

Top-pair and single-top differential cross sections and unfolding techniques



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Overview of unfolding

- algorithms used in top quark analyses
- problems of unfolding
- tests of unfolding

Differential $t\bar{t}$ quark cross sections:

- have been measured in dilepton, $e/\mu + \text{jets}$, and all-hadronic events
- in resolved and boosted regimes
- at parton and particle level

Differential single top quark cross sections

- in t-channel and tW

These measurements provide:

- precision tests of the standard model top quark production
usually full covariance matrices of statistical and systematic uncertainties provided
→ facilitates quantitative comparisons to theory predictions
- PDF constraints, extractions of m_t , α_s

Maximize likelihood:

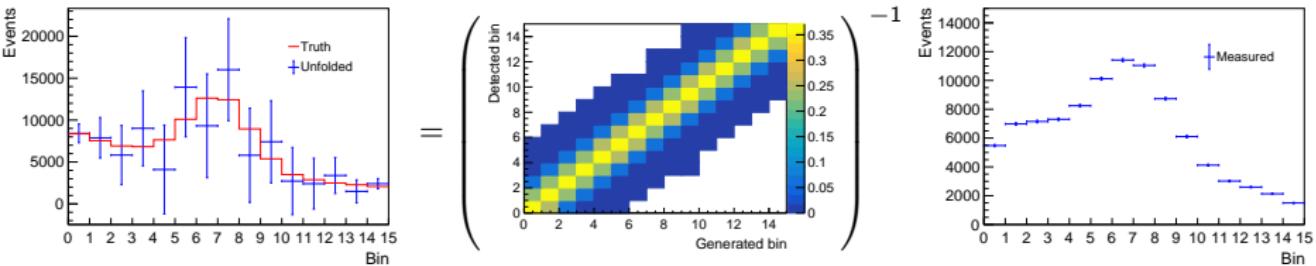
$$\log(p(\mathbf{d}|\boldsymbol{\lambda})) = \sum_i \left(d_i \log\left(\sum_j M_{ij}\lambda_j + b_i\right) - \left(\sum_j M_{ij}\lambda_j + b_i\right) \right),$$

where \mathbf{d} ($\boldsymbol{\lambda}$) is the observed (unfolded) spectra and M the migration matrix, \mathbf{b} backgrounds.
 If M is square/invertible the MLE is:

$$\boldsymbol{\lambda} = M^{-1}(\mathbf{d} - \mathbf{b}).$$

This represents an unbiased result, but statistical uncertainties in \mathbf{d} can be extremely amplified in the unfolded spectrum

→ large oscillations with strongly anti-correlated adjacent bins.



Regularization

Iterative D'Agostini method [[arxiv:1010.0632](https://arxiv.org/abs/1010.0632)]
solves the problem iteratively:

$$\lambda_j^{(n+1)} = \frac{\lambda_j^{(n)}}{\sum_i M_{ij}} \sum_i \frac{M_{ij}(d_i - b_i)}{\sum_k M_{ik} \lambda_k^{(n)}},$$

$\lambda_j^{(0)}$ is a guess, e.g., the MC or flat spectrum.

Stopping the iterative algorithm early will remove large unphysical oscillations, but can introduce a bias.

Used in all ATLAS analyses and in several CMS.

χ^2 Unfolding

Minimize:

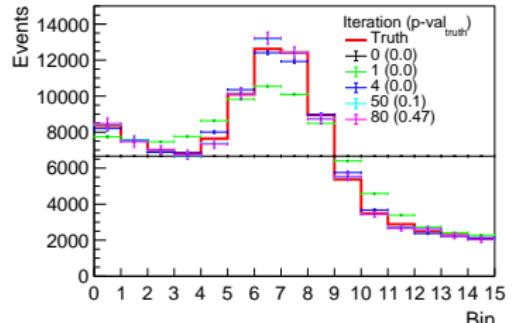
$$\chi^2 = (\mathbf{d} - M\boldsymbol{\lambda})^T C^{-1} (\mathbf{d} - M\boldsymbol{\lambda}) + \tau(\boldsymbol{\lambda} - \boldsymbol{\lambda}_0)^T L^T L (\boldsymbol{\lambda} - \boldsymbol{\lambda}_0)$$

with Covariance matrix C , often more bins in \mathbf{d} than in $\boldsymbol{\lambda}$.

Regularization: (Tikhonov)

- the second term penalizes differences in curvature (L is discretized 2nd derivative operator) between $\boldsymbol{\lambda}$ and a distribution $\boldsymbol{\lambda}_0$, usually the MC prediction.
- the regularization parameter τ often chosen to minimize the global correlation [[arxiv:1611.01927](https://arxiv.org/abs/1611.01927)] coefficient. Heuristic criterion → to be tested.

Used in many CMS analyses.



Measurement of running m_t using $d\sigma/dM(t\bar{t})$ in $e\mu$ -events

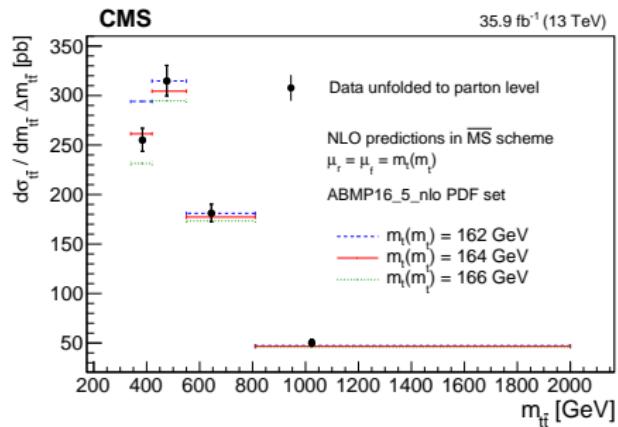
When the likelihood is maximized for the unfolding, there are usually no (effective) degrees of freedom left to constrain uncertainties in the response matrix.

Most analyses propagate uncertainties by repeating the unfolding with altered matrices.

→ provide more information by introducing categories or auxiliary distributions per measured bin.

