Event generator setups and definition of modelling uncertainties

TOP2020

September 15th, 2020

Simone Amoroso (DESY)
on behalf of
the ATLAS and CMS Collaborations

Introduction

* MC event generators are ubiquitous in LHC physics

Unfolding, Bkg. subtraction, Selection Optimisation

Need good modelling of the data, and uncertainties not in tensions with it

Extrapolation, Interpretations

Need high accuracy predictions, and well-defined uncertainties (as small as possible too)

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Modeling uncertainties					
JEC flavor (linear sum)	-0.35	$+0.1$	-0.31	-0.34	0.0
– light quarks (uds)	$+0.10$	-0.1	-0.01	$+0.07$	-0.1
– charm	$+0.03$	0.0	-0.01	$+0.02$	0.0
– bottom	-0.29	0.0	-0.29	-0.29	0.0
– gluon	-0.19	$+0.2$	$+0.03$	-0.13	$+0.2$
b jet modeling (quad. sum)	0.09	0.0	0.09	0.09	0.0
– b frag. Bowler–Lund	-0.07	0.0	-0.07	-0.07	0.0
– b frag. Peterson	-0.05	0.0	-0.04	-0.05	0.0
– semileptonic b hadron decays	-0.03	0.0	-0.03	-0.03	0.0
PDF	0.01	0.0	0.01	0.01	0.0
Ren. and fact. scales	0.05	0.0	0.04	0.04	0.0
ME/PS matching	$+0.32 \pm 0.20$	-0.3	-0.05 ± 0.14	$+0.24 \pm 0.18$	-0.2
ISR PS scale	$+0.17 \pm 0.17$	-0.2	$+0.13 \pm 0.12$	$+0.12 \pm 0.14$	-0.1
FSR PS scale	$+0.22 \pm 0.12$	-0.2	$+0.11 \pm 0.08$	$+0.18 \pm 0.11$	-0.1
Top quark p_T	$+0.03$	0.0	$+0.02$	$+0.03$	0.0
Underlying event	$+0.16 \pm 0.19$	-0.3	-0.07 ± 0.14	$+0.10 \pm 0.17$	-0.2
Early resonance decays	$+0.02 \pm 0.28$	$+0.4$	$+0.38 \pm 0.19$	$+0.13 \pm 0.24$	$+0.3$
CR modeling (max. shift)	$+0.41 \pm 0.29$	-0.4	-0.43 ± 0.20	-0.36 ± 0.25	-0.3
– "gluon move" (ERD on)	$+0.41 \pm 0.29$	-0.4	$+0.10 \pm 0.20$	$+0.32 \pm 0.25$	-0.3
– "QCD inspired" (ERD on)	-0.32 ± 0.29	-0.1	-0.43 ± 0.20	-0.36 ± 0.25	-0.1
Total systematic	0.81	0.9	1.03	0.70	0.7
Statistical (expected)	0.21	0.2	0.16	0.20	0.1
Total (expected)	0.83	0.9	1.04	0.72	0.7

Submitted to PRD

Source	Unc. on m_t [GeV]	Stat. precision [GeV]
Data statistics	0.40	
Signal and background model statistics	0.16	
Monte Carlo generator	0.04	±0.07
Parton shower and hadronisation	0.07	±0.07
Initial-state QCD radiation	0.17	±0.07
Parton shower α_S^{FSR}	0.09	±0.04
b-quark fragmentation	0.19	±0.02
HF-hadron production fractions	0.11	±0.01
HF-hadron decay modelling	0.39	±0.01
Underlying event	< 0.01	±0.02
Colour reconnection	< 0.01	±0.02
Choice of PDFs	0.06	±0.01
Total systematic uncertainty	0.67	±0.04
Total uncertainty	0.78	±0.03

ATLAS-CONF-2019-046

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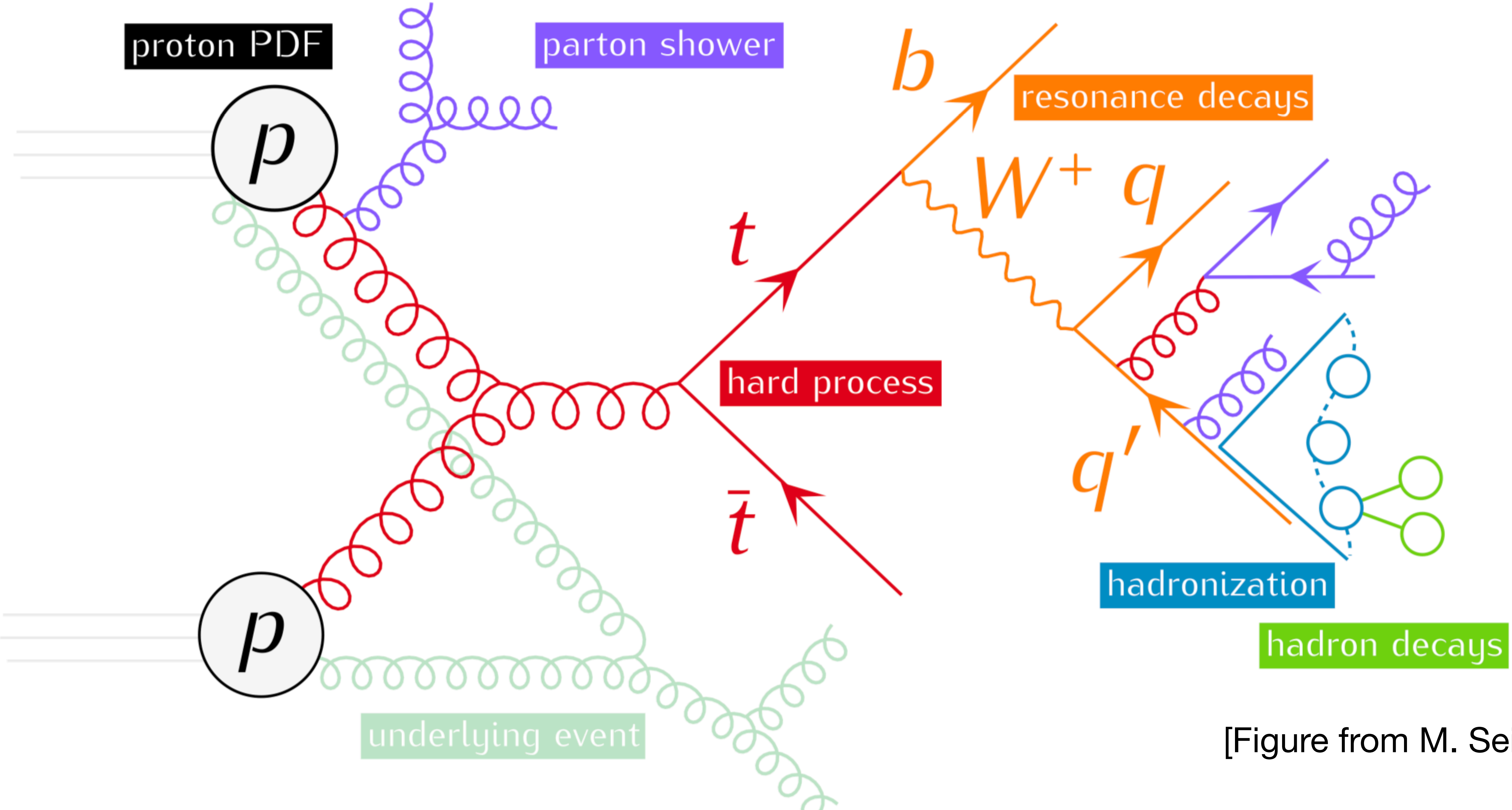
Need a long-term strategy to reduce them

Outline

* This presentation will focus on modelling of ttbar production
  * Complex coloured multiscale problem, probing all the different aspects of a Monte Carlo event generator
  * But conclusions mostly apply to other processes involving tops where we already use the same uncertainties prescriptions
* I will discuss the ***nominal generator configurations*** used by the ATLAS and CMS Collaborations
* Compare the different ***modelling uncertainty prescriptions***, (some) of their known limitations and new relevant studies
  * In particular the outcome of several discussions in the TOPLHCWG and some recent ATLAS studies
* And finally discuss proposed ***avenues for reducing modelling uncertainties*** in future analyses

Simulating top-quark pair production



[Figure from M. Seidel]

- **NLO Matrix Elements** for ttbar production in the Narrow Width Approximation
- **LO+Matrix Element Corrections** for the top decay
- Soft/collinear radiation from the **parton shower at LL accuracy**
- Phenomenological models of **hadronization** and **underlying event**

NLO matrix-elements

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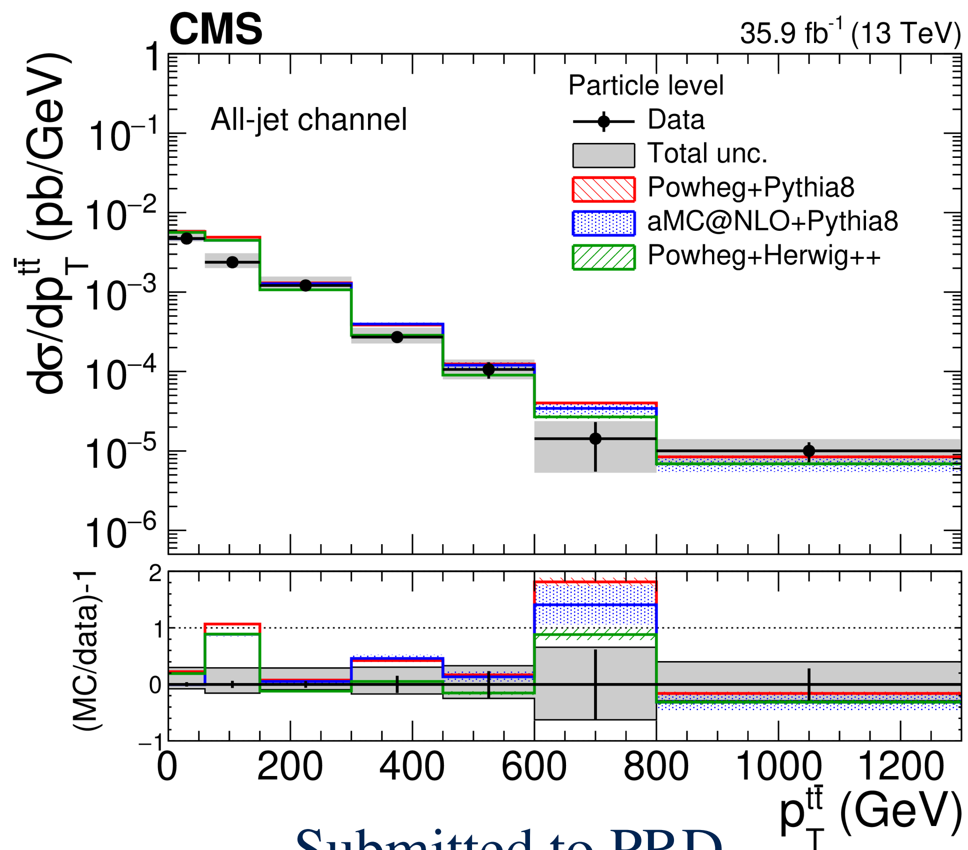
  - Scales set to $\mu_R = \mu_F = \sqrt{m_t^2 + p_T^2}$
  - Slightly different choices of h_{damp}:
    ATLAS $h_{damp} = 1.5 m_t$
    CMS $h_{damp} = 1.58 m_t$



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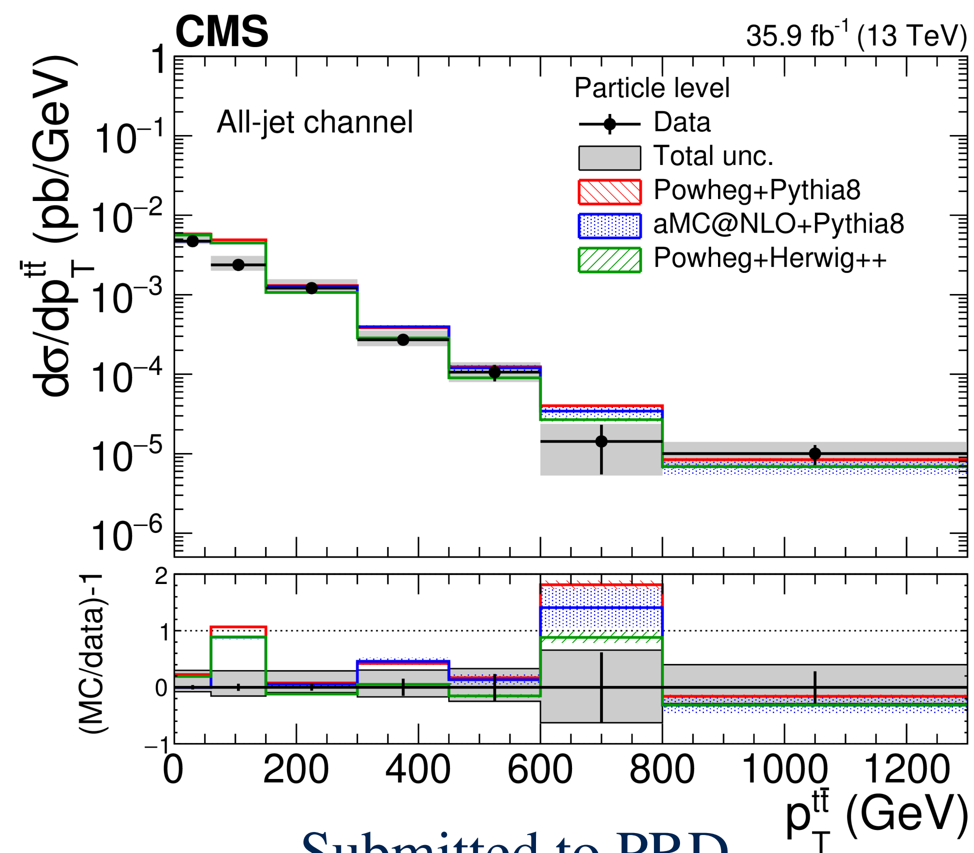

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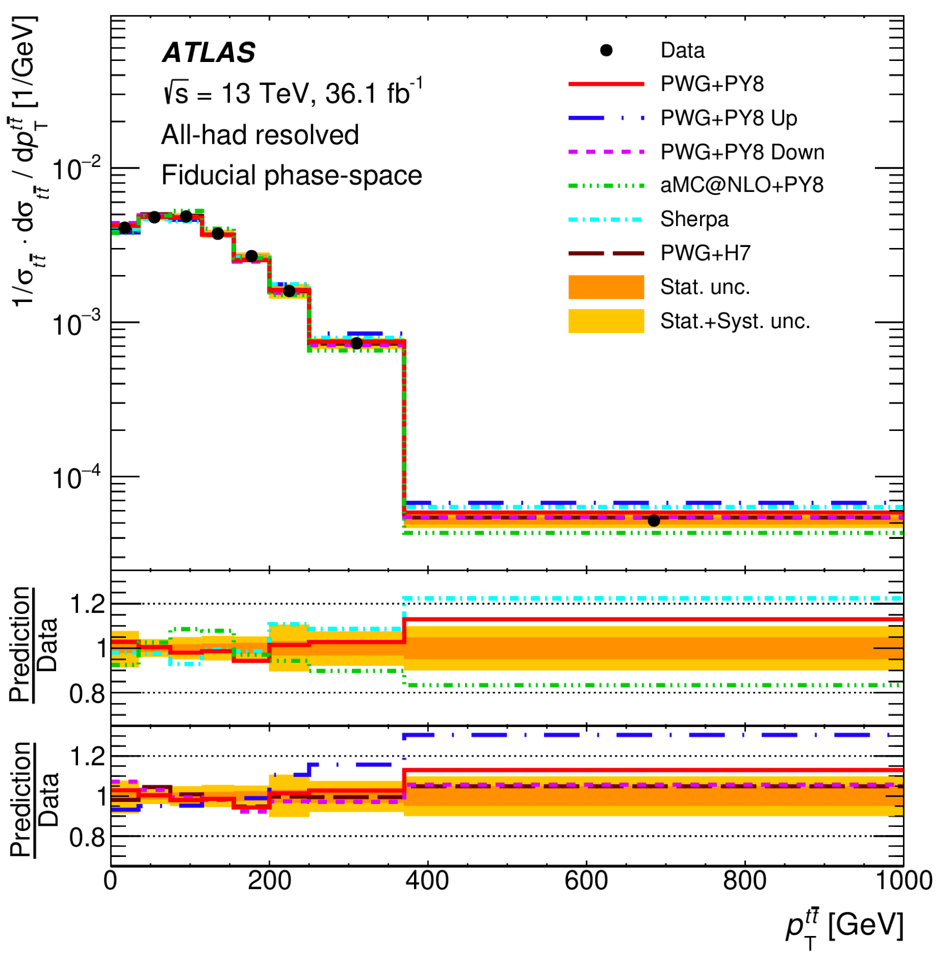

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- Alternative samples with **MC@NLO** matching used for systematic studies
  - MG5_aMC@NLO NLO/FxFx in CMS
  - MG5_aMC@NLO NLO and Sherpa MEPS@NLO in ATLAS

Interfaced to parton showers

Parameter	CMS	ATLAS
POWHEG		
vetoCount	100	3
pTdef	1	2
pThard	0	0
pTemt	0	0
emitted.	0	0
MPIveto	0	0
SpaceShower		
alphaSorder	2	1
alphaSvalue	0.118	0.127
rapidityOrder	off	on
pT0Ref	2.0	1.56
TimeShower		
alphaSorder	2	1
alphaSvalue	0.118	0.127
MultipartonInteractions		
alphaSvalue	0.118	0.126
alphaSorder	2	1
pT0Ref	1.44	2.09
ecmPow	0.03344	0.215
bProfile	2	3
coreRadius	0.7634	-
coreFraction	0.63	-
ColourReconnection		
range	5.176	1.77

