Top-quark (pole) mass extraction at NNLO accuracy

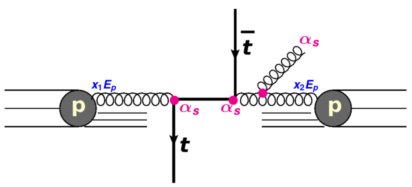
S. Alekhin[1], Maria Vittoria Garzelli[1], J. Mazzitelli[2], S.-O. Moch[1], O. Zenaiev[1]

[1] II Institut für Theoretische Physik, Universität Hamburg
[2] PSI, Villigen

On the basis of
arXiv:2311.05509
published in JHEP
+ work in progress

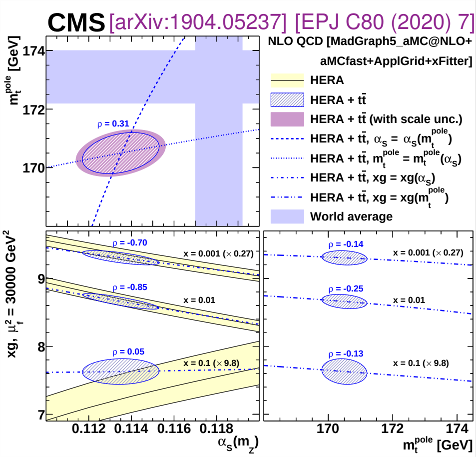
LHCP Conference, Boston, MA
June 3-8, 2024

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



- m_t provides a hard scale
  ⇒ ultimate probe of pQCD
  (NLO, aNNLO, NNLO, ...)
- Produced mainly via *gg*
  ⇒ 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 our work

- Extraction of m_t (+ proton PDFs, α_s), by comparing double-(triple-)differential $pp \to t\bar{t} + X$ cross sections with NNLO calculations
  - however, for 3D cross sections in $M(t\bar{t})$, $y(t\bar{t})$, N_{jet} [CMS arXiv:1904.05237], NNLO calculations are not yet available for $t\bar{t}$ + jets + X

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

- We also consider the most recent results for total cross sections.

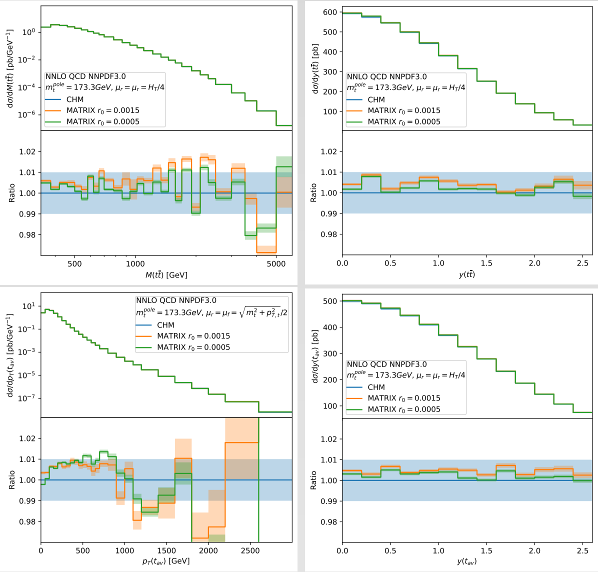
- NNLO computations for total inclusive $pp \to t\bar{t} + X$ cross sections can be obtained with theory tools already publicly available since long.

- 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.

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 (with accuracy well below 1% in all bins)
  - interface implemented privately and only for the $pp \to t\bar{t} + X$ process
- Further modifications to MATRIX to make possible runs with $\Delta\sigma_{t\bar{t}} < 0.1\%$
  - adapted to DESY Bird Condor cluster and local multicore machines
  - 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 $\Delta\sigma_{t\bar{t}} = 0.02\%$
  - $\approx$ 60000 CPU hours/run ($\sim$5 years/run on a single CPU)
  - for differential distributions, statistical uncertainties in bins are $\lesssim 0.5\%$ $\to$ not negligible compared to data precision and included in χ^2 calculation
- Differential distributions obtained with fixed $r_{cut} = 0.0015$ (q_T subtraction: see talks by S. Kallweit and S. Devoto)
  - 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
- $\mu_r = \mu_f = H_T/4$, $H_T = \sqrt{m_t^2 + p_T^2(t)} + \sqrt{m_t^2 + p_T^2(\bar{t})}$, 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 (assuming that CHM also have uncertainty $\sim 1\%$)

