MC and MC uncertainties - ATLAS perspective -

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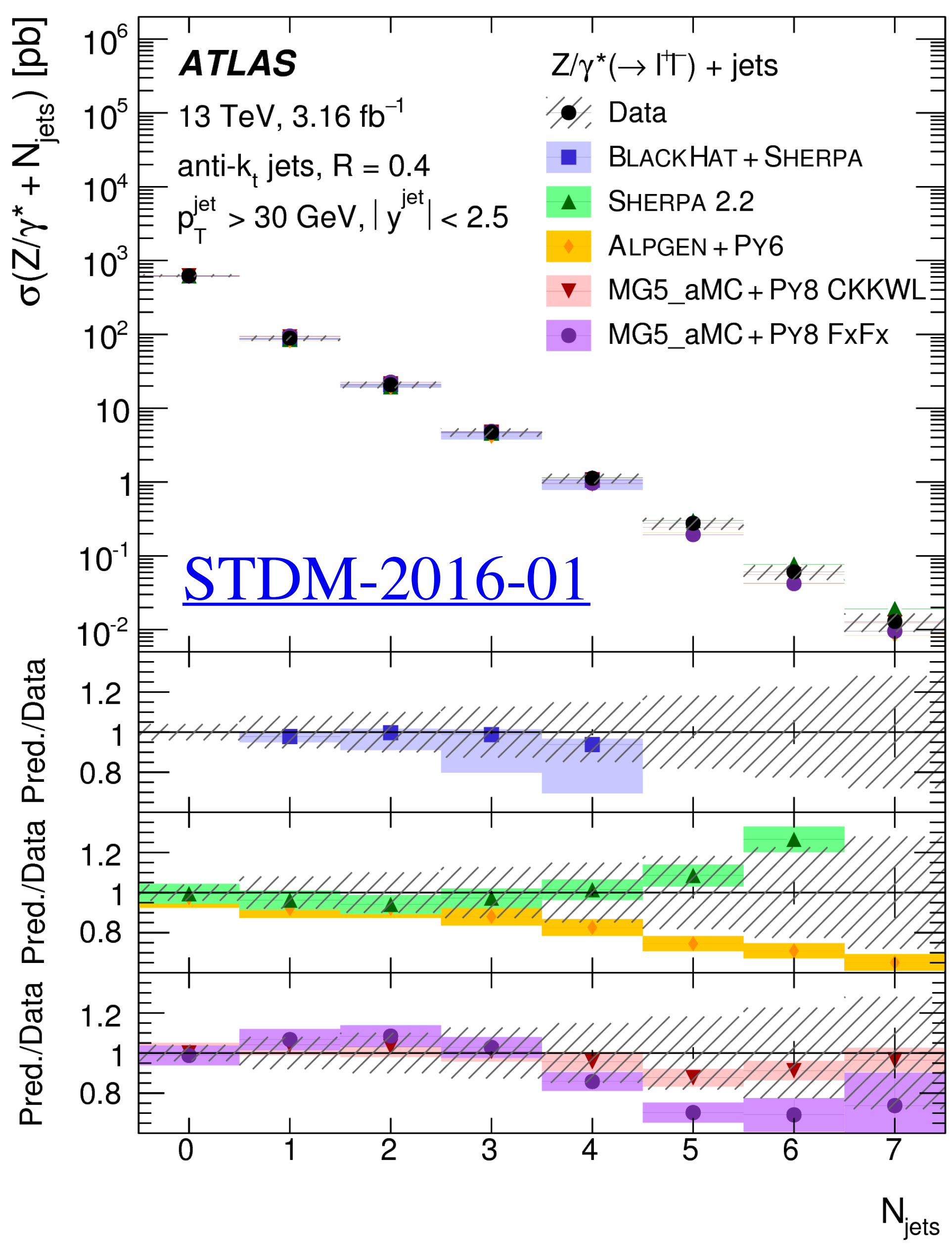
Introduction

* With a wealth of statistics collected by the LHC most of our measurements and searches are now systematics limited
* Detector calibrations typically rely on data samples and (to some extent) will also scale with the luminosity
* For theory uncertainties this is not (trivially) the case and they will be a limiting factors in both the LHC and HL-LHC physics program

* I will give an overview of the current way theory uncertainties are estimated in ATLAS analyses
* Describe where we have identified obvious bottlenecks as well as promising theory developments
* And point out where more effort from theory might be needed

Higher orders (QCD)

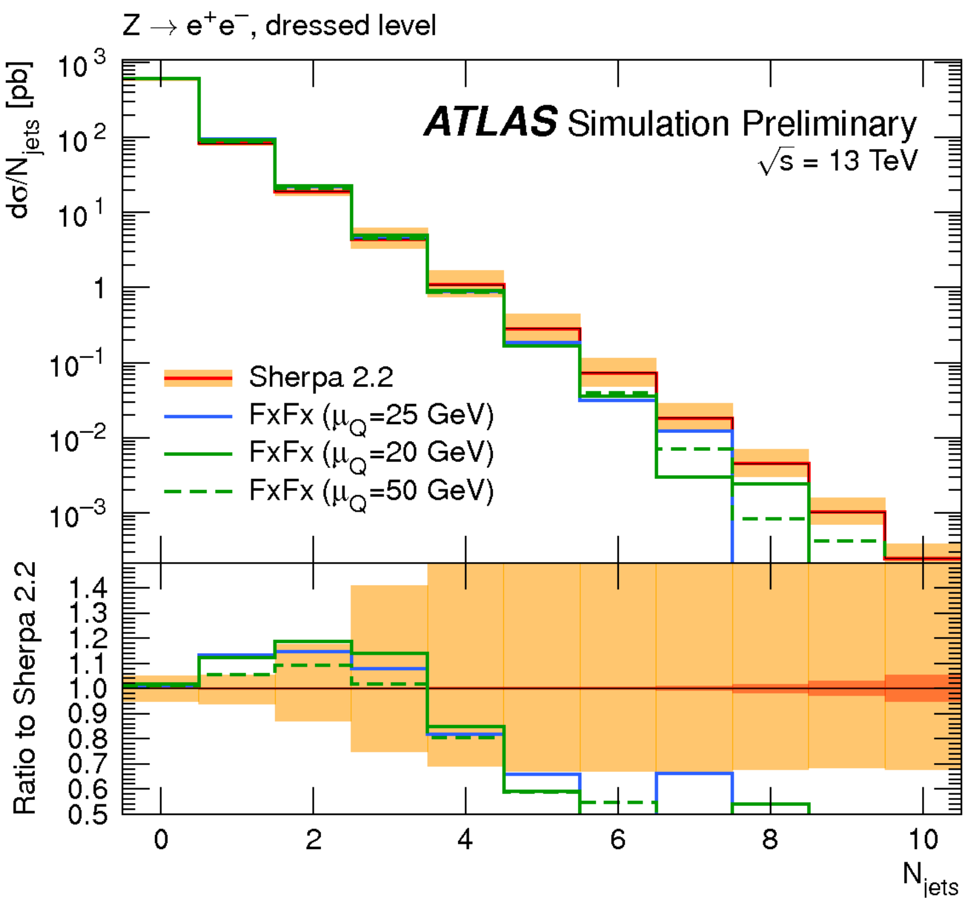
- For optimising analyses and estimate SM backgrounds we rely on state-of-the-art NLO-merged accurate MC samples which are passed through a simulation of the ATLAS detector
  - They provide a good description of data up to the high jet multiplicities probed by searches, and a reasonably “small” perturbative uncertainty



- e.g. V+jet production in ATLAS is simulated with Sherpa MC with 0+1jet@NLO, 2+3jets@LO
- As we extend our searches to even higher jet multiplicities and more exclusive phase-spaces, we go back to regions dominated by the LO MEs or by the PS
- Reaching even higher multiplicities would be useful but these simulations are already extremely expensive in terms of computing resources, and might not scale well to the needs of the HL-LHC

