Compatibility between theoretical predictions at NNLO QCD accuracy and experimental data for top-antitop hadroproduction at the LHC

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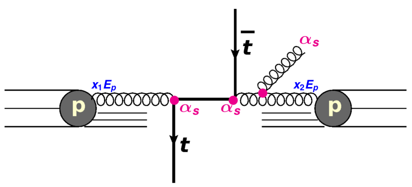
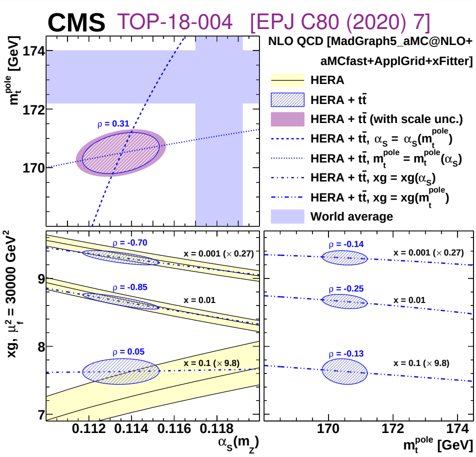
Why studying $t\bar{t}$ production?



- m_t provides a hard scale
  $\Rightarrow$ ultimate probe of pQCD
  (NLO, aNNLO, NNLO, ...)
- Produced mainly via *gg*
  $\Rightarrow$ constrain gluon PDF at high x
- Production sensitive to α_s and m_t
- May provide insight into possible new physics

Example:



- Simultaneous extraction of PDFs, α_s, m_t^{pole} using normalised triple-differential cross sections at NLO
- Extended to $\overline{\text{MS}}$, MSR schemes in JHEP 04 (2021) 043 [Garzelli, Kemmler, Moch, Zenaiev]

Scope of this work

- NNLO computations for total and multi-differential $pp \to t\bar{t} + X$ cross-sections can now be performed thanks to the publicly available MATRIX framework [Catani, Devoto, Grazzini, Kallweit, Mazzitelli Phys.Rev.D 99 (2019) 5, 051501; JHEP 07 (2019) 100]
  - fully differential NNLO calculations were also published in JHEP 04 (2017) 071 [Czakon, Heymes, Mitov], but no public code available. Part of their predictions can however now be accessed through the HighTEA (database) platform

- Comparing double-(triple-)differential $pp \to t\bar{t} + X$ x-sections with NNLO calculations makes it possible to extract proton PDFs, α_s, m_t^{pole}
  - however, for 3D x-sections in $M(t\bar{t})$, $y(t\bar{t})$, N_{jet} [CMS TOP-18-004] NNLO calculations are not yet available for $t\bar{t}$ + jets + X

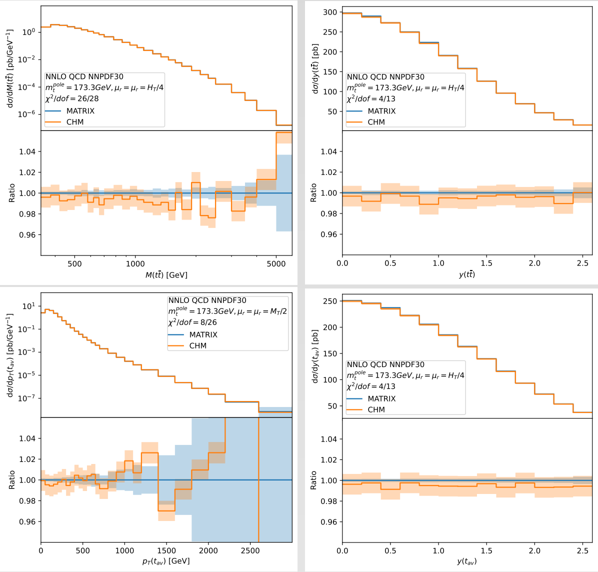
- For the time being, we focus on PDF and m_t^{pole} sensitivity and look at double-differential $M(t\bar{t})$, $y(t\bar{t})$ x-sections
  - $M(t\bar{t})$ provides sensitivity to m_t via threshold effects
  - $y(t\bar{t})$ provides sensitivity to PDFs via relation to partonic momentum fraction x: at LO $x_{1,2} = (M(t\bar{t})/\sqrt{s}) \exp[\pm y(t\bar{t})]$

- We also consider the most recent results for total cross-sections (for which theory tools are already publicly available since long)

Theoretical calculations with MATRIX + PineAPPL framework

- Using private version of MATRIX [Grazzini, Kallweit, Wiesemann, EPJC 78 (2018) 537]
- Interfaced to PineAPPL [Carrazza at al., JHEP 12 (2020) 108] to produce interpolation grids which are further used in xFitter https://gitlab.com/fitters/xfitter
  - reproduce NNLO calculations using any PDF + $\alpha_s(M_Z)$ set and/or varied μ_r, μ_f in $\sim$ seconds
  - interface implemented privately and only for the $pp \to t\bar{t} + X$ process
- Further modifications to MATRIX to make possible runs with $\Delta\sigma_{t\bar{t}} = 0.05\%$
  - recycling of parts of computations already done, instead of repeating them (tailored for $t\bar{t}$)
  - adapted to DESY Bird Condor cluster
  - technical fixes related to memory and disk space usage, etc.
- We did runs with different m_t^{pole} values 165–177.5 GeV with step of 2.5 GeV and $\Delta\sigma_{t\bar{t}} = 0.05\%$
  - $\approx$ 60000 CPU hours/run ($\sim$5 years on a single CPU)
  - for differential distributions, statistical uncertainties in bins are $\sim 1\%$ $\to$ not negligible compared to data precision and included in χ^2 calculation
  - currently exploring the possibility to improve further to $\Delta\sigma_{t\bar{t}} = 0.02\%$
- Differential distributions obtained with fixed $r_{cut} = 0.0015$ (q_T subtraction)
  - checked that extrapolation to $r_{cut} = 0$ for total $\sigma(t\bar{t} + X)$ produces differences $< 1\%$, see also S. Catani et al., JHEP 07 (2019) 100
- $\mu_r = \mu_f = H_T/4$, $H_T = \sqrt{m_t^2 + p_T^2(t)} + \sqrt{m_{\bar{t}}^2 + p_T^2(\bar{t})}$, varied up and down by factor 2 with $0.5 \leq \mu_r/\mu_f \leq 2$ (7-point variation)