ATLAS and CMS datasets used in this work: total cross sections

experiment	decay channel	dataset	luminosity	$\sqrt{s}$
ATLAS & CMS	combined	2011	5 fb^{-1}	7 TeV
ATLAS & CMS	combined	2012	20 fb^{-1}	8 TeV
ATLAS	dileptonic, semileptonic	2011	257 pb^{-1}	5.02 TeV
CMS	dileptonic	2011	302 pb^{-1}	5.02 TeV
ATLAS	dileptonic	2015-2018	140 fb^{-1}	13 TeV
ATLAS	semileptonic	2015-2018	139 fb^{-1}	13 TeV
CMS	dileptonic	2016	35.9 fb^{-1}	13 TeV
CMS	semileptonic	2016-2018	137 fb^{-1}	13 TeV
ATLAS	dileptonic	2022	11.3 fb^{-1}	13.6 TeV
CMS	dileptonic, semileptonic	2022	1.21 fb^{-1}	13.6 TeV

Selection criteria:

- Data considered in the LHC Top Working Group (June 2023, there is a 2024 update that however we expect to play only a minor role on our results).

ATLAS and CMS datasets used in this work: single- and double-differential distributons

Experiment	decay channel	dataset	luminosity	$\sqrt{s}$	observable(s)	n
CMS	semileptonic	2016–2018	137 fb^{-1}	13 TeV	$M(t\bar{t})$, $\lvert y(t\bar{t})\rvert$	34
CMS	dileptonic	2016	35.9 fb^{-1}	13 TeV	$M(t\bar{t})$, $\lvert y(t\bar{t})\rvert$	15
ATLAS	semileptonic	2015–2016	36 fb^{-1}	13 TeV	$M(t\bar{t})$, $\lvert y(t\bar{t})\rvert$	19
ATLAS	all-hadronic	2015–2016	36.1 fb^{-1}	13 TeV	$M(t\bar{t})$, $\lvert y(t\bar{t})\rvert$	10
CMS	dileptonic	2012	19.7 fb^{-1}	8 TeV	$M(t\bar{t})$, $\lvert y(t\bar{t})\rvert$	15
ATLAS	semileptonic	2012	20.3 fb^{-1}	8 TeV	$M(t\bar{t})$	6
ATLAS	dileptonic	2012	20.2 fb^{-1}	8 TeV	$M(t\bar{t})$	5
ATLAS	dileptonic	2011	4.6 fb^{-1}	7 TeV	$M(t\bar{t})$	4
ATLAS	semileptonic	2011	4.6 fb^{-1}	7 TeV	$M(t\bar{t})$	4

Selection criteria:

- we focus on $d\sigma/dM(t\bar{t})$ and $d^2\sigma/dM(t\bar{t})dy(t\bar{t})$ distributions.
- We use measurements where the experimental collaborations provide unfolding to the inclusive parton level ($t\bar{t}$) (MATRIX is being extended at decayed-top level only now (see talk by S. Kallweit), LHCb data so far only available at the particle level).
- We used measurements normalized, to reduce the effect of lack of information concerning correlations of uncertainties between different experimental analyses (source by source available only in CMS dilepton analyses!).
- we used measurements for which info on bin-by-bin correlated uncertainties are available.

More on the ATLAS and CMS datasets used in this work

- We focus especially on measurements at 13 TeV where double-differential $M(t\bar{t})$, $y(t\bar{t})$ cross sections at parton level are available not considered so far in any top-quark pole-mass extraction at NNLO

  (1) CMS EPJ C80 (2020) 658 [1904.05237, TOP-18-004]:
  2D cross sections in dileptonic channel, $L = 35.9\ \text{pb}^{-1}$