Categories and distributions fitted per bin:

	$N_b = 1$	$N_b = 2$	Other N_b
$N_{\text{jets}} < 2$	N_{events}	n.a.	N_{events}
$m_{t\bar{t}}^{\text{reco}} 1$	$m_{\ell b}^{\min}$	jet p_T^{\min}	N_{events}
$m_{t\bar{t}}^{\text{reco}} 2$	$m_{\ell b}^{\min}$	jet p_T^{\min}	N_{events}
$m_{t\bar{t}}^{\text{reco}} 3$	$m_{\ell b}^{\min}$	jet p_T^{\min}	N_{events}
$m_{t\bar{t}}^{\text{reco}} 4$	N_{events}	N_{events}	N_{events}

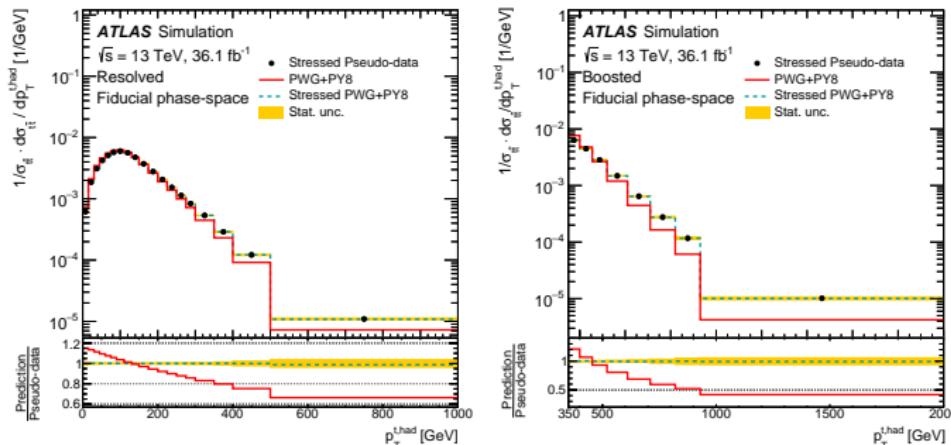


Uncertainty constraints: N_b : b tagging, $m_{\ell b}$: top mass in MC, jet- p_T jet: energy scale

No explicit regularization method used, but implicit regularization due to coarse binning.

Problems of unfolding

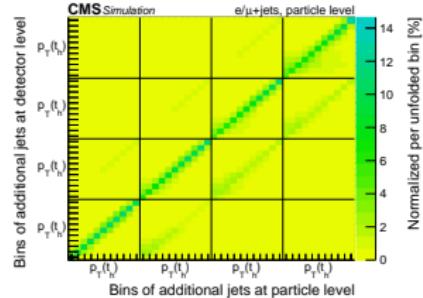
- **Estimate regularization bias** (should be much smaller than uncertainty in measurement):
 - compare (χ^2 -tests) regularized and unregularized results to predictions
- **But even an unregularized result can be biased due to generator assumptions entering the response matrix:** (Example: n -jets is mismodelled in MC, but has direct impact on reconstruction/resolution of X)
 - multidimensional unfolding reduces the impact of modelling assumptions.
(→ measure n -jets vs. X)
 - compare (χ^2 -tests) unfolded and folded distributions to corresponding predictions
→ agreements at both levels should be similar.
 - unfold reweighted MC with default response:
→ bias due to the choice of the migration matrix should be covered by modelling uncertainties.



Double-Differential $t\bar{t}$ cross sections measurements in $e/\mu+jets$ events: resolved

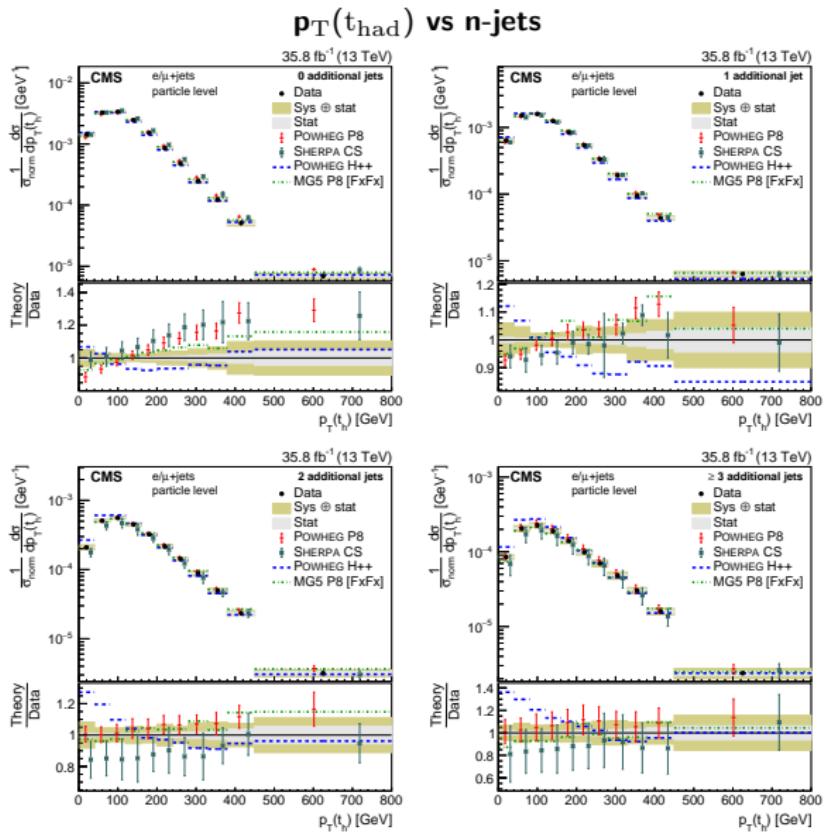
36 fb^{-1} , 13 TeV, CMS: PRD 97 (2018) 112003