Validation of NNLO computations vs JHEP 04 (2017) 071 by Czakon, Heymes, Mitov [CHM]



- Good agreement (assume that CHM also have uncertainty $\sim 1\%$); LO and NLO in BACKUP

ATLAS and CMS data

- For the time being: only measurements at 13 TeV where double-differential $M(t\bar{t})$, $y(t\bar{t})$ cross sections at parton level are available

  (1) CMS EPJ C80 (2020) 658 [1904.05237, TOP-18-004]:
  2D x-sections in dileptonic channel, $L = 35.9\ \mathrm{pb}^{-1}$
  - for 3D $M(t\bar{t})$, $y(t\bar{t})$, N_{jet} x-sections, NNLO is not available for $t\bar{t}$ + jets + X

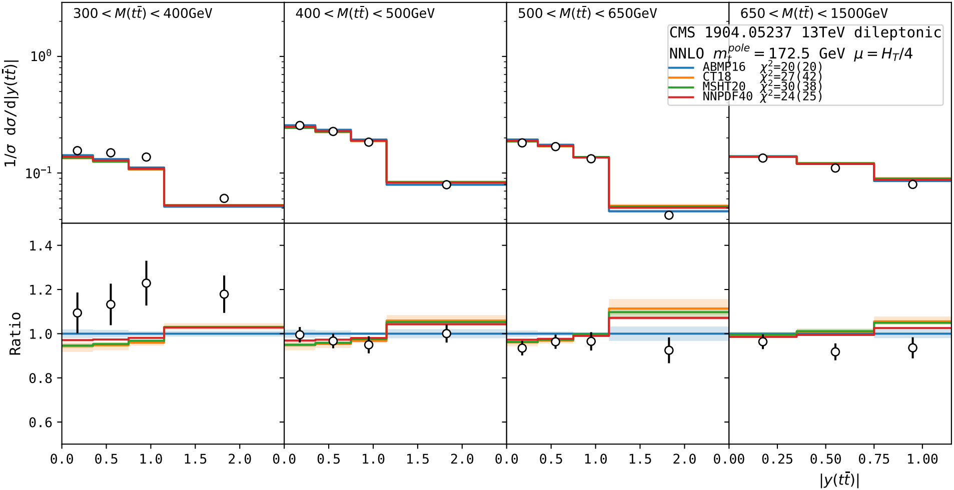
  (2) CMS Phys.Rev.D104 (2021) 9, 092013 [2108.02803, TOP-20-001]:
  2D x-sections in l+jets channel, $L = 137\ \mathrm{pb}^{-1}$

  (3) ATLAS EPJ C79 (2019) 1028 [1908.07305]:
  2D x-sections in l+jets channel, $L = 36\ \mathrm{pb}^{-1}$

  (4) ATLAS JHEP 01 (2021) 033 [2006.09274]:
  2D x-sections in all-hadronic channel, $L = 36.1\ \mathrm{pb}^{-1}$

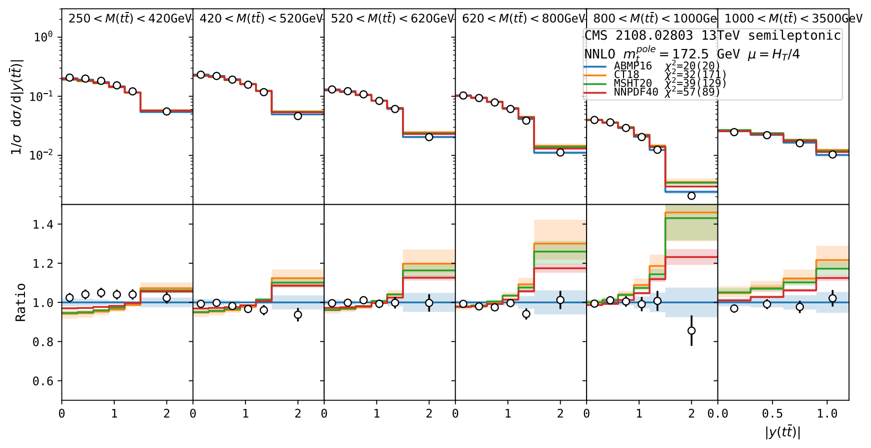
- For all measurements, we use normalised x-sections unfolded to the final-state parton level
- We use information on correlations of experimental uncertainties as provided in the paper (1) or in the HEPDATA database (2,3,4)
  - assumed no correlation between different measurements
    (reasonable assumption for normalised x-sections)
- Additionally, comparisons with measurements at other centre-of-mass energy (Run 1), and also total $t\bar{t} + X$ x-section