* **Powheg** parton-level events are interfaced to **Pythia8** for parton showering including effects from MPI, CR and hadronization
  - Pythia emissions at scales higher than the Powheg radiation are vetoed
* Different choice of Pythia8 settings/tunes
  - ATLAS tune of shower and MPI to 7 TeV UE/jets/Z/ttbar data - ***A14***
  - CMS tune of shower and MPI to 13 TeV UE measurements - ***CP5***
* Outstanding agreement with data, well beyond expectations for an NLOPS generator (thanks to years of tuning)
* But also plenty of regions with large mismodellings

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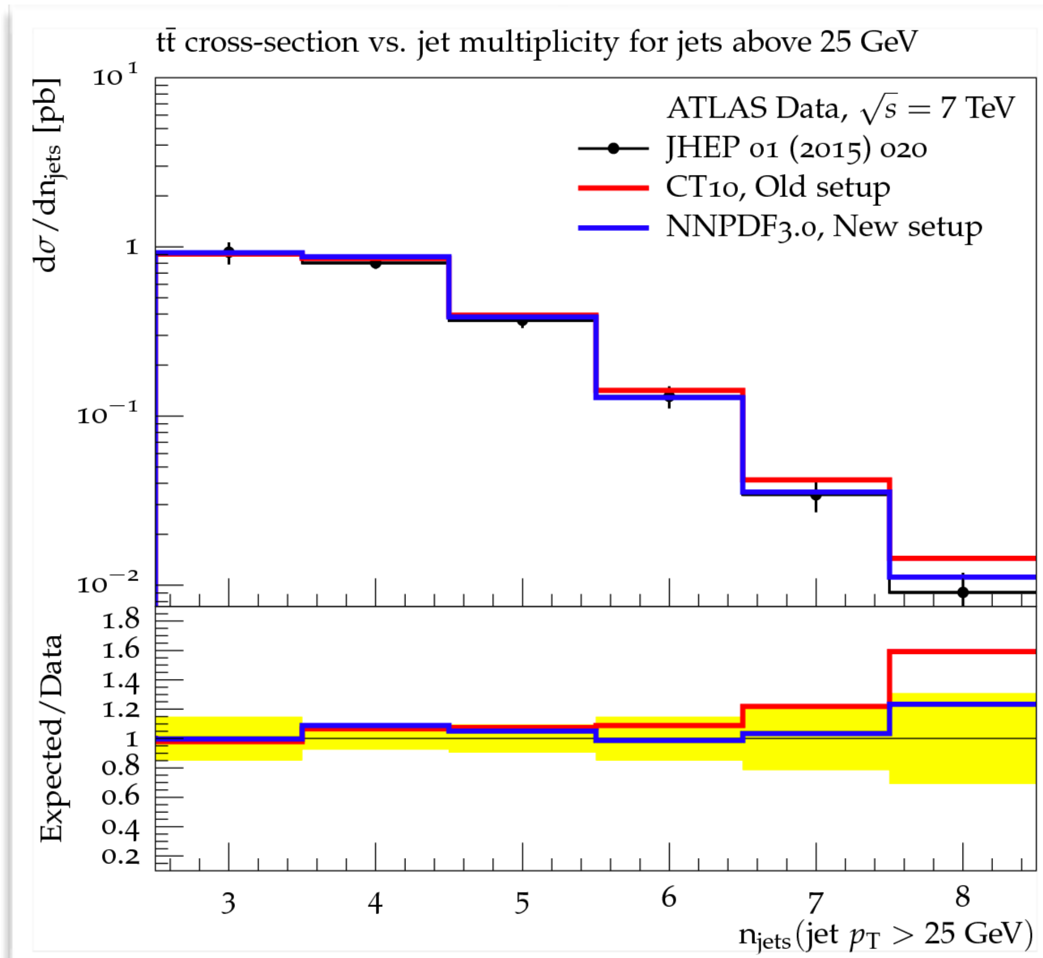
NLOPS matching parameters

vetoed showers and main31, but exact settings do differ



ATL-PHYS-PUB-2016-004

Interfaced to parton showers

Parameter	CMS	ATLAS
POWHEG		
vetoCount	100	3
pTdef	1	2
pThard	0	0
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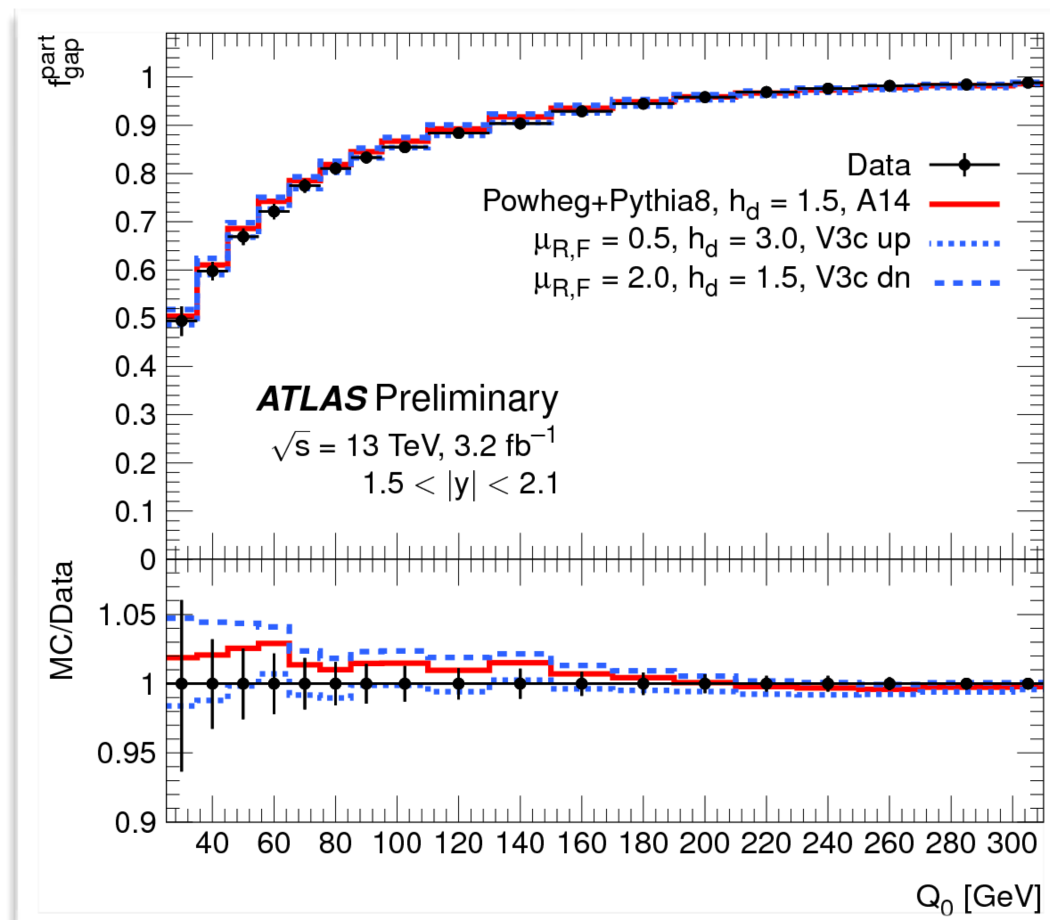
Perturbative shower parameters

Shower scales, evolution, and IR cut-off, as well as ordering of emissions



ATL-PHYS-PUB-2018-009

Interfaced to parton showers

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POWHEG		
vetoCount	100	3
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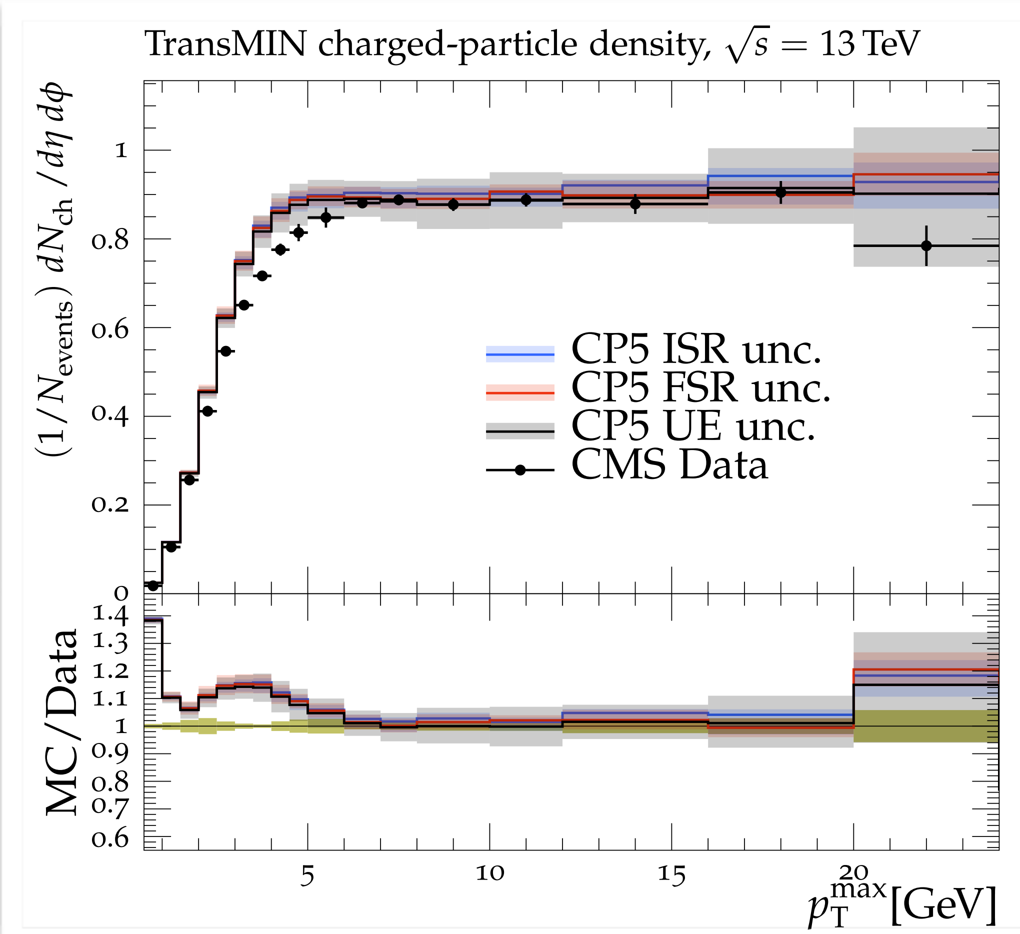
MPI and CR parameters

UE and CR tune parameters



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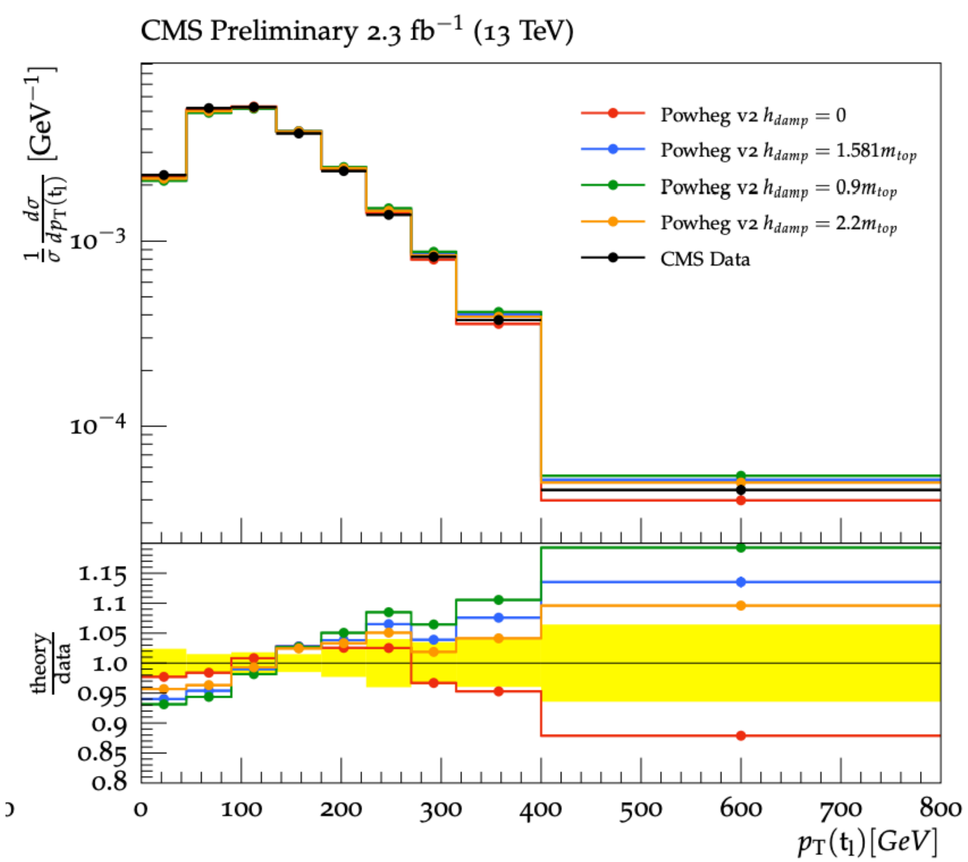
And uncertainties

Systematic	**ATLAS**	**CMS**
Nominal	PowhegPythia8	
PDFs	PDF4LHC recommendations	
NLO matching	Powheg vs MC@NLO	MC@NLO as cross-check but reweights top p_T to NNLO
Initial State Radiation	7-point variations of $\mu_R^{\mathrm{ME}}, \mu_F^{\mathrm{ME}}$ + independent variations of $h_{\mathrm{damp}}, \mu_R^{\mathrm{PS,ISR}}$	
Final State Radiation	Variations of $\mu_R^{\mathrm{PS,FSR}}$	
Underlying Event	Tune variations (*A14*/*CP5*) + different CR models	
B-fragmentation	Variations of r_B parameter in Pythia8 (CMS also compares to Peterson fragmentation)	
Fragmentation/ Hadronisation	Pythia8 vs Herwig7	Pythia6 vs Herwig++ (only impact on jet response)
ttbar/Wt interference	DR vs DS in Powheg	

h_{damp} CHOICE

- In Powheg matching we have additionally an ambiguity in the amount of real radiation to exponentiate, which is regulated by the factor $h^2_{\text{damp}}/(h^2_{\text{damp}} + p_T^2)$, with h_{damp} a tunable parameter determined using ttbar data (N_{jets}, p_T^{top}, p_T^{jet1})
- CMS obtains $h_{\text{damp}} = 1.58^{+0.66}_{-0.59}$, ATLAS uses $h_{\text{damp}} = 1.5$ with an uncertainty from a symmetrised $h_{\text{damp}} = 3.0$ variation



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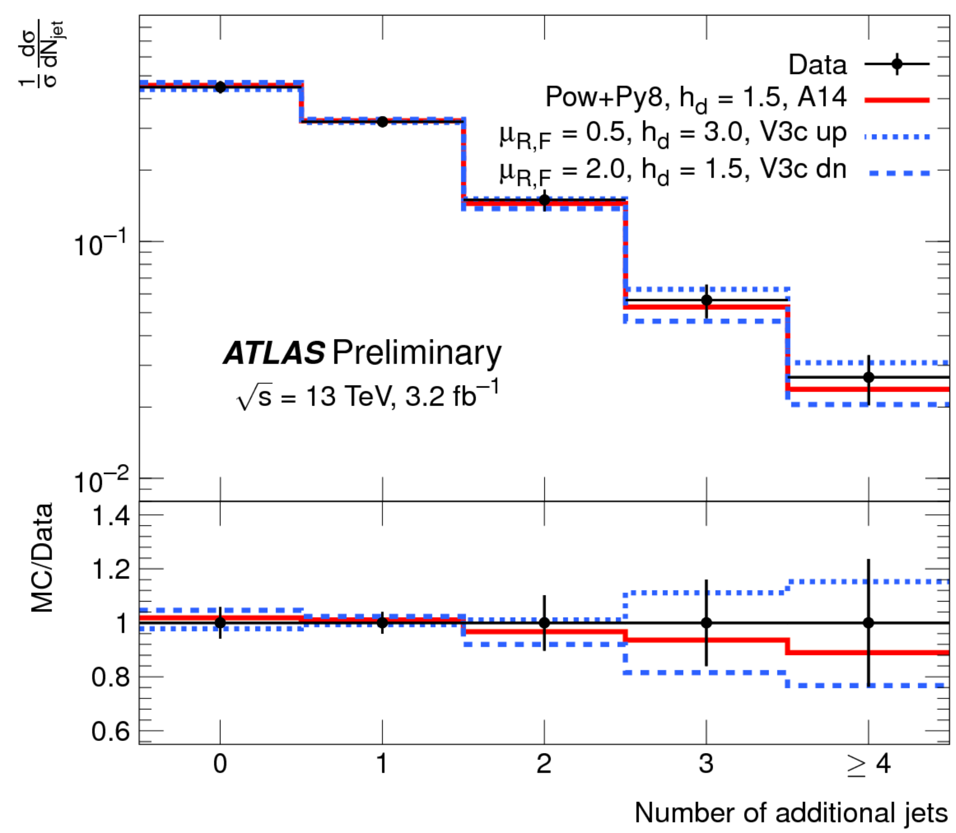