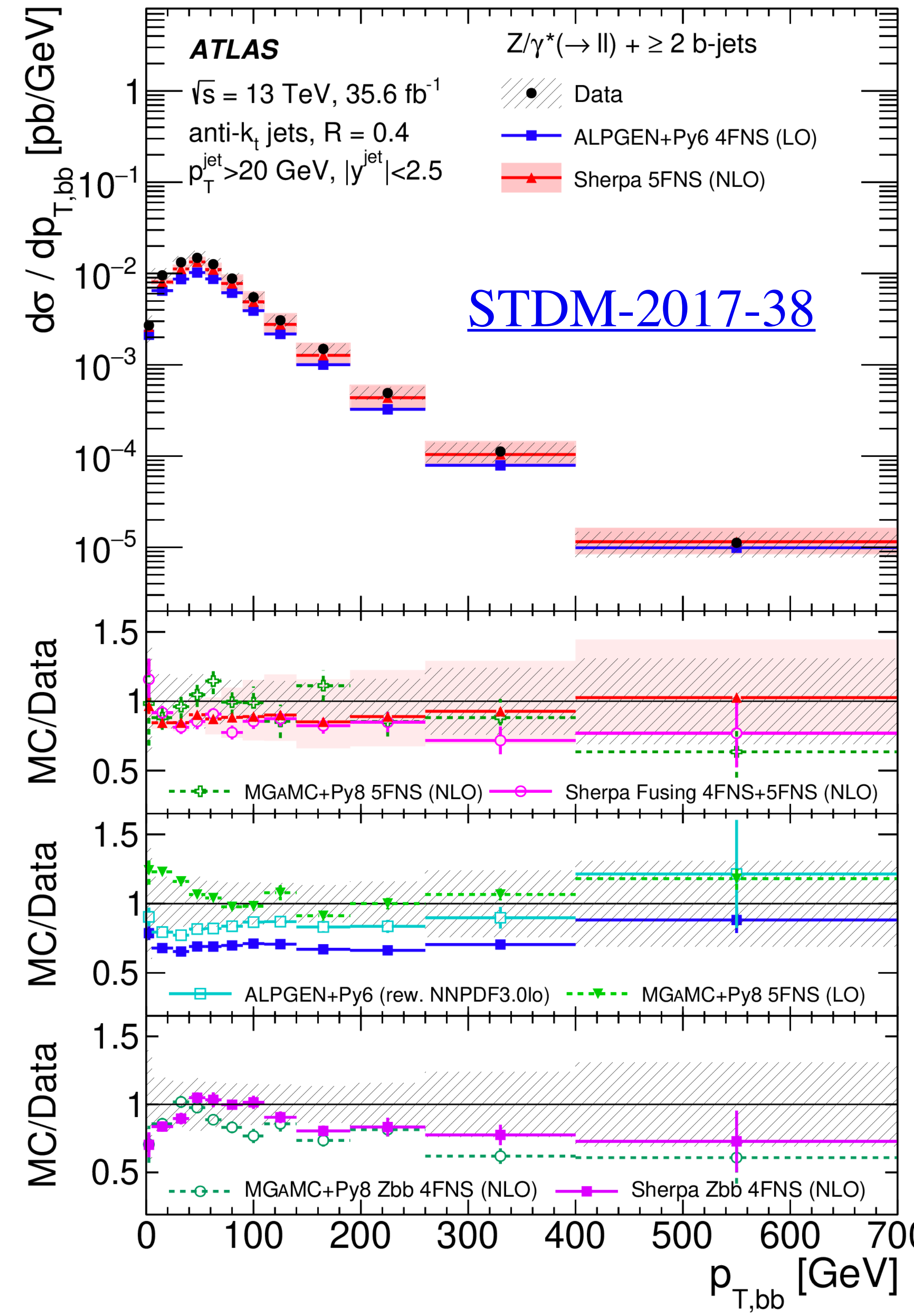
Higher orders (QCD)

- Scales and PDF variations are now routinely included in MC samples as on-the-fly weights and used to estimate MHOU/PDF uncertainties
- Other explicit variations, related to the specific merging algorithm, are also often used in evaluating uncertainties
  - merging and resummation scale in Sherpa, shower starting scale in MC@NLO, h_{damp} in Powheg
- And whenever possible we compare also to a different program with a similar level of accuracy
- But we often find different programs to disagree well beyond the MHOU band
- And that many (formally subleading) algorithmic choices can have large effects Shower histories, scale assignments, …



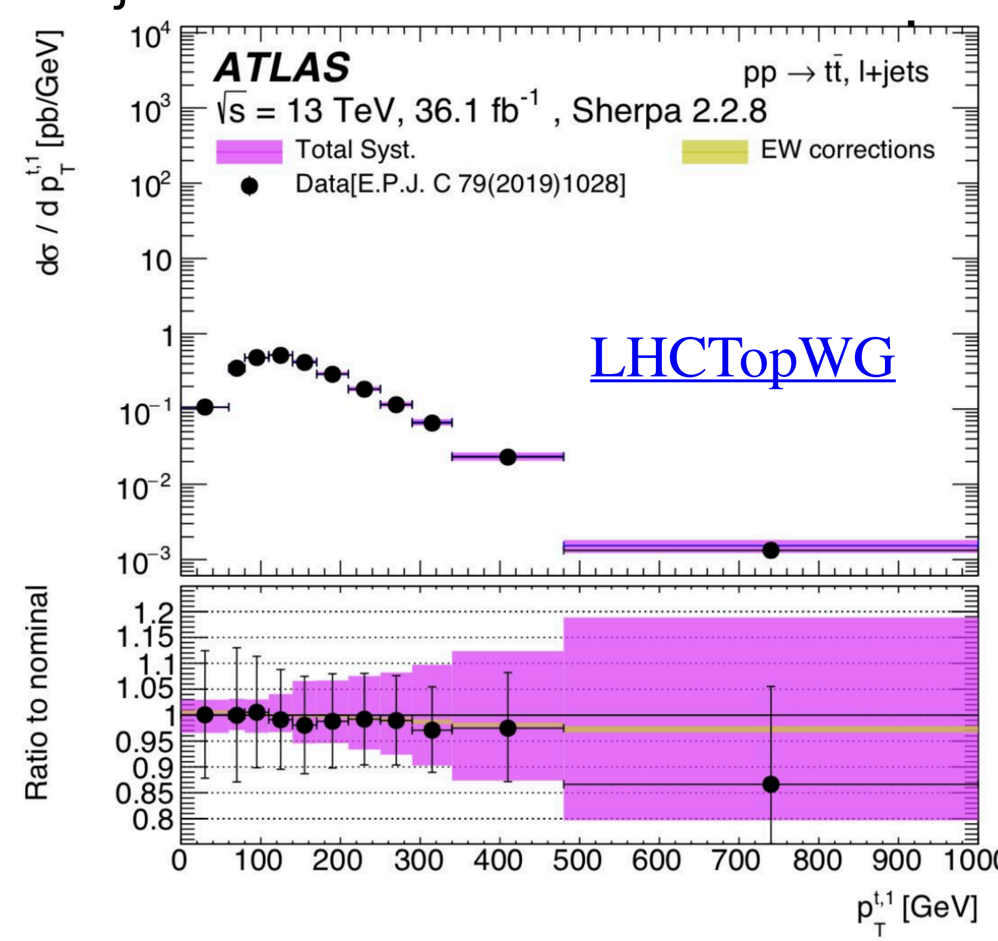
Heavy Flavours

- Description of heavy flavours crucial to model backgrounds in many important measurements and searches
  - Z/W+bb for H->bb
  - tt+bb for ttH/4-top
- Typically modelled by 5FS MC samples as the contribution of HF from the shower cannot be neglected
- Often complex reweightings of flavour-fractions to either HO calculations or to data are used to obtain an acceptable modelling and constraint the MHOU
- Recently some approaches to combine 4FS with 5FS calculations have been developed
  - Sherpa "fusing" of 4FS/5FS in multijet-merged MC is likely to become the ATLAS standard for modelling HF final-states
- In general raises the question of what is the relevant scale choice one should use in a MC



