Bottlenecks in precision top-quark measurements

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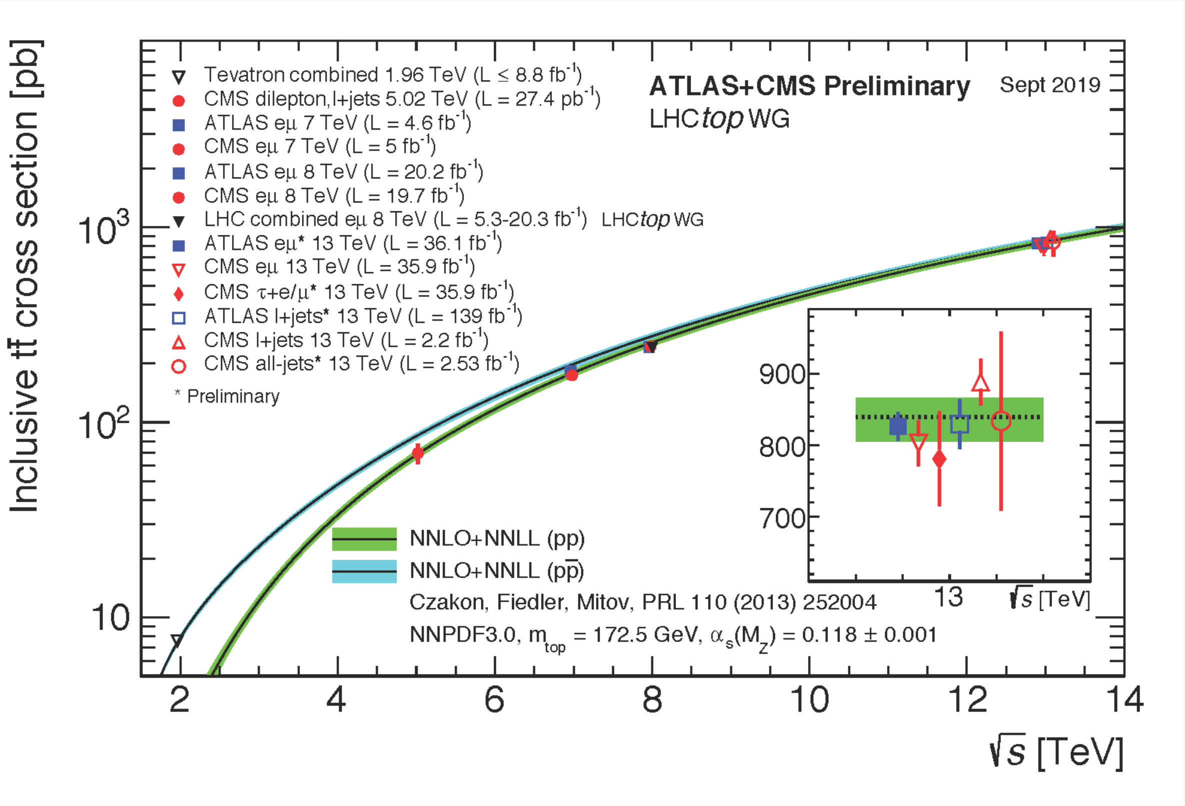
The top precision measurements era

Since the discovery of the ttbar (1995) and single top (2009) processes at Tevatron:

- LHC entered a new era of precision measurements
- During Run 1 and 2 LHC delivered millions of top-quark events
- Statistical uncertainty is no more an issue for inclusive cross-section and differential cross-section measurements in the ‘low' p_T region



Top quark properties are extensively measured to test SM and to search for BSM → modelling effects dominate the final result

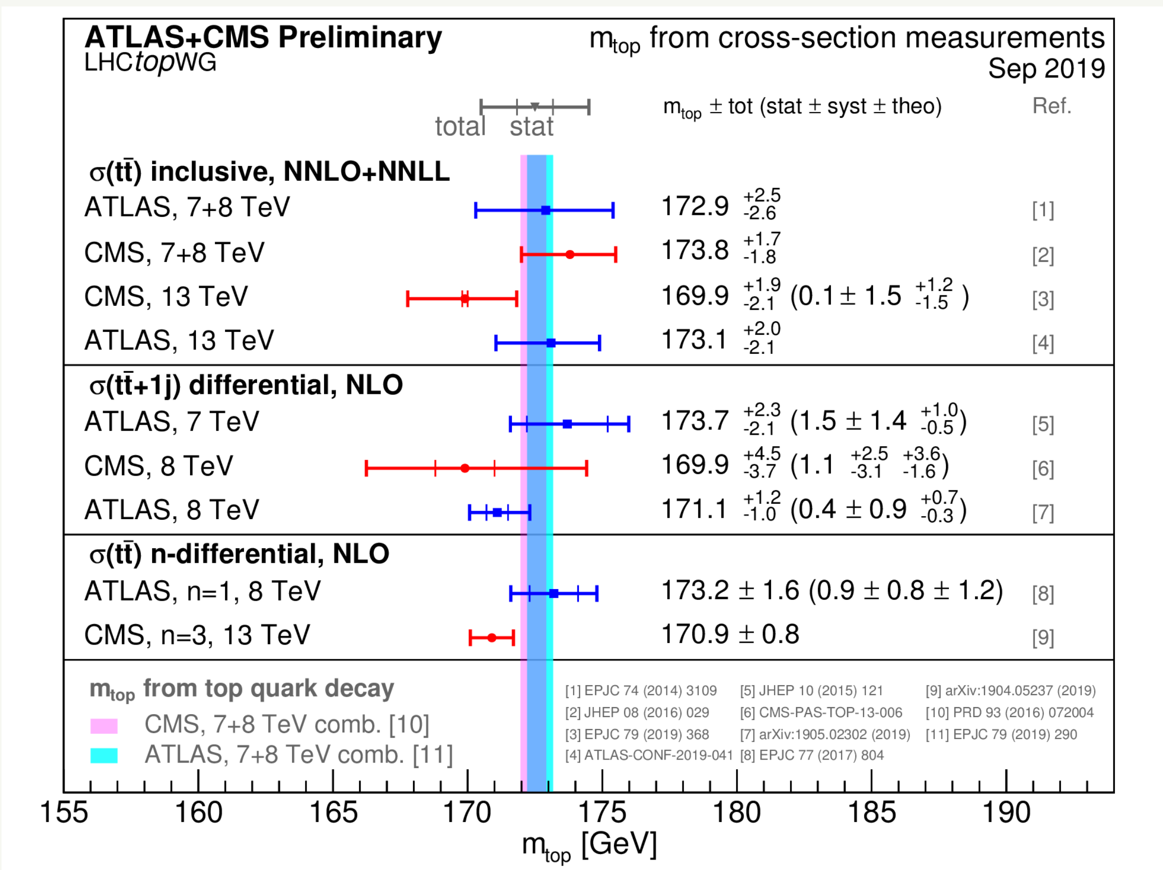
There has been a big effort to improve the treatment of the modelling uncertainties from both the theoretical and experimental side:

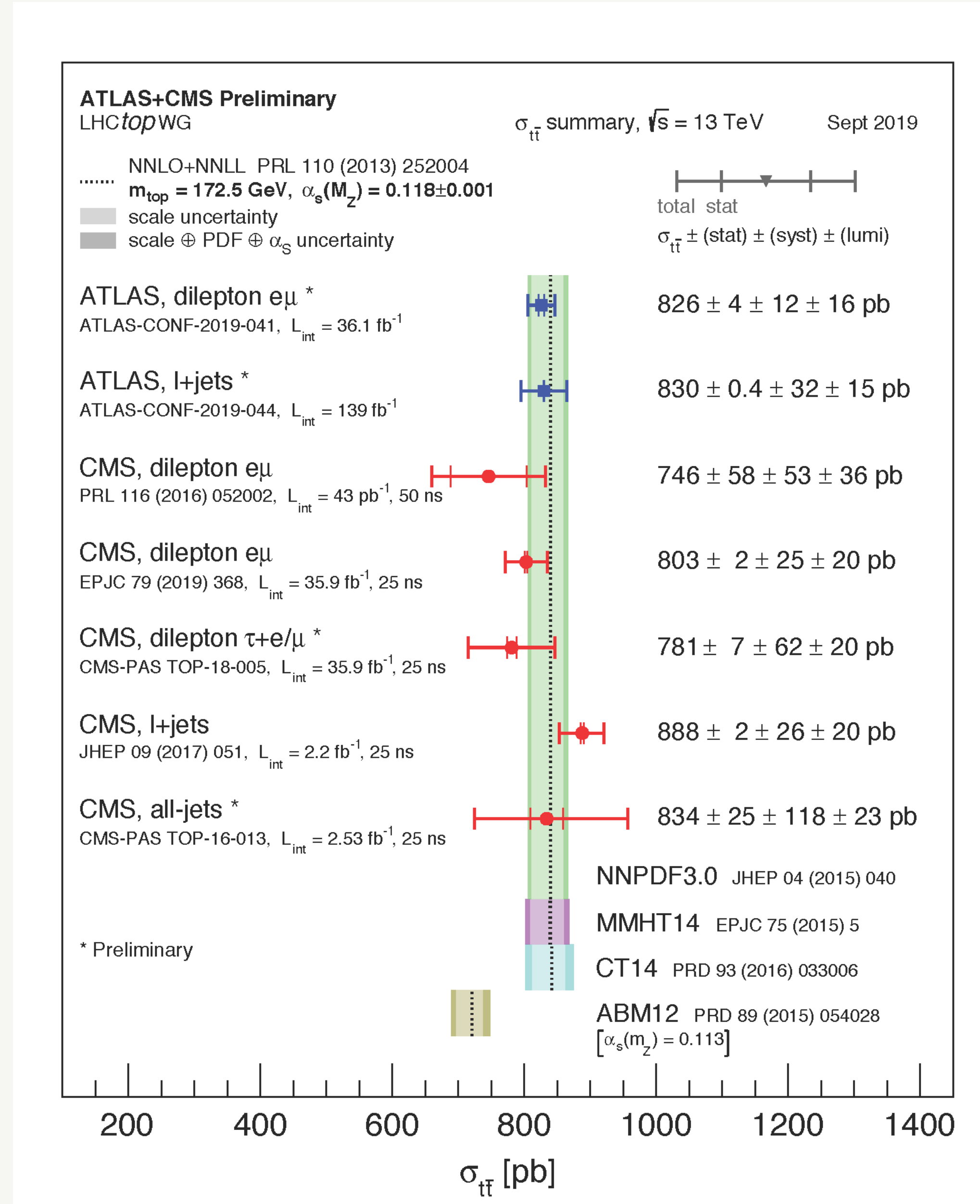
- Higher order calculations
- Tuning of models using data

‘To profile or not to profile’

Top precision measurements:

- Differential and inclusive cross sections
  - Fiducial and full phase space
- SM parameters measurements





Also informations on the systematic uncertainties can be extracted from data (profiled) with the aim of reducing them. However, a general recipe for when to profile or not does not exist.

Uncertainties are **profiled** in:

- **Inclusive** cross section measurements (see Olga Bessidskaia Bylund’s talk)
- Rare processes and **properties** measurements

Differential cross section measurements usually **don’t profile** their uncertainties

- First unfolded measurements with profiled uncertainties

Contents

Building a Profile Likelihood Fit:

- Systematics treatment via Nuisance Parameters
- Prevention of unphysical systematic uncertainties reduction
  - Smoothing, Bootstrapping, decorrelation and factorisation
- Interpreting uncertainties reduction

Differential cross sections:

- Profiling and Unfolding
- Results from normalised cross sections
  - Covariance Matrix for single and multiple variables

Measurement of inclusive cross section

Measurement of ttbar cross section in l+jets (ATLAS) and dilepton (CMS) final state

- Fiducial and full phase space
- Fit runs on several variables of different signal regions

$$\sigma_{fid} = A_{fid} \cdot \sigma_{incl}, \quad A_{fid} = \frac{N_{fid}}{N_{tot}}$$

FIDUCIAL CROSS SECTION

Extraction of fiducial cross section from data using profile likelihood fit

INCLUSIVE CROSS SECTION

ATLAS performs fit

- Impact of modelling encoded in A
- Cross check on result by extrapolation to full phase space

CMS extrapolates from fiducial cross section

- Fixed uncertainties to fiducial post fit values and evaluated impact on A

Both measurements externalise luminosity uncertainty:

No NP defined, the fit is repeated for up and down variation

ATLAS ttbar(l+jets) inclusive cross-section arXiv:2006.13076

CMS ttbar(dilepton) inclusive cross-section Eur. Phys. J. C (2019) 79:368

Profile Likelihood Method

A Profile Likelihood Fit is a statistical tool largely used to estimate various top quark properties (xsec, width, mass…)

- Given a probability model $F(x_i)$ for the variable under study x_i
  - Prediction model depends on:
    - parameter of interest μ
    - variations due to systematic effects (encoded in nuisance parameters, θ)
- Likelihood quantifies the 'likeness' of observed data and this model, $F(x_i^{data})$

$$\mathscr{L}(\mu, \overrightarrow{\theta}) = \prod_{i=1} \mathscr{P}(x_i(\mu, \overrightarrow{\theta}), x_i^{data}) \prod_{t=1} \pi(\theta_t),$$

where $\pi(\theta_t)$ represents the PDF of a Nuisance Parameter, encoding the systematic variation θ_t of the models bins:

- Assumed to have a Gaussian distribution for most of the uncertainties
- Sometimes log-normal or gamma functions also are used

Different types of systematics

DETECTOR UNCERTAINTIES

Originate at any point in the **detector simulation**:

- Trigger Efficiency
- Lepton identification and isolation
- Jet flavour tagging efficiency
- Objects' momentum/energy scale

The quantity that might be mis-modelled is usually well defined and also measured in dedicated regions

Re-weighting of simulation

Changing the properties of final state objects

N.B. Detector uncertainties have modelling components (i.e. calibration of b-jets uses ttbar events)

Different types of systematics

PHYSICS MODELLING UNCERTAINTIES*

Originate at any other step of the simulation:

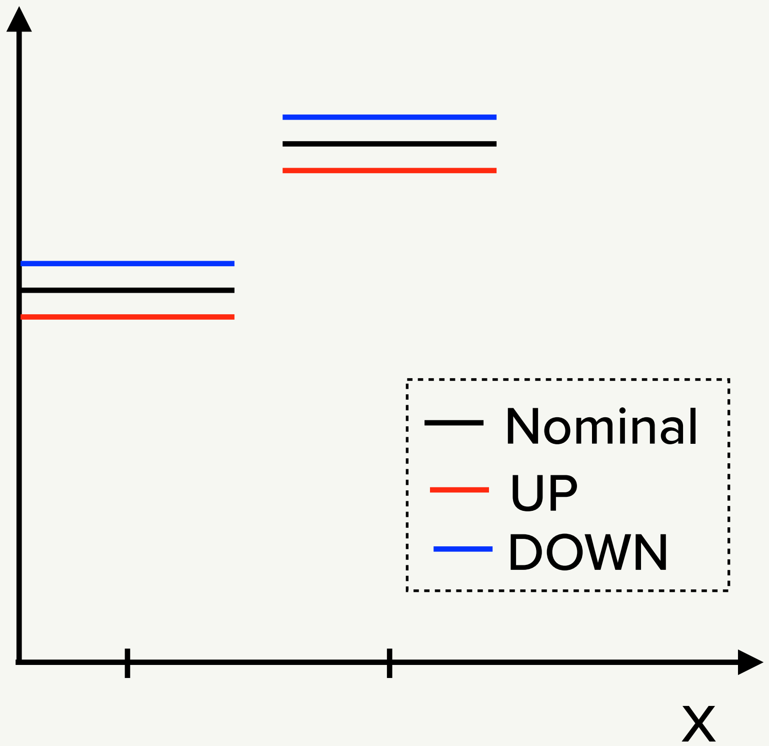
- **P**arton **D**ensity **F**unction
- **Perturbative** calculations
  - Matrix Element
  - Parton Shower
  - ME+PS matching
- **Non-perturbative** calculations
  - Hadronisation
  - Underlying events

*More details about the definition of the modelling uncertainties in Simone Amoroso's talk

Alternative simulations

Comparison of different generators or variation of nominal simulation parameters

Nuisance Parameters



Example: measurement of the b-tagging efficiency ε_b:

- The ε_b in the simulation is re-weighted to match value found in data
- Up and down variations by varying correction factors within calibration uncertainty

↓

Effect on our model for the variable X given by the systematic variation is used to build NP

If θ_0 is the best estimate of θ given by the calibration and $\Delta\theta$ the corresponding uncertainty, we apply the coordinates transformation $\theta \to \alpha(\theta)$ to get normalised pulls

$$\alpha = (\theta - \theta_0)/\Delta\theta$$

Before running our PL Fit

- $\theta = \theta_0, \alpha = 0$
- Up and Down variations correspond to $\Delta\alpha = \pm 1$

After the PL Fit

- Available $\hat{\theta}$ and $\Delta\hat{\theta}$ as extracted from data

PULL
$|\hat{\alpha}| > 1$

CONSTRAIN
$\Delta\hat{\alpha} < 1$

Prevention of spurious pulls and constrains

The probability model for the variable being examined is estimated using Monte Carlo simulations:

- This model is affected by systematic uncertainties which can distort it at any simulation step
- **To prevent unphysical pulls and constrains of NPs due to MC statistical fluctuations:**

The probability model of x_i is provided for the systematic variation

↓

The systematic distribution might have different normalisation and/or shape w.r.t. the nominal prediction

↓

SMOOTHING	DECORRELATION
BOOTSTRAPPING	FACTORISATION

Profiling modelling uncertainties

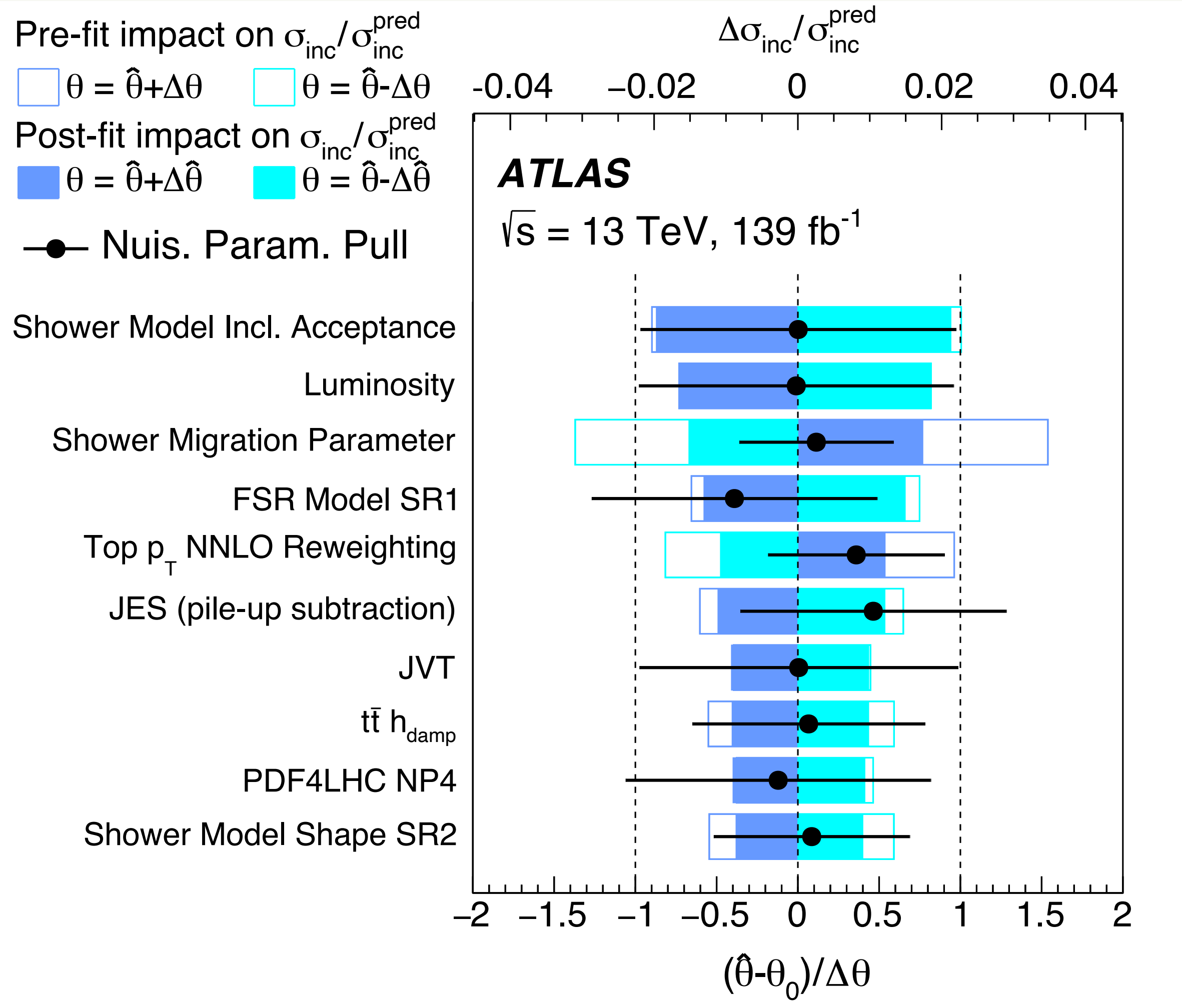
Top p_T re-weighting NP pulled towards NNLO prediction

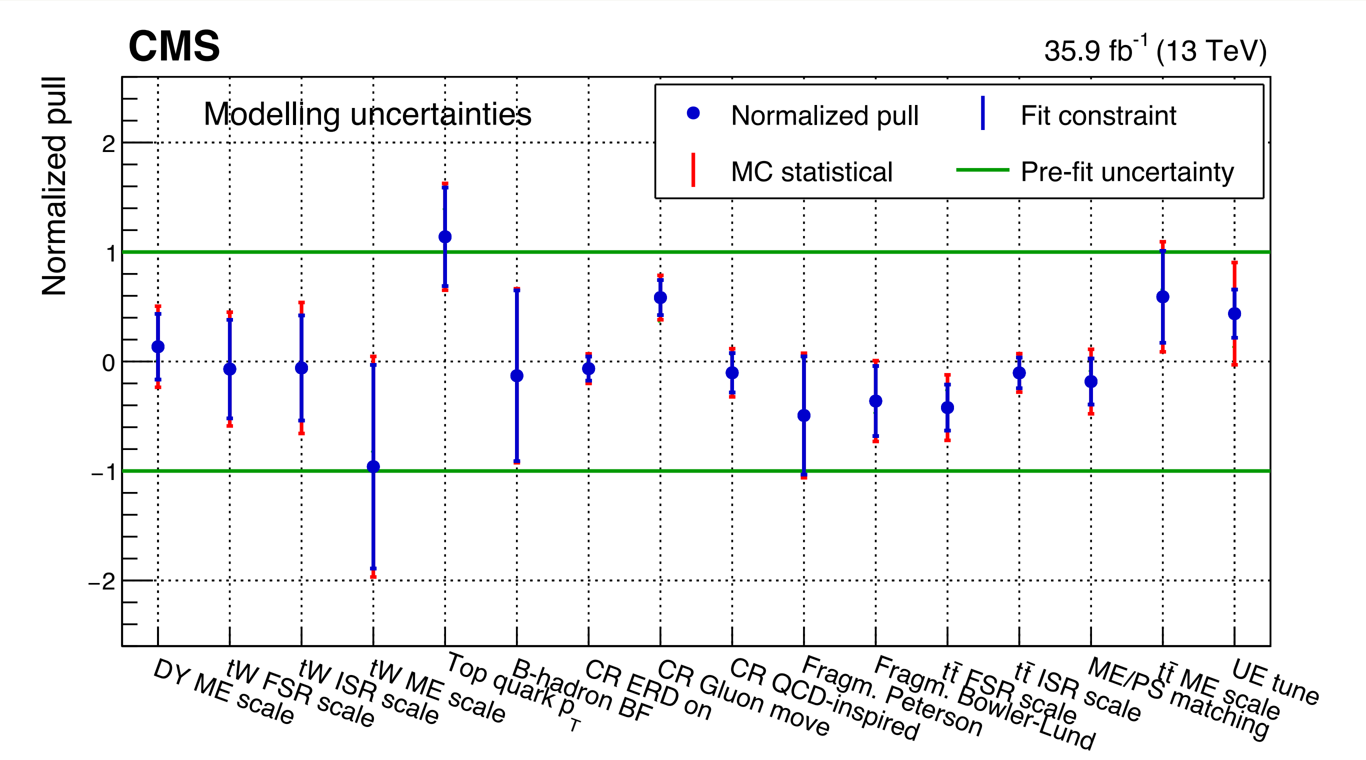
ATLAS constrain of Shower Migration Parameter due to difference w.r.t nominal larger than data uncertainty

- Cross-check via **decorrelation** of different SRs and decoupling of normalisation and shape

CMS assigned statistical uncertainty on NPs using **toy experiments**:

- Estimated spurious component of constrains





ATLAS ttbar(l+jets) inclusive cross-section arXiv:2006.13076

CMS ttbar(dilepton) inclusive cross-section Eur. Phys. J. C (2019) 79:368

Towards better ttbar modelling

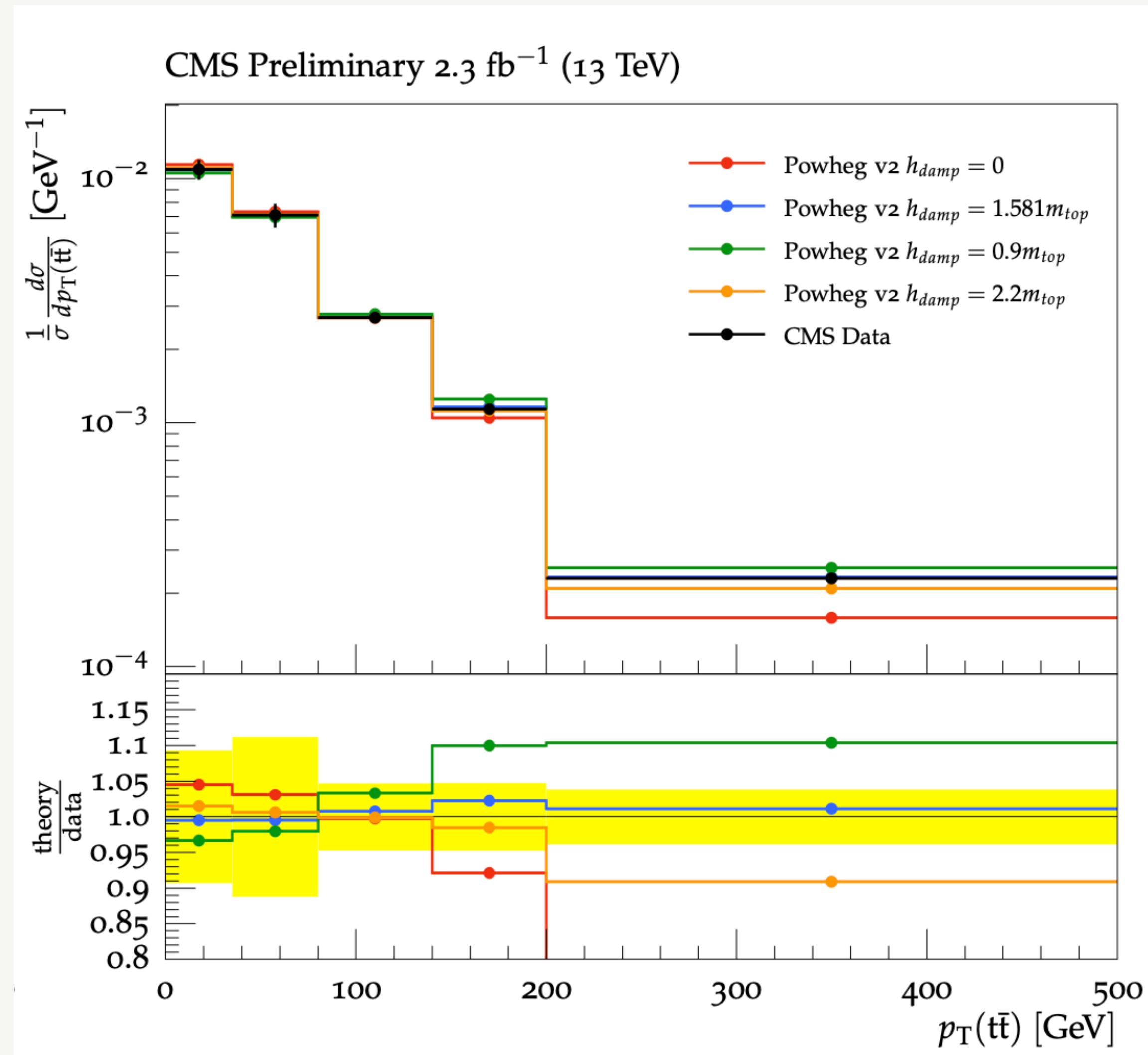
CMS

- Compared unfolded data to different hdamp values, tuned hdamp = 1.581m_{top}
- Uncertainty obtained by varying hdamp within $0.996m_{top} < hdamp < 2.239m_{top}$

ATLAS*

The ISR uncertainty is decorrelated into different components:

1. Split in scale variations and alternative *hdamp* parameters
   - Tuned value of hdamp = 1.5m_{top}
   - Symmetrisation of hdamp = 3.0 m_{top}
2. Studied effect of correlating the HS scale variations with the PS tune
   - Envelope of the HS and PS independent variations gives larger uncertainty

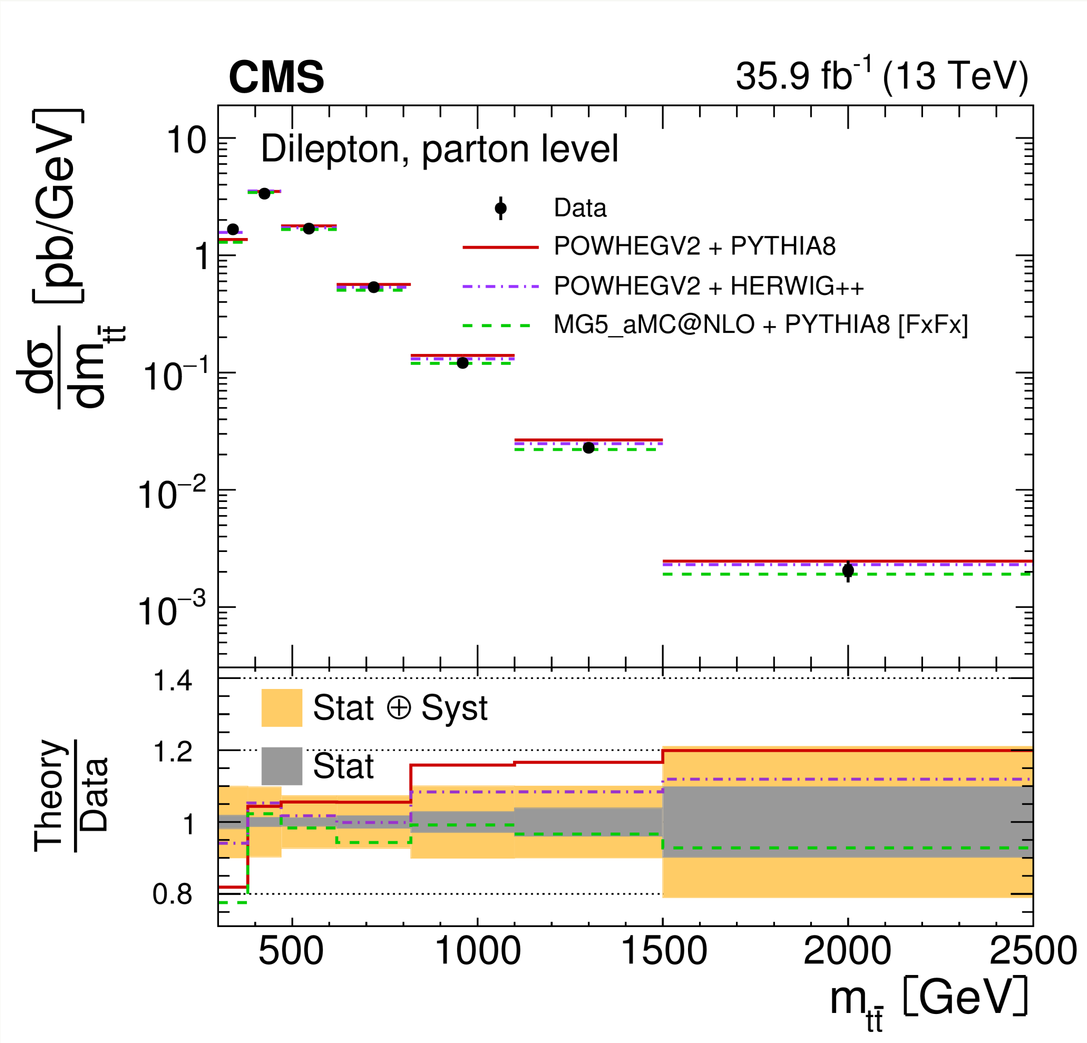


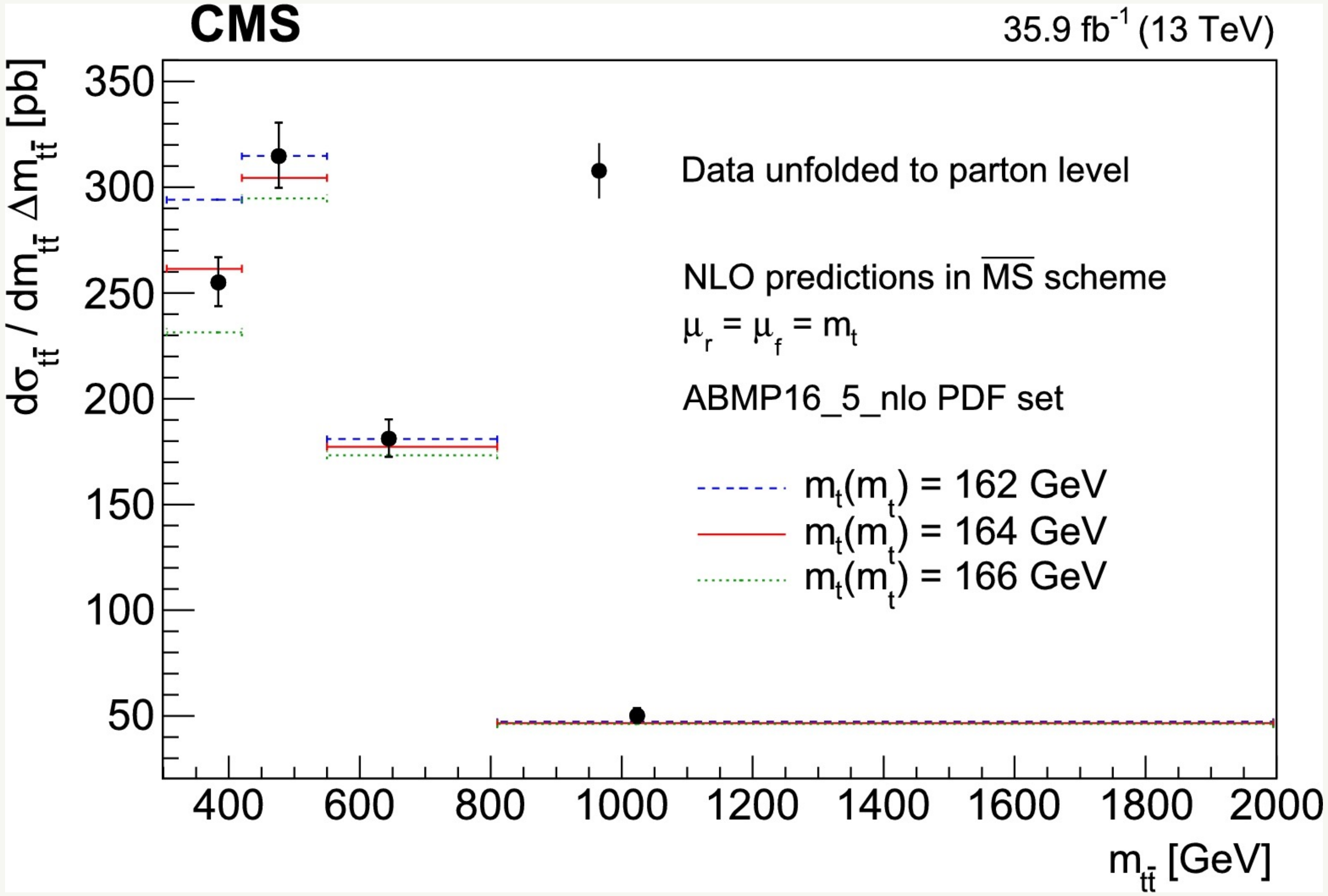
*More details about this in Simone Amoroso's talk

ATLAS ttbar(l+jets) inclusive cross-section arXiv:2006.13076

CMS parton shower tuning CMS PAS TOP-16-021

Combining Unfolding and Profiling





CMS Maximum Likelihood Unfolding

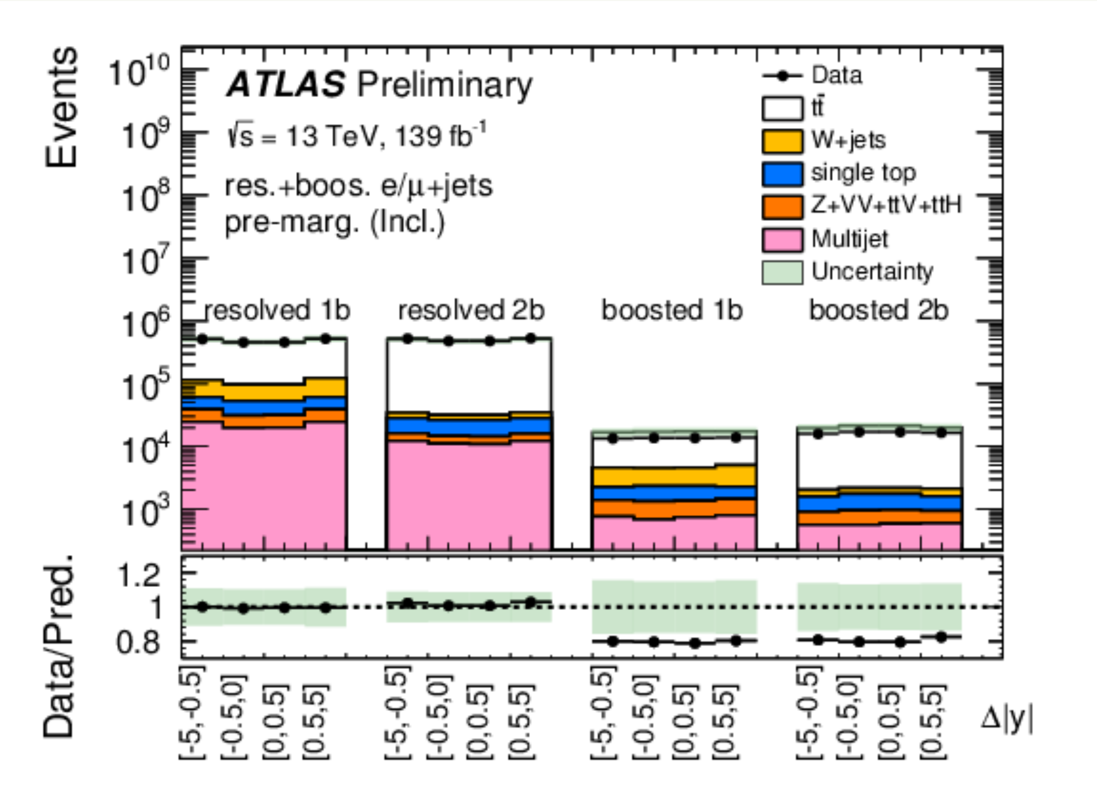
- The unfolding problem was found to be well-conditioned, and therefore no regularisation is needed
- Acceptance and efficiencies not free parameters
- Improved uncertainty on unfolded m(tt) thanks uncertainty profiling