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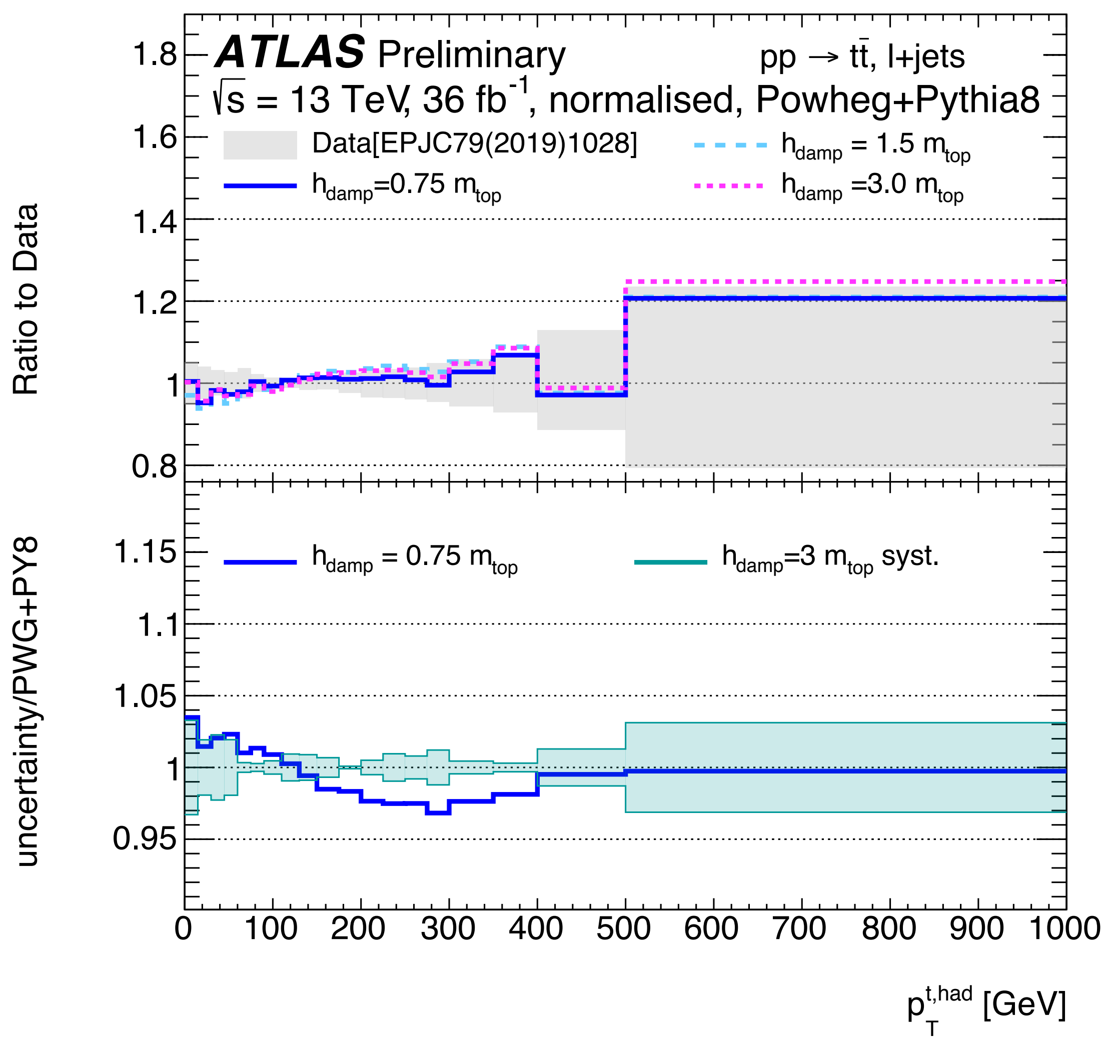
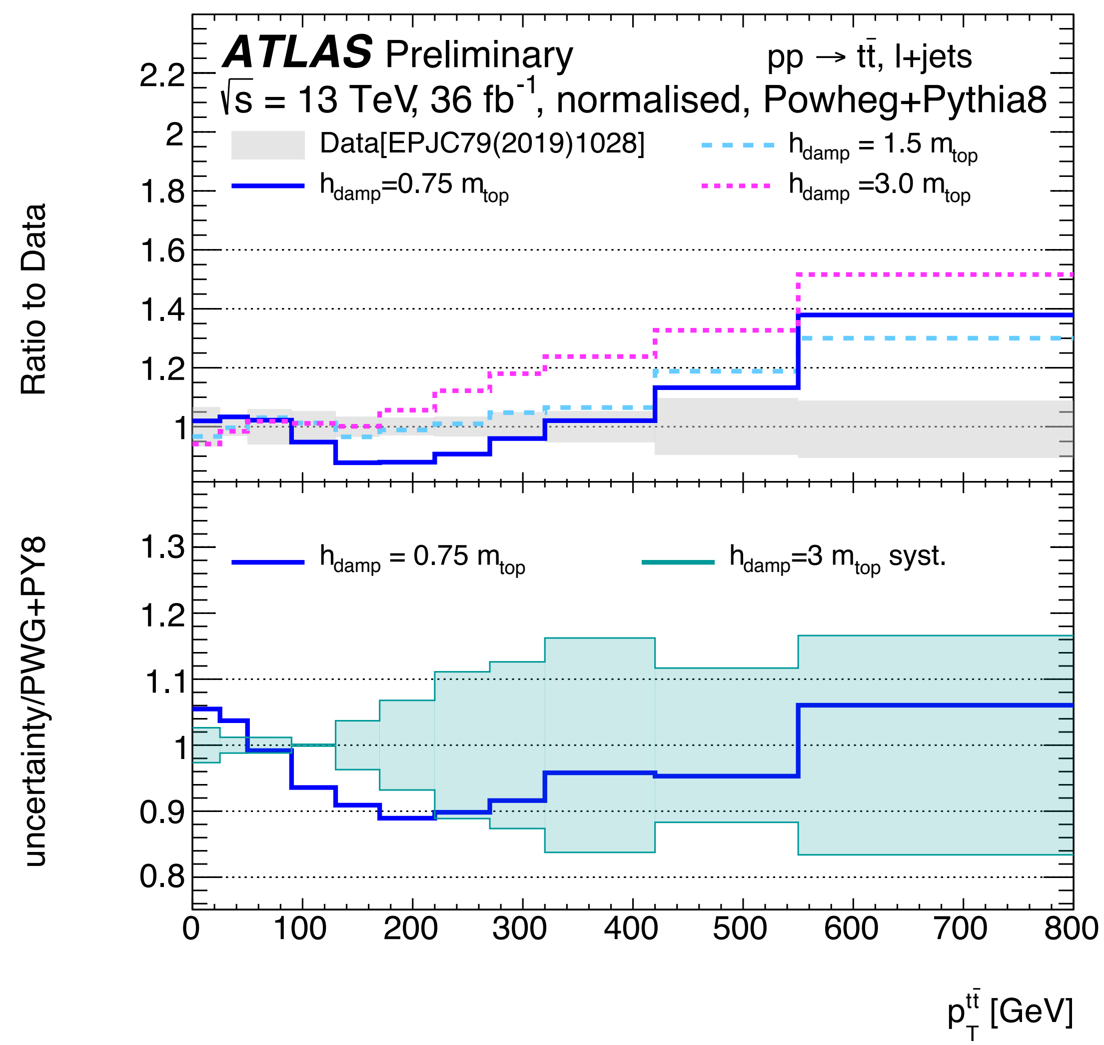
h_{damp} Uncertainties

- h_{damp} variation affects the $p_T(t\bar{t})$ at intermediate values
  - ATLAS uses a one-sided h_{damp} variation symmetrised
  - CMS a two sided variation from the tune
  - Only minor differences between the two approaches

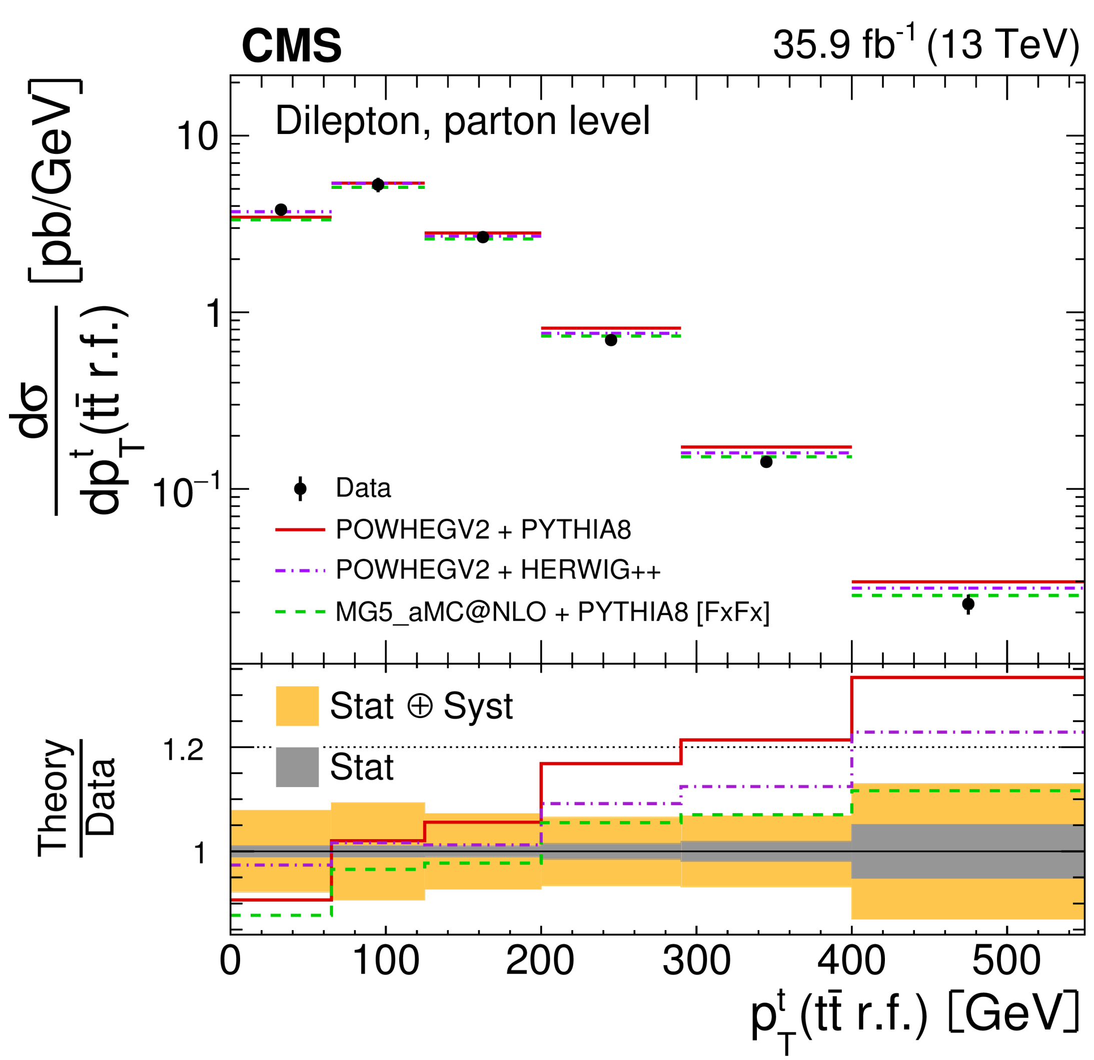




ATL-PHYS-PUB-2020-023

NLO generator uncertainty

- Important to validate the nominal prediction with independent samples using different codes and different algorithms
- This is done by comparing to MC@NLO matched samples
  - In ATLAS often included as an additional "matching" uncertainty
- Comparison often gives a large uncertainty (or is the dominant one)



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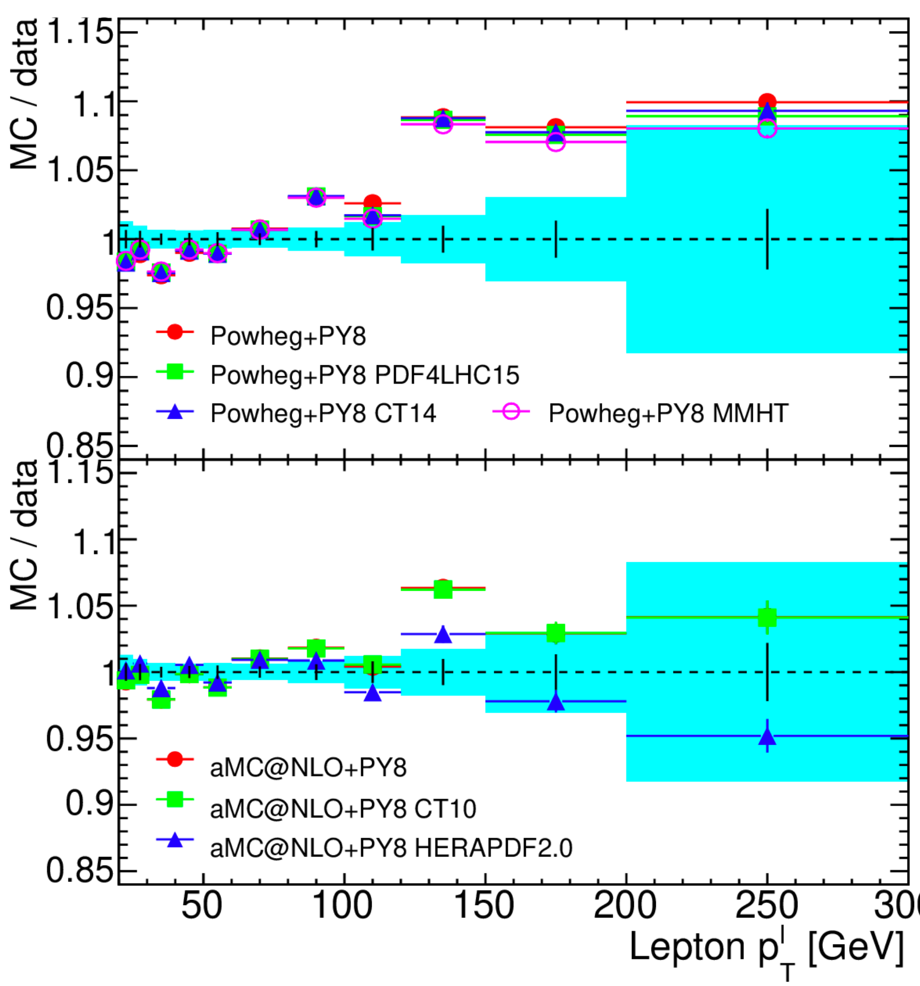

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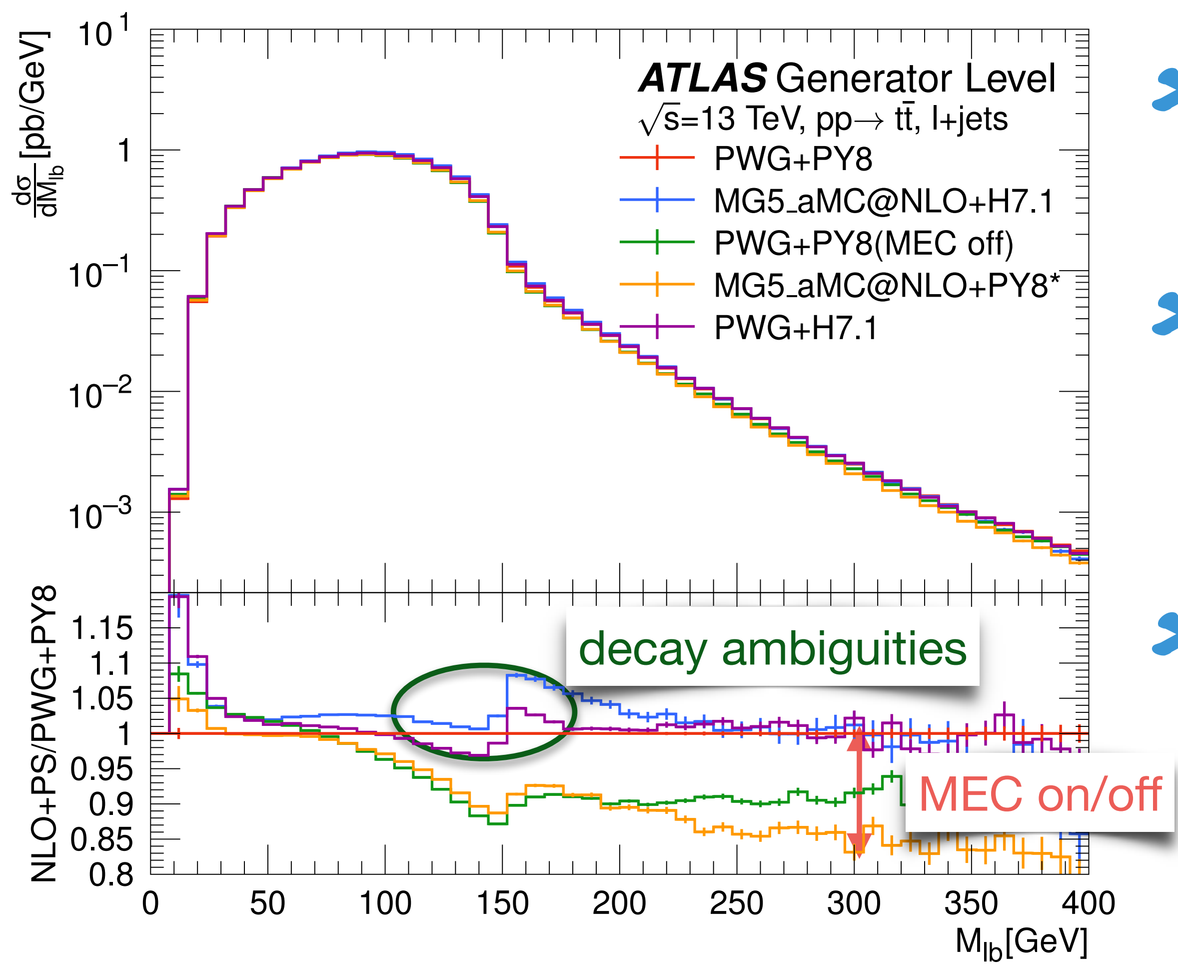
NLO generator uncertainty