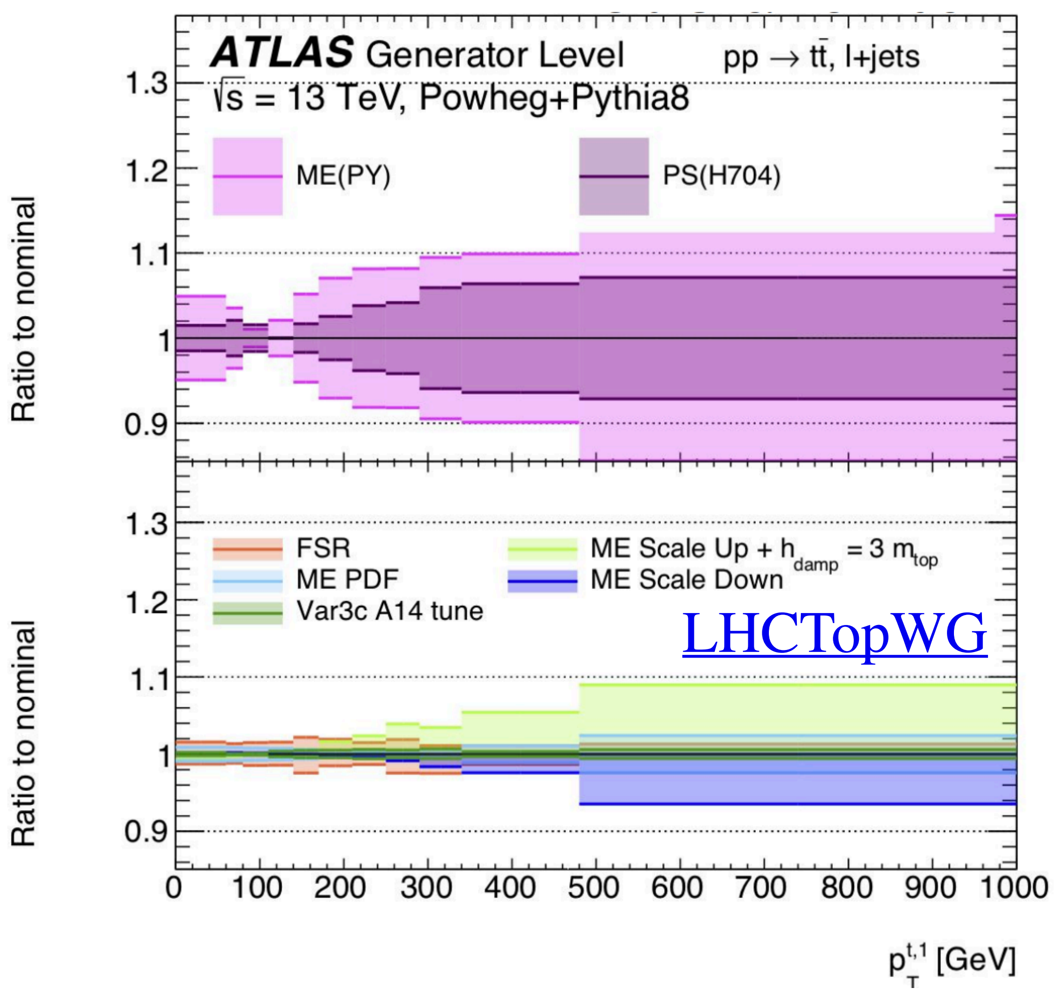
Higher orders (EW)

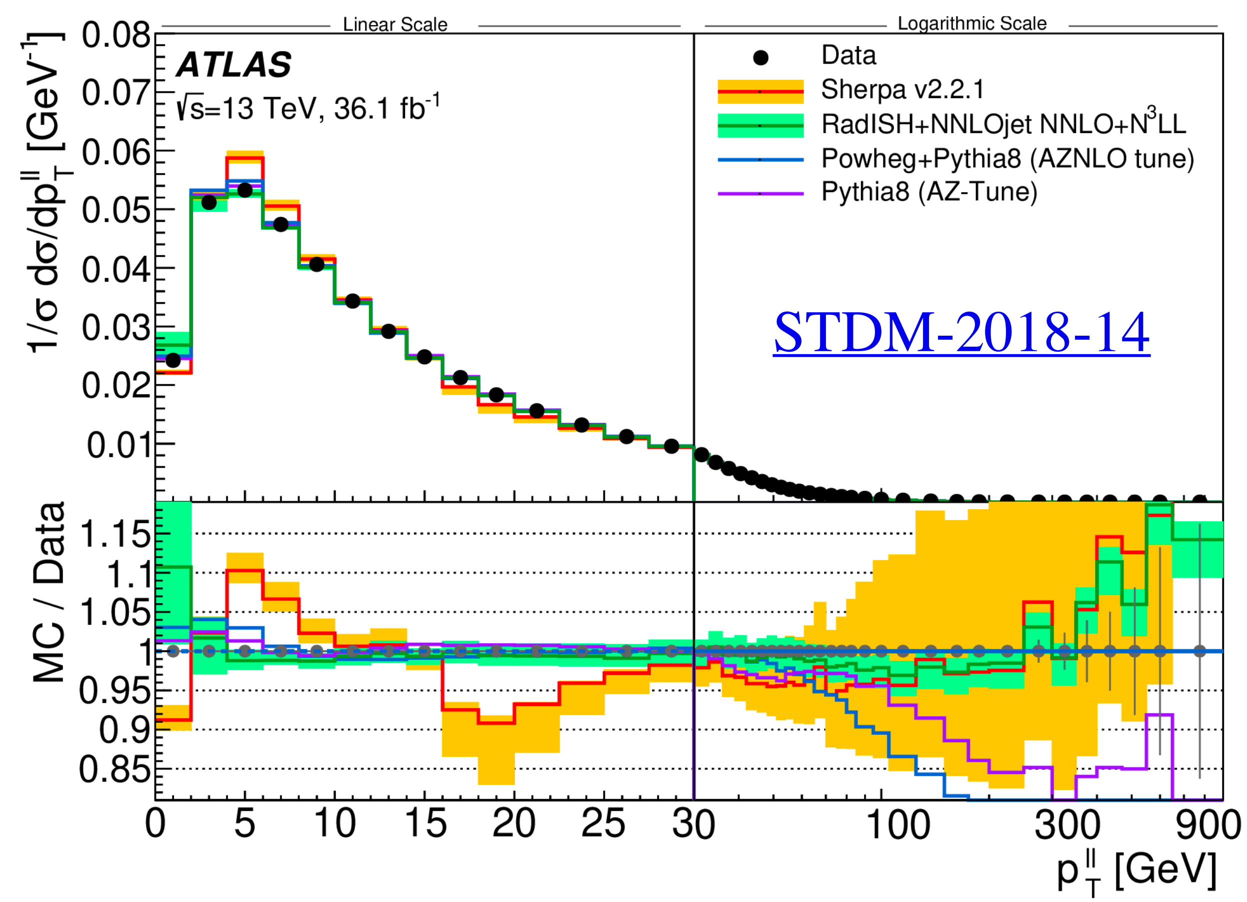
* Higher orders in EW couplings are becoming more and more important for both precision measurements and searches
  * In measurements these are typically computed with external codes applied as additive/multiplicative k-factors on top of a FO or MC prediction
  * In searches these effects are mostly neglected, often on the ground that they would be reabsorbed in data-driven bkg. estimates (but some exceptions like Z'/W' or monojet)
* QED lepton FSR is instead essential and included in our simulation with PHOTOS or by the parton shower, often in conjunction with QED ISR
* Only recently available in MC programs
  * Powheg implements NLO QCD + NLO EW corrections interfaced to shower for selected processes
  * Sherpa implements app. EW virtual corrections within its NLO-merging
* Crucial development for future analyses as EW Sudakov logs large at high-pT