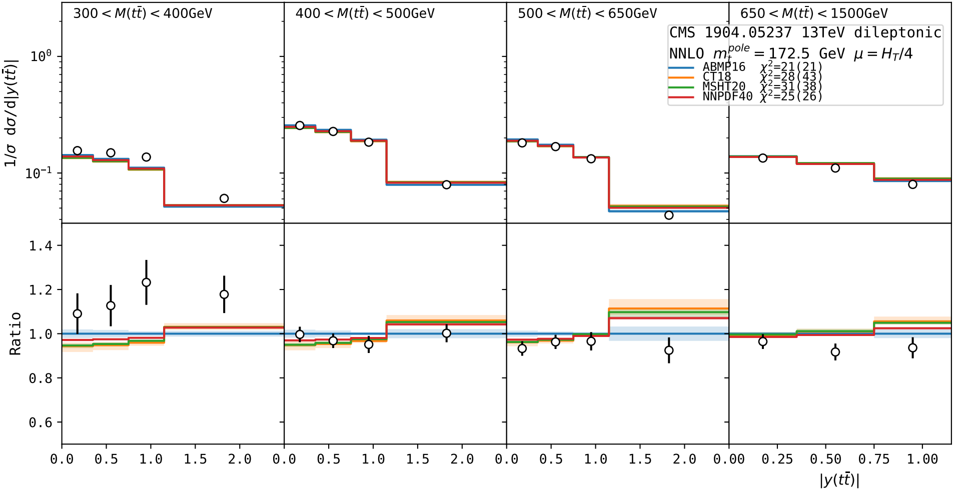
  - for 3D $M(t\bar{t})$, $y(t\bar{t})$, N_{jet} cross sections, NNLO is not available for $t\bar{t}$ + jets + X

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

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

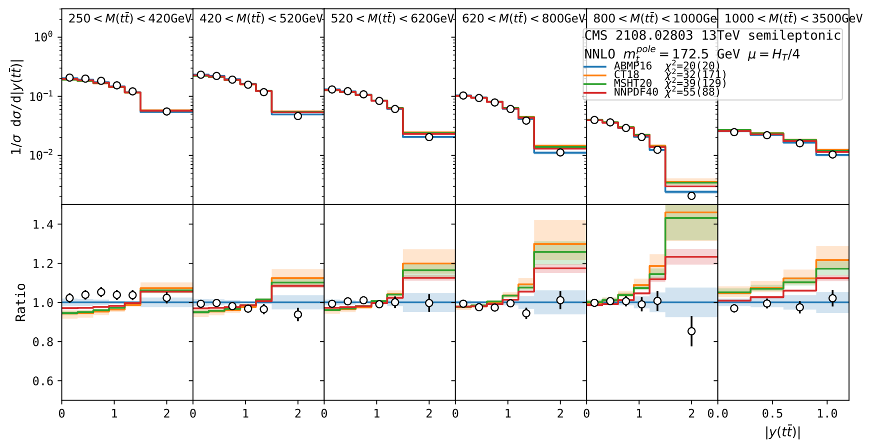
  (4) ATLAS JHEP 01 (2021) 033 [2006.09274]:
  2D cross sections in all-hadronic channel, $L = 36.1\ \text{pb}^{-1}$

CMS [arXiv:1904.05237] vs NNLO predictions using different PDFs



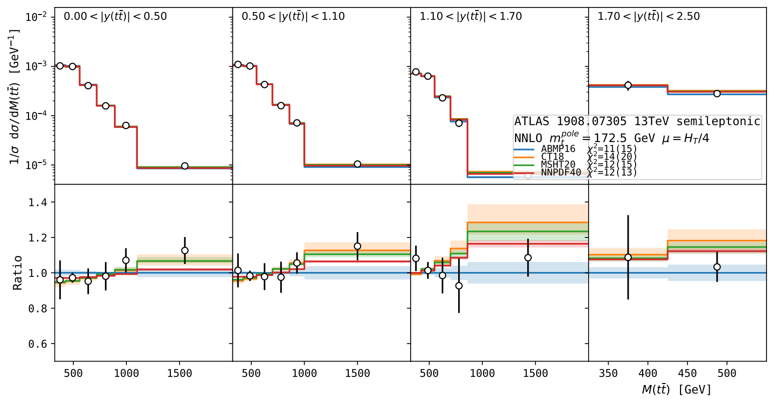
- Fixed $m_t^{\text{pole}} = 172.5$ GeV, $\mu_r = \mu_f = H_T/4$
- Reported χ^2 values with (and without) PDF uncertainties
- All PDF sets describe data reasonably well, with best description by ABMP16