- 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



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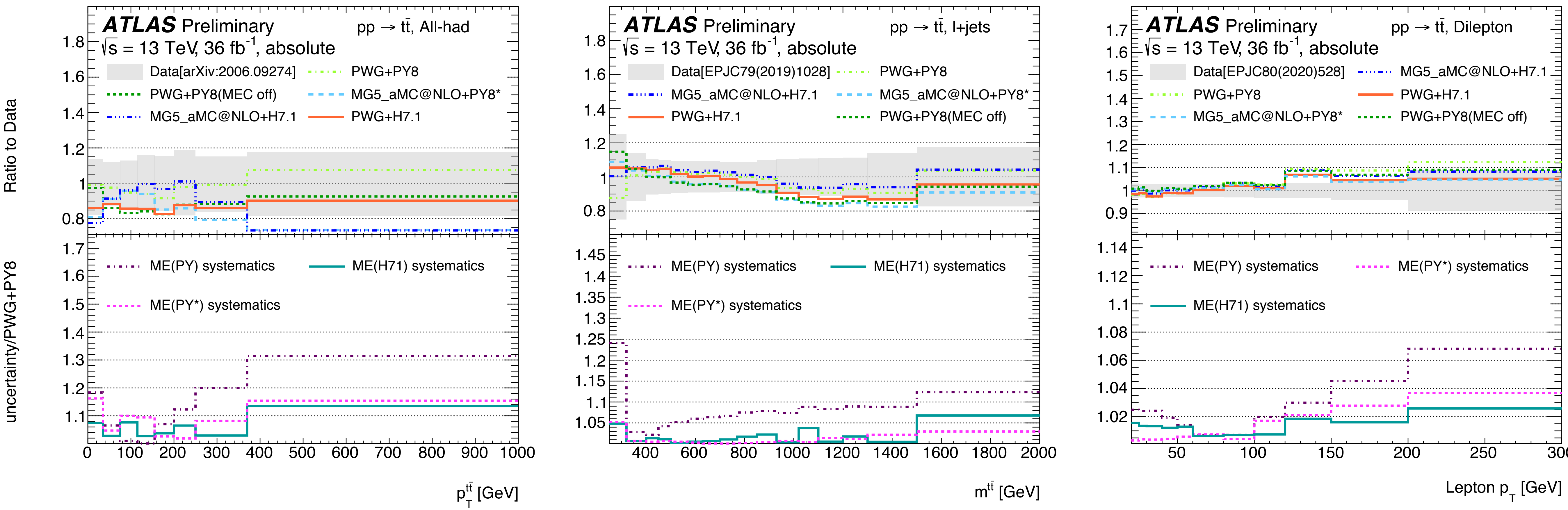
- Huge effect when considering top decay sensitive observables
- Disabling MEC to the decay in Powheg restores agreement with mg5_aMC@NLO
- H7 adds MEC in MC@NLO matching, unclear if this adds some double-counting

NLO GENERATOR UNCERTAINTY

- Considered two ways to factorise the effect of MEC in the decay from the Powheg/mg5_aMC@NLO comparison
  - ME(PY*) - Switch off the decay MEC in PowhegPythia
  - ME(H7) - Interface both codes to H7.1 (which adds decay MEC for both codes)
- Reduced differences with respect to the old recipe, yet somewhat selection and generator dependent



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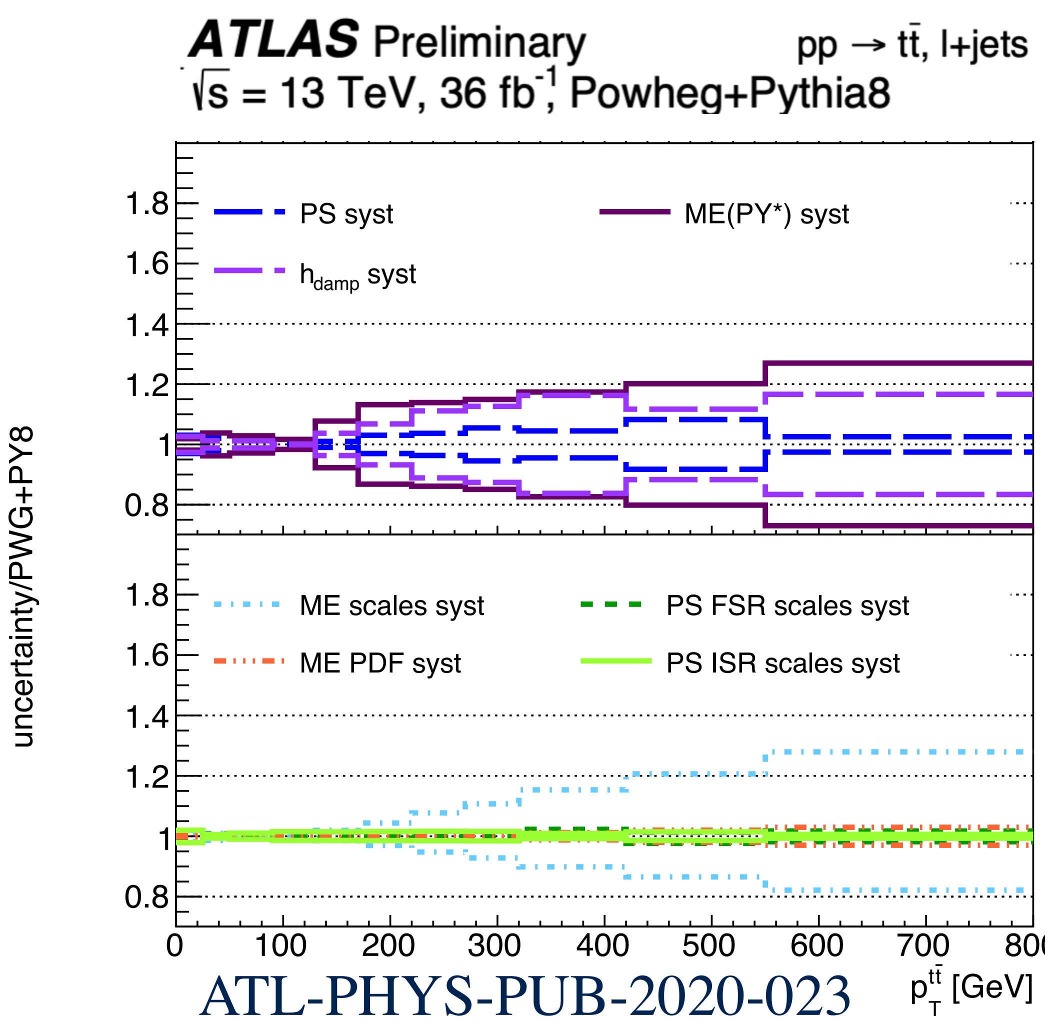
Shower uncertainties

- Parton shower perturbative uncertainties are obtained through variations of the scale at which the emission is evaluated (p_T)
  - Available in all generators as **“on-the-fly” weights** and usually including an O(α_S^2) compensation term to preserve the soft gluon limit
  - Typically separated into independent ISR and FSR variations
  - Usually small, but in exclusive phase-spaces can be larger than ME uncertainties (i.e. when looking at radiation in decay)



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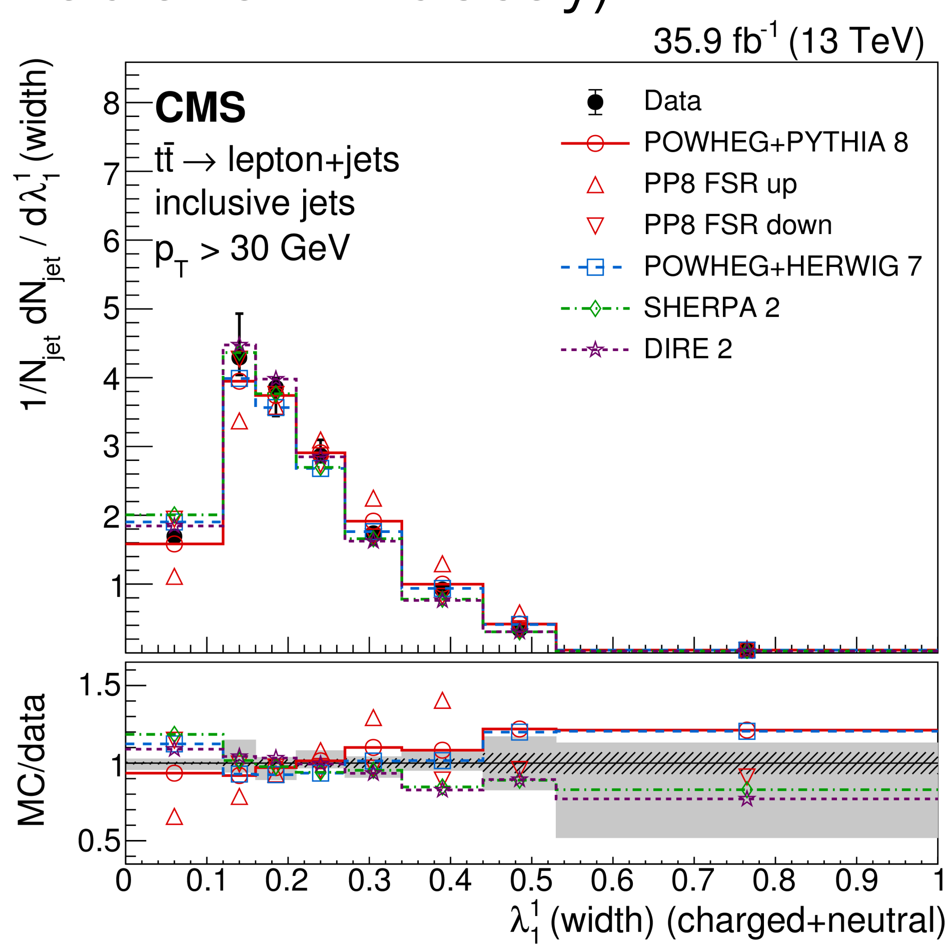
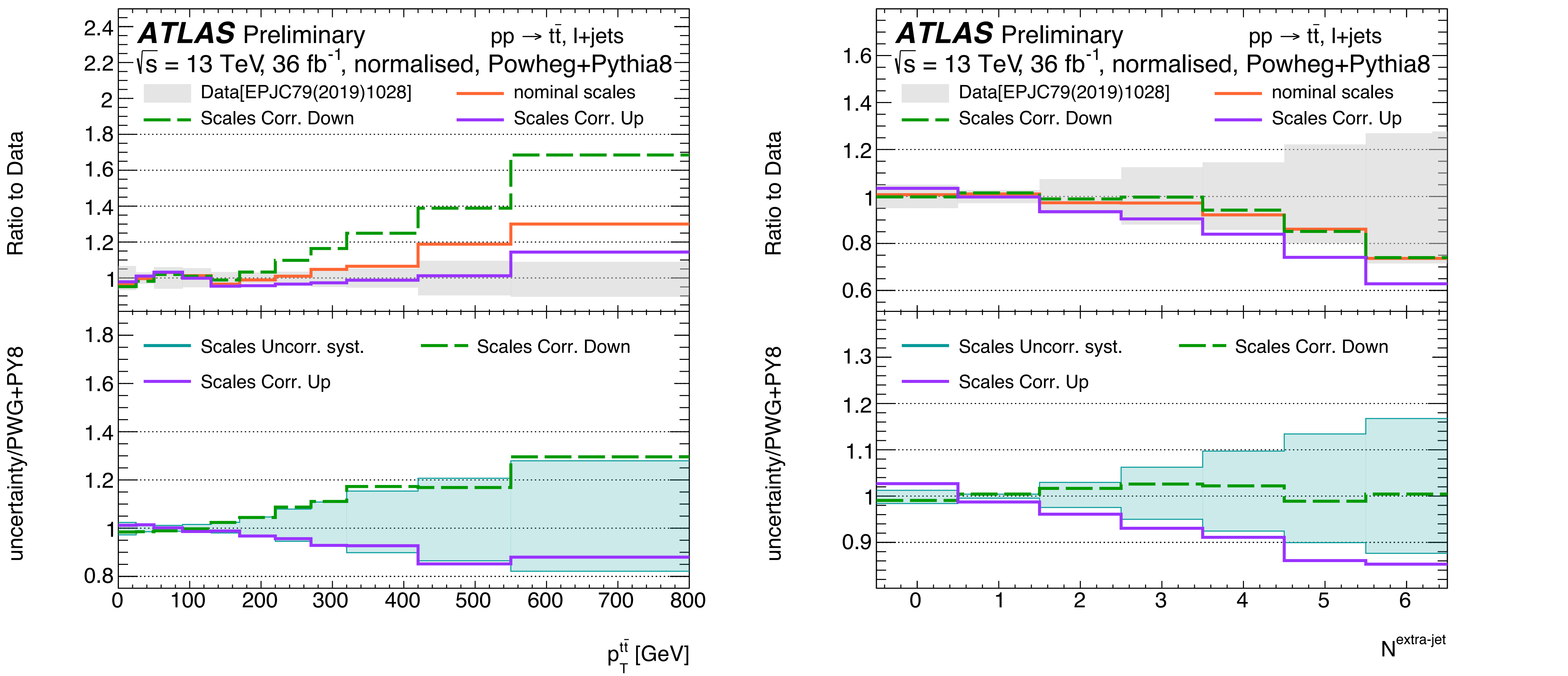


Phys. Rev. D 98 (2018) 092014

To correlate scales or not?

- ATLAS used to correlate the ISR variations ($\mu_R^{\mathrm{ME}}, h_{\mathrm{damp}}, \mu_R^{\mathrm{PS,ISR}}$)
  - Seen to provide coverage of differential ttbar cross-sections data
  - Several studies (see LesHouches17) also suggest this approach
- What is the impact of correlating or not ME and PS scales?
- Almost no difference for p_T(ttbar) while at high jet multiplicities correlating the scales gives a smaller MHOU (aggressive?)



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Parton shower Recoils

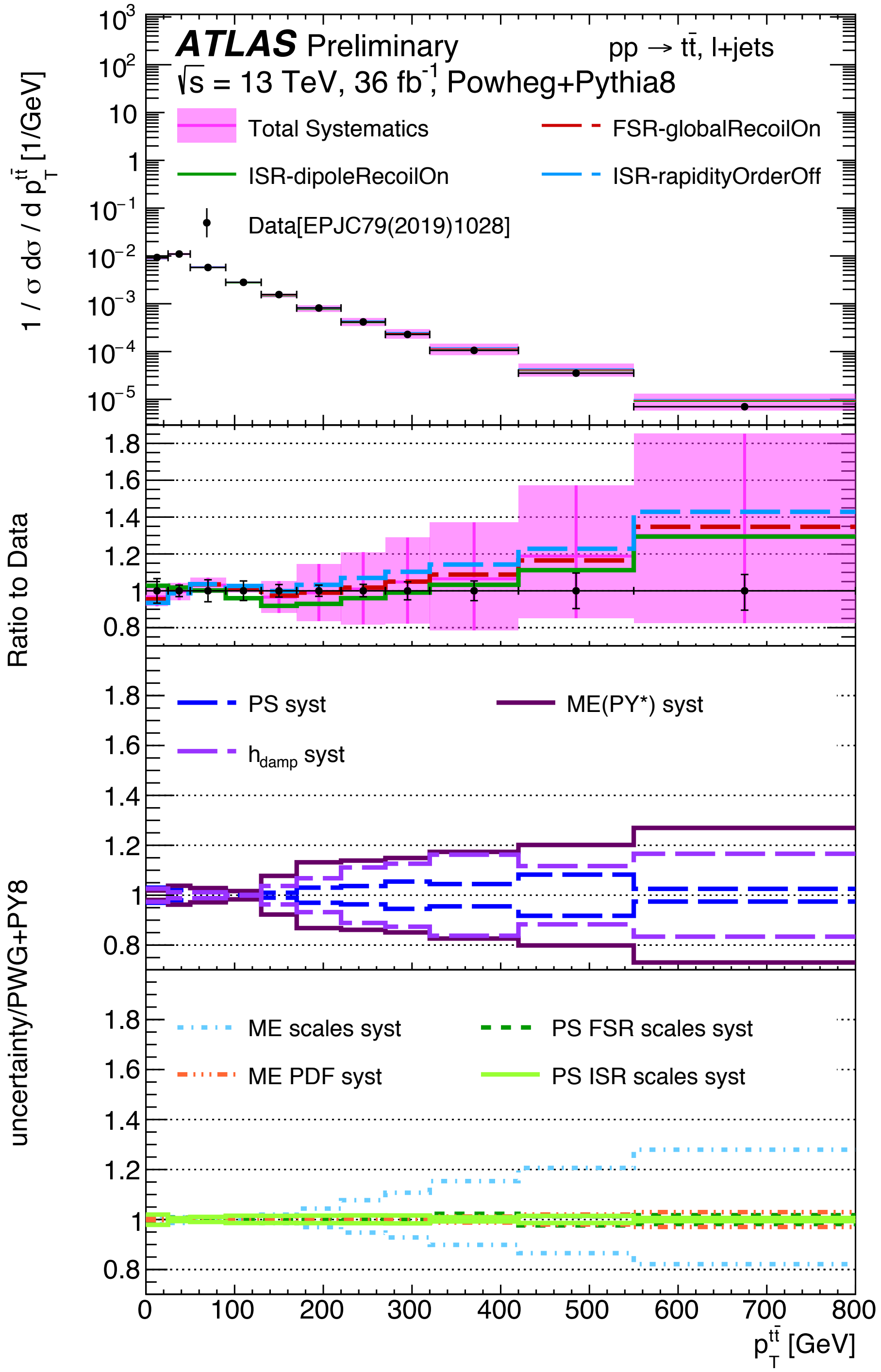
- Besides variations of μ_R many other ambiguities enter the construction of a parton shower
  - Ordering variable, recoils, treatment of splittings in the non-singular region, phase-space mapping, α_s evolution, …
  - Cannot be reweighted, and require dedicated MC runs