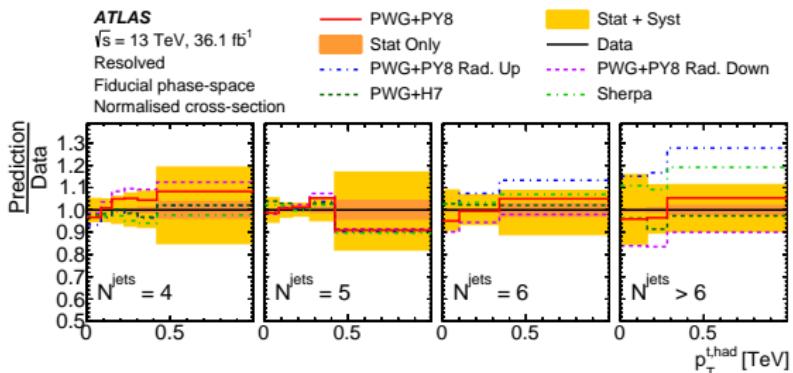
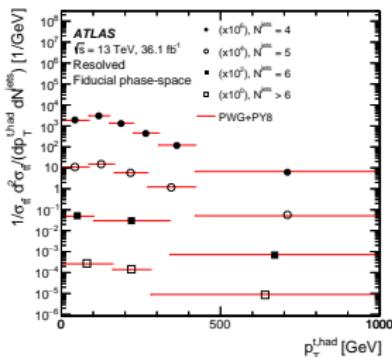
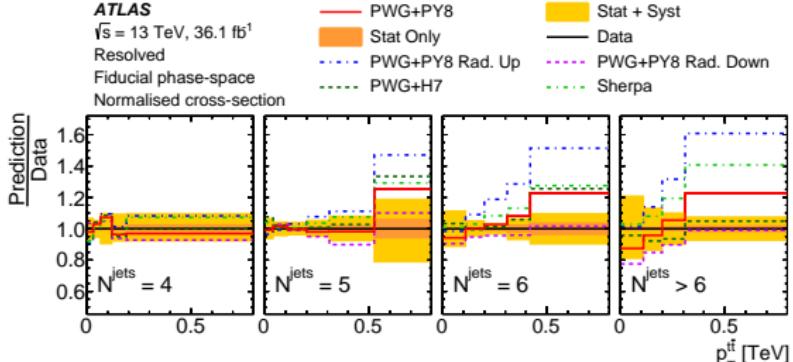
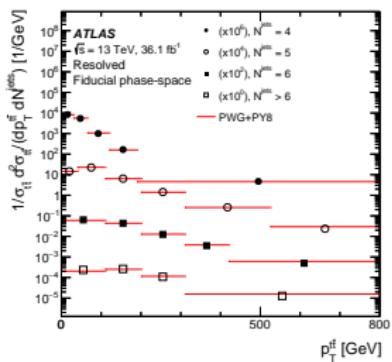
Results unfolded in 2 dim.



Resolution worse at higher jet multiplicity.

- $p_T(t)$ better described at higher multiplicities by POWHEG+PYTHIA8
- $0.01 < p\text{-values} < 0.83$



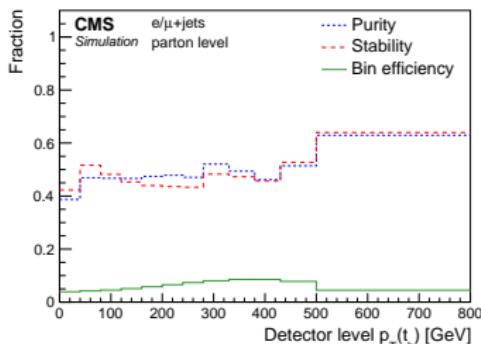
$p_T(t)$ in bins of jet multiplicity $p_T(t\bar{t})$ in bins of jet multiplicity

- The slope in p_T disappears for events with higher jet multiplicity, but becomes steeper for $p_T(t\bar{t})$.

Parton level

Extract properties of top quarks before their decays.

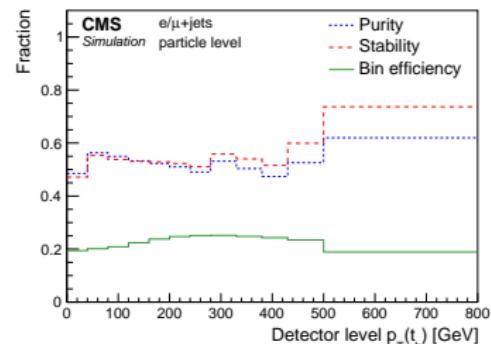
- available at NNLO QCD + NLO EW precision.
- in general not a well defined observable (WWbb production ...)



Particle level

Define proxy of top quark based on leptons, jets, ... within experimental acceptance:

- clean definition of “top quark” observable.
- avoids theoretical extrapolations.



Particle-level measurements:

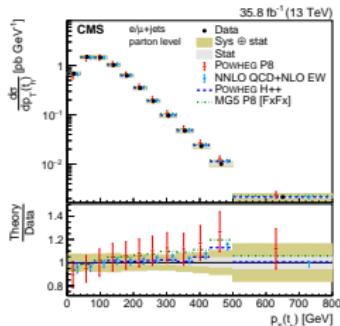
- typically more diagonal response matrix (high purity and stability)
- significantly higher bin efficiencies due to reduced acceptance corrections

purity: correct fraction of events in reconstructed bin, stability: correct fraction in generated bin

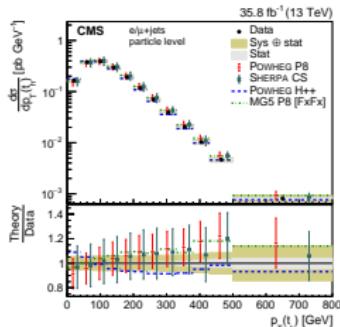
Differential $t\bar{t}$ cross sections in $e/\mu+jets$ events: resolved

