tagged jets. Since same-flavour channels are not included in the $bb4\ell$ event generation, the $\tau\tau$ channel is vetoed in all samples. H_T is defined as the scalar sum p_T of both leptons, both b-jets and missing transverse momentum. The comparison is performed at stable particle level with $\tau > 30$ ps. A description of the $bb4\ell$ generator can be found in Eur. Phys. J. C 76, 691 (2016).

NEW

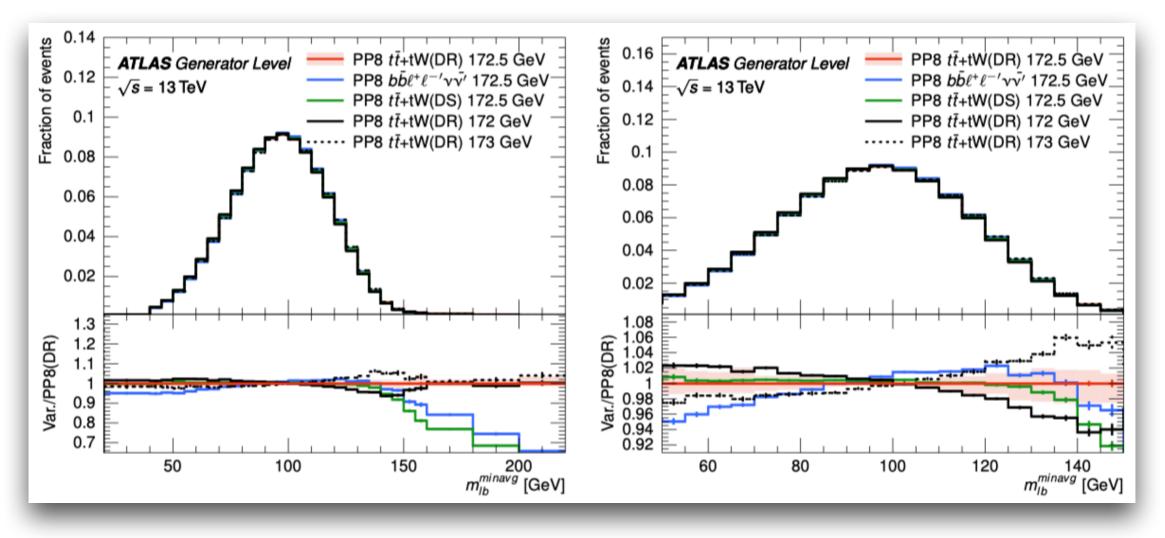


Figure: Shape comparison between the sum of $t\bar{t}$ and tW (diagram removal) distributions generated with POWHEG+PYTHIA 8 hvq (red line) and the $b\bar{b}\ell^+\ell^-'\nu\bar{\nu}'$ sample generated with the POWHEG+PYTHIA 8 bb4 ℓ generator (blue line) and distributions generated with POWHEG+PYTHIA 8 hvq using the diagram-subtraction scheme in the tW production, for the invariant mass of the lepton-*b*-jet combination with the lowest average $m_{\ell b}$ value. In addition, $t\bar{t}+tW$ samples generated with POWHEG+PYTHIA 8 hvq are shown, which have a higher/lower top-quark mass (black, 172 and 173 GeV) than the $t\bar{t}+tW$ setup shown in red as well as the $t\bar{t} + tW$ (DS) setup (green). All events must have exactly one electron and one muon with opposite sign, at least two jets and exactly two *b*-tagged jets. Scale variations in the matrix element and the parton shower (ISR and FSR) are combined in the red uncertainty band for the $t\bar{t}+tW$ (DR) setup. Since same-flavour channels are not included in the $bb4\ell$ event generation, the $\tau\tau$ channel is vetoed in all samples. The right-hand plot shows a typical mass range used for an m_{top} measurement with the template method. The comparison is performed at stable particle level with $\tau > 30$ ps. A description of the $bb4\ell$ generator can be found in Eur. Phys. J. C 76, 691 (2016).

Colour reconnection **CMS-PAS-GEN-17-002**

- Model used in default CMS Pythia8 UE tune:
 - <u>MPI-based model</u> (CP5)= simplest model with only one tunable parameter

$$P = \frac{p_{\mathrm{T}_{\mathrm{Rec}}}^2}{(p_{\mathrm{T}_{\mathrm{Rec}}}^2 + p_{\mathrm{T}}^2)}$$

 $p_{\mathrm{T}_{\mathrm{Rec}}} = R \cdot p_{\mathrm{T0}}$, where *R* is a tunable parameter

 $\lambda = \ln(1 + \sqrt{2}\frac{E_1}{m_0}) + \ln(1 + \sqrt{2}\frac{E_2}{m_0})$

- New models implemented in Pythia8:
 - <u>QCD-inspired model</u> (CP5-CR1): adds the QCD colour rules on top of the minimisation of the string length
 - <u>Gluon-move model</u> (CP5-CR2): moves the final-state gluons to a string piece belonging to different colour connected partons

Tune obtained by constraining simultaneously the parameters controlling the contributions of the MPI and of the CR model