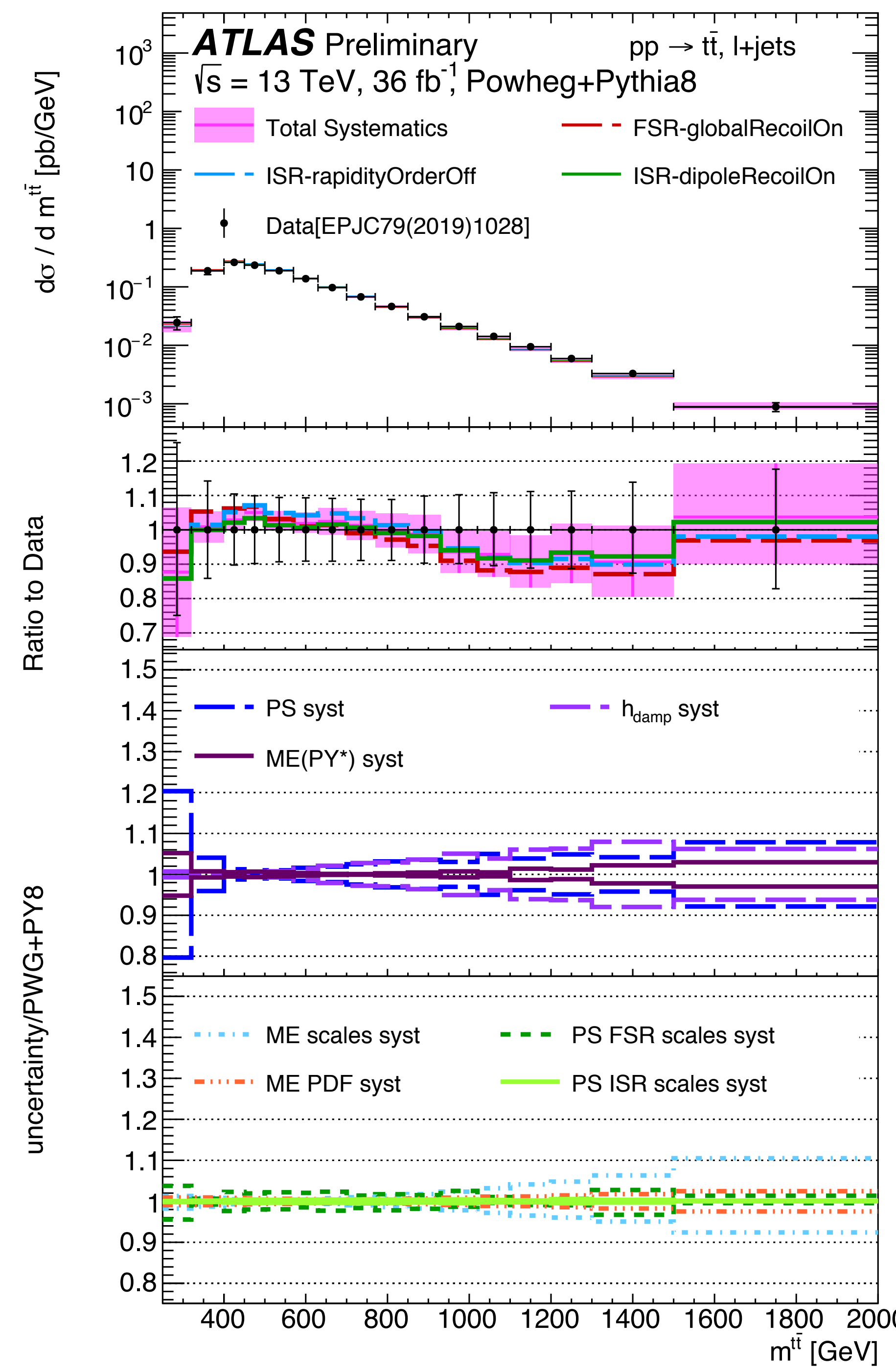
- Started to look at Pythia8 variations in ATLAS study
  - ISR:dipoleRecoil - pass from a global to a local recoil for ISR
  - ISR:rapidityOrdering - force rapidity ordering of ISR emissions
  - FSR:globalRecoil - pass from a local to a global recoil for FSR

- Important step towards constructing a full uncertainty band on a generator prediction using “in-house” variations

Parton shower recoils

- Effect of the recoil well within the quoted uncertainties
  - Hints of a better description of data with dipole recoils





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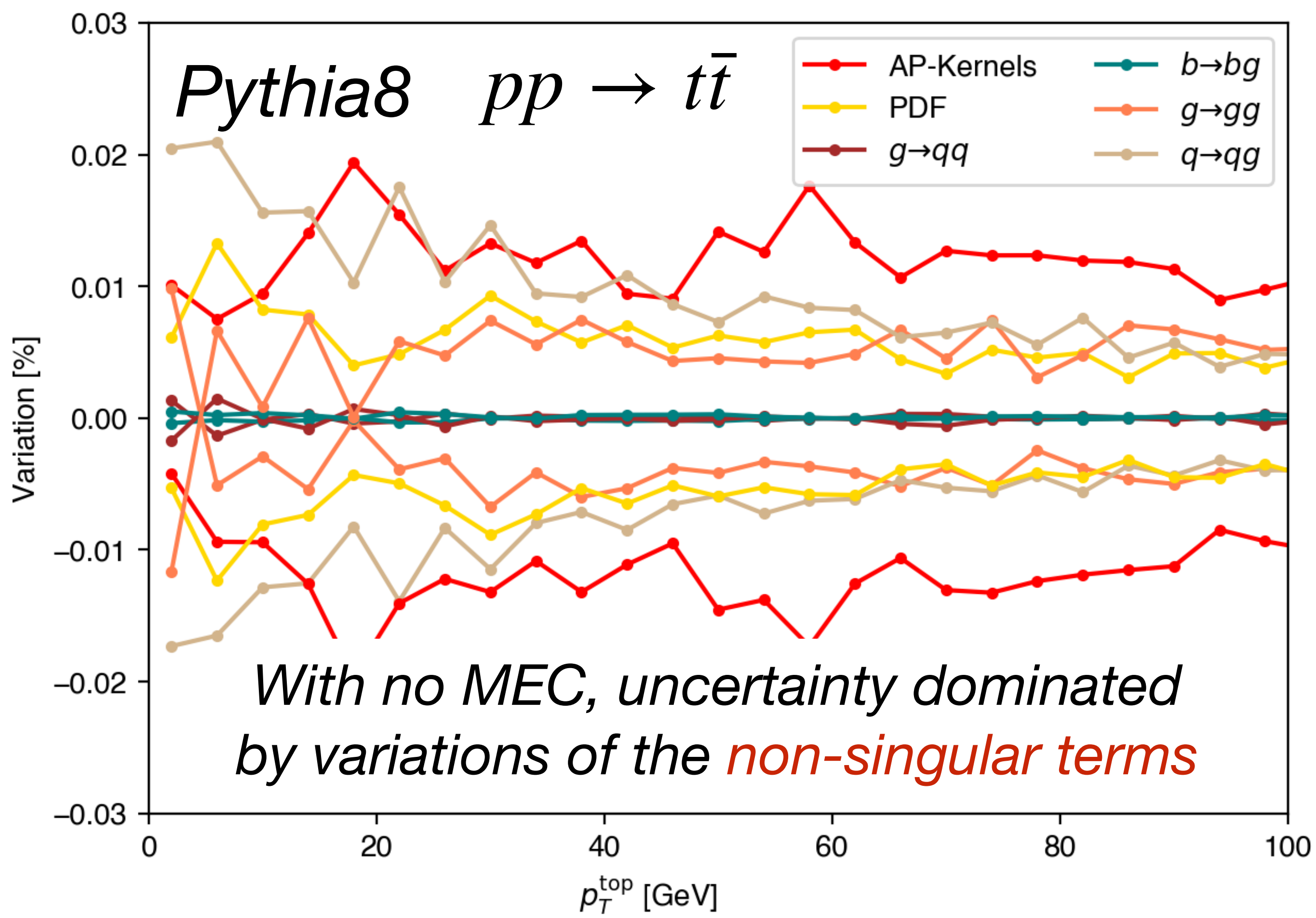
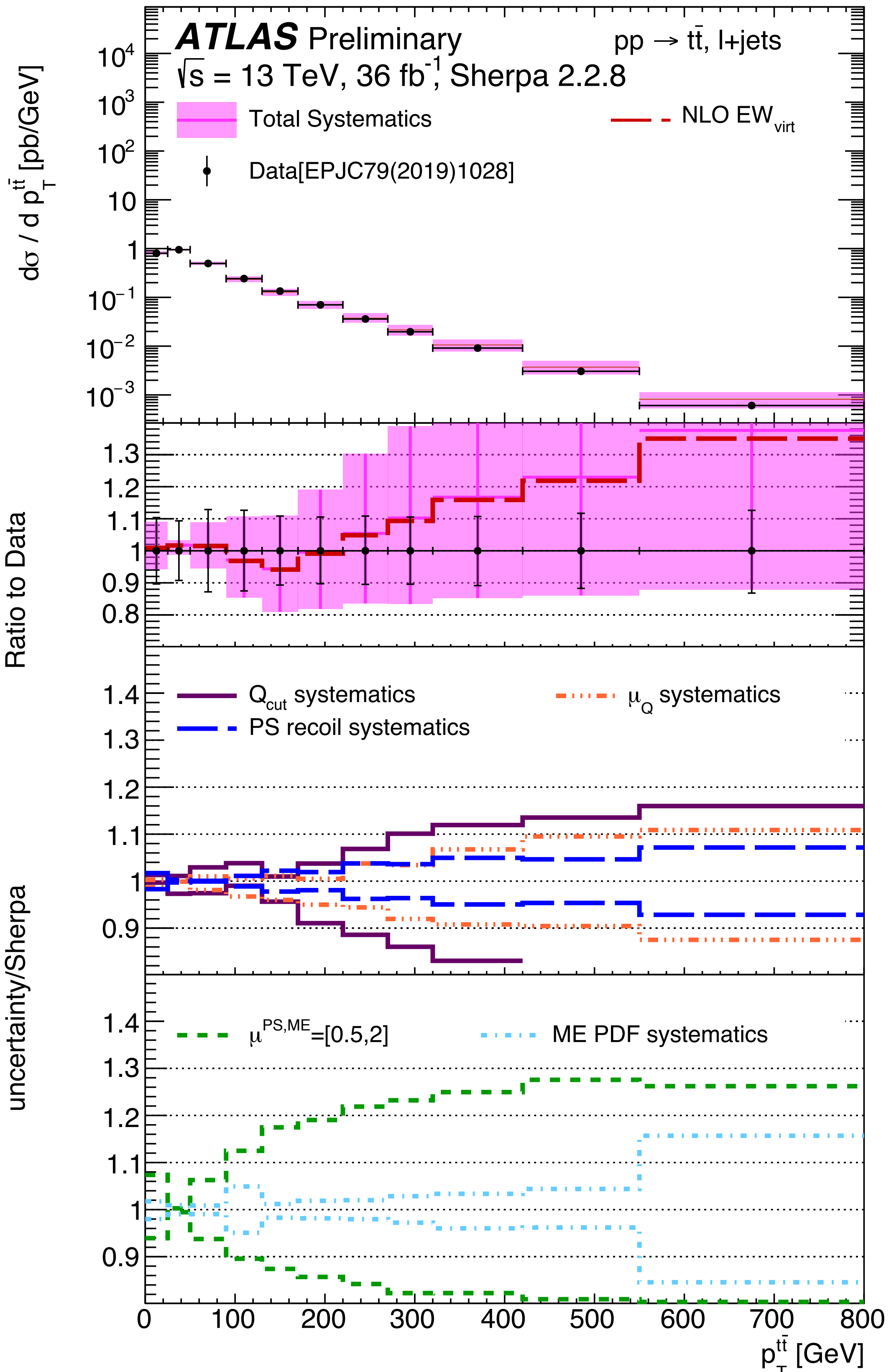
PS uncertainties - the future?

- Pythia8 has recently introduced the possibility of including "decorrelated shower variations" as on-the-fly weights
  - Independent μ_R variations for each splitting kernel
  - Variations of the DGLAP splittings in the non-singular region
- Would allow to propagate (and constrain) the decorrelated μ_R variations as nuisance parameters in likelihood fits



  - Avoids spurious constraints like having a b-quark from top decays constraints the scale of an ISR gluon
- Strong interest by both collaborations in exploiting this approach

Sherpa NLO-merged ttbar



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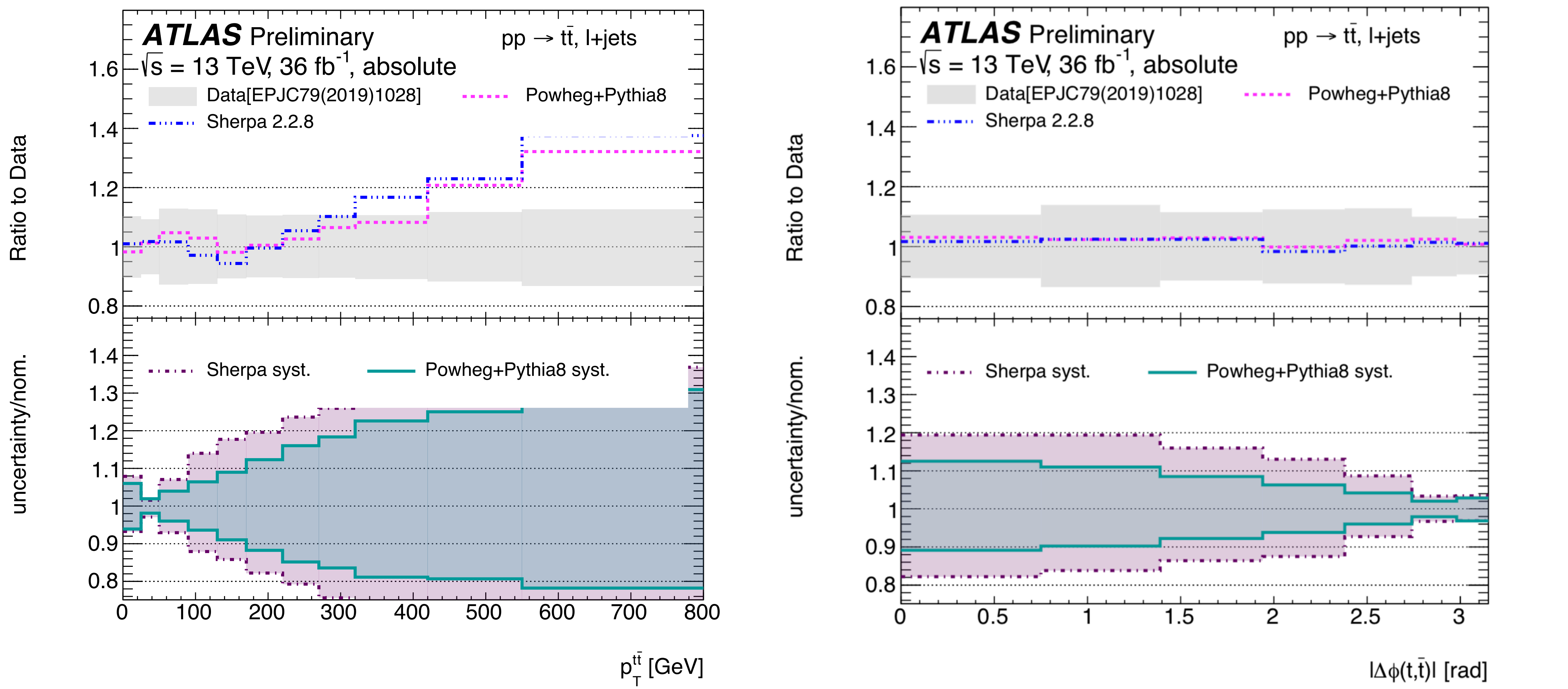
- Sherpa2.2.8 MEPS@NLO ttbar sample
  - ttbar+0,1jet@NLO+2,3,4jet@LO
  - Including NLO EW_{virt} corr. as weights
- Very good description of data, with no visible impact (yet) of NLO EW effects
- Construct a perturbative uncertainty band considering the following variations
  - 7-point variations of ME+PS scales
  - Merging scale variations Q_{cut} [20, 50] GeV
  - Shower starting scale variations [0.5,2.0]
  - Variation of the shower recoils

Do we understand perturbative uncertainties ?

- We can now compare the Sherpa and Powheg predictions
  - Adjusted the Powheg uncertainty band to contain similar variations
- Sherpa uncertainty consistently larger than PowhegPythia8
  - Would expect NLO-merging to significantly decrease uncertainties
  - Missing uncertainties in PowhegPythia8 or Sherpa too conservative?