RESUMMATION (SHOWER)

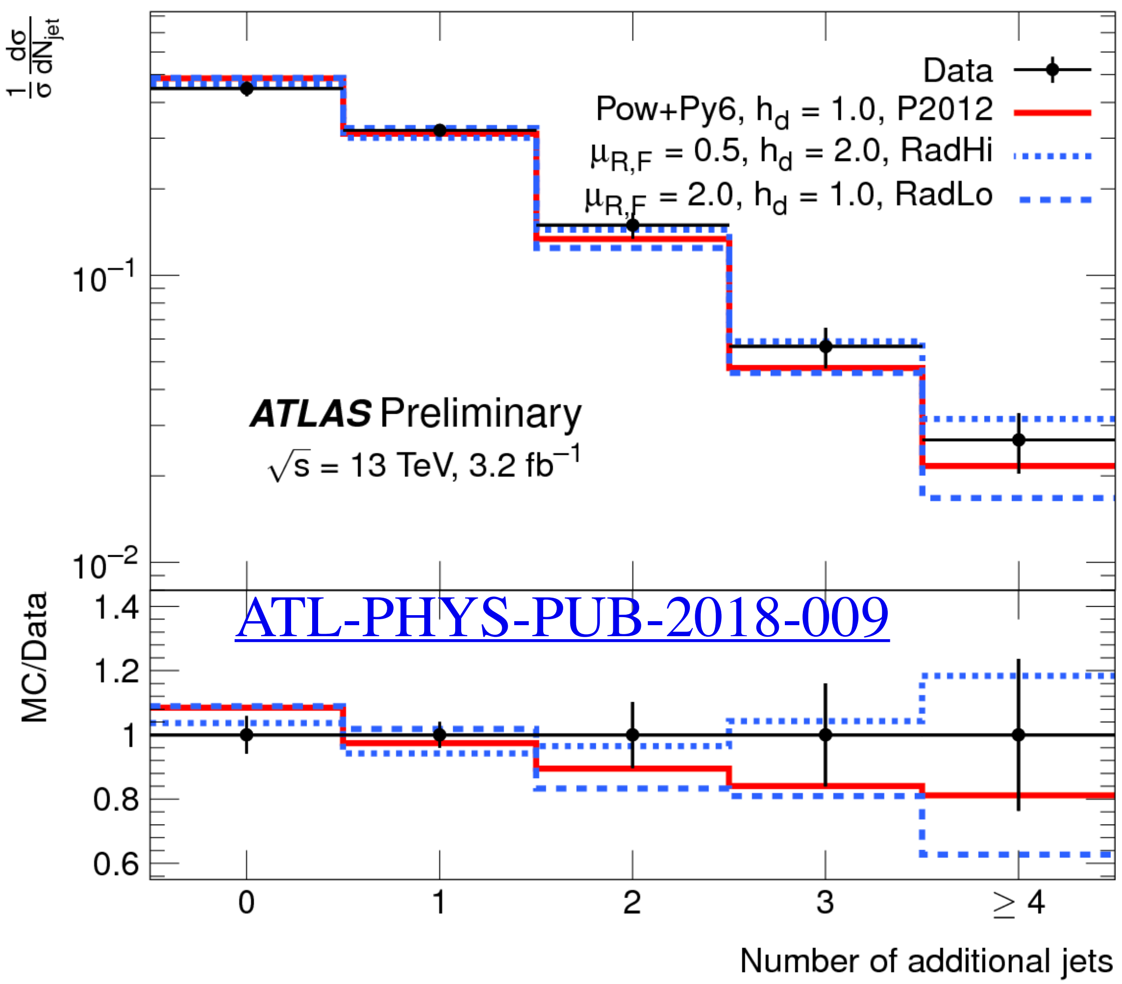
- Parton shower perturbative uncertainties are often a dominant source of uncertainty
  - For top and DY precision measurements we still rely on NLO+PS samples for an accurate description of inclusive quantities and uncertainties in the resummation region are (large and) important
  - NLO-merged samples often do not provide a good description of inclusive quantities (can this be fixed?) hence cannot/are not used

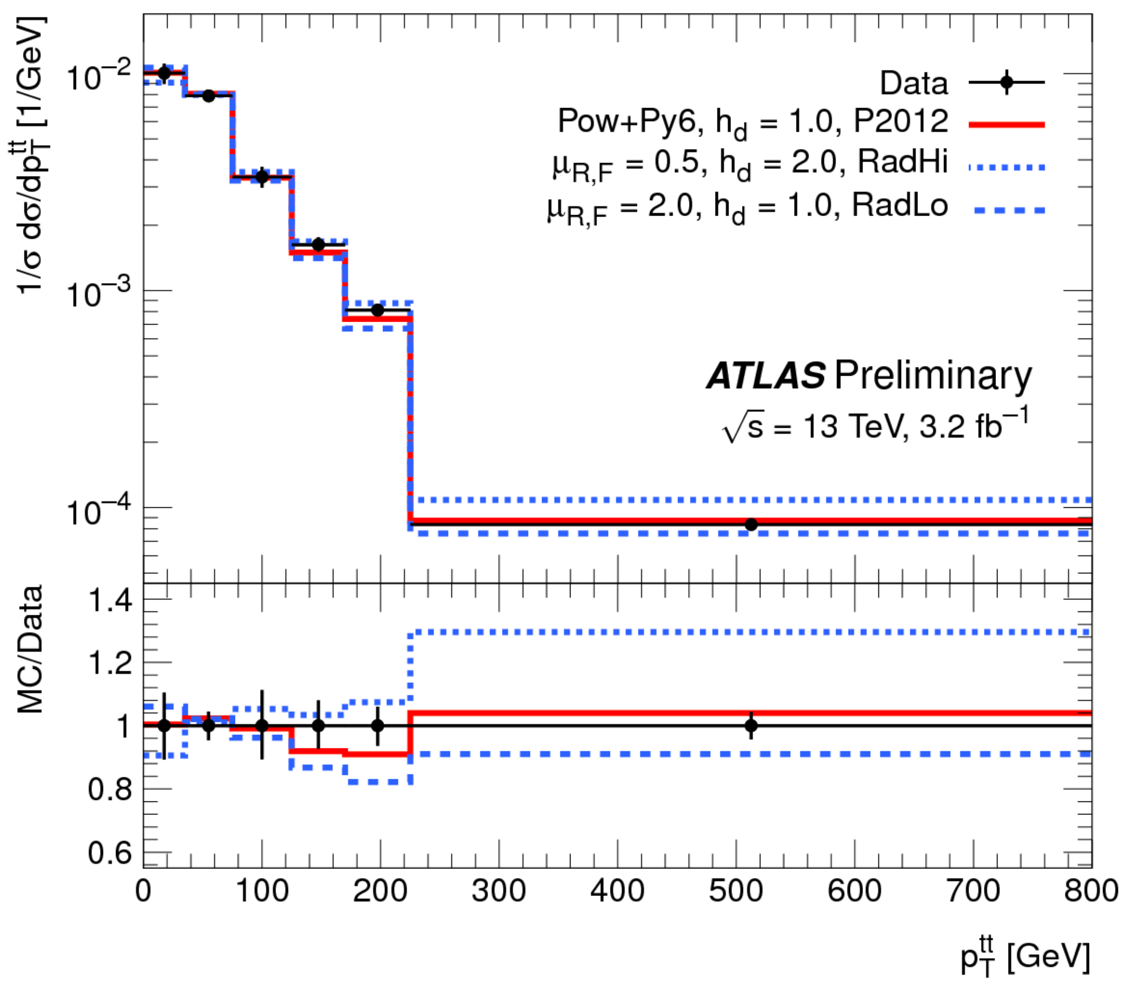




Shower uncertainties

- Uncertainties on parton shower predictions are typically estimated by varying the ren. scale at which the emission is computed
  - Either by some variations determined by data or by factors 0.5,2
  - These are now available as OTF weights, and included in most samples
- Top production might be the best example, as our nominal MC sample is an NLOPS sample with a “tuned” PowhegPythia8