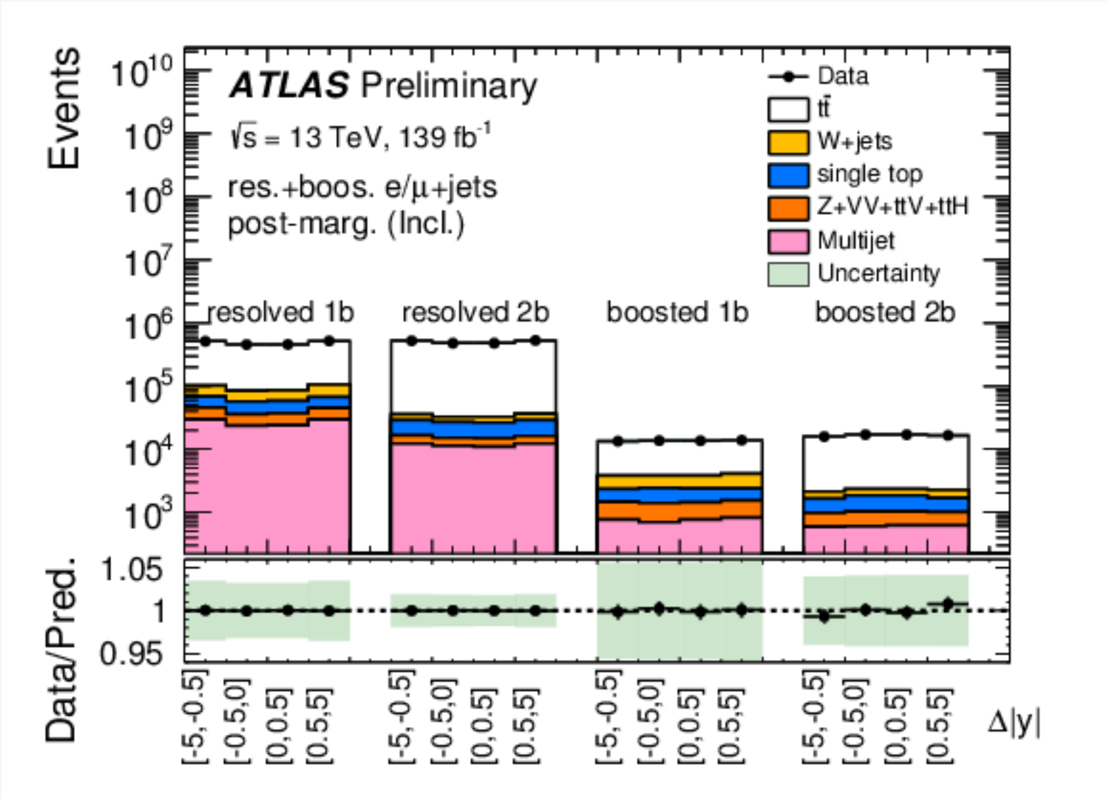
Profiling results

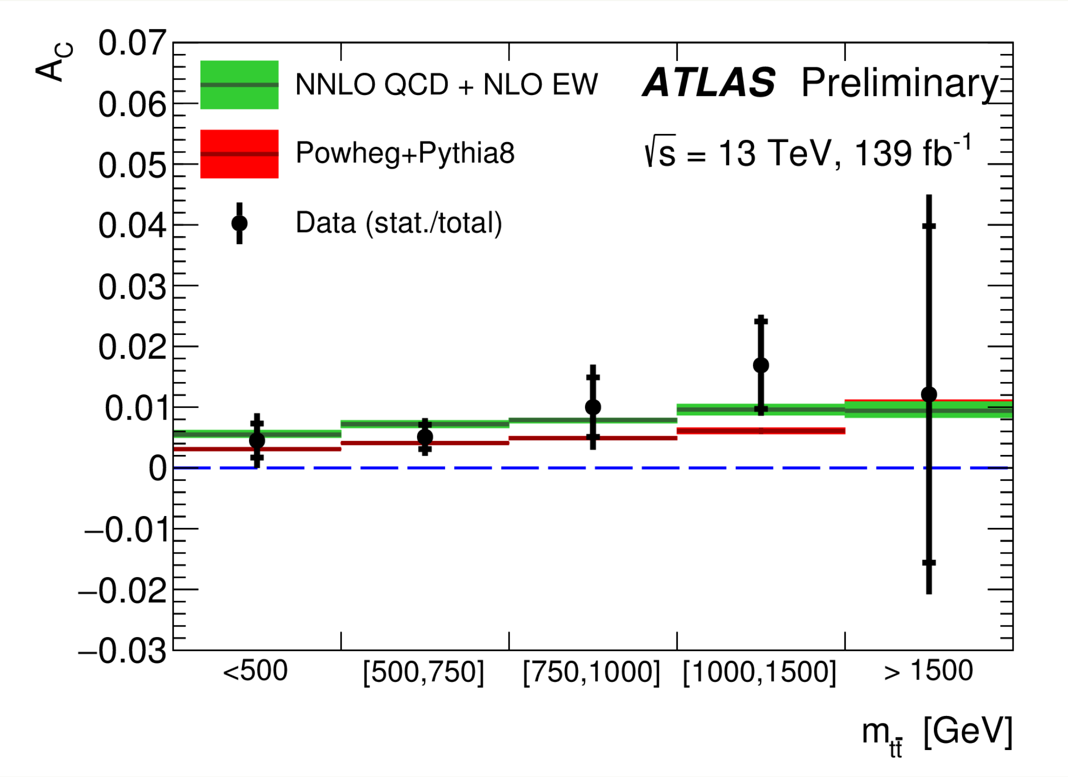
M(tt) bin	1	2	3	4
Total Uncert	+4.7 -4.4	+5.0 - 4.8	+5.0 - 4.8	+7.2 -6.9

CMS dilepton differential + running mass Phys. Lett. B 803 (2020) 135263
CMS dilepton differential JHEP 02 (2019) 149

Combining Unfolding and Profiling







ATLAS Fully Bayesian Unfolding

- Asymmetry measurement @13 TeV combine resolved and boosted measurements
- Exploits profile likelihood framework to perform extraction in different regions of the phase space
- Reduction of the uncertainty in the different regions probed by the analysis

Statistical and systematic uncertainties: Covariance Matrix

Quantification of the agreement between measured normalised unfolded distributions* and theoretical predictions

$$\chi^2 = V^T_{N_{b-1}} \cdot Cov^{-1}_{N_{b-1}} \cdot V_{N_{b-1}},$$

where $V_{N_{b-1}}$ is the vector of differences between data and prediction and $Cov_{N_{b-1}}$ is the sub-matrix derived from the full covariance matrix.

Proper definition of covariance matrix is crucial to test the available models
Different solutions proposed by the analyses

Covariance Matrix expressed as the sum of **two matrices**:

1. Statistical, detector systematics and background modelling
2. Signal modelling (generator, PS, ISR/FSR and PDF)

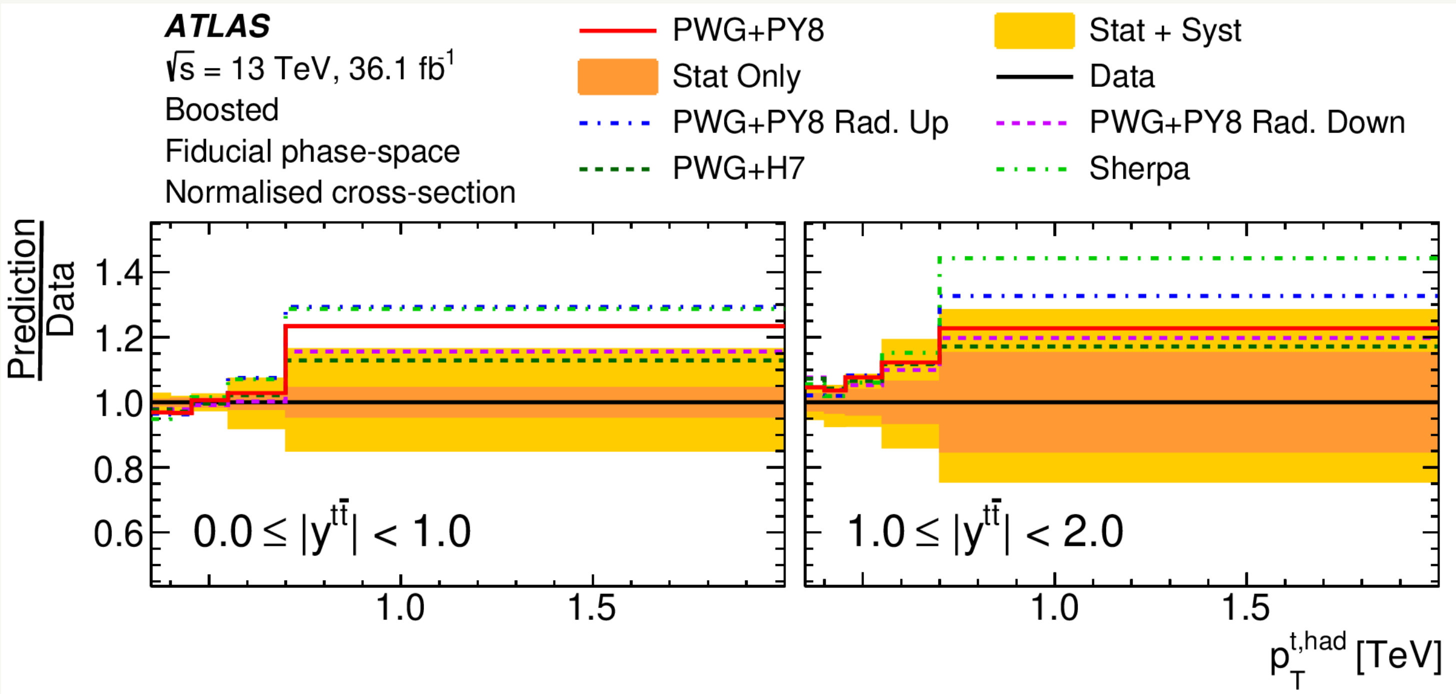
Two different approaches for the detector systematic and background uncertainties:

- Correlations estimated from **toy experiments**
- Evaluated bins **systematic uncertainty shift** and “assumed” correlation

NB: This is independent from the number of unfolded variables we want to test

*More details about unfolding in Otto Heinz Hindrichs’ talk

Statistical and systematic uncertainties: Covariance Matrix - single variable

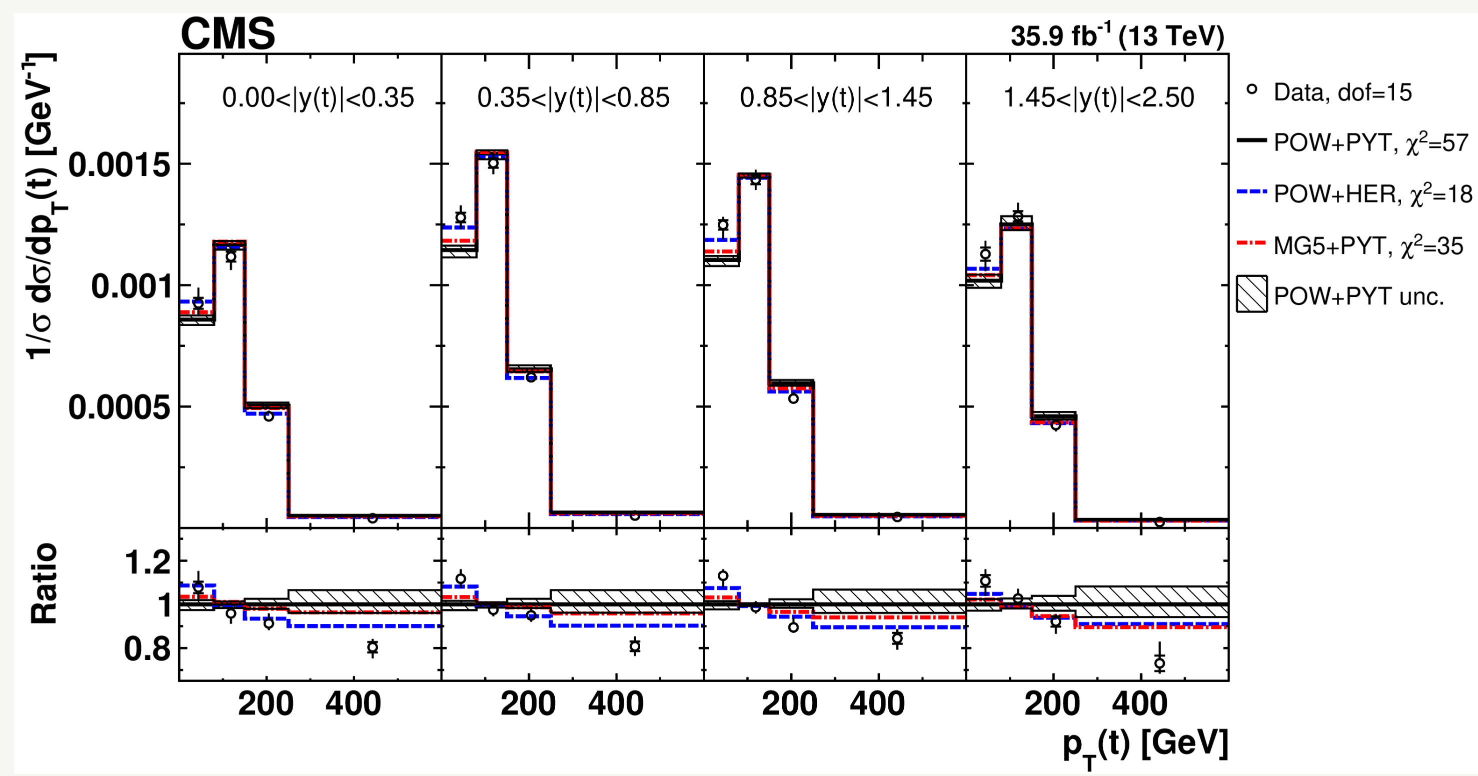


Toy experiments for both statistical and systematic uncertainties:

- Statistical and systematic correlation matrix derived from toy events

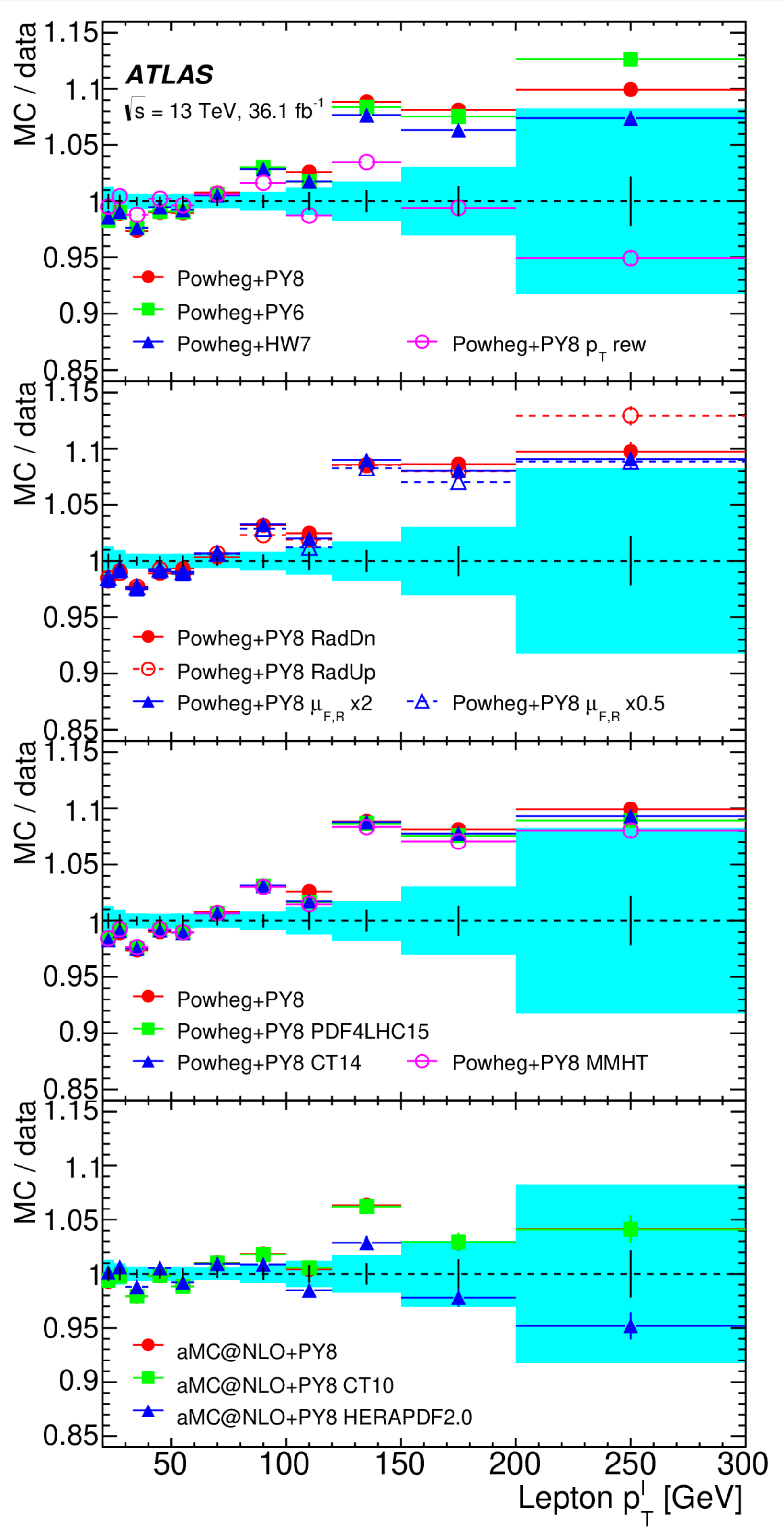
Difference between systematic and nominal is taken as standard deviation

- Correlations between bins by looking at systematic shifts direction



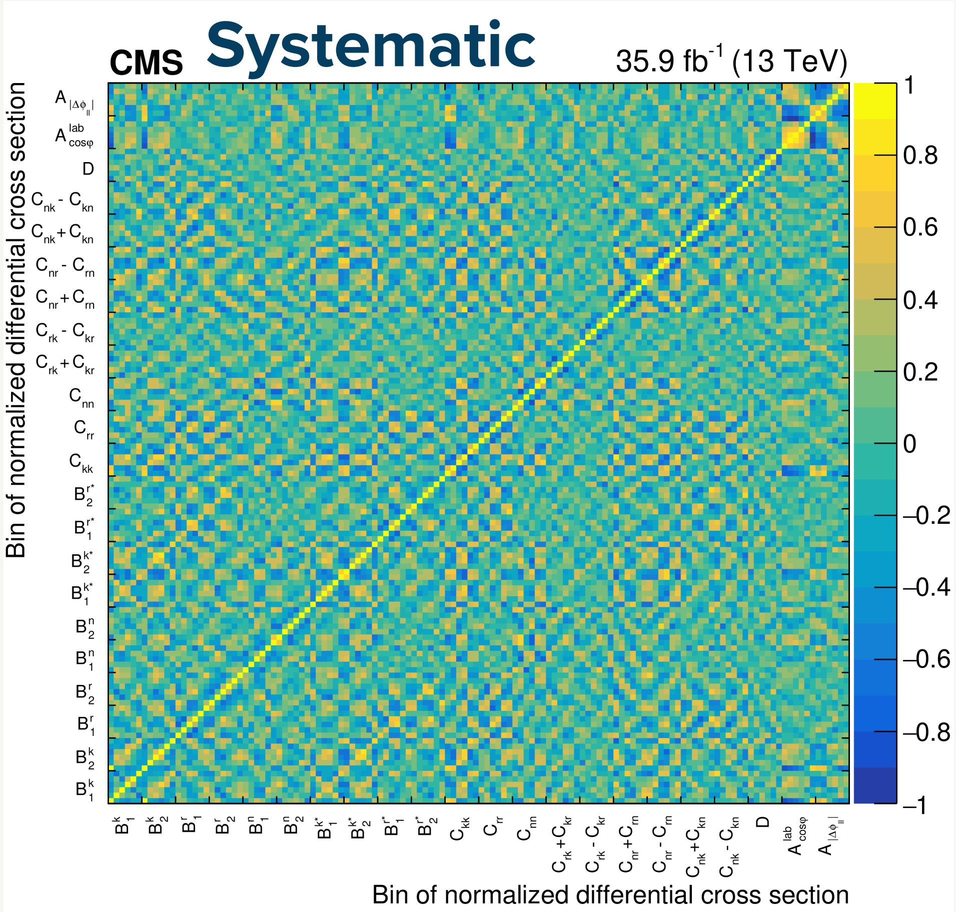
ATLAS ttbar(l+jets) differential cross-section Eur. Phys. J. C (2019) 79:1028
CMS normalised multi-differential cross sections arXiv:1904.05237

Statistical and systematic uncertainties: Covariance Matrix - multiple variables



ATLAS ttbar dilepton differential Eur. Phys. J. C (2020) 80:528

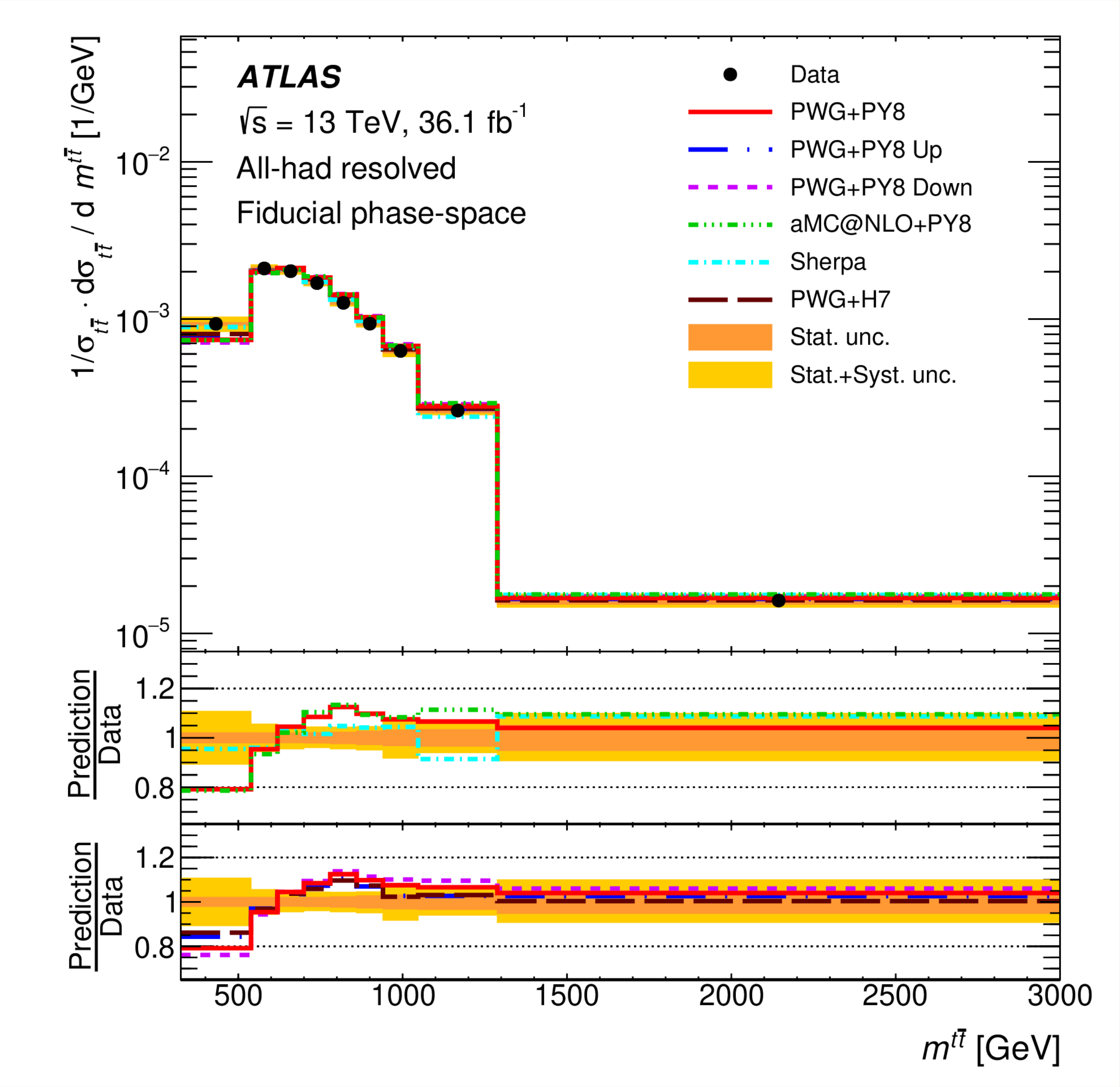
- Different lepton variables tested
- The statistical correlations between distributions were evaluated using pseudo-experiments
- Systematic uncertainties were assumed to be correlated between distributions



CMS spin correlation and polarisation Phys. Rev. D 100 (2019) 072002

- Measured coefficients from different normalised differential xsec
- Systematic covariance matrices derived by looking to shifts direction and assigning ±100% correlation between bins of different distributions

Statistical and systematic uncertainties: Covariance Matrix - normalised variables



In the newly released ttbar all-hadronic differential cross-section measurement calculation of covariance matrix slightly changed for normalised results:

- The **signal-modelling shifts** are derived by using the **expected relative variations** from the associated systematic uncertainty **to scale each bin of the Poisson-fluctuated distribution** unfolded with nominal corrections
- Varied distributions are normalised to unity after all effects are included
- Correlation properly handled

This new method for the calculation of modelling covariance matrix found to improve p-value results in some variables

Summary

Most of the top quark related measurements are nowadays limited by the systematic uncertainty:

- Modelling of the top events plays a big role in most of the results
- Effort in the community to improve these uncertainties
  - Here we presented the treatment of the systematic uncertainty in the context of Profile Likelihood Fits
    - ATLAS and CMS agree on similar procedure
      - ✓ How to prevent unphysical constrain and pull of NP
      - ✓ Real constrains and pulls from fit to data
    - In the future we might want to tune better the available models
  - Unfolded data used to test predictions
    - First results published with profiled uncertainties within unfolding analyses
    - χ^2 test uses covariance matrix defined in similar way
      - ✓ Both single and multiple variables tested

The road ahead

Given the observed constrains on the systematic uncertainties in the future we might want to invest time in model improvement:

- How to better **tune** them from data?
- Better estimates of the uncertainties by **varying model parameters** within a given generator instead of comparing different generators
- Study the correlations between different effects

BACKUP

‘To profile or not to profile’

We consider as top precision measurements those which uncertainty is mainly systematic such as:

- Differential and inclusive cross sections
  - Fiducial and full phase space
- SM parameters measurements

Also informations on the systematic uncertainties can be extracted from data (profiled) with the aim of reducing them.