CMS TOP-18-004 vs NNLO predictions using different PDFs



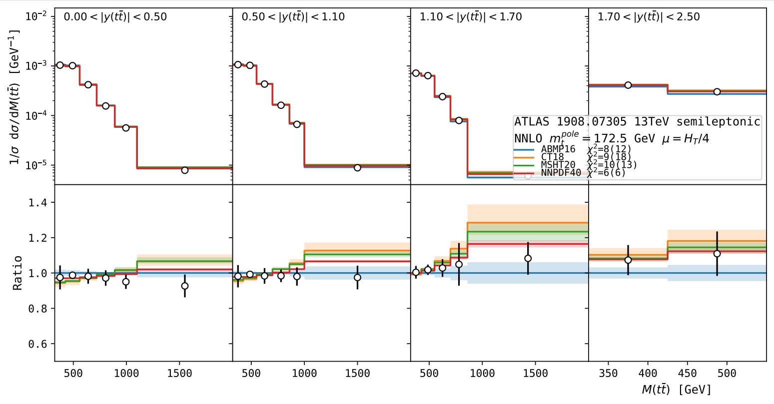
- Fixed $m_t^{\text{pole}} = 172.5$ GeV, $\mu_r = \mu_f = H_T/4$
- Reported χ^2 values with (and without) PDF uncertainties
- All PDF sets describe data reasonably well, with best description by ABMP16

CMS TOP-20-001 vs NNLO predictions using different PDFs



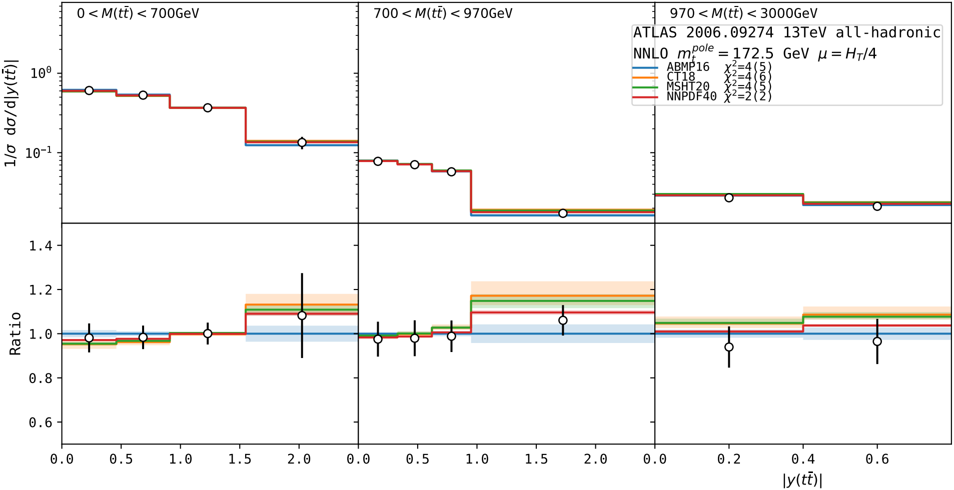
- Fixed $m_t^{\text{pole}} = 172.5$ GeV, $\mu_r = \mu_f = H_T/4$
- Reported χ^2 values with (and without) PDF uncertainties
- All PDF sets describe data reasonably well, with best description by ABMP16
  - CT18, MSHT20 and NNPDF40 show clear trend w.r.t data at high $y(t\bar{t})$ (large x)
- This is most precise currently available dataset with finest bins

ATLAS 1908.07305 vs NNLO predictions using different PDFs



- Fixed $m_t^{\text{pole}} = 172.5$ GeV, $\mu_r = \mu_f = H_T/4$
- Reported χ^2 values with (and without) PDF uncertainties
- All PDF sets describe data equally well
- $\chi^2/\text{dof} < 1$ indicating possible overestimation of experimental uncertainties (additionally, the data covariance matrix is not singular, i.e. det(cov) $\neq 0$: to be checked if this is related to some numerical inaccuracy or other reasons. This affects estimates of correlated uncertainties. Same issue in the $\sqrt{s} = 8$TeV ATLAS analysis [arXiv:1607.07281].

ATLAS 2006.09274 vs NNLO predictions using different PDFs



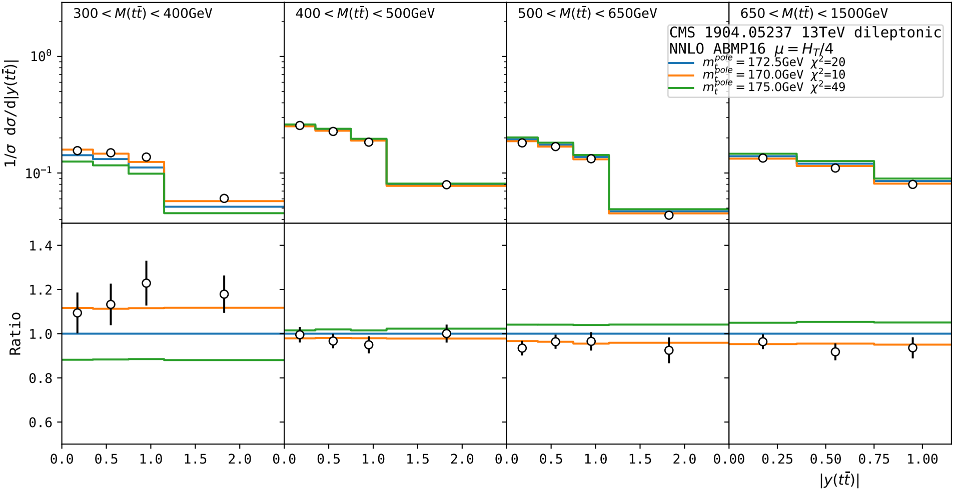
- Fixed $m_t^{\text{pole}} = 172.5$ GeV, $\mu_r = \mu_f = H_T/4$
- Reported χ^2 values with (and without) PDF uncertainties
- All PDF sets describe data equally well
- $\chi^2/\text{dof} < 1$ indicating possible overestimation of experimental uncertainties