36 fb^{-1} , 13 TeV, CMS: PRD 97 (2018) 112003, ATLAS: EPJC 79 (2019) 1028

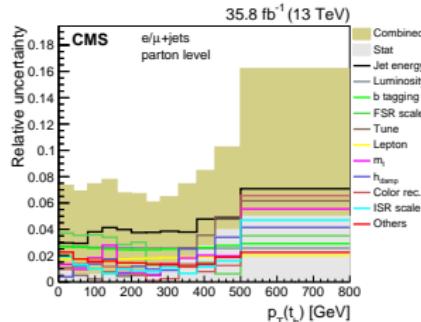
$p\text{-val}_{POW+P8} = 0.18$



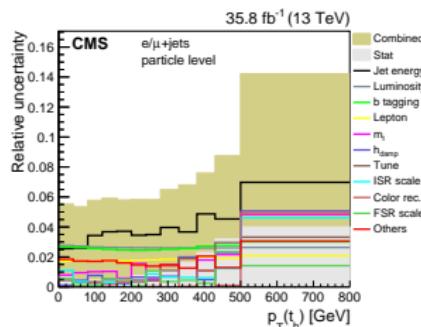
$p\text{-val}_{POW+P8} = 0.20$



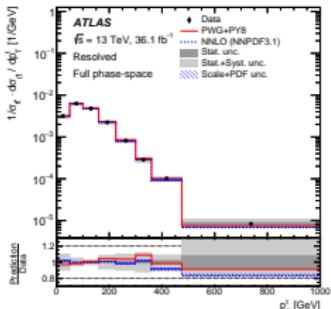
Parton level



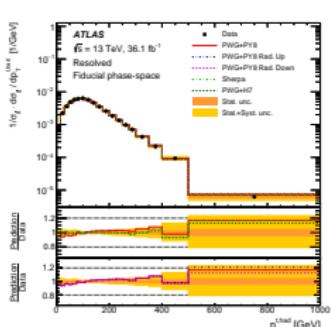
Particle level



$p\text{-val}_{POW+P8} = 0.49$



$p\text{-val}_{POW+P8} = 0.86$



- softer $p_T(t)$ compared to POWHEG/MG5(FxFx)+PYTHIA8 and SHERPA at parton and particle levels
 - reduced modelling uncertainties in particle-level measurement
- ATLAS p-values exclude uncertainties in prediction

Differential $t\bar{t}$ cross sections in $e/\mu + \text{jets}$ events: boosted

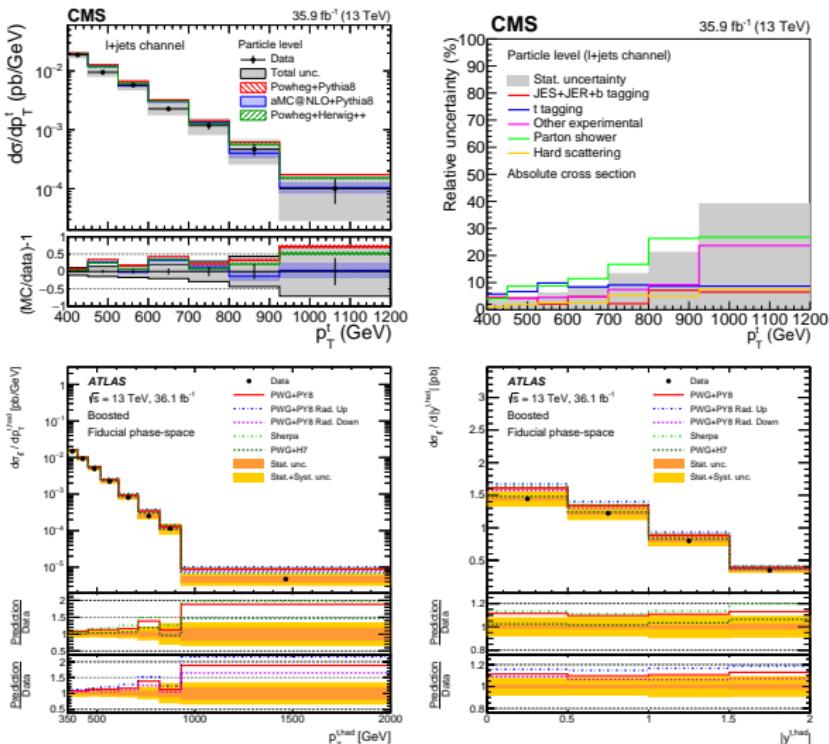
36 fb^{-1} , 13 TeV, CMS: arXiv:2008.07860 sub. PRD, ATLAS: EPJC 79 (2019) 1028

Selection:

- t_{lep}^{\perp} : 1 e/μ , at least 1 b jet
- t_{had}^{\perp} :
 - CMS: 1 anti- k_T jet (size: 0.8), $105 < m_{\text{sd}} < 220 \text{ GeV}$
 - ATLAS: anti- k_T (size: 1) applied to 0.4-size jets, soft jets removed ($p_T < 5\%$), mass 120–220 GeV

Cross section $p_T(t_{\text{had}}^{\perp})$

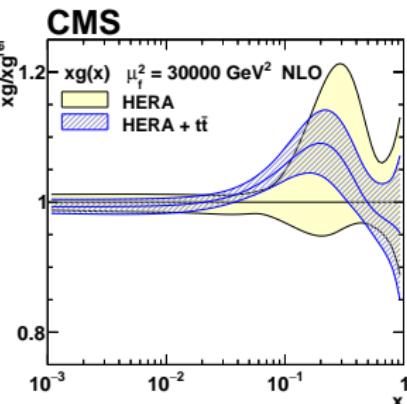
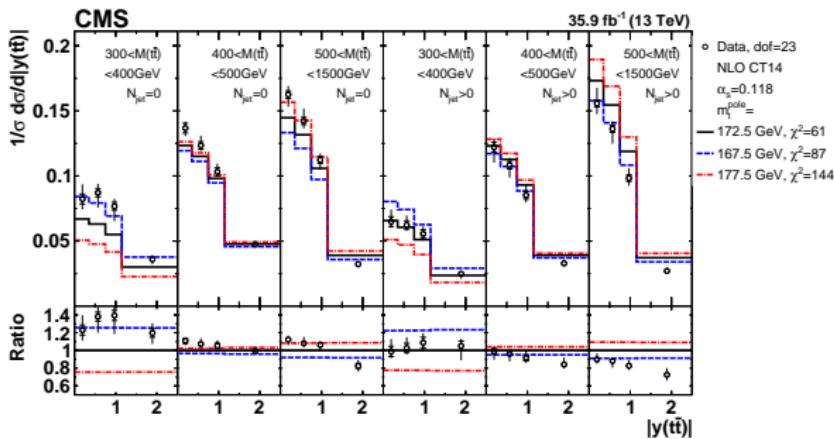
- absolute cross section lower than predicted (slope continued?)
- even in the boosted region mostly dominated by systematics