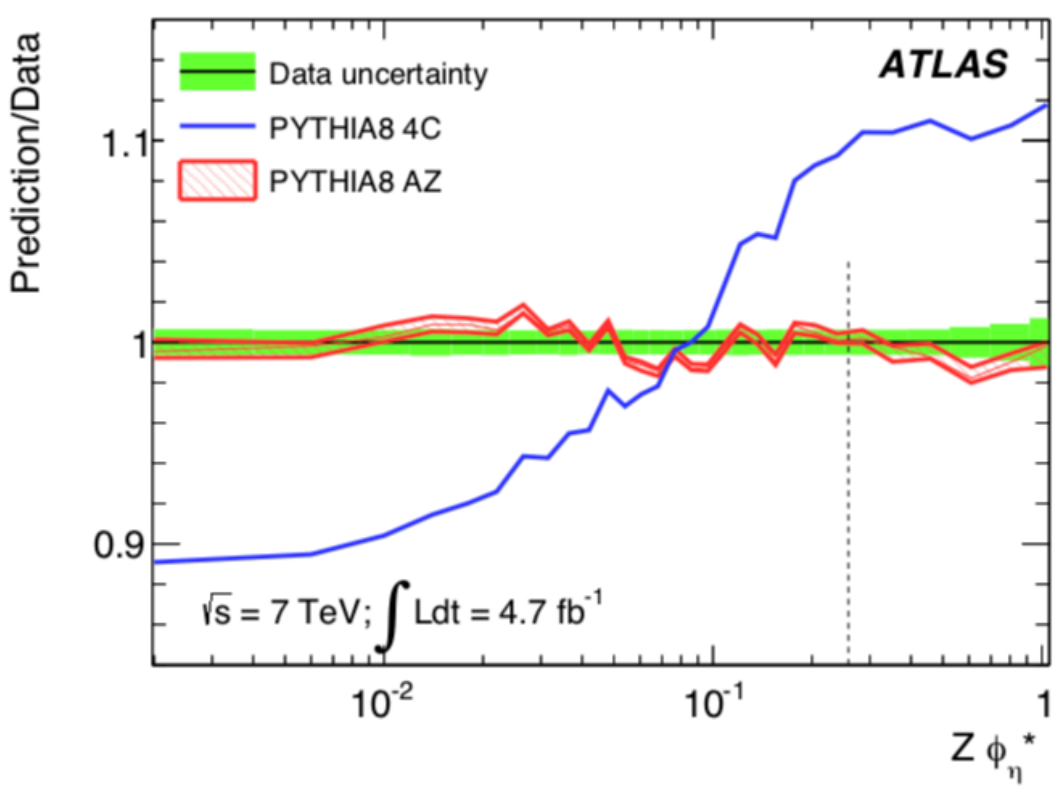


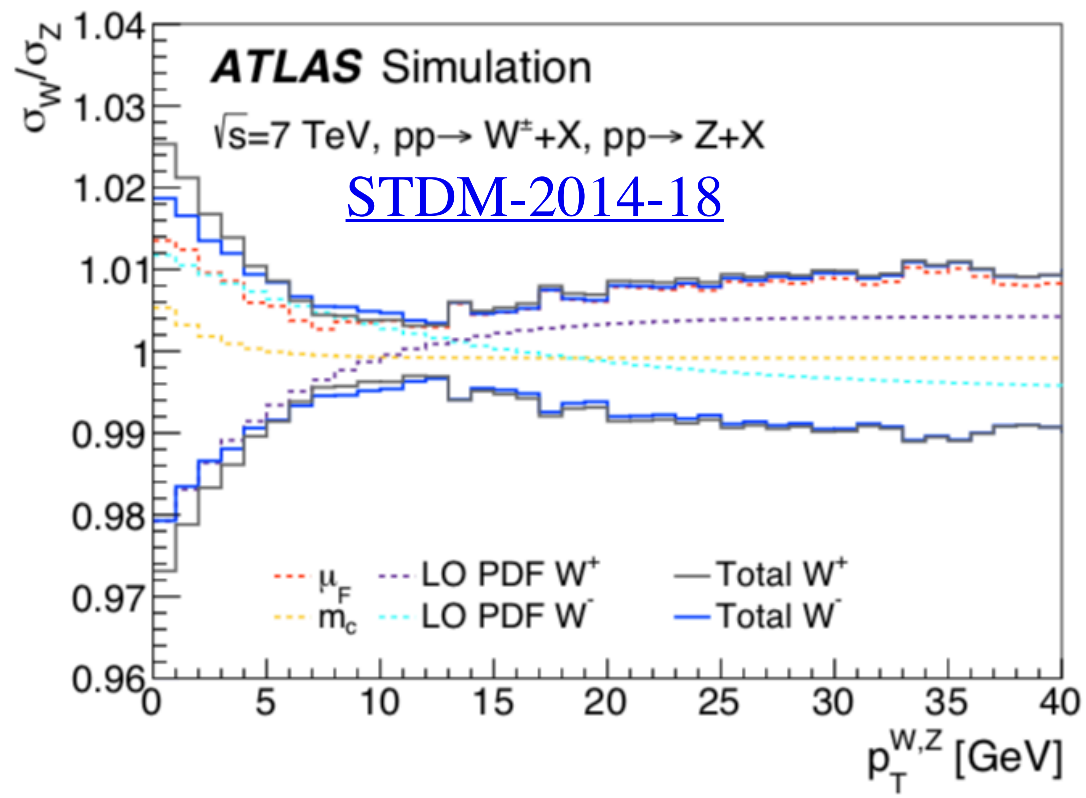
Shower uncertainties

* PS scale variations are handled differently by different programs
  * Sherpa varies scales coherently with the ME variations (and FSR,ISR)
  * Pythia includes and “NLO” compensation term and allows to vary ISR/FSR scales independently (but cannot coherently change them in the ME)
  * We typically use whatever is the default in a given generator
* We often find that differences between programs are not covered by these uncertainties, and that other (formally subleading) effects give large variations
  * E.g. evolution variable, shower recoils, alphaS evolution, …
* Most of the times a comparison with a different shower program is included to account for both algorithmic choices in the PS construction and to account for an uncertainty on MPI/had.
* Can we get some better understanding on the approximation that enter the shower constructions and how to build a realistic uncertainty band?