Data vs NNLO predictions using different PDFs: summary

PDF	$t\bar{t}$ data in PDF fit	χ^2/dof (all data)	
		w/ PDF unc.	w/o PDF unc.
ABMP16	only total $\sigma(t\bar{t}+X)$	$52/78$	$57/78$
CT18	total and diff. $\sigma(t\bar{t}+X)$	$72/78$	$237/78$
MSHT20	total and diff. $\sigma(t\bar{t}+X)$	$83/78$	$185/78$
NNPDF4.0	total and diff. $\sigma(t\bar{t}+X)$	$89/78$	$122/78$

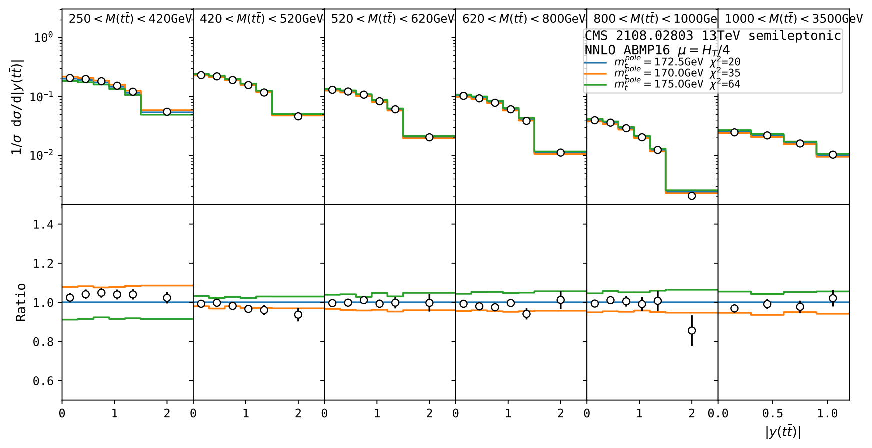
- No PDF fit include the datasets (1)-(4) that we considered
  - NNPDF4.0 include single-differential data from CMS studies [1803.08856, 1811.06625], using 2016 events, with partial overlap with the events used in the independent CMS Run 2 analyses that we considered. Additionally they include the double-differential Run 1 CMS dataset [arXiv:1703.01630], that we also include in our fits.

CMS TOP-18-004 vs NNLO predictions using different m_t^{pole}



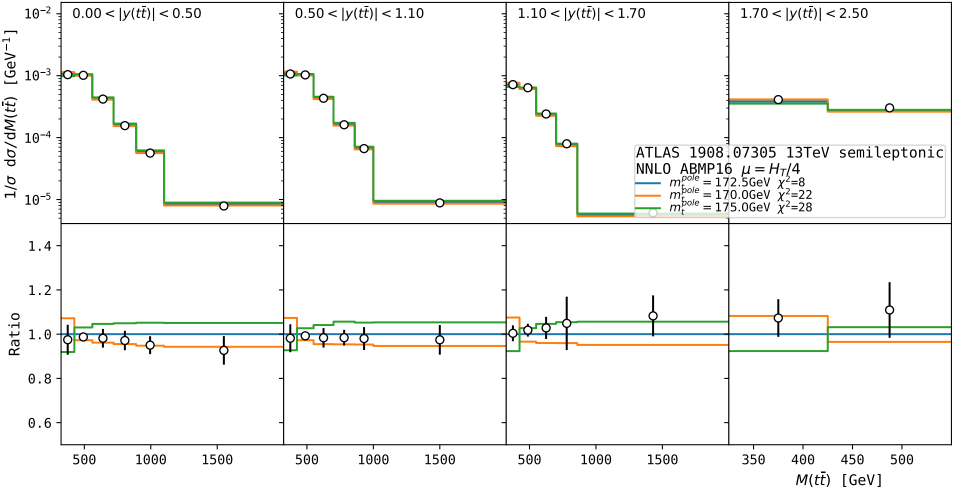
- Using ABMP16, $\mu_r = \mu_f = H_T/4$
- Reported χ^2 values with PDF uncertainties
- Large sensitivity to m_t^{pole} in the first $M(t\bar{t})$ bin (and due to x-section normalisation, also in other $M(t\bar{t})$ bins)