Interpretations of multi-differential $t\bar{t}$ cross sections in dilepton events

36 fb^{-1} , 13 TeV, CMS: arXiv:1904.05237 acc. by EPJC

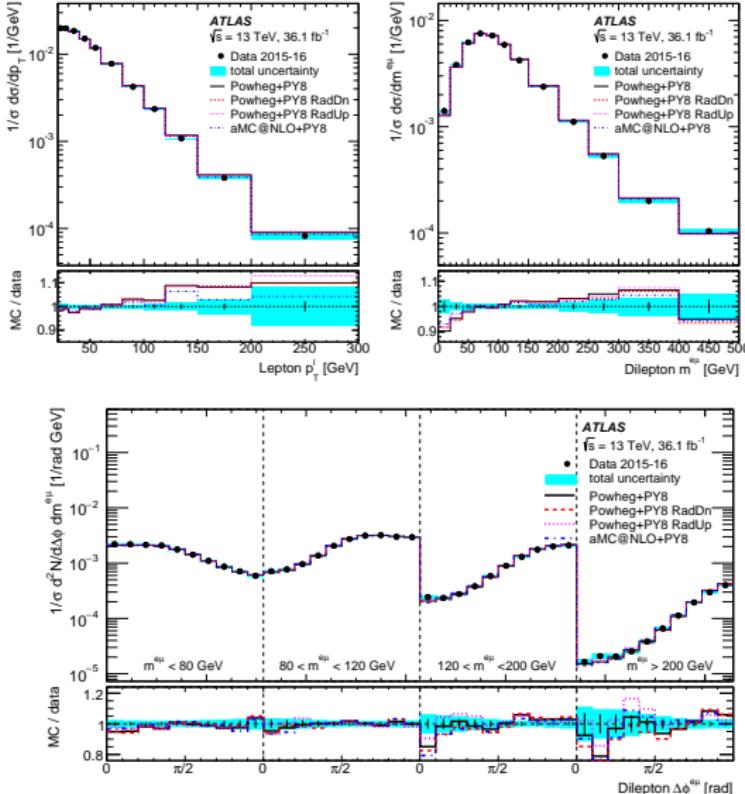
- Selection: ee, $e\mu$, $\mu\mu$ at least 2 jets, at least 1 b jet.
- The kinematics of the $t\bar{t}$ system (not of the individual top quarks) are reconstructed without using m_t to avoid a reconstruction bias: $p_z(\nu\bar{\nu}) = p_z(\ell^+\ell^-)$



- PDF parameterization similar to HERAPDF2.0 using xFITTER
- m_t and α_s are free parameters
- comparisons with NLO cross section taking into account scale and PDF uncertainties
- combined fit with HERA DIS data
- extracted: $m_t^{\text{pole}} = 170.5 \pm 0.8 \text{ GeV}$ $\alpha_s(m_Z) = 0.1135^{+0.0021}_{-0.0017}$

Differential cross sections of e/μ in dilepton events

36 fb^{-1} , 13 TeV, ATLAS: EPJC 80 (2020) 528



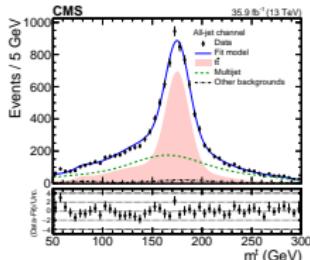
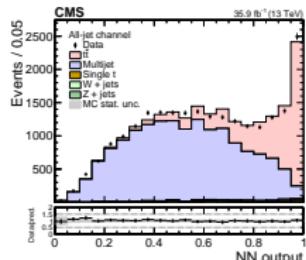
- lepton observables: advantage of reduced uncertainties from parton shower modelling
- deviation also observed in lepton p_T
- similar trend toward lower masses also observed in $m(t\bar{t})$
- $\phi^{e\mu}$: decent agreement in bins of $m^{e\mu}$

Differential $t\bar{t}$ cross sections in all-hadronic events: boosted

CMS

36 fb^{-1} , 13 TeV, arXiv:2008.07860 sub. PRD

- 2 jet (size: 0.8) $p_T > 400 \text{ GeV}$, soft-drop mass: $120 - 220 \text{ GeV}$, b-tagged
- neural network based on n-subjettiness used to define signal and control region:



CR: $NN < 0.8$ normalized using m_t fit

- unregularized unfolding (matrix inversion)

ATLAS

36 fb^{-1} , 13 TeV, PRD 98 (2018) 012003

- 2 jet (size: 1.0) $p_T > 350(500) \text{ GeV}$, trimmed mass: $m_t \pm 50 \text{ GeV}$, b-tagged, top-tagged (based on n-subjettiness and jet mass)
- multipjet background estimated from 16 CRs:

numbers: $t\bar{t}$ contamination

2nd large- R jet	1t1b	J (7.6%)	K (21%)	L (42%)	S
0t1b	B (2.2%)	D (5.8%)	H (13%)	N (47%)	
1t0b	E (0.7%)	F (2.4%)	G (6.4%)	M (30%)	
0t0b	A (0.2%)	C (0.8%)	I (2.2%)	O (11%)	
	0t0b	1t0b	0t1b	1t1b	

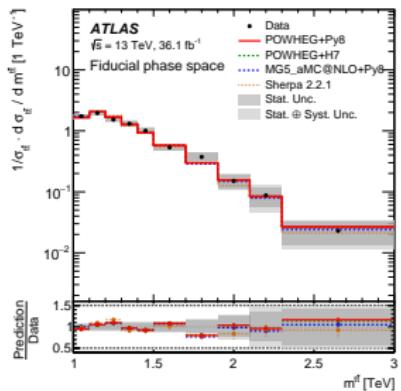
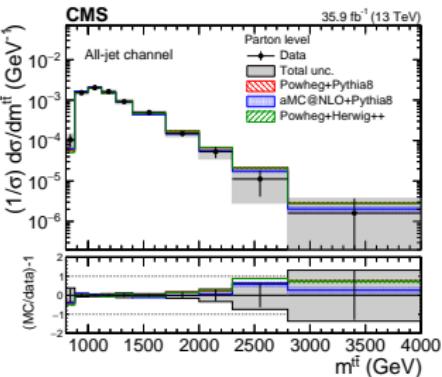
Leading large- R jet

$$S = \frac{J \times O}{A} \cdot \frac{D \times A}{B \times C} \cdot \frac{G \times A}{E \times I} \cdot \frac{F \times A}{E \times C} \cdot \frac{H \times A}{B \times I},$$