An example: W-mass

- W-mass measurement crucially relies on the description of the W pT
- For the 7 TeV ATLAS measurement a prediction for the W pT was obtained by "tuning" a Pythia8 prediction to the 7 TeV Z pT measurement data and letting the program extrapolate it to W pT

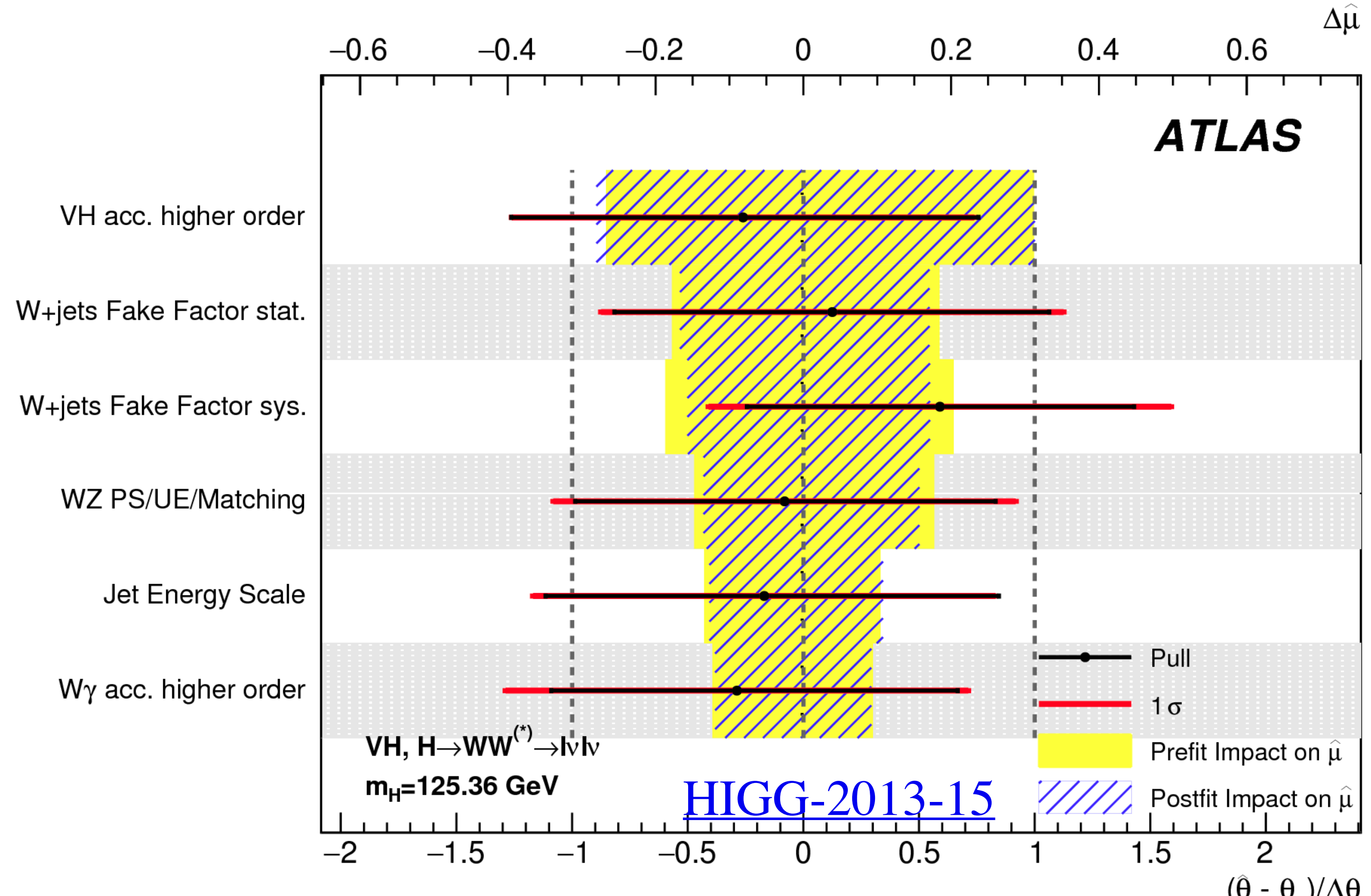




- Crucial to obtain an estimate of effects which decorrelate between Z and W (e.g. HF)
  - obtained varying the PS PDFs and m_C and with independent variations of μ_F for each initial state process

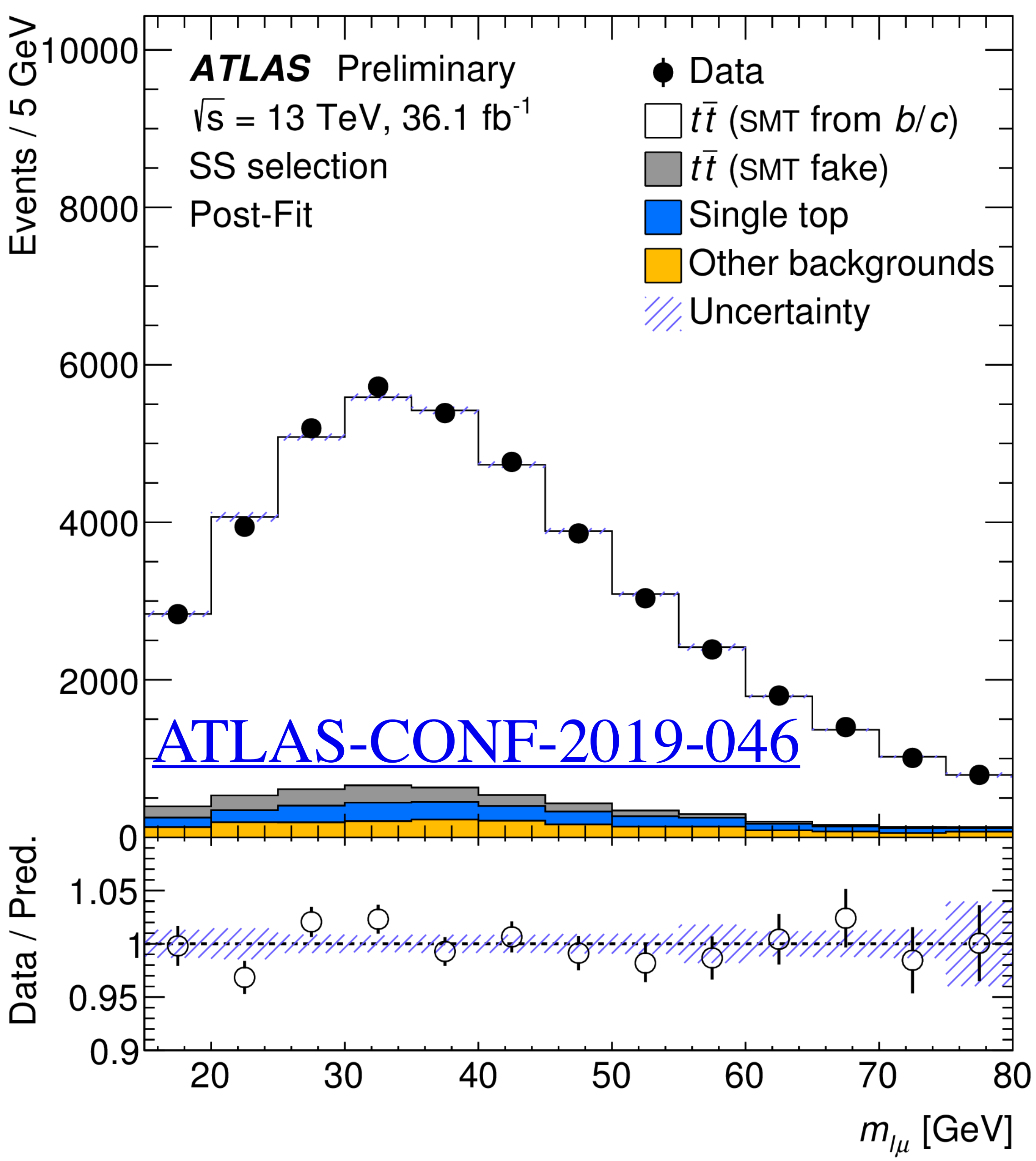
Fragmentation/hadronization

- Typically included with the "usual" Pythia/Herwig sandwich which convolves the effect of many things
  - Perturbative physics, fragmentation, hadronization, MPI, CR and the tune
- Currently a bottleneck for many analyses, although usually unclear which component is dominating the uncertainty
  - More acurrate estimates can be achieved, but usually require a significant amount of effort/physics studies (examples later)