However, a general recipe for when to profile or not does not exist

Uncertainties are **profiled** in:

- **Inclusive** cross section measurements
- Rare processes and **properties** measurements

Differential cross section measurements usually **don’t profile** their uncertainties

- First unfolded measurements with profiled uncertainties

Inclusive cross section measurements
Uncertainties are profiled
CMS - tt+bb PLB 803 (2020) 135285, tt+jets JHEP 07 (2020) 125 and tt(e/mu +tau) JHEP 02 (2020) 191 in the fiducial phase space and EPJC 79 (2019) 368
ATLAS - tt(l+jets) arXiv:2006.13076 in fiducial and full phase space, tt+bb JHEP 04 (2019) 046

Rare processes, properties and search-oriented analyses
Uncertainties are profiled
CMS - CKM matrix elements PLB 808 (2020) 135609 and tZq Observation PRL 122 (2019) 132003
ATLAS - Top Width ATLAS-CONF-2019-038, Top mass (soft muon) ATLAS-CONF-2019-046, tZq observation JHEP 07 (2020) 124, FCNC tqgamma Phys. Lett. B 800 (2019) 135082

Differential cross section measurements
Uncertainties not profiled
CMS - arXiv:2008.07860, arXiv:1904.05237 arXiv:1911.03800
ATLAS - Eur. Phys. J. C 80 (2020) 528, Eur. Phys. J. C 79 (2019) 1028, Phys. Rev. D 98 (2018) 012003

Partially profiled
CMS - EPJC 80 (2020) 370 (t-ch differential measurement) in which experimental uncertainties and background normalisations are profiled and the rest externalised.

Profiling within Unfolding
CMS - Phys. Lett. B 803 (2020) 135263
ATLAS - ATLAS-CONF-2019-026

Prevention of spurious pulls and constrains

✳ Smoothing algorithms act on systematic histograms to make them *smoother*

- Computationally faster (easier example: re-binning)
- Applied to most of the systematic uncertainties '*a priori*'

✳ Decorrelation of NPs among the regions

- This might either reduce or increase the systematic uncertainty

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✳ Bootstrapping smooths systematic histograms from statistical fluctuations, generating N replicas of the event

- Correlation between nominal and systematic
- More CPU consuming

✳ Factorization of components

- If alternative model is discrepant with data consider re-weighting an observable before building the systematic variation
- Top pT re-weight applied to all alternative samples

Unfolding techniques

Unfolding techniques are used in the top sector to measure differential distributions at the particle and parton level:

- Unfolded data used to test theoretical predictions
- Possible to extract physical parameters
  - Spin correlation and polarisation
  - Top-antitop charge asymmetry

Determination of the distribution *F(x)* of a stochastic variable *x* using a sample of data $x_1,\ldots,x_n$

- Each observation *i* is characterised by a measured value y_i corresponding to a true value x_i
- Measured values y_i distorted by measurement errors
- *y* and *x* are related by the response function *R(y|x)*

$$F_{obs}(y) = \int R(y\,|\,x)\; F_{true}(x)\; dx$$

We measure number of data events in a bin ΔX_k of a variable histogram

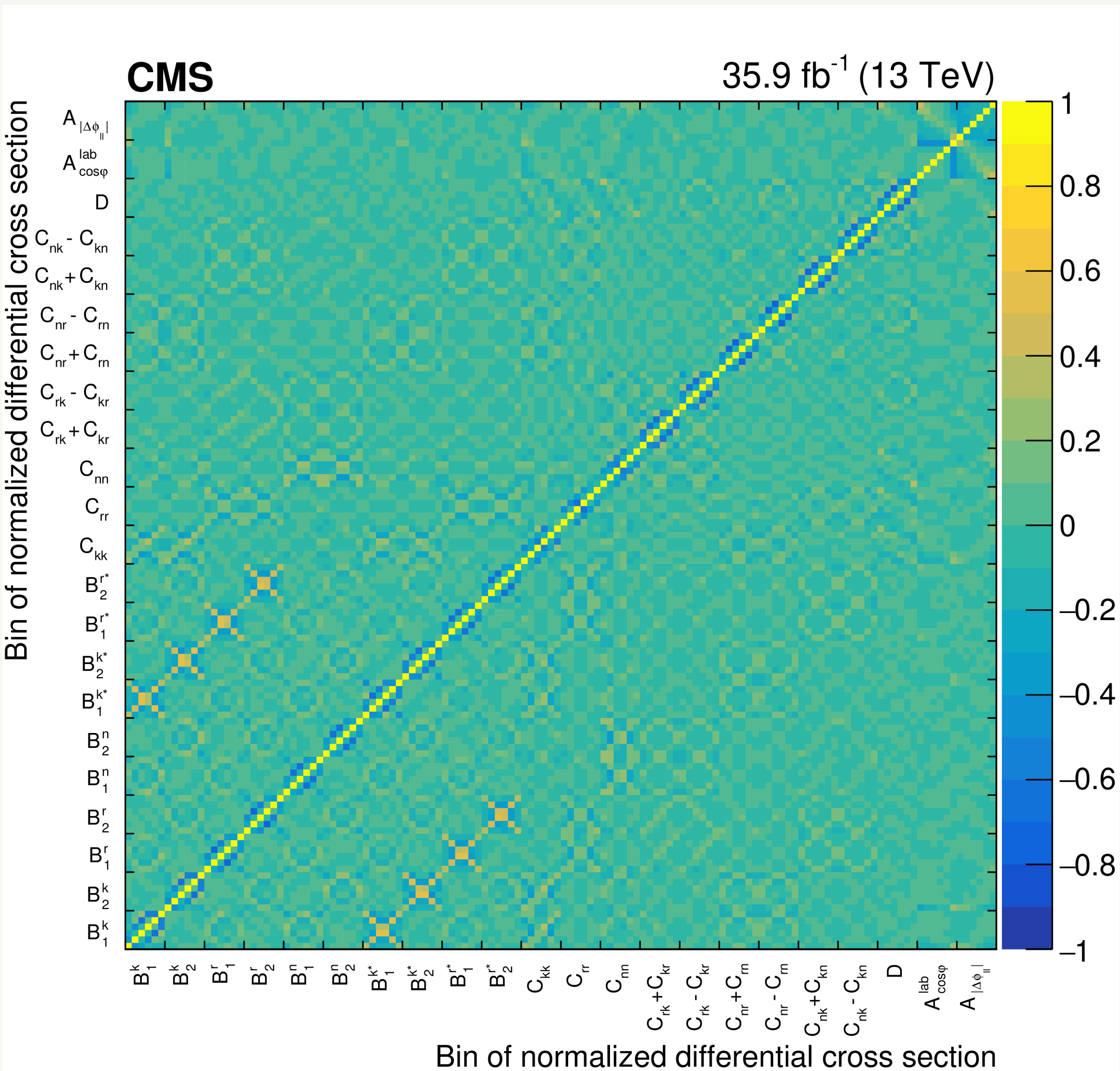
$$N_k^{reco} = \Sigma_j\; R_{kj}\; N_j^{unf} + N_k^{bkg} \longrightarrow \left(\frac{d\sigma}{dX}\right)_j = \frac{N_j^{unf}}{L \cdot \Delta X_j}$$

Multiple normalised distributions

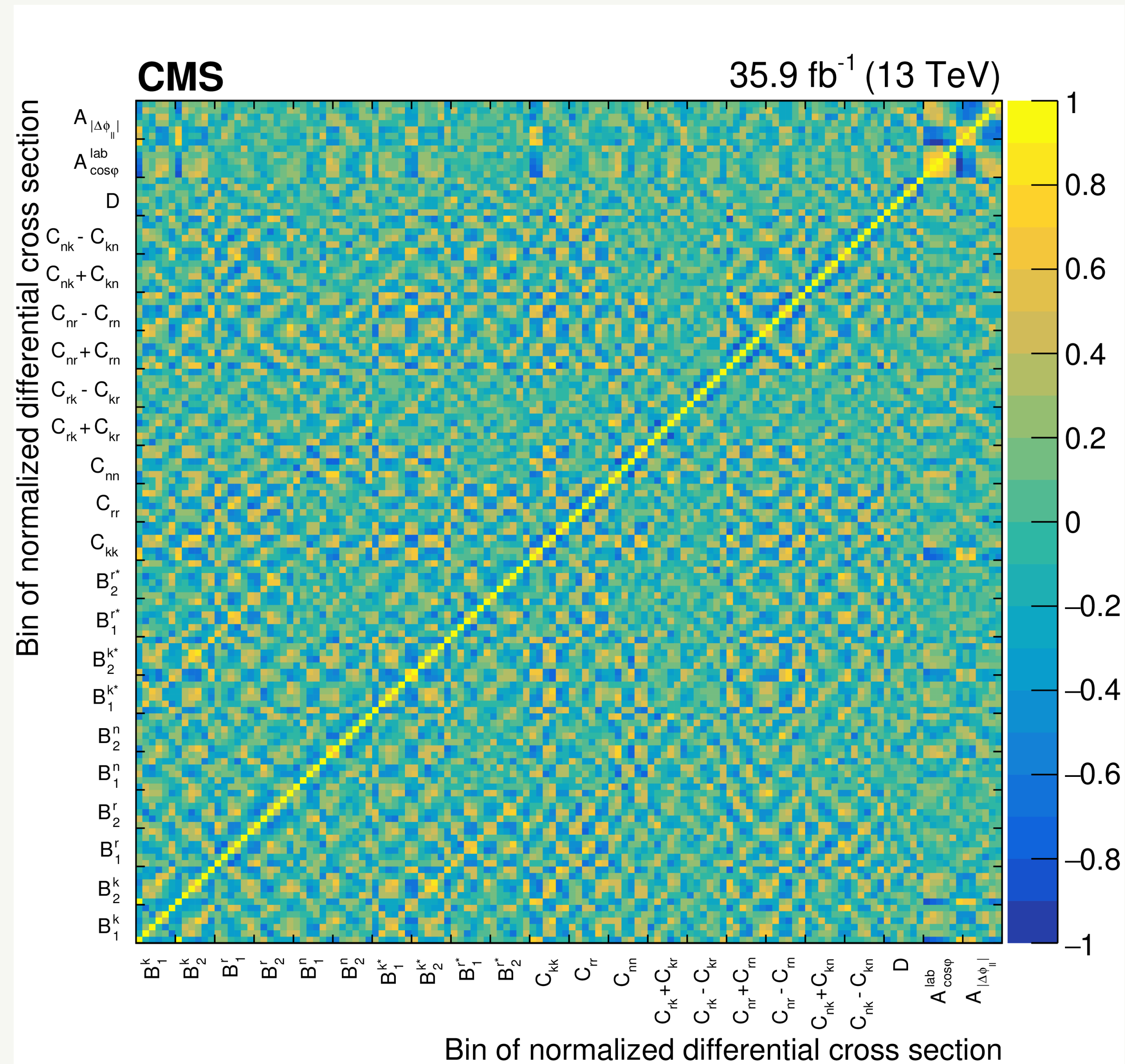
It is possible to perform a χ^2 test simultaneously on various normalised differential cross sections:

- Correlation between bins of different unfolded distributions is under study

Statistical

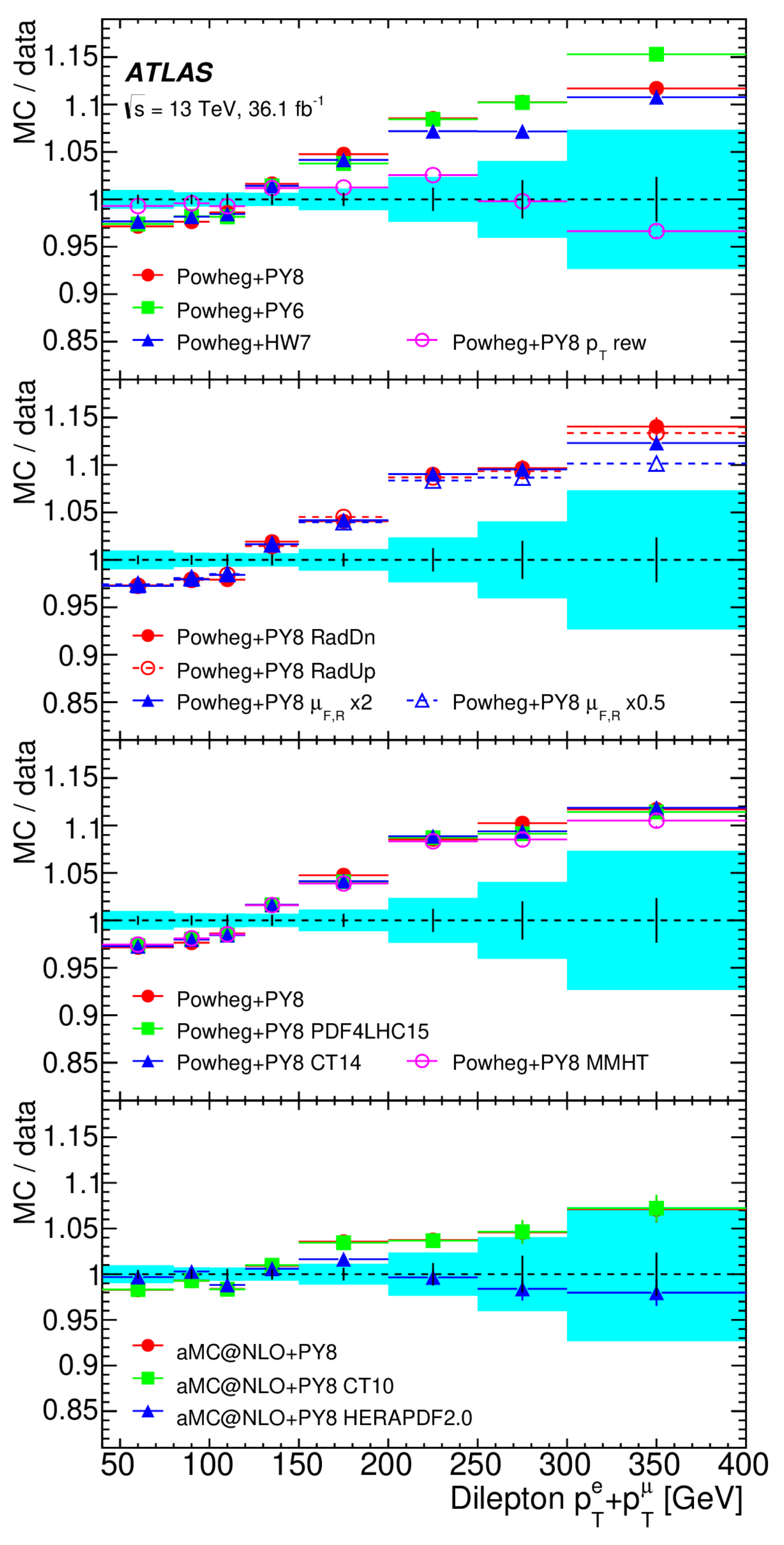


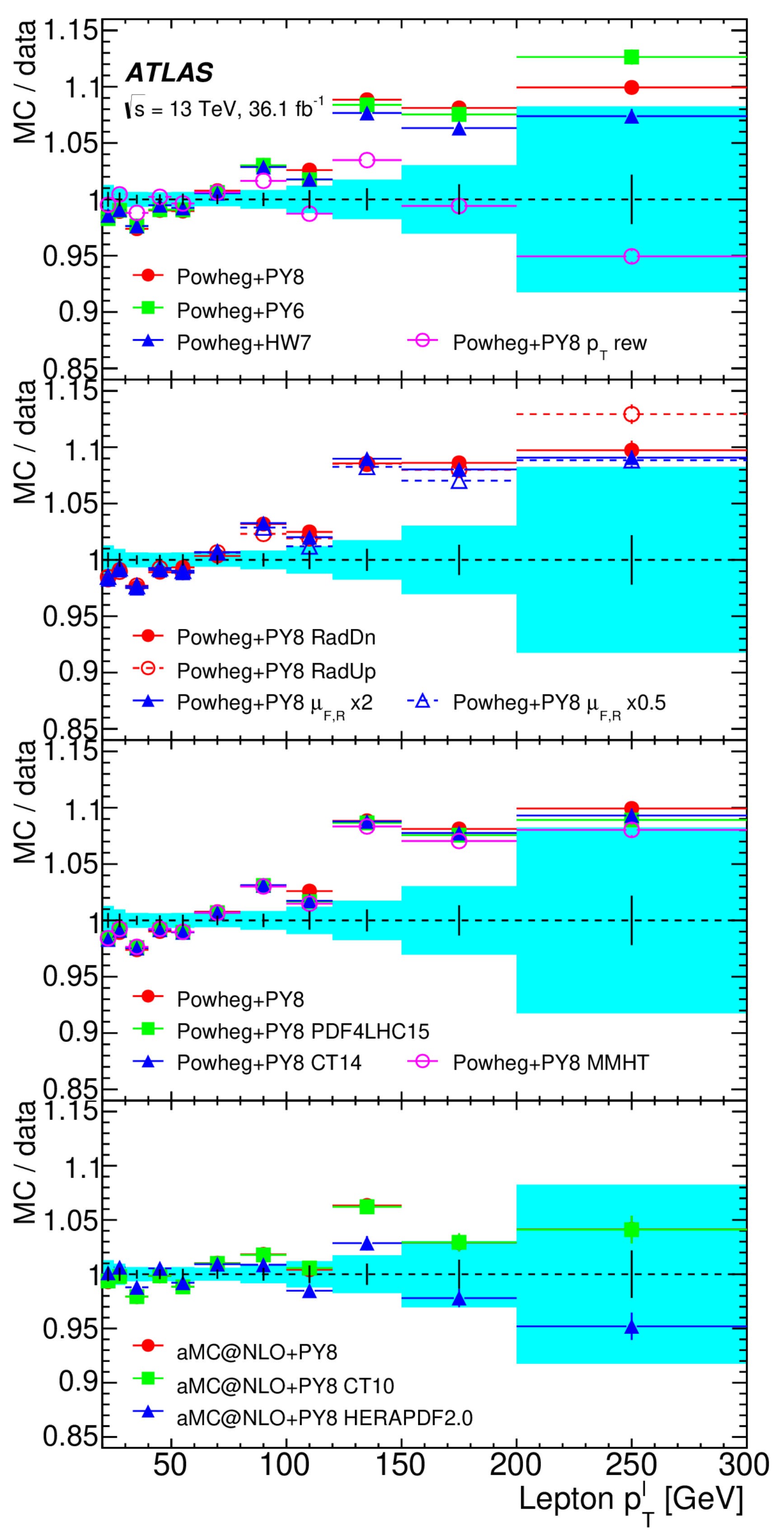
Systematic



CMS spin correlation and polarisation Phys. Rev. D 100 (2019) 072002

Multiple normalised distributions





ATLAS ttbar dilepton differential
Eur. Phys. J. C (2020) 80:528

- The statistical correlations between distributions were evaluated using pseudo-experiments
- Systematic uncertainties were assumed to be correlated between distributions

Improvement of ttbar modelling

ATLAS procedure for Initial State Radiation uncertainty:

- Compare nominal ttbar to alternative samples with different settings of *hdamp*, normalisation and factorisation scales and different PS tune
    - Choice based looking at variables measured at 8 TeV
- In ttbar(l+jets) measurement the NP associated to the envelope of these variations significantly constrained

↓

DECORRELATION PROCEDURE

ATLAS ttbar(l+jets) inclusive cross-section arXiv:2006.13076

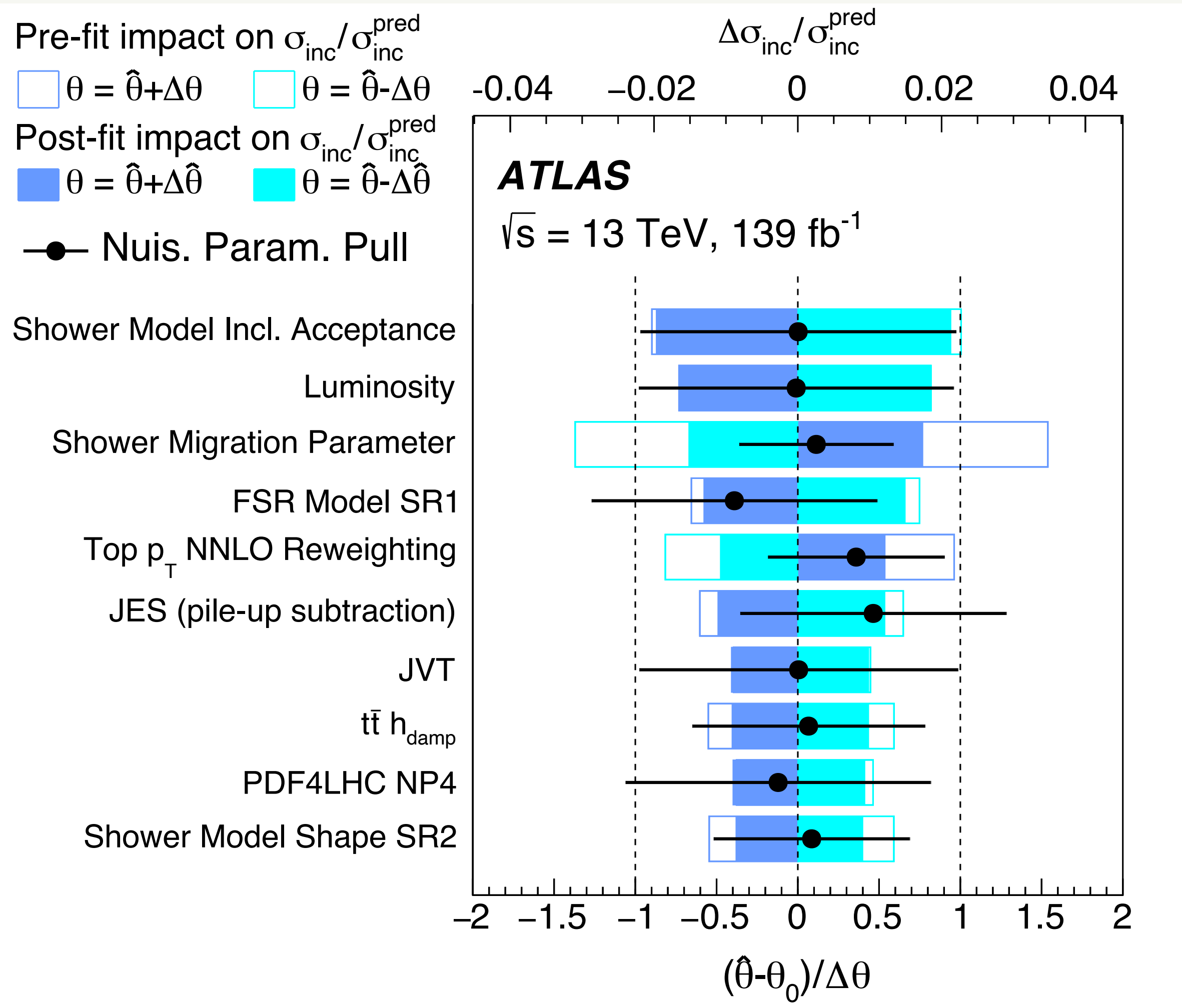
Improvement of ttbar modelling

Measurement of ttbar cross section in l+jets final state

- Fit on three variables of three independent signal regions
- Both fiducial and inclusive cross sections extracted from fit

$$\sigma_{fid} = A_{fid} \cdot \sigma_{incl}, \quad A_{fid} = \frac{N_{fid}}{N_{tot}}$$

$$\sigma_{incl} = \frac{N_{data} - N_{bkg}}{L_{int} \cdot A_{fid} \cdot C}, \quad C = \frac{N_{reco}}{N_{fid}}$$



Reduction of modelling uncertainties via renormalisation of varied distributions

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FIDUCIAL FIT: all distributions scaled to same fiducial acceptance

- Remaining normalisation uncertainty in C

INCLUSIVE FIT: all distributions scaled to same inclusive cross section

- Impact of modelling encoded in A

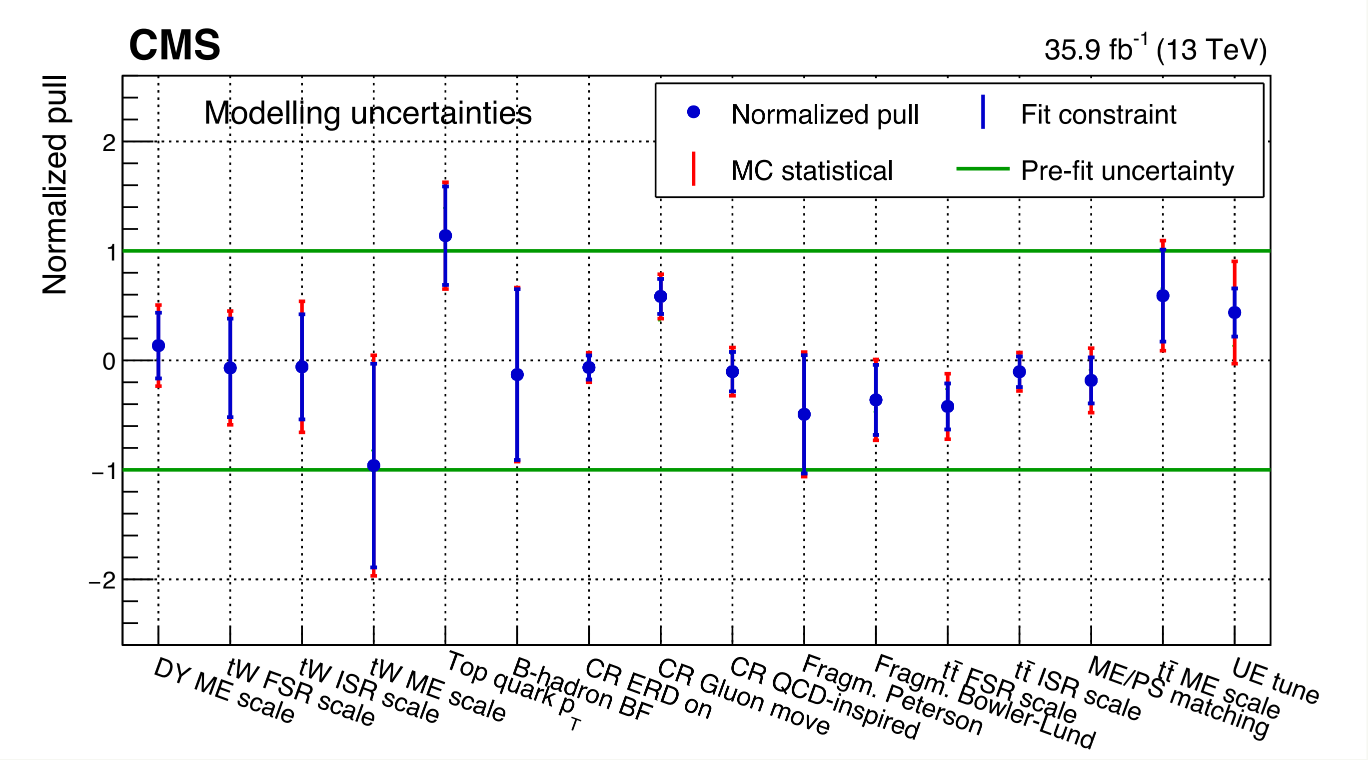
$$\sigma_{t\bar{t}} = 830 \pm 0.4(stat) \pm 36(syst) \pm 14(lumi)\ pb$$