CMS TOP-20-001 vs NNLO predictions using different m_t^{pole}



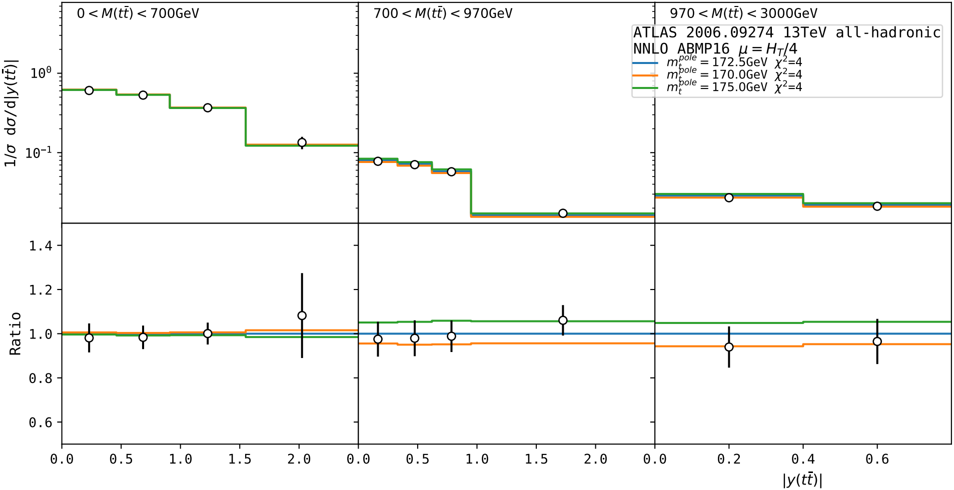
- Using ABMP16, $\mu_r = \mu_f = H_T/4$
- Reported χ^2 values with PDF uncertainties
- Large sensitivity to m_t^{pole} in the first $M(t\bar{t})$ bin (and due to x-section normalisation, also in other $M(t\bar{t})$ bins)
- Fluctuations of theory predictions are $\lesssim 1\%$ and covered by the assigned uncertainty of 1%

ATLAS 1908.07305 vs NNLO predictions using different m_t^{pole}



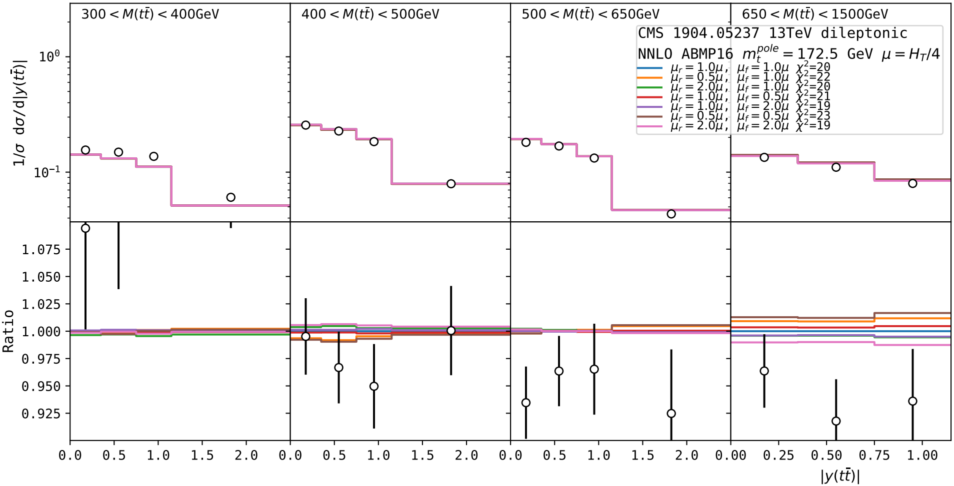
- Using ABMP16, $\mu_r = \mu_f = H_T/4$
- Reported χ^2 values with PDF uncertainties
- Large sensitivity to m_t^{pole} in the first $M(t\bar{t})$ bin (and due to x-section normalisation, also in other $M(t\bar{t})$ bins)

ATLAS 2006.09274 vs NNLO predictions using different m_t^{pole}



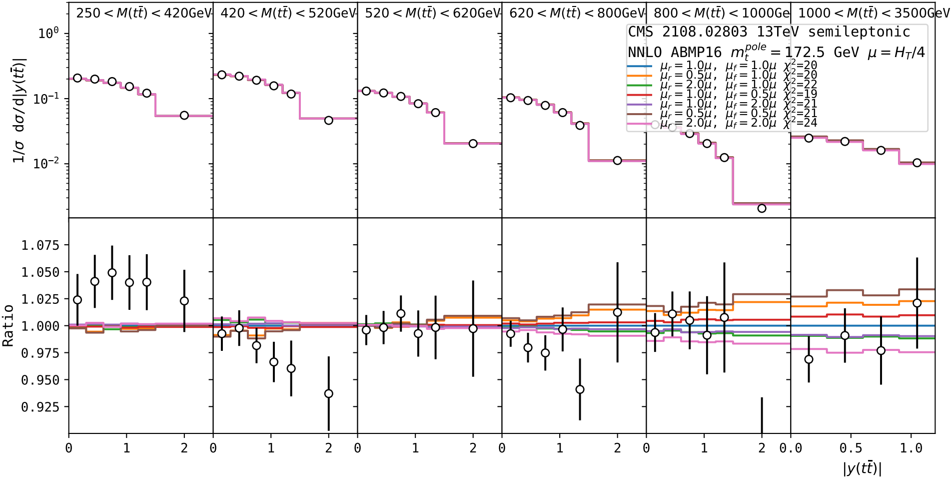
- Using ABMP16, $\mu_r = \mu_f = H_T/4$
- Reported χ^2 values with PDF uncertainties
- Limited sensitivity to m_t^{pole} due to wide $0 < M(t\bar{t}) < 700$ GeV bin: this dataset is not used as standalone, but is still used in our global fits for m_t^{pole} extraction