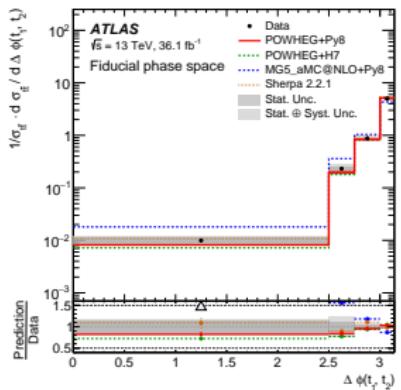
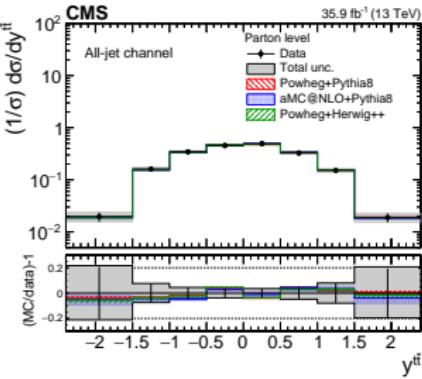
$$= \frac{J \times O \times H \times F \times D \times G \times A^3}{(B \times E \times C \times I)^2},$$

- iterative D'Agostini unfolding

- nice agreements of shapes between predictions and measurements in boosted regime
- absolute cross sections lower than expected similar to $e/\mu + \text{jets}$ measurements



$0.35 < \text{p-val} < 0.91$



$0.01 < \text{p-val} < 0.89$

p-values exclude uncertainties in prediction

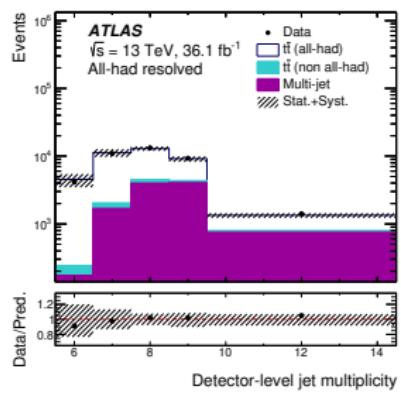
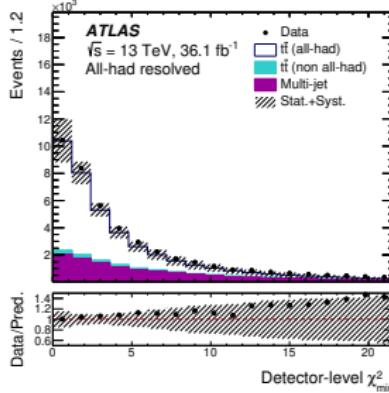
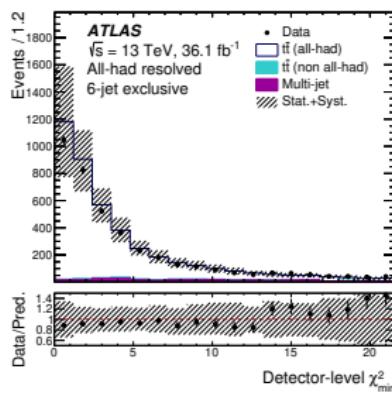
Differential $t\bar{t}$ cross sections in all-hadronic events: resolved

36 fb^{-1} , 13 TeV, ATLAS: [arXiv:2006.09274](https://arxiv.org/abs/2006.09274) sub. JHEP

- 6 jets $p_T > 55 \text{ GeV}$, exactly 2 b-tagged
- reconstruction:

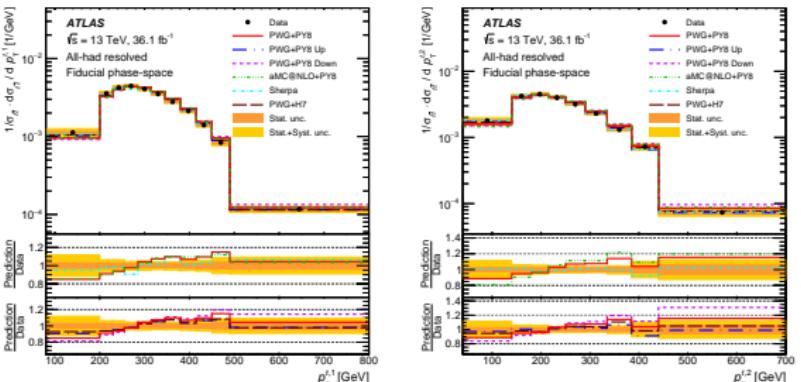
$$\chi^2 = \frac{(m_{b_1 j_1 j_2} - m_{b_2 j_3 j_4})^2}{\sigma_t^2} + \frac{(m_{j_1 j_2} - m_W)^2}{\sigma_W^2} + \frac{(m_{j_3 j_4} - m_W)^2}{\sigma_W^2},$$

60% of 6 jets events correctly reconstructed. $130 < m_t < 200 \text{ GeV}$



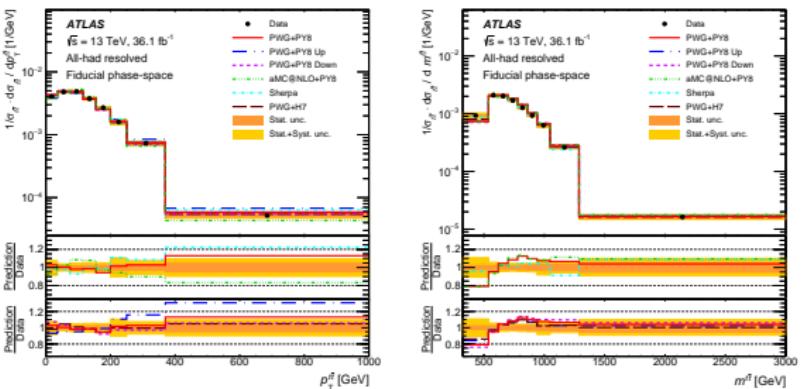
High purity in 6 jet bin.