Top mass and fragmentation

- Recent ATLAS top mass measurement using a soft muon from a semileptonic decay of a b-hadron
- Reduce the uncertainty from the JES but introduces an uncertainty on the modelling of the b-quark—>soft-muon transition



- This transition consists of a perturbative evolution down to a NP scale, a NP contribution from hadronization, and the modelling of the decay
- Standard μ_R variation in the FSR shower would dominate the uncertainty and make the measurement not competitive
- An H7/Py8 comparison is included and gives a small uncertainty, but of difficult interpretation

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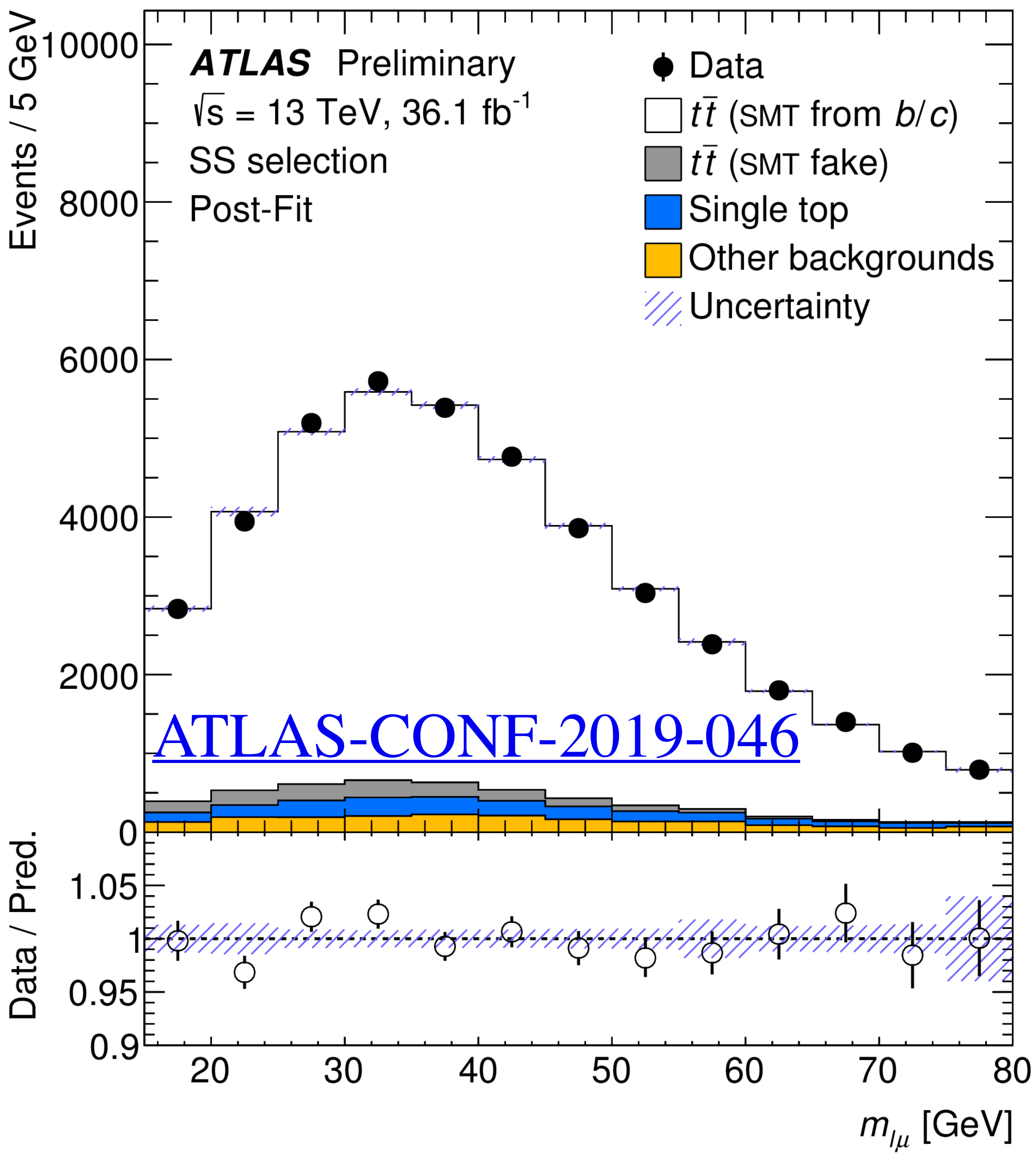
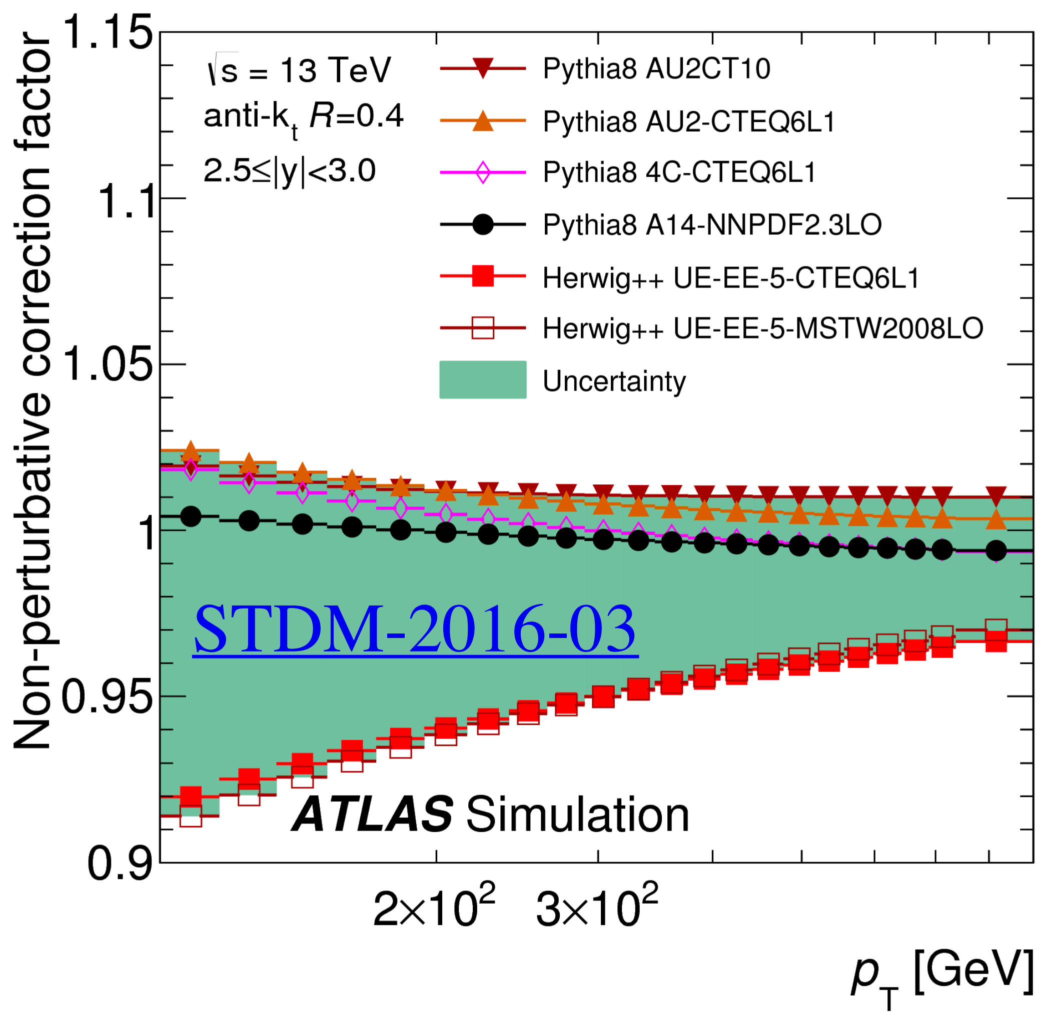