CMS TOP-18-004 vs NNLO predictions with scale variations



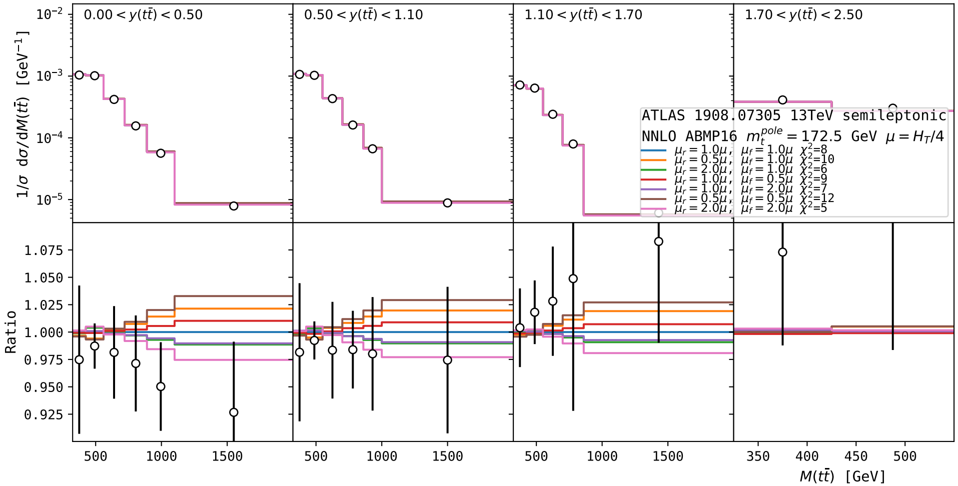
- Using ABMP16, $m_t^{\text{pole}} = 172.5$ GeV, $\mu = H_T/4$
- Reported χ^2 values with PDF uncertainties
- Effect of scale variations at NNLO $< 2.5\%$ (at low $M(t\bar{t}) < 1\%$) in these large bins.

CMS TOP-20-001 vs NNLO predictions with scale variations



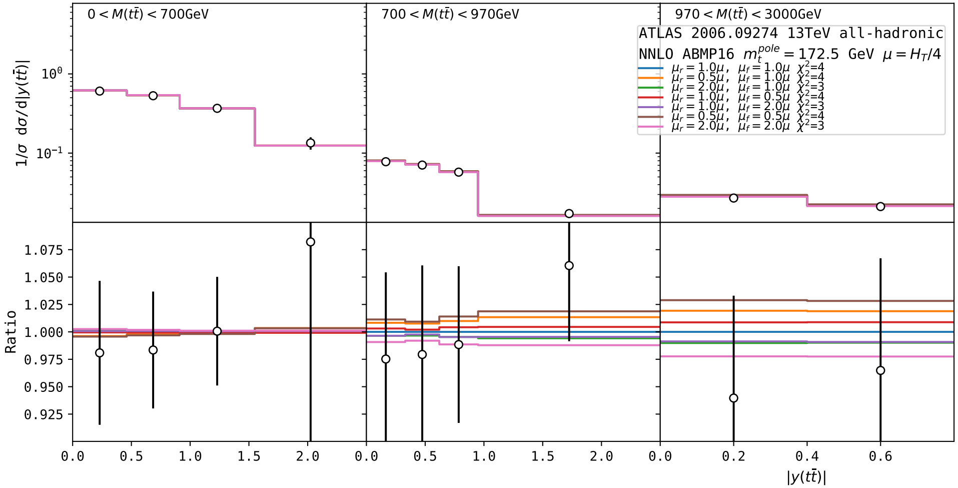
- Using ABMP16, $m_t^{\rm pole} = 172.5$ GeV, $\mu = H_T/4$
- Reported χ^2 values with PDF uncertainties
- Effect of scale variations at NNLO $< 4\%$ (at low $M(t\bar{t}) < 1\%$)

ATLAS 1908.07305 vs NNLO predictions with scale variations



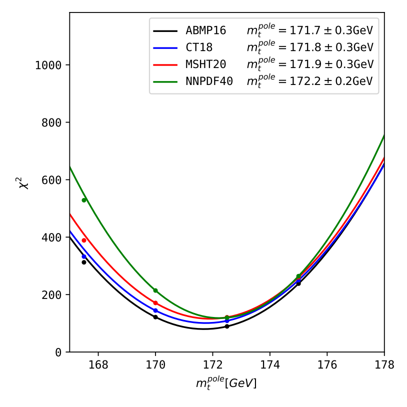
- Using ABMP16, $m_t^{\text{pole}} = 172.5$ GeV, $\mu = H_T/4$
- Reported χ^2 values with PDF uncertainties
- Effect of scale variations at NNLO $< 4\%$ (at low $M(t\bar{t}) < 1\%$)

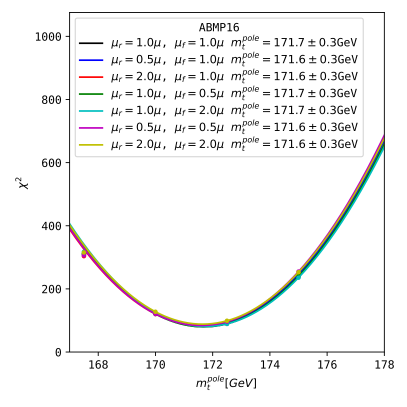
ATLAS 2006.09274 vs NNLO predictions with scale variations



- Using ABMP16, $m_t^{\rm pole} = 172.5$ GeV, $\mu = H_T/4$
- Reported χ^2 values with PDF uncertainties
- Effect of scale variations at NNLO $< 4\%$ (at low $M(t\bar{t}) < 1\%$)