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UE and CR Uncertainties

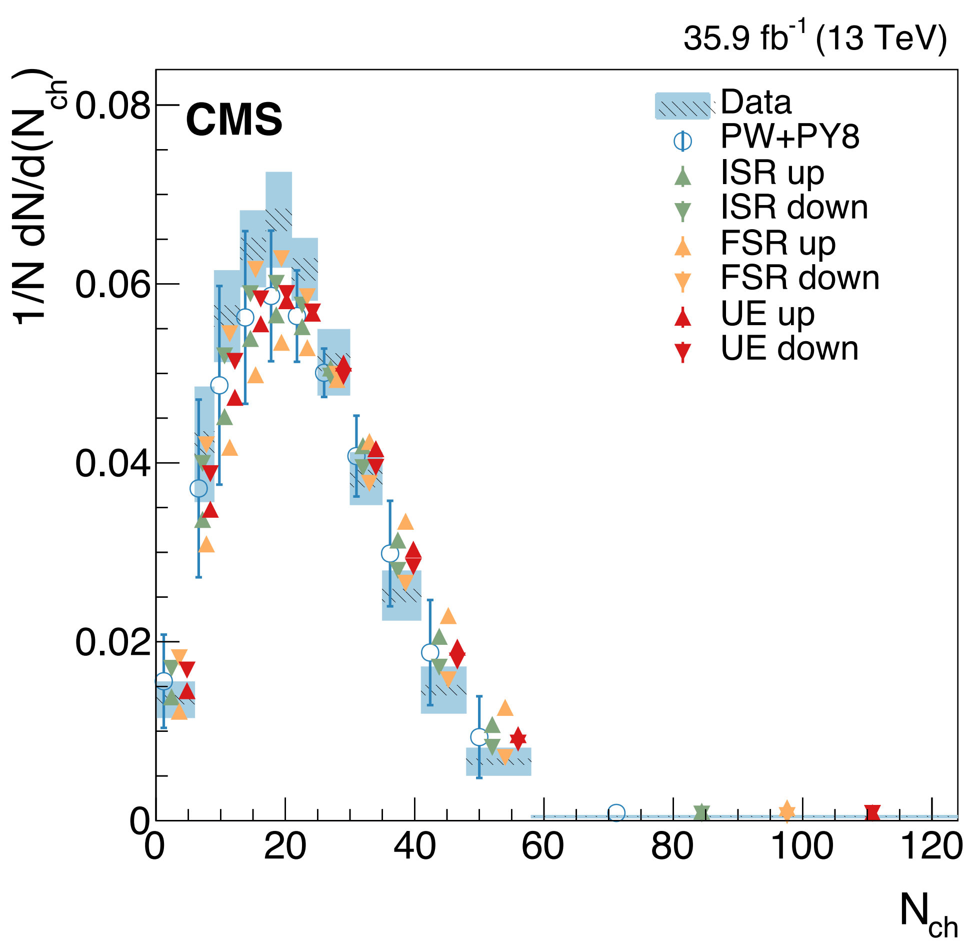
- CR reconnection significant uncertainty for mass measurements
  - Special role in top as decay width comparable to hadronization
  - Non-perturbative reshuffling of hadrons momenta, effects of $O(\Lambda_{QCD})$

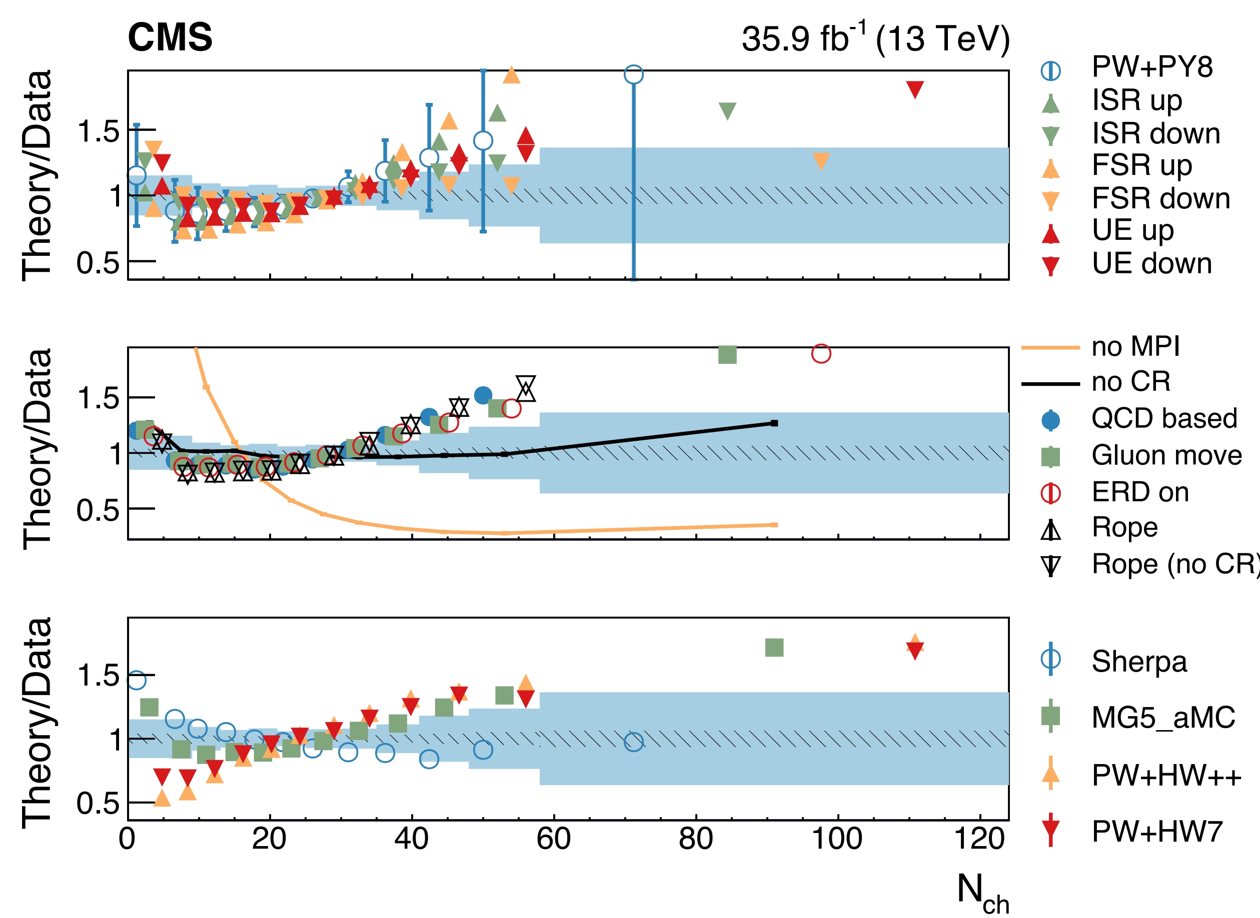
- New models have recently been implemented in Pythia8
  - ***MPI-model:*** default simple model, with a single “range” parameter
  - ***Gluon-move:*** very flexible, up to 1GeV effect on m_{top}
  - ***QCD-inspired:*** more realistic, small effects at LEP (and in top?)
  - And for each option for the top decay products can reconnect

- Both ATLAS and CMS now consider comparisons of some of these models in addition to parameter variations of the MPI-based one
  - Spread of Pythia8 models resulted in ~0.4 GeV uncertainty in the CMS 13 TeV direct mass measurement in the all had. channel

UE and CR measurements

- CMS measured of charged particle multiplicities in ttbar at 13 TeV, sensitive to FSR, MPI and CR
  - In general, overproduction of N_{ch} by all generators
  - Hard to disentangle MPI and CR effects, as interpretation is dominated by variations in the FSR shower scales
- Still, important (and only) input to test MPI universality





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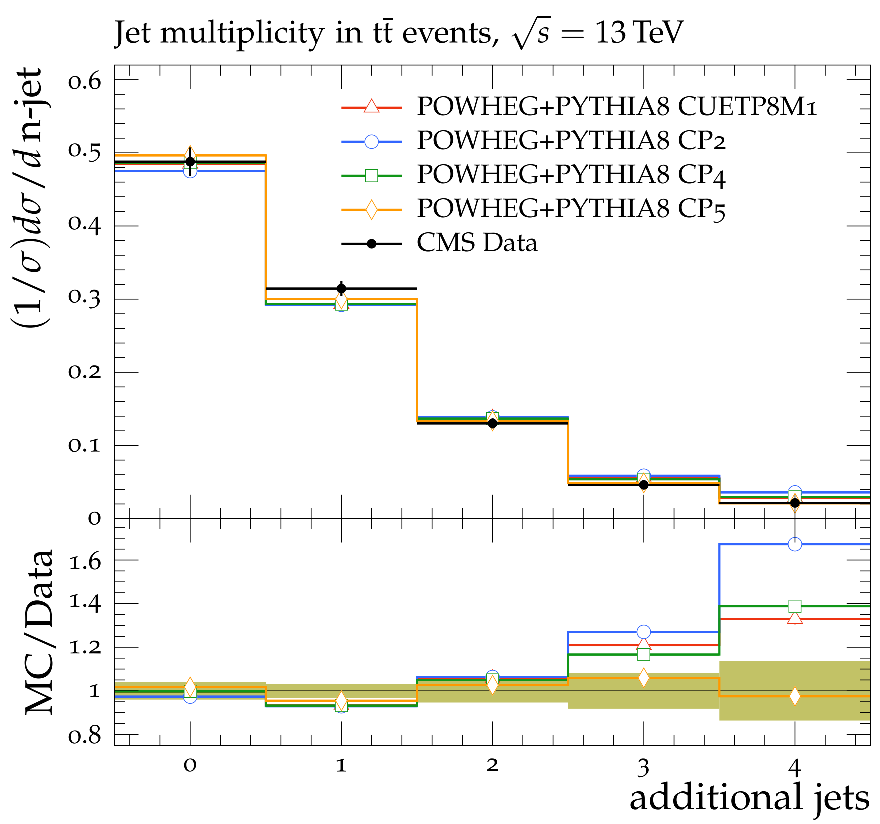
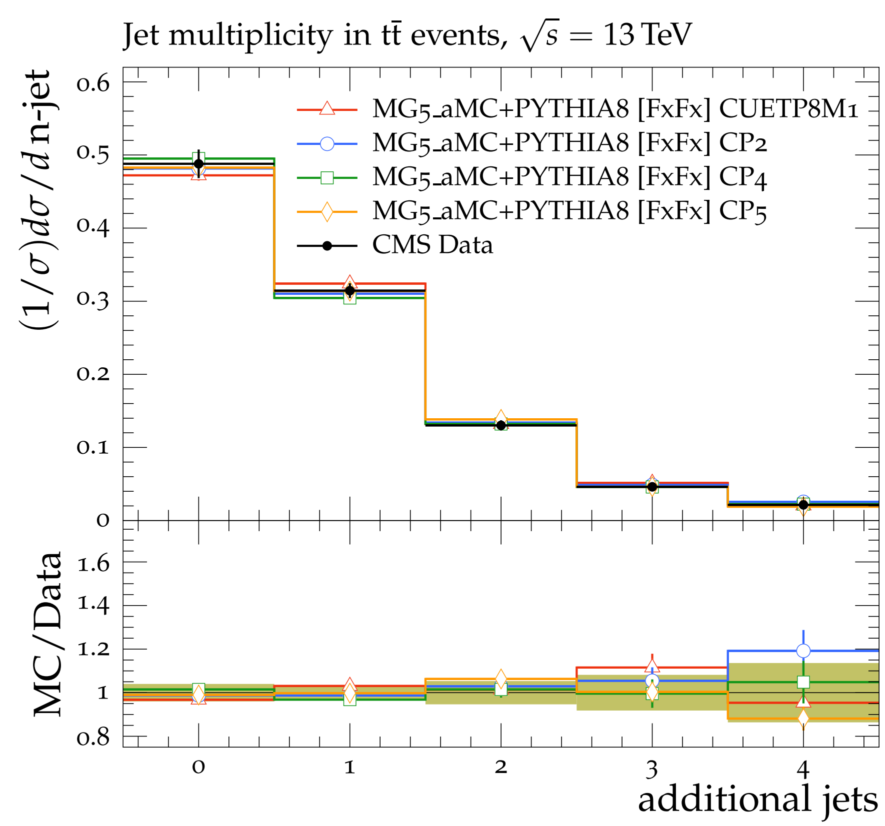
CMS Py8 tunes and TTbar

- CMS tune(s) of shower and MPI in Pythia8 to 13 TeV UE data
  - Explore different PS α_S and PDF order (LO, NLO, NNLO)
  - After tuning all options provide a similar description of UE data





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- Compared to measurements of ttbar production
  - Nominal CP5 tune best in the shower dominated region
  - But small differences when merging additional NLO MEs (FxFx)

CMS H7 tunes vs Ttbar

* New CMS tune(s) of shower/ MPI parameters in H7
  * To allow "tuned comparison" of Pythia/Herwig MPI models
  * Use NNLO PDFs and $\alpha_S = 0.118$ in the shower
  * Varying them in the MPI model, LO PDFs favoured by data

		SoftTune	CH1	CH2	CH3
	$\alpha_S(m_Z)$	0.1262	0.118	0.118	0.118
PS	PDF set	MMHT2014 LO	NNPDF3.1 NNLO	NNPDF3.1 NNLO	NNPDF3.1 NNLO
	$\alpha_S^{PDF}(m_Z)$	0.135	0.118	0.118	0.118
MPI	PDF set	MMHT2014 LO	NNPDF3.1 NNLO	NNPDF3.1 LO	NNPDF3.1 LO
	$\alpha_S^{PDF}(m_Z)$	0.135	0.118	0.118	0.130
	$p_{\perp,0}^{min}$	3.502	2.322	3.138	3.040
	b	0.416	0.157	0.120	0.136
	μ^2	1.402	1.532	1.174	1.284
	p_{reco}	0.5	0.4002	0.479	0.471
	χ^2/N_{dof} (fit)	-	4.15	1.54	1.71
	χ^2/N_{bins}	12.5	5.11	1.50	1.67

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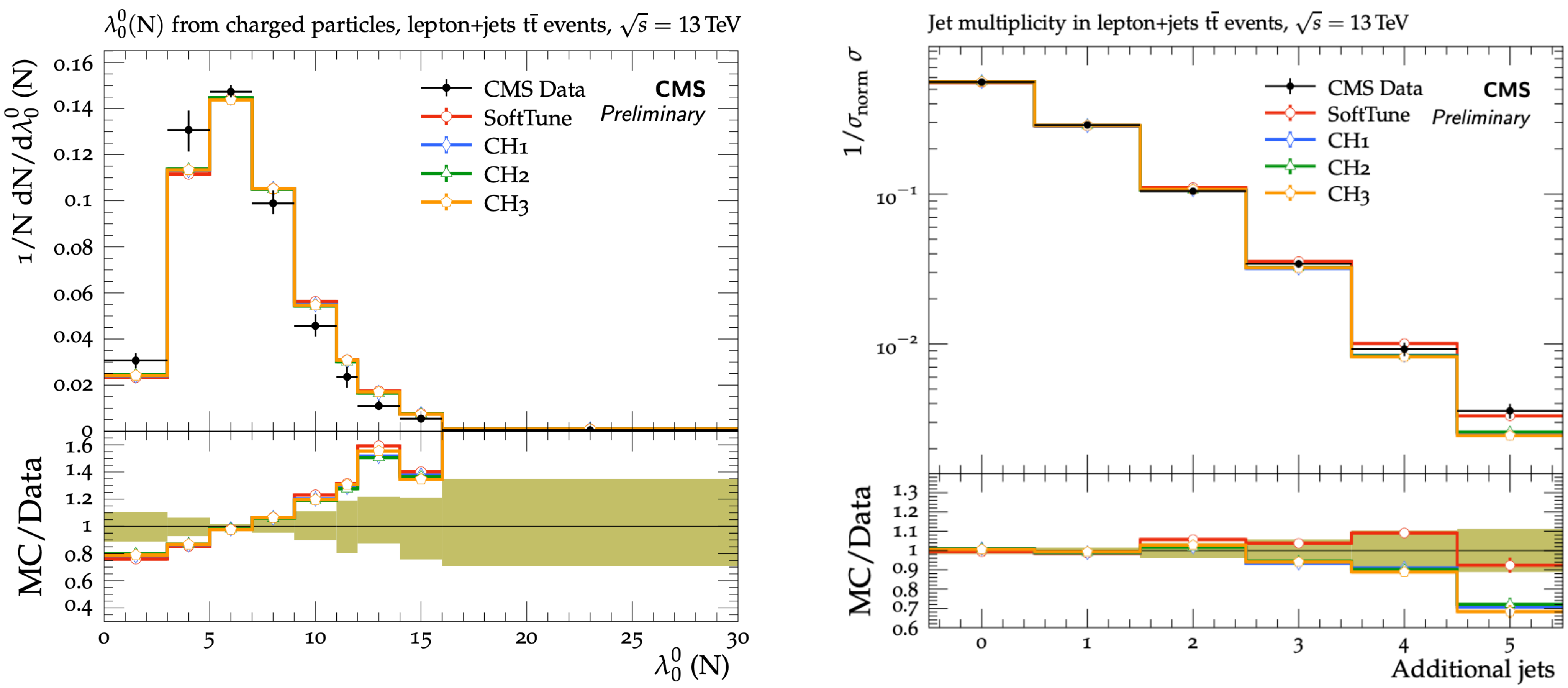
CMS H7 tunes vs TTbar

* Results compared to ttbar measurements (Powheg+H7)
  * Very good description of ttbar kinematics
  * Overprediction of charged particle multiplicities in ttbar