- A dedicated shower uncertainty is derived by fitting the parameters of the NP Lund hadronization model to LEP measurements of b-quark fragmentation
- These are "retuned" also for the 2x, 0.5x variations of μ_R to compensate the perturbative changes significantly reducing their impact
- The residual uncertainty from PS scales on the evolution becomes subleading

Non-perturbative effects

- To compare jet measurements to fixed-order prediction we need to correct our particle-level measurement to parton-level
  - Done by deriving a correction factor as: σ(PS+had.+MPI)/ σ(PS)



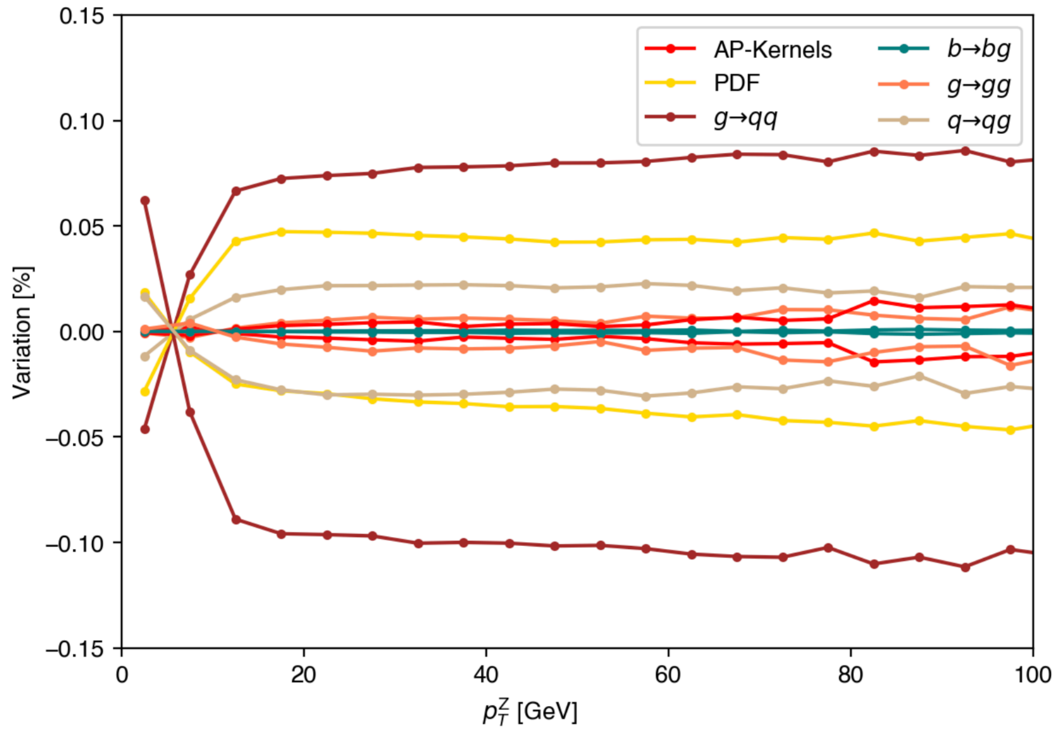
- Large differences are observed in the size of these corrections between different MC programs (Py8/H++),
- Well beyond the spread given by using a different shower tune
- Should be possible to overcome by constraining the relevant MC parameters "in-situ" using jet-shapes or R-scan measurements
- But would be nice to have some understanding of the MPI/had. effect through "analytic" models as developed for LEP event shapes

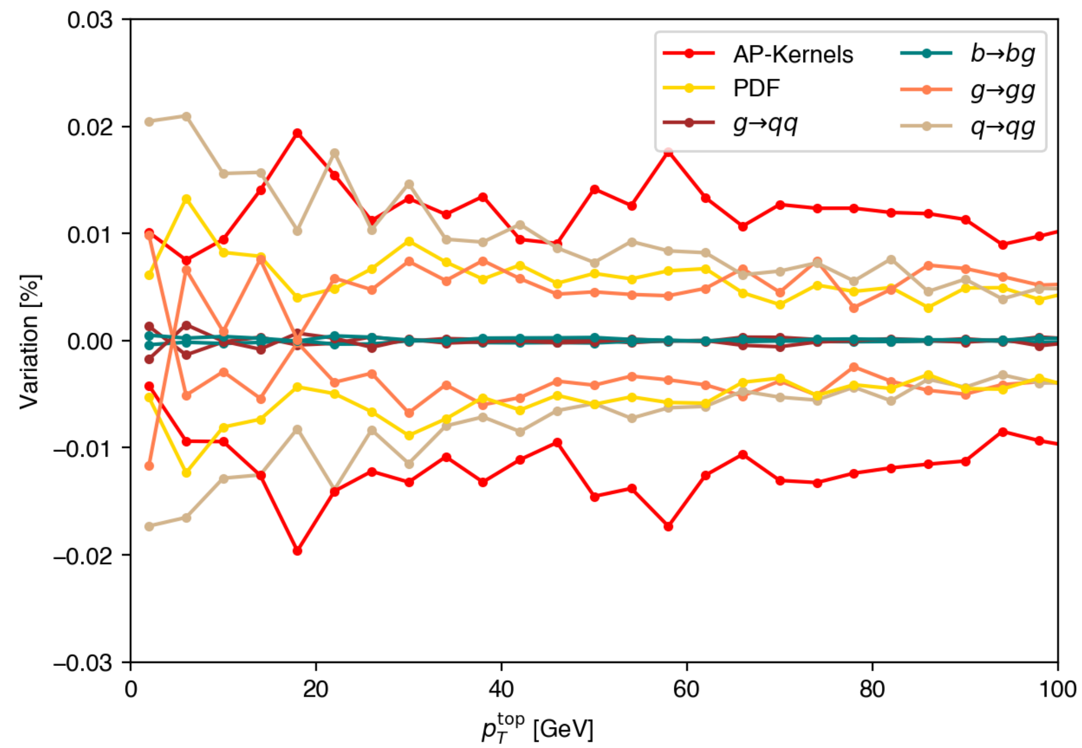
Statistical interpretation of theory uncertainties

- Our analyses typically require a simultaneous statistical interpretation of different phase-spaces and processes
- While we might have an estimate of the uncertainty band around our predictions we have (almost) no theory guidance into how these uncertainties should enter our statistical analyses
- And this is becoming a limiting factor even more than the size of the uncertainties themselves
- Typical questions that arise are:
  - Should we treat scale variations as (symmetric?) Gaussian nuisance parameters
  - Should MHOU be correlated across the phase-space?
  - And for numerator and denominator in normalised cross-sections?
  - And for different (similar) processes, e.g. W and Z?
  - Should MHOU in ME and PS (ISR/FSR) be correlated? And NP effects?
  - And can we rely on the event generator pattern of correlations for MPI/had.?

Statistical interpretation of PS uncertainties

- A recent interesting development introduced by Pythia8 has been to make available variations of the individual DGLAP splitting kernels, and separate the contribution of their non-singular part
- We could then think of the scale variations in the singular terms to be universal, and allow them to be constrained by data or calculations with higher log accuracy while keeping the non-singular term variations as process-specific
- Is this something that can be "elevated" to a general recommendation for shower uncertainties?





SUMMARY

- Theory progress is essential for the success of the LHC/HL-LHC physics program
- And event generators remain the unavoidable theory tool for most of the analyses we do
- Important to make simultaneous progress on several aspects:
  - Matching to higher-orders (NNLO)
  - Coherent inclusion of EW higher orders in QCD MC
  - Impact of subheading choices both in the matching/merging and shower
  - What is the PS accuracy and can it be improved
  - How to construct an event generator uncertainty band
  - Interplay with PDFs (e.g. for MPI and ISR)
  - How should these uncertainties be treated in statistical analyses?
- All this while keeping the computational cost under control