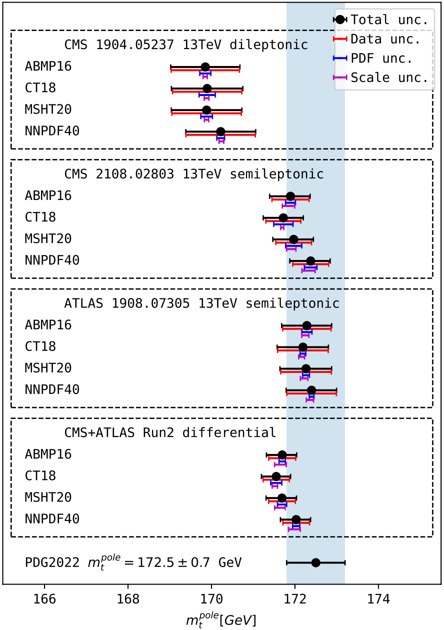
Extraction of m_t^{pole}





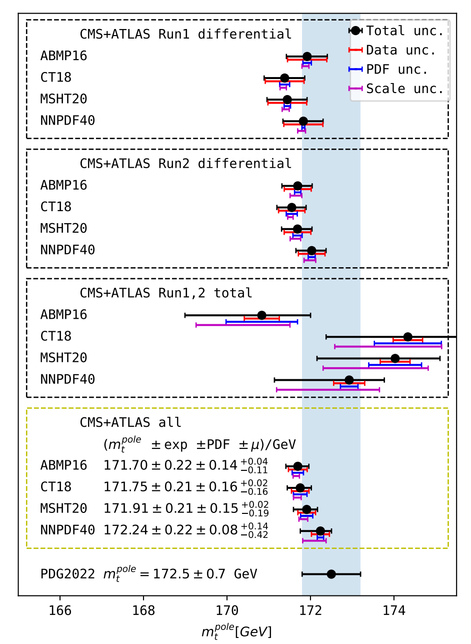
- χ^2 minimum is determined using parabolic interpolation of 3 points with lowest χ^2 values
- Both experimental and PDF uncertainties included in χ^2
- Δm_t^{pole} uncertainty $\sim \pm$ 0.3 GeV quoted in the plots takes into account all uncertainties included in the covariance matrix.
- Scale variations are not included in χ^2 (the uncertainties do not follow a gaussian distribution) but they are done explicitly (offset method) (typically amount to $\pm 0.1 - 0.2$ GeV)

Extraction of m_t^{pole}: summary from Run-2



- Global Run-2 fit: extracted m_t^{pole} values with precision ± 0.4 GeV are consistent with PDG value 172.5 ± 0.7 GeV
  - data uncertainty $\sim$ 0.3 GeV
  - PDF uncertainty $\sim$ 0.1 GeV
  - NNLO scale uncertainty $\sim$ 0.2 GeV
- Significant dependence on PDFs ($\sim$ 0.5 GeV):
  - different m_t^{pole} used in different PDFs
  - PDFs, m_t^{pole}, α_s should be determined simultaneously
- For the fit to the TOP-18-004 dataset, our NNLO results are consistent with the NLO ones published in the experimental paper itself.
  - $\sim 2\sigma$ difference w.r.t other LHC data (unfolding effect ?)
- Coulomb and soft-gluon resummation effects near the $t\bar{t}$ production threshold are neglected: expected correction $\sim \mathcal{O}$(1 GeV) can be regarded as additional theoretical uncertainty [CMS Coll. EPJ C80 (2020) 658; Kiyo, Kuhn, Moch, Steinhauser, Uwer EPJ C60 (2009) 375; Mäkelä, Hoang, Lipka, Moch 2301.03546]
  - having these corrections will make possible m_t^{pole} extraction with uncertainty $\lesssim$ 0.4 GeV

Extraction of m_t^{pole}: summary from Run-1+Run-2



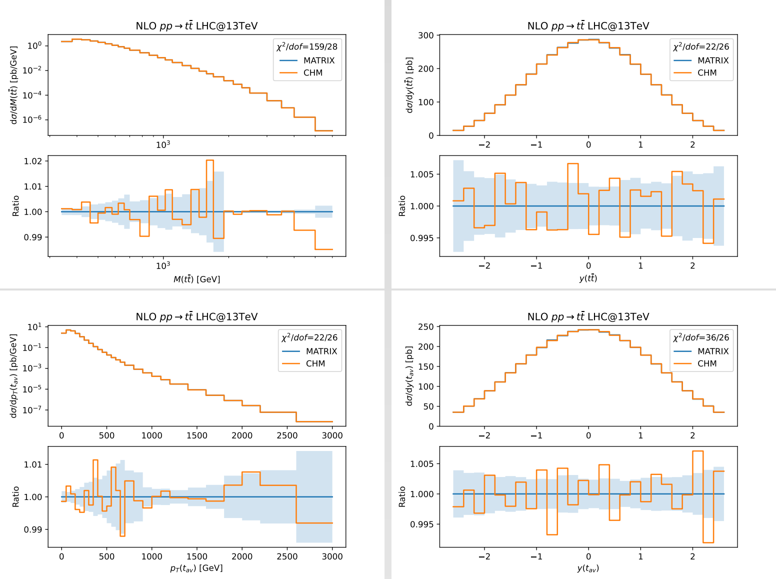
- Global Run-1 + Run-2 fit:
  extracted m_t^{pole} values with precision ± 0.3 GeV are consistent with PDG value 172.5 ± 0.3 GeV
  - data uncertainty ~ 0.2 GeV
  - PDF uncertainty $\sim 0.1 - 0.2$ GeV
  - NNLO scale uncertainty $\sim 0.1 - 0.2$ GeV