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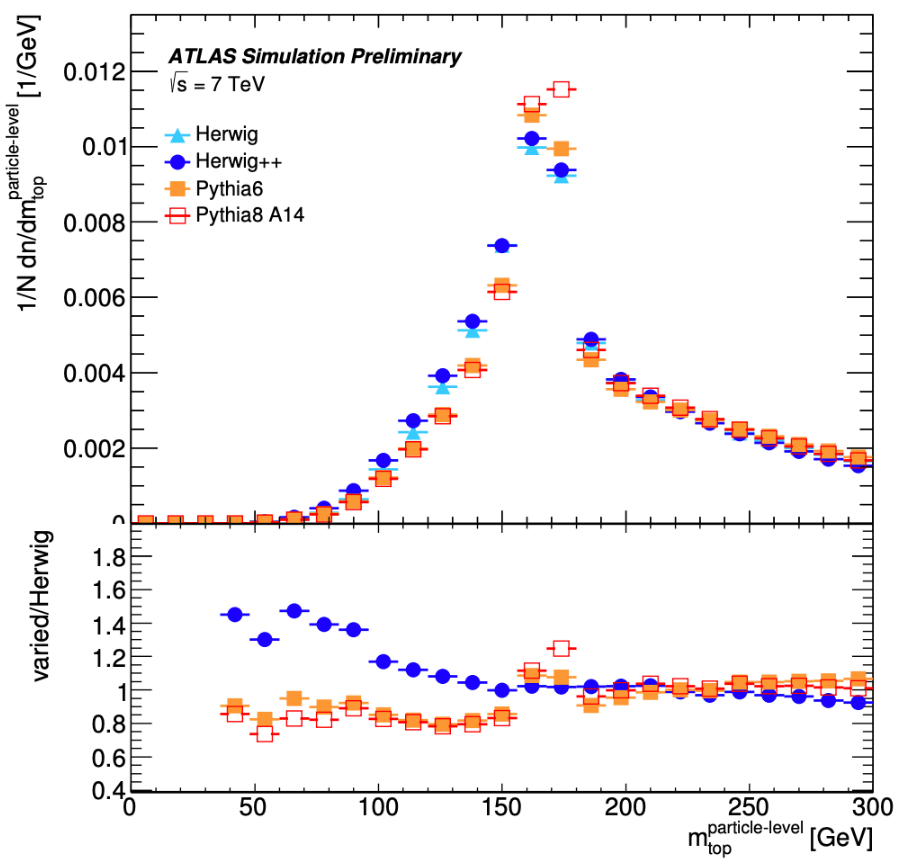
Hadronization

- No explicit hadronization uncertainties, rely on authors tunes and the usual Pythia/Herwig sandwich to cover them
  - Mix a change in shower (ordering variable, recoils), MPI and hadronization model, as well as the tune
- Important source of uncertainties in most mass measurements
  - In CMS consider only impact on the jet flavour response
  - ATLAS evaluates them both in the jet response and in the analysis, as old 7 TeV studies indicate jet response effect not sufficient



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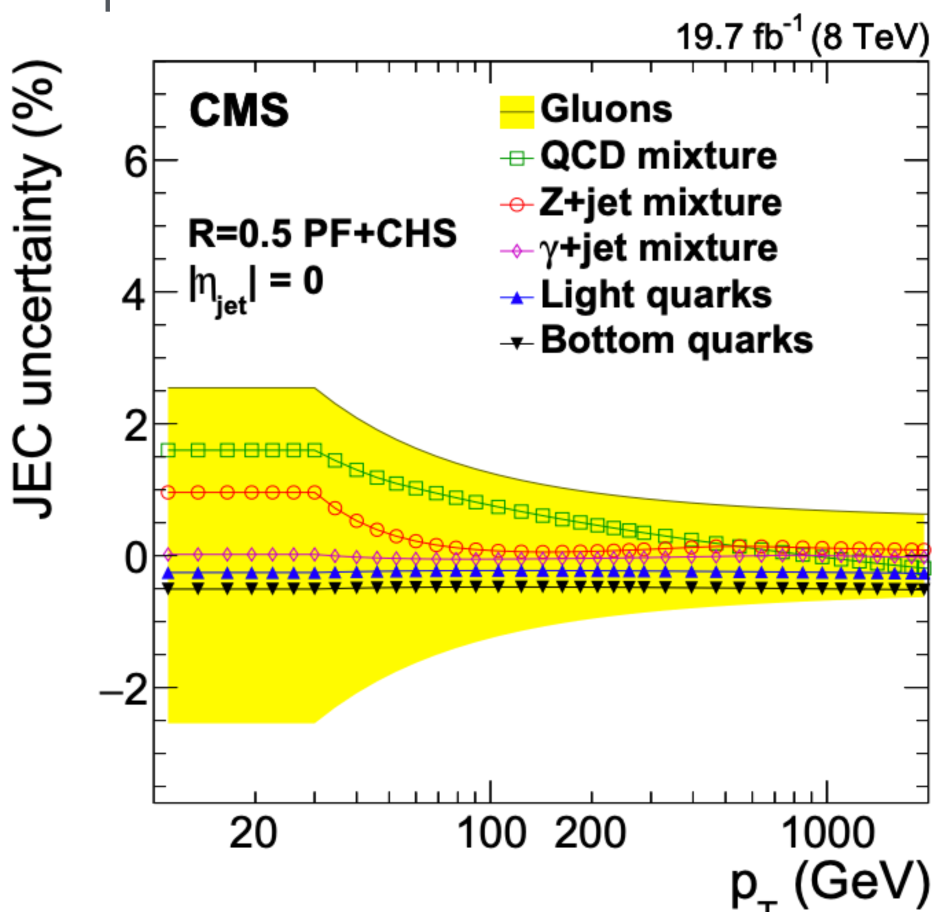
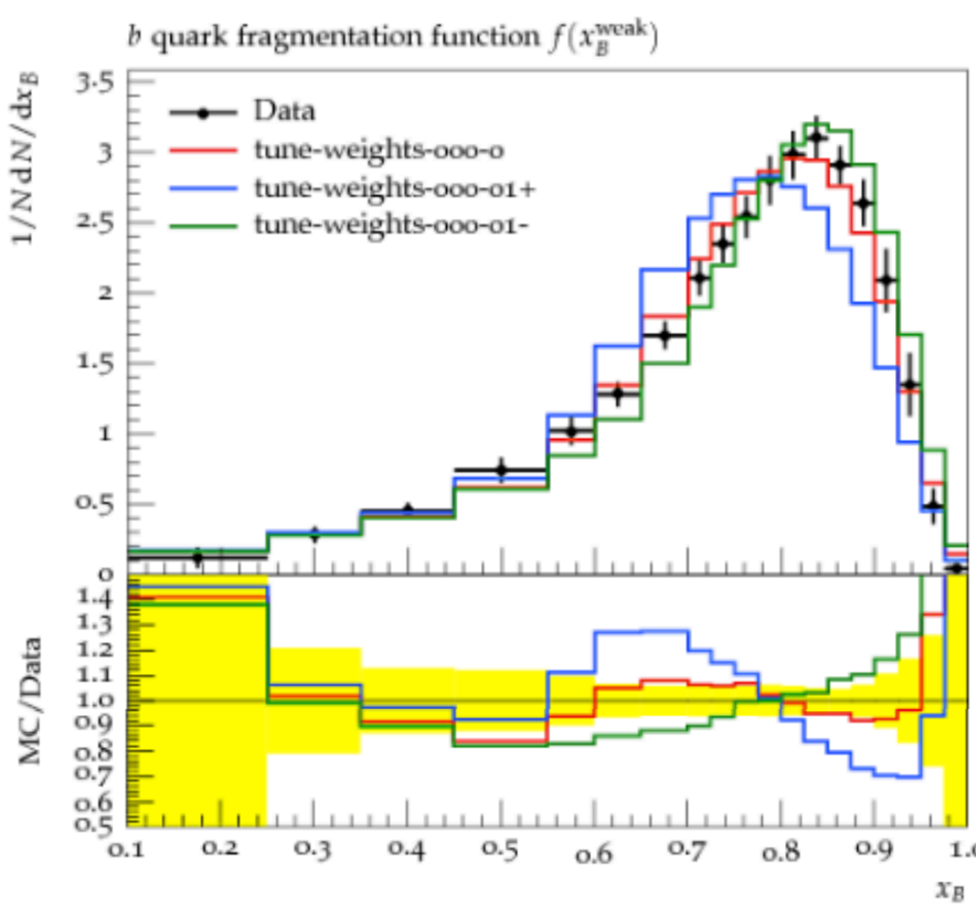


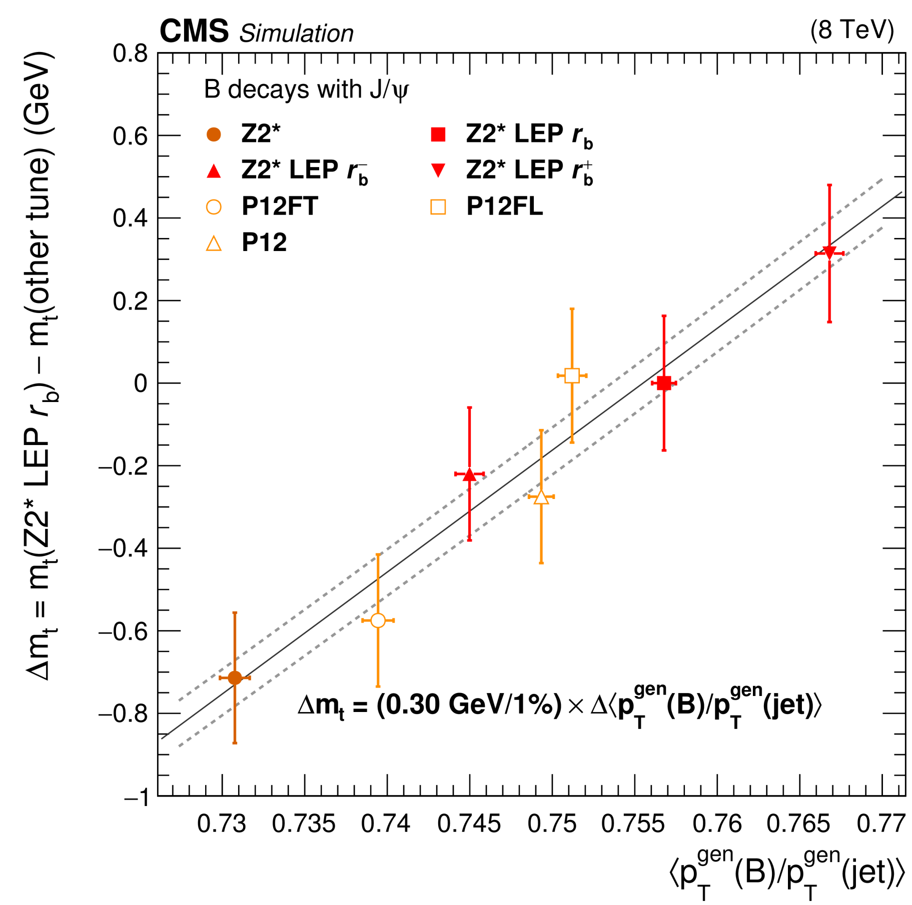
JINST 12 (2017) P02014

Bottom fragmentation

- Heavy-quark fragmentation described in Pythia by the Lund-Bowler string, introducing a mass suppression parameter, r_Q
  - Both ATLAS and CMS tuned this parameter to LEP/SLD data
  - Uncertainty from eigentunes, CMS in addition compares to the Peterson fragmentation function



[M. Seidel at HXSWG]

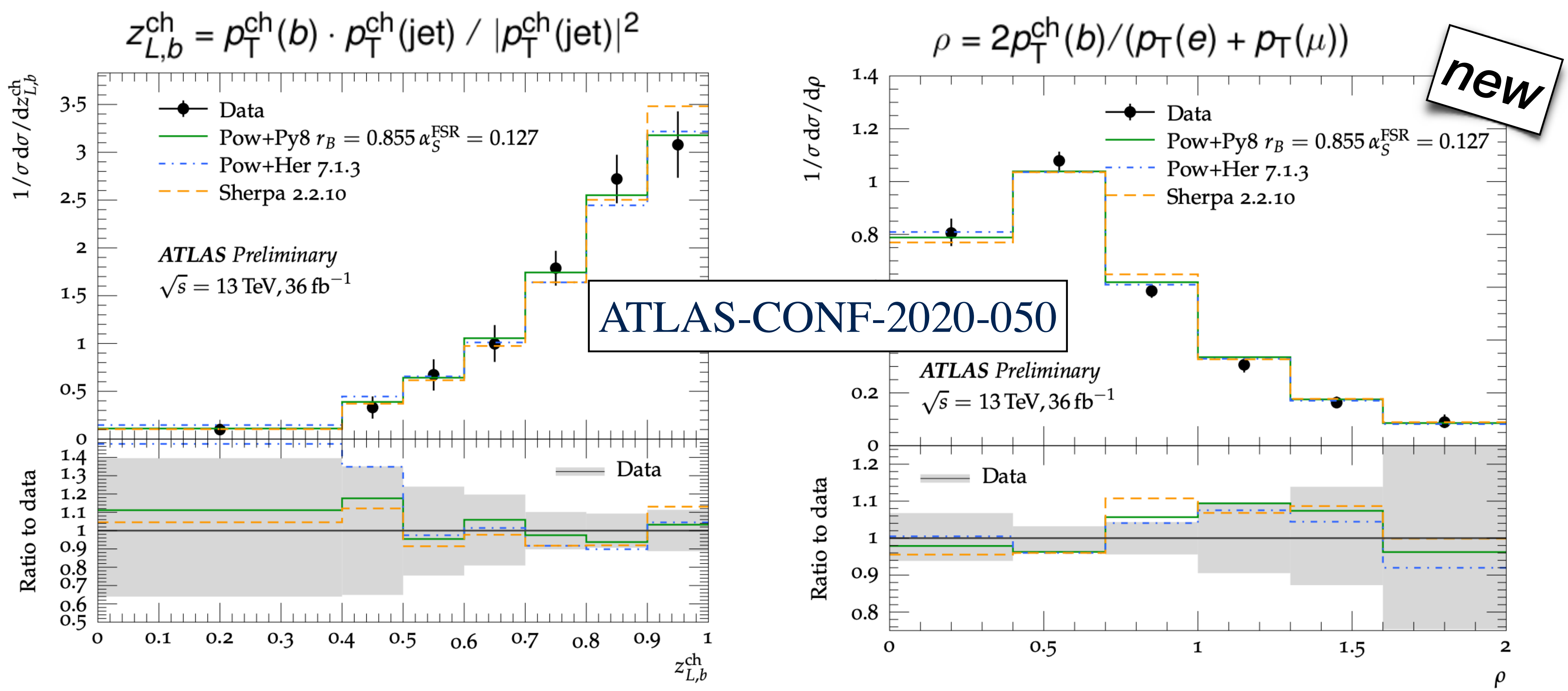


JHEP 12 (2016) 123

- B-fragmentation in top decays might be different from Z->bb, in-situ test in ttbar decays crucial!

Bottom fragmentation

- Heavy-quark fragmentation described in Pythia by the Lund-Bowler string, introducing a mass suppression parameter, r_B
  - Both ATLAS and CMS tuned this parameter to LEP/SLD data
  - Uncertainty from eigentunes, CMS in addition compares to the Peterson fragmentation function
  - New ATLAS measurement of fragmentation observables in ttbar, models consistent with data at this level of precision



Summary

- Reducing modelling systematics crucial to reduce uncertainties in top precision measurements (mass, cross-section, width, …)

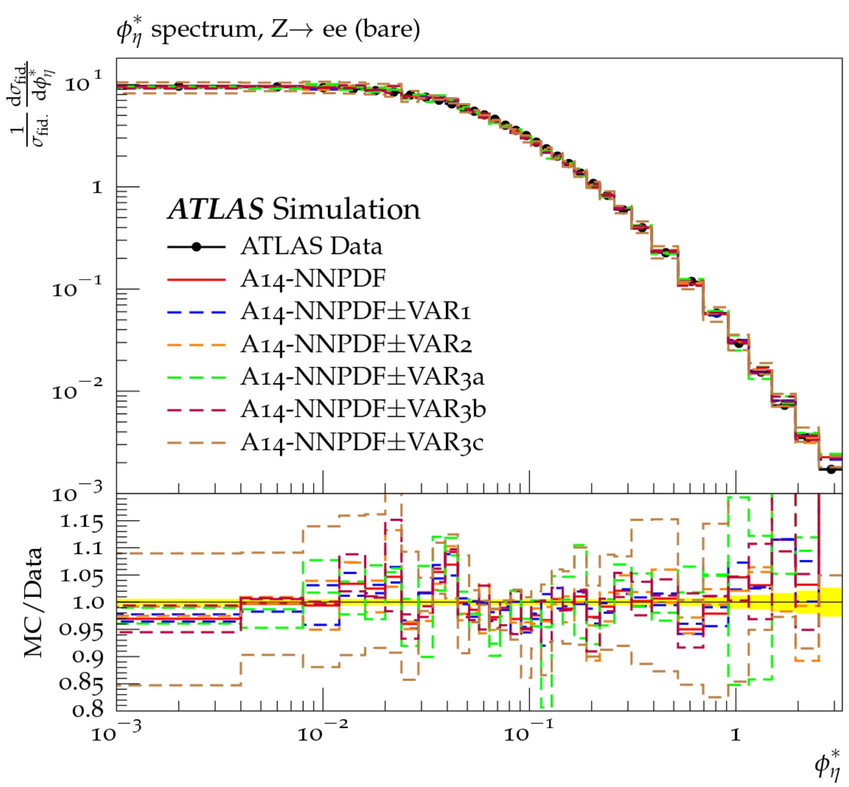
- Experiments still rely on “old” NLOPS generators, but we have seen significant theory improvements in the last years
  - NLO-merging ttbar production with MEPS@NLO, FxFx
  - NLO top decay in Powheg, H7.1
  - NLO finite width (and Wt interference) effects in Powheg
  - Higher accuracy showers and better models of MPI,CR
- Yet no single tool can seamlessly incorporate them all