ATLAS ttbar(l+jets) inclusive cross-section arXiv:2006.13076

Improvement of ttbar modelling

Measurement of ttbar cross section in the dileptonic final state

- Events categorised as function of number of b-tagged and non-b-tagged jets



Extrapolation uncertainty determined by :

1. Fixing all NPs to post-fit value
2. NP under study set to ± 1
3. Recorded variation on A
4. Sum in quadrature to derive uncertainty on inclusive cross section

Uncertainties in the inclusive phase space are not fully profiled

$$\sigma_{t\bar{t}} = 803 \pm 2(stat) \pm 25(syst) \pm 20(lumi)\ pb$$

Combining Unfolding and Profiling

Both ATLAS and CMS gave an example of Unfolding with Profiled systematic uncertainties:

- The main idea is to perform a maximum likelihood fit
- Comparing data to prediction for both spectrum unfolding and uncertainty constrains

X = TRUE DISTRIBUTION

Y = RECO DISTRIBUTION

$$\mathscr{L}(Y\,|\,X, B) = \prod_{i=1}^{n} \mathscr{P}(y_i, r_i(X, \mathscr{M}) + b_i)$$

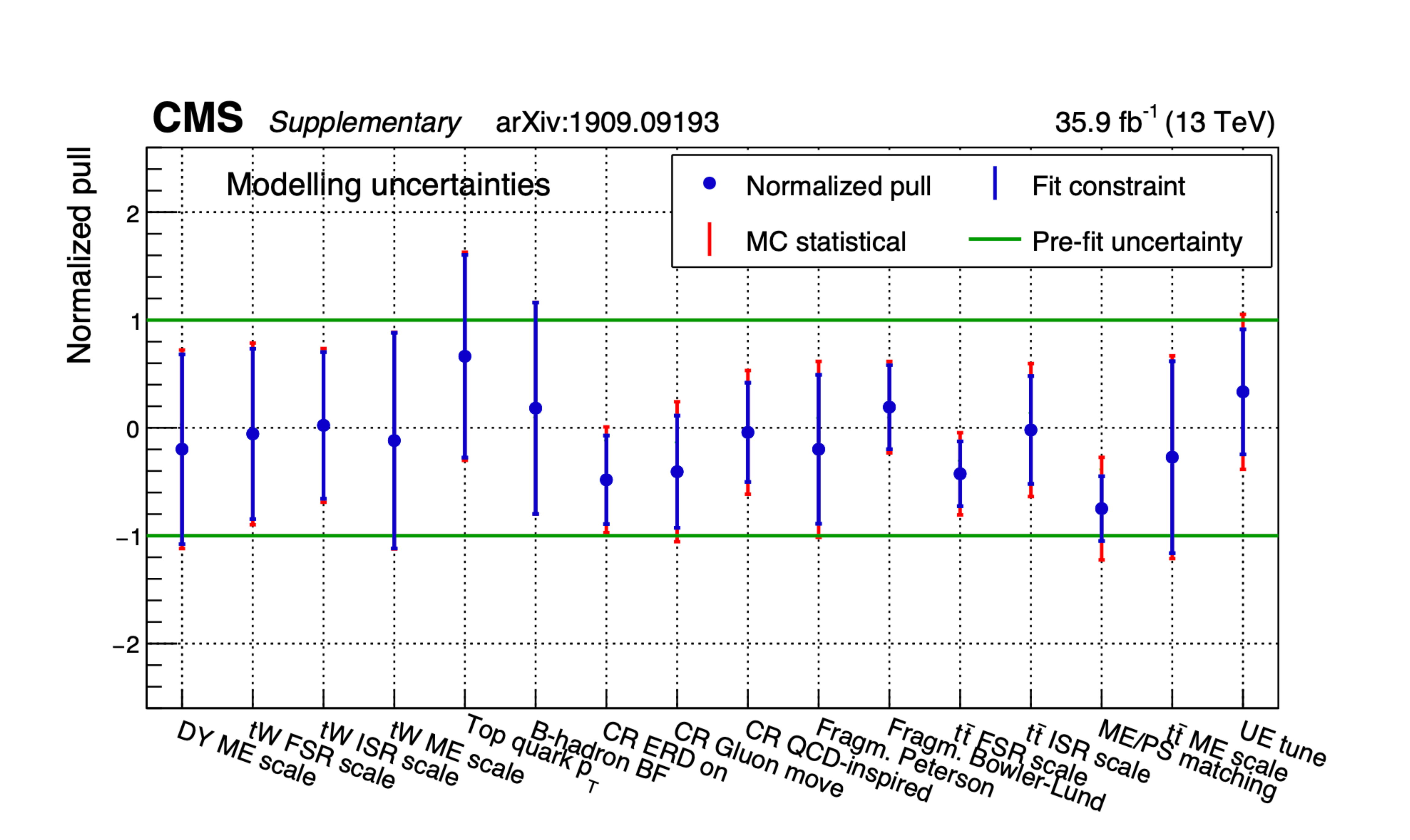
Reco data in a bin *i* follows a Poissonian distribution with predicted value given by true distribution and migration matrix

- Does not involve an explicit matrix inversion
- Prior choice determines bias
- "automatic" handling of systematics and correlations

ATLAS charge asymmetry ATLAS-CONF-2019-026

CMS running mass Phys. Lett. B 803 (2020) 135263

Combining Unfolding and Profiling



CMS dilepton differential + running mass [Phys. Lett. B 803 (2020) 135263]

Fully Bayesian Unfolding

Choice of the prior corresponds to applying a regularisation with strength:

- Curvature prior corresponds to a generalisation of Tikhonov regularisation

Systematics are marginalised in the Bayesian inference framework:

- Posterior probability integrated over NPs

$$\mathscr{L}(Y|X) = \int \mathscr{L}(Y|X,\theta)\ \mathscr{N}(\theta)\ d\theta$$

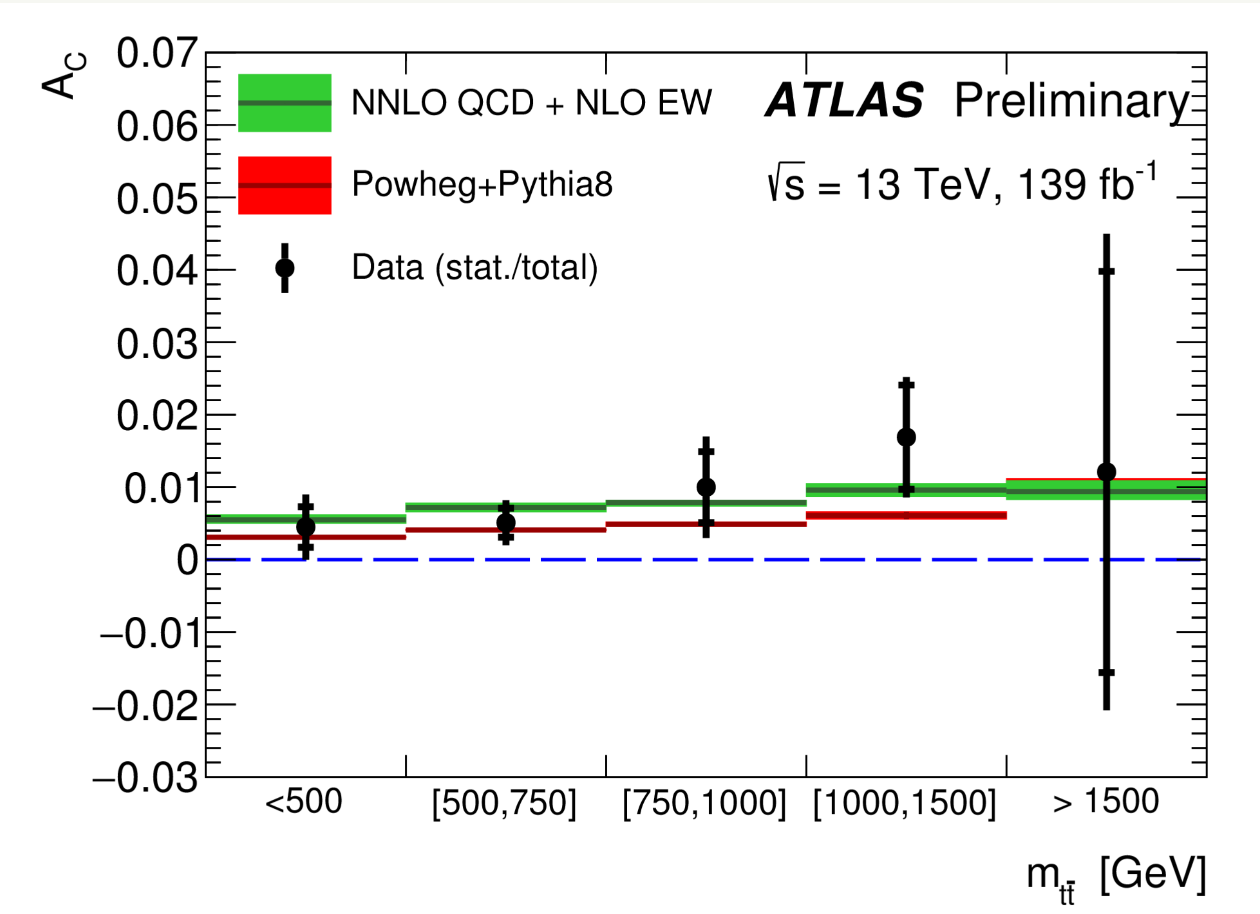
NP prior

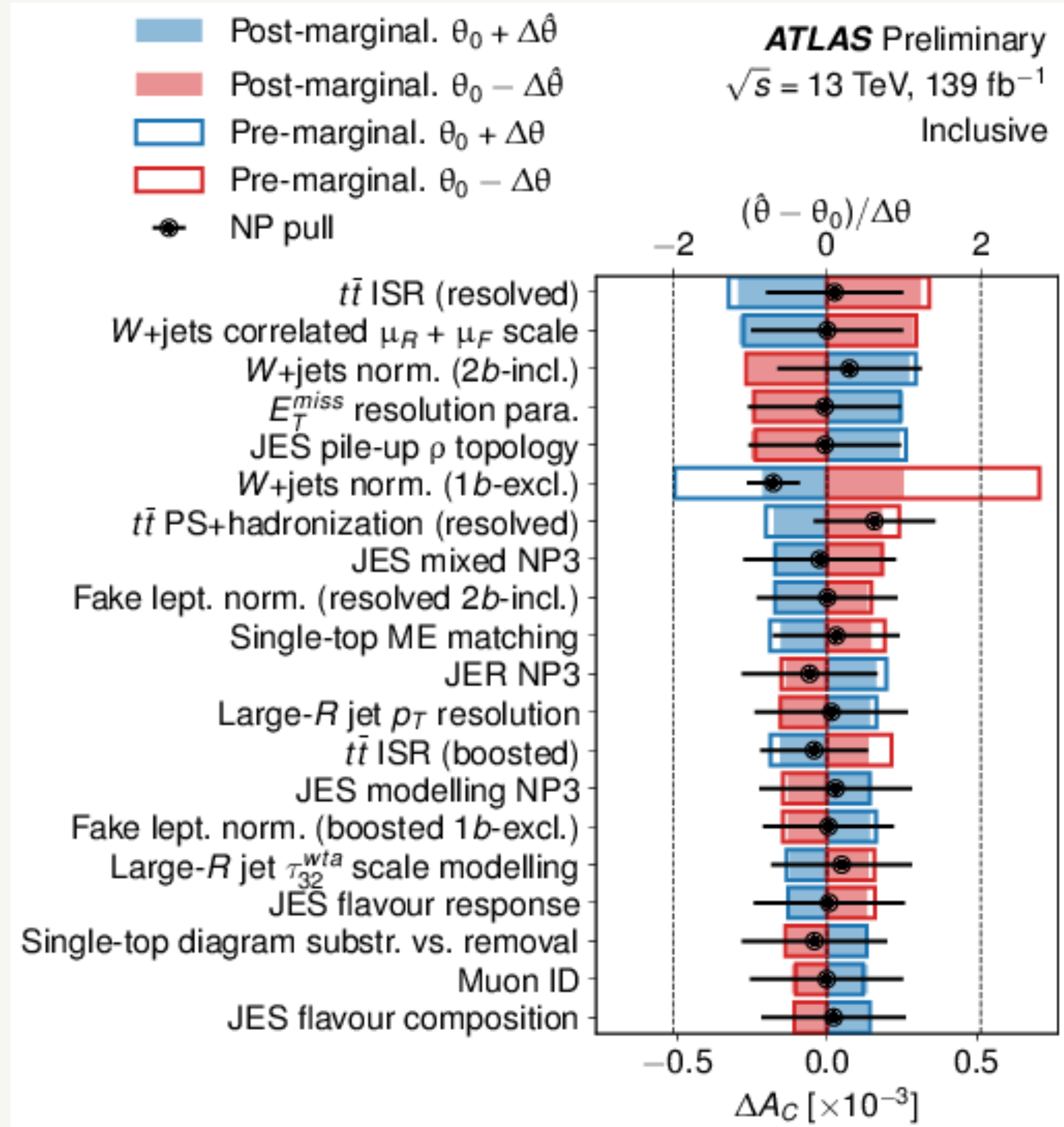
Formalism is flexible also when it comes to combining different channels:

- Correlation of NPs handled
- Possibility to add CRs for background processes

$$\mathscr{L}(Y_1, \ldots, Y_{N_{ch}}|X) = \int \prod_{h=1}^{N_{ch}} \mathscr{L}(Y_h|X,\theta)\ \mathscr{N}(\theta)\ d\theta$$

Charge Asymmetry with FBU





Statistical uncertainties are mostly dominating

Non-zero inclusive asymmetry observed at 4σ