Summary and outlook

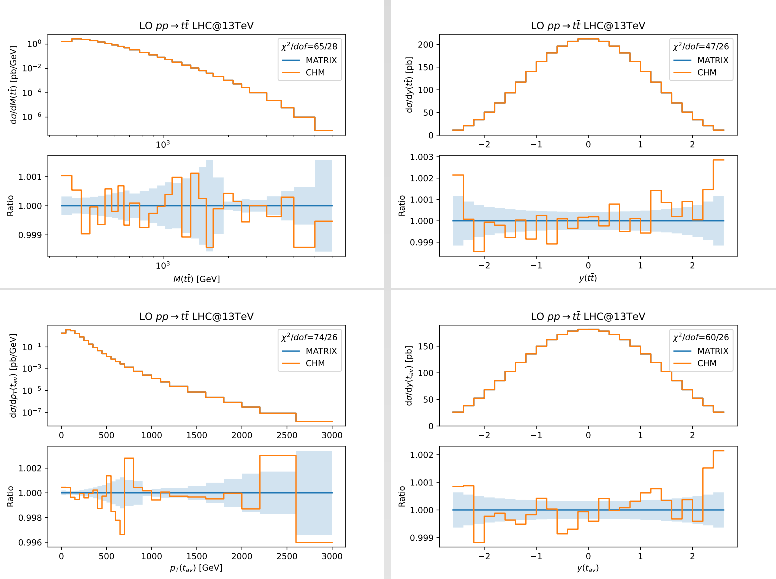
- Compared latest LHC $t\bar{t} + X$ differential measurements with NNLO QCD predictions using the modified `MATRIX` framework
  - interfaced with `PineAPPL` to produce interpolation tables for convolution with different PDFs + $\alpha_s(M_Z)$
  - used further in `xFitter` to benchmark vs experimental data
- Double-differential $M(t\bar{t})$, $y(t\bar{t})$ x-sections are able to distinguish between modern PDF sets by ABMP, CT, MSHT, NNPDF
  - reasonable description by all PDF sets, with best description by ABMP16
  - including these data in a PDF fit will make it possible to further reduce gluon PDF uncertainties at high x
- $M(t\bar{t})$ x-section near production threshold provides great sensitivity to m_t^{pole}
  - extracted m_t^{pole} values with precision ± 0.3 GeV and consistent with PDG value: e.g. using ABMP16 $m_t^{pole} = 171.7 \pm 0.22(\text{exp}) \pm 0.14(\text{PDF})^{+0.04}_{-0.11}(\mu)$ GeV
  - missing Coulomb and soft-gluon resummation effects: additional ~ 1 GeV uncertainty
  - additional dependence on PDFs ~ 0.5 GeV should be resolved in a simultaneous PDF + $\alpha_s\ (M_Z)$ + m_t^{pole} fit
- the considered distributions, especially those of Run 2, have much larger constraining power on m_t than the total cross-sections, where the effects of correlations between $\alpha_s(M_z)$ and m_t are much larger.

BACKUP

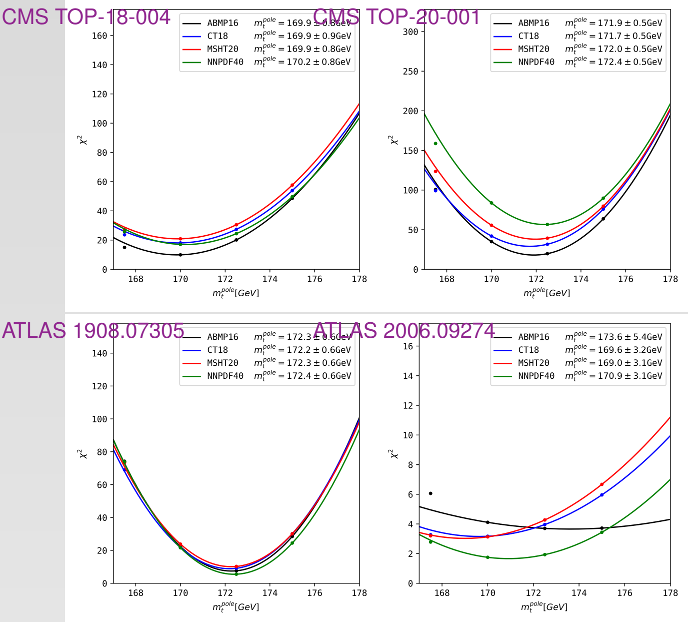
Validation of NLO calculations vs JHEP 04 (2017) 071 [CHM]



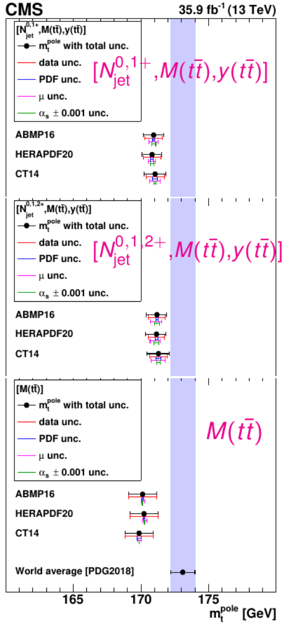
Validation of LO calculations vs JHEP 04 (2017) 071 [CHM]



Extraction of m_t^{pole}



TOP-18-004 checks



DESY 2018 summer school, L. Materne, bachelor thesis "Differential Top-Pair Production Cross Section with the CMS Detector - Optimization of Measurement Information", Karlsruher Institut für Technologie (KIT), Bachelorarbeit, 2018 [ETP-Bachelor-KA/2018-11]