- Ambiguities in MC predictions likely to dominate top measurements also in the future
  - Development of better models is essential
  - Need deeper understanding of theory uncertainties and “correlations"

Backup

ATLAS A14 Eigentunes

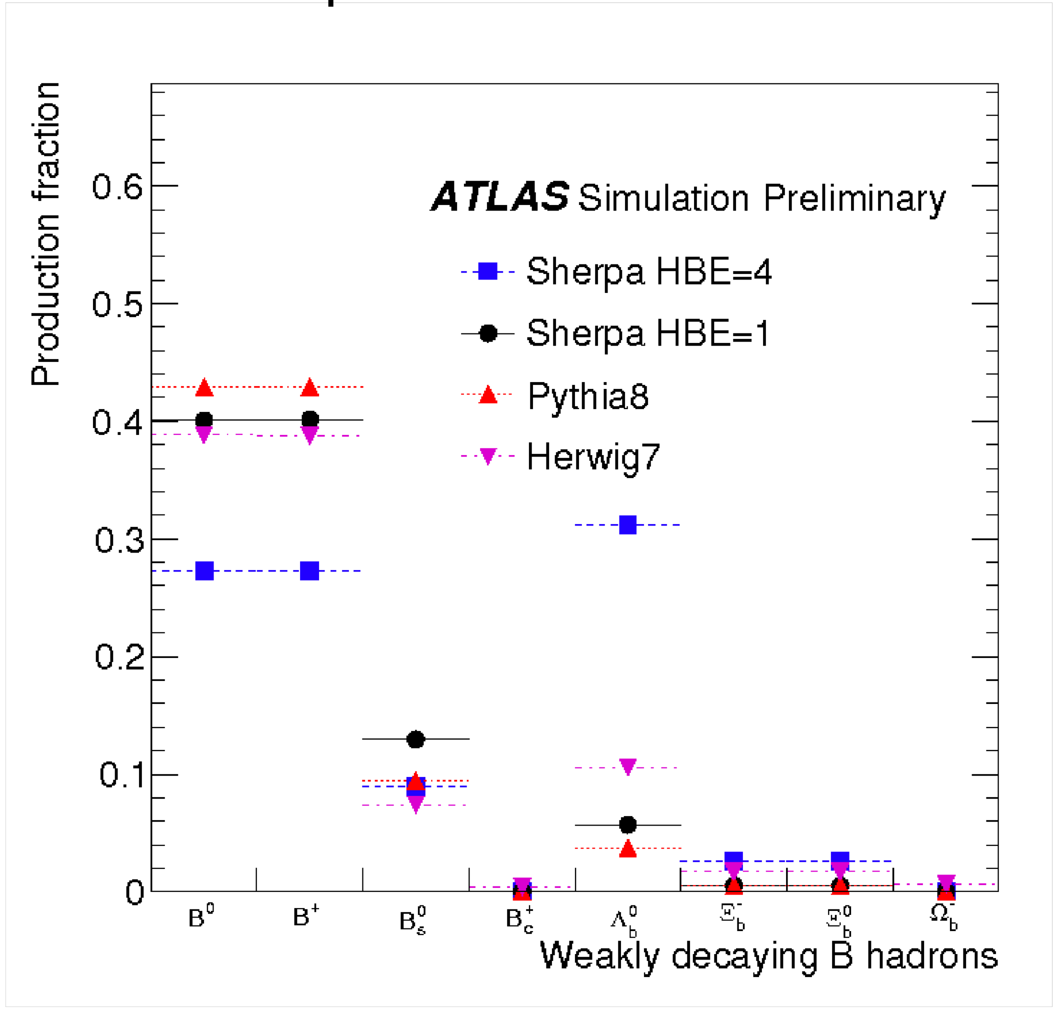
- Systematic variations (for A14-NNPDF23) are obtained using the eigentunes approach of Professor
  - Two variations per parameter (up/down), obtained by varying $\Delta\chi^2$ by a fixed amount until data uncertainties are covered
- 20 variations unmanageable, reduced to three by hand
  - Var1 for UE (MPI)
  - Var2 for jet substructure (FSR)
  - Three different Var3 to cover jet production (ISR), analysis and physics process dependent



Param	+ variation	− variation
VAR1: MPI+CR (UE activity and incl jet shapes)		
`BeamRemnants:reconnectRange`	1.73	1.69
`MultipartonInteractions:alphaSvalue`	0.131	0.121
VAR2: ISR/FSR (jet shapes and substructure)		
`SpaceShower:pT0Ref`	1.60	1.50
`SpaceShower:pTdampFudge`	1.04	1.08
`TimeShower:alphaSvalue`	0.139	0.111
VAR3a: ISR/FSR ($t\bar{t}$ gap)		
`MultipartonInteractions:alphaSvalue`	0.125	0.127
`SpaceShower:pT0Ref`	1.67	1.51
`SpaceShower:pTdampFudge`	1.36	0.93
`SpaceShower:pTmaxFudge`	0.98	0.88
`TimeShower:alphaSvalue`	0.136	0.124
VAR3b: ISR/FSR (jet 3/2 ratio)		
`SpaceShower:alphaSvalue`	0.129	0.126
`SpaceShower:pTdampFudge`	1.04	1.07
`SpaceShower:pTmaxFudge`	1.00	0.83
`TimeShower:alphaSvalue`	0.114	0.138
VAR3c: ISR ($t\bar{t}$ gap, dijet decorrelation and Z-boson p_T)		
`SpaceShower:alphaSvalue`	0.140	0.115

Decay Tables

- ATLAS using EvtGen-1.6 to decay heavy-flavour hadrons in all generators but for Sherpa
  - Reduce differences in HF-tagging efficiency across generators
  - Generally no dedicated uncertainty used
- CMS considering an envelope of Pythia8 and PDG values for leptonic B-hadron decays



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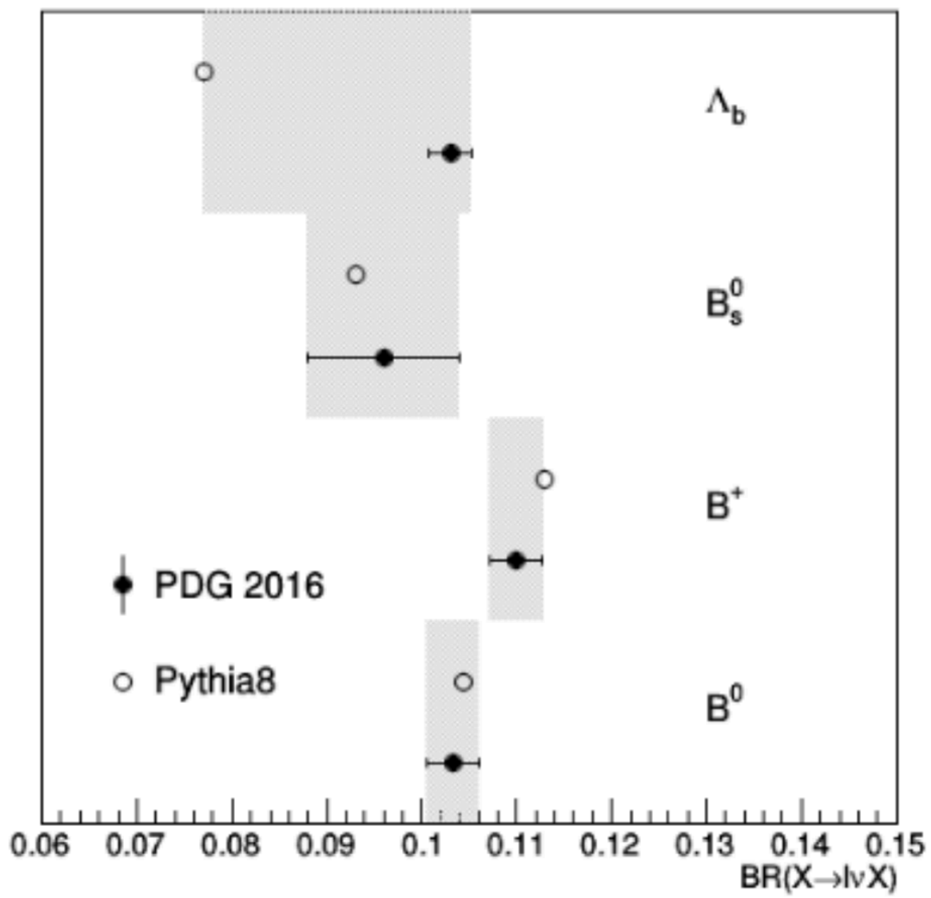
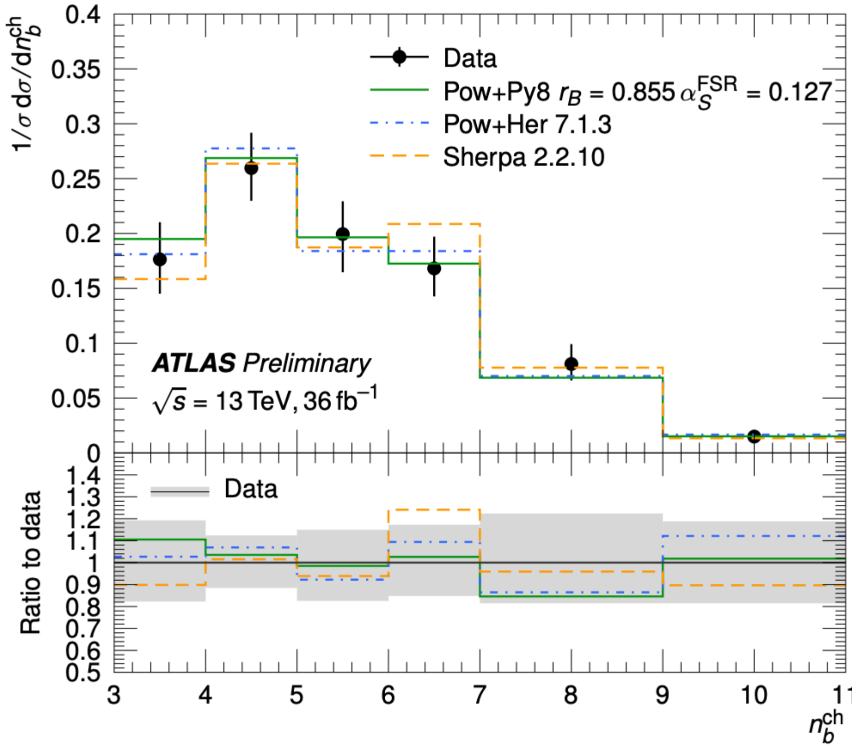
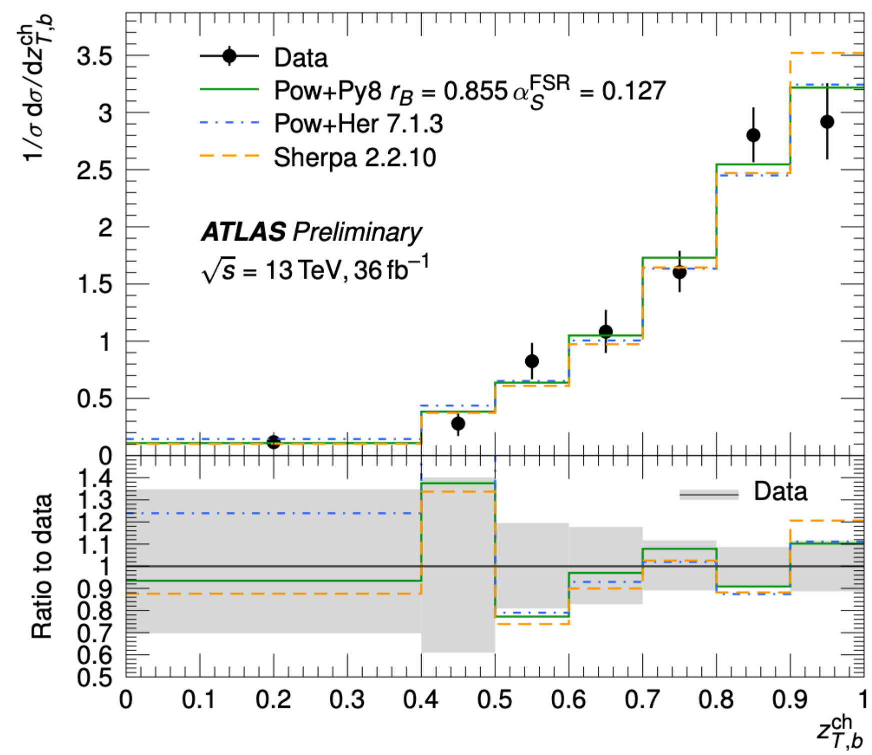
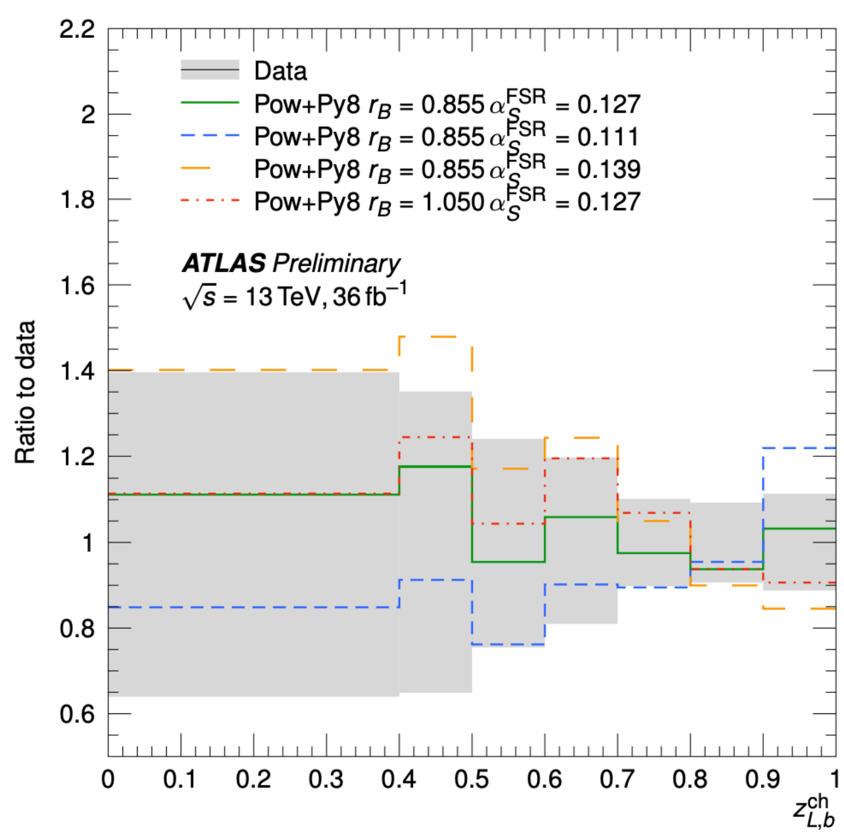


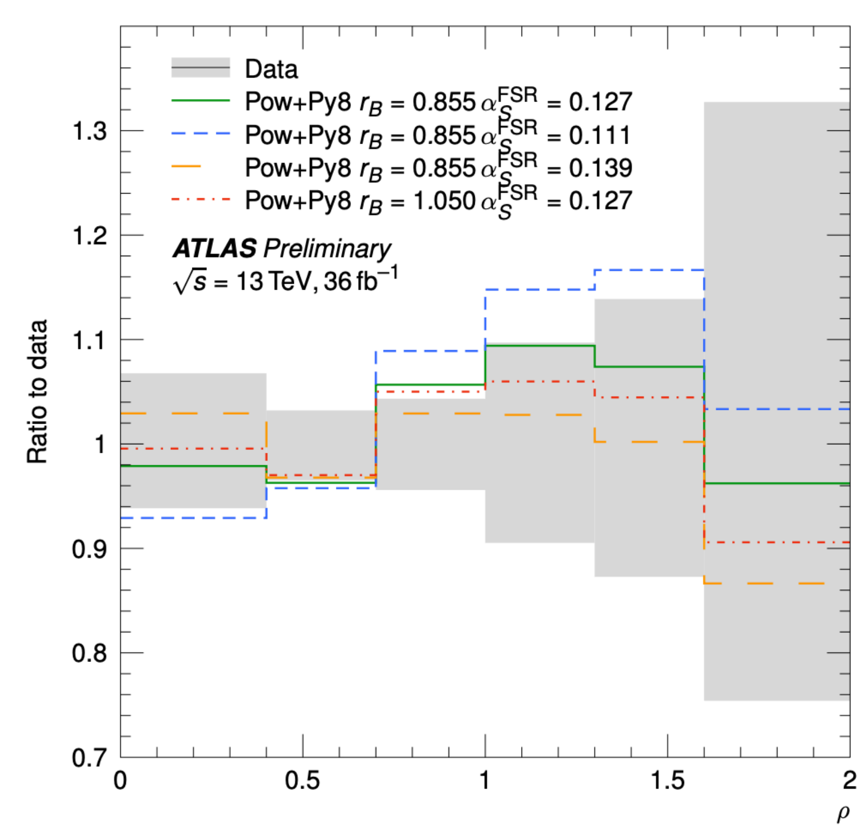
[M. Seidel at HXSWG]

B-RAGMENTATION MEASUREMENT









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