- confirmation of softer p_T spectrum in all-hadronic channel
- but there are also other deviations, also observed in $e/\mu+jets$ and dilepton:
 - modulation in $p_T(t\bar{t})$
(deficit in data for very low and high $p_T(t\bar{t})$)
 - mismodelling at threshold and low $M(t\bar{t})$



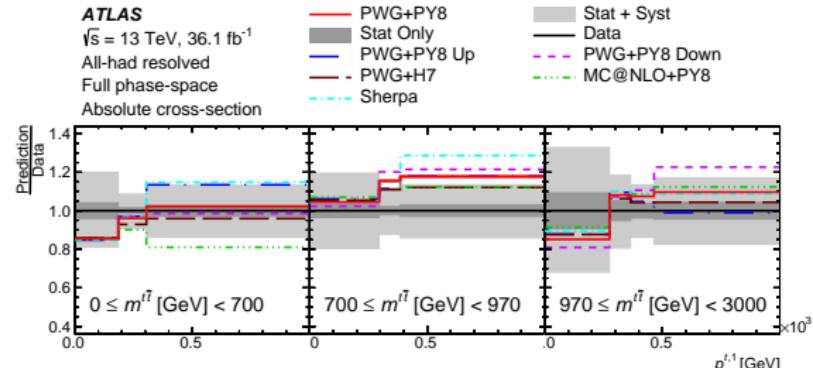
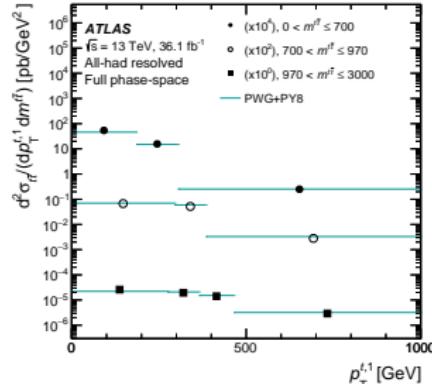
0.01 < p-val < 0.33

0.01 < p-val < 0.97



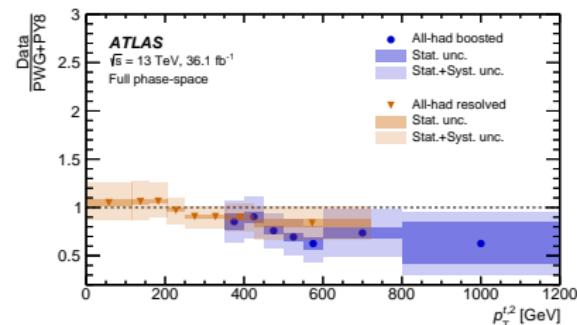
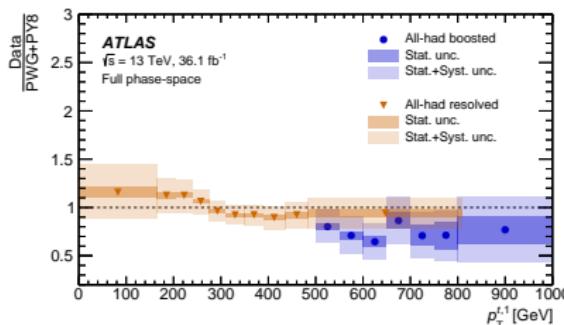
0.01 < p-val < 0.67

0.02 < p-val < 0.58



$0.01 < p\text{-val} < 0.27$

– double-differential cross section measured in all-hadronic



– reasonable consistency between resolved and boosted reconstruction at medium p_T

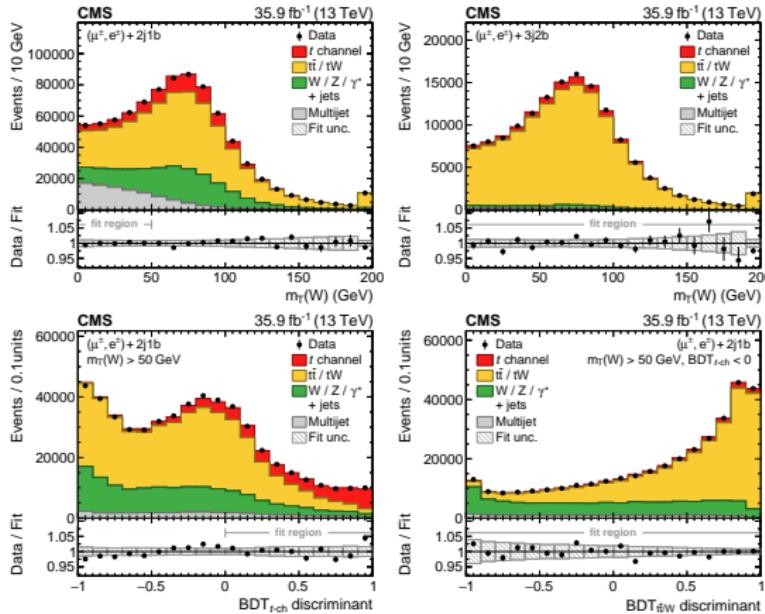
Single top quark differential cross sections

36 fb^{-1} , 13 TeV, CMS: EPJC 80 (2020) 370

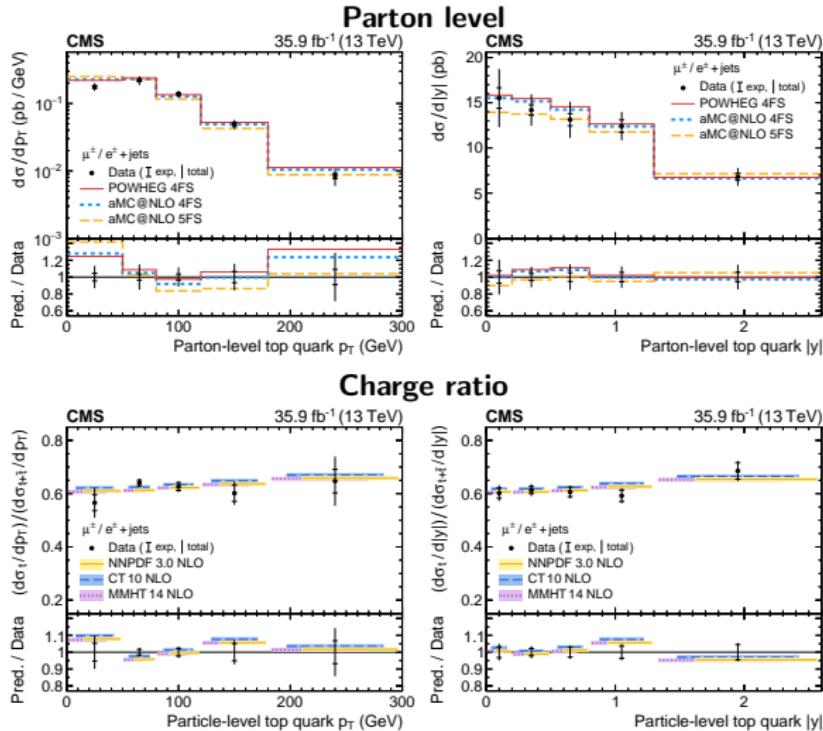
Measurement of t -channel single top quark production

- 1 isolated electron/muon + 2 jets, 1 b jet (signal region)
- top quark reconstructed as momentum sum of b jet, e/μ , and neutrino (calculated from p_T^{miss} and e/μ using m_W constraint)

Signal extraction

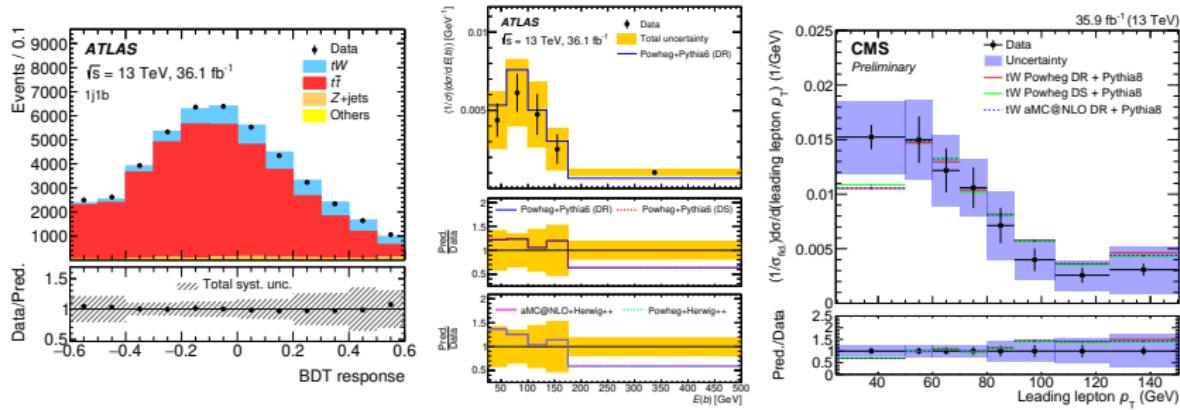


- ML fit of four (per lepton charge and flavor) distributions: $M_T(W)$ in 2j1b and 3j2b categories, two BDTs based on kinematic variables
- BDT _{t -ch} signal vs background
- BDT _{$t\bar{t}/W$} discrimination between $t\bar{t}$ and W backgrounds
- uncertainties profiled in fit
- the total log-likelihood is the sum over all bins of the differential measurement



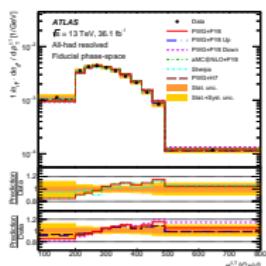
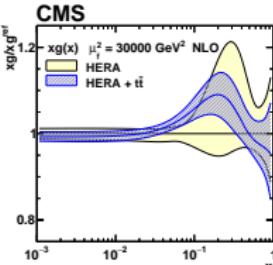
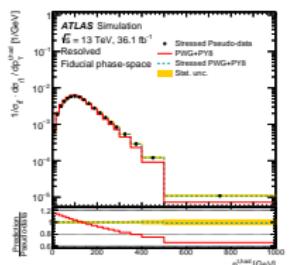
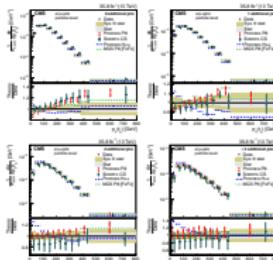
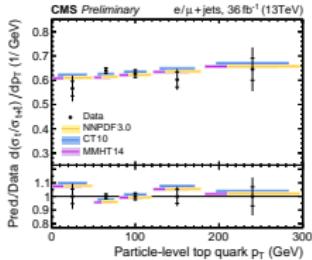
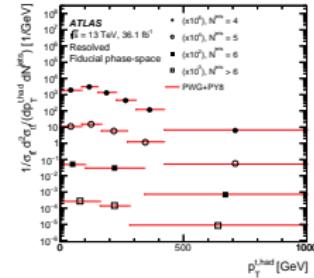
- extracted event yields are unfolded to parton and particle level based on χ^2 minimization (most distributions without regularization).
- the various predictions show reasonable agreement with the data: POWHEG 4FS, MADGRAPH 4FS/5FS.
- charge ratios in agreement with expectations → test of proton composition

Measurement of tW



- observables measured at particle level
- large uncertainties due to $t\bar{t}$ background (statistical and $t\bar{t}$ modelling)
- unfolding: χ^2 (CMS), D'Agostini (ATLAS)

Conclusion



Unfolding

- risk of mismeasurement due to:
 - regularization
 - generator mismodelling of response matrix
- perform consistency/stress tests to estimate effects

Differential $t\bar{t}$ cross sections

- all measurements give consistent results. Some deviations from predictions, but not significant.
- a softer $p_T(t)$ spectrum is observed in all channels.

Differential single top quark cross sections

- well described by NLO MCs

Backup