CMS [arXiv:2108.02803] vs NNLO predictions using different PDFs



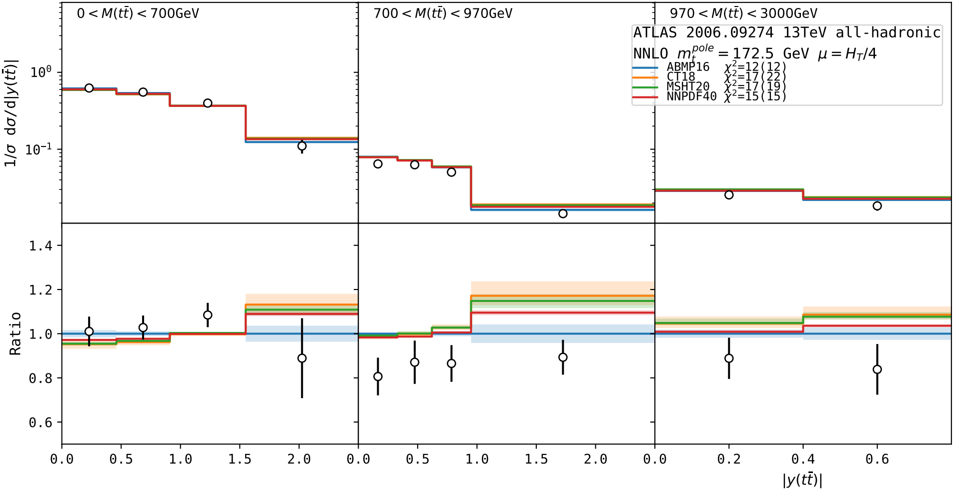
- Fixed $m_t^{\text{pole}} = 172.5$ GeV, $\mu_r = \mu_f = H_T/4$
- Reported χ^2 values with (and without) PDF uncertainties
- All PDF sets describe data reasonably well
  - But CT18, MSHT20 and NNPDF40 show clear trend w.r.t data at high $y(t\bar{t})$ (large x)
- This is the most precise currently available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

ATLAS [arXiv: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 reasonably well.
- $\chi^2/\text{dof} < 1$ indicating possible overestimation of experimental uncertainties (additionally, the data covariance matrix is not singular, i.e. $\det(\text{cov}) \neq 0$: 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 [arXiv:2006.09274] vs NNLO predictions using different PDFs



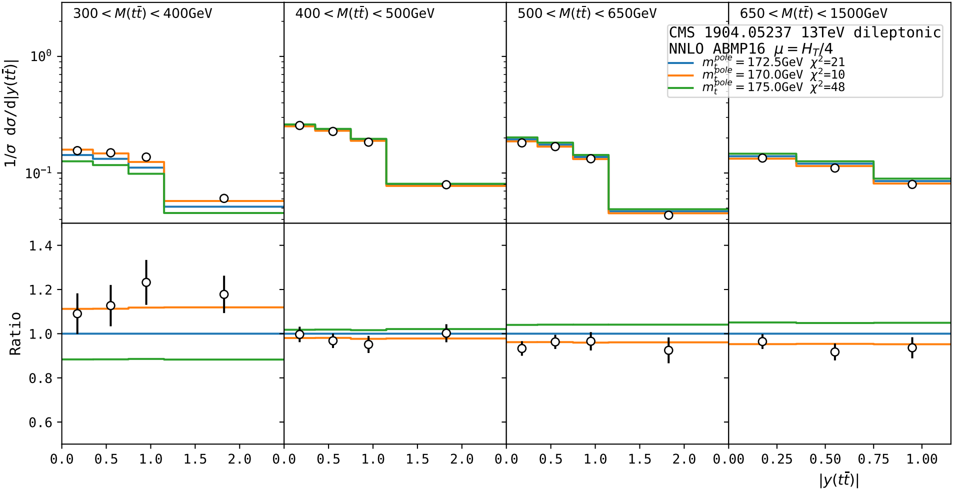
- Fixed $m_t^{\text{pole}} = 172.5$ GeV, $\mu_r = \mu_f = H_T/4$
- Reported χ^2 values with (and without) PDF uncertainties
- All PDF sets describe data reasonably well
- $\chi^2/\text{dof} < 1$ indicating possible overestimation of experimental uncertainties

Data vs double-diff NNLO predictions at $\sqrt{s} = 13$ TeV using different PDFs: summary

PDF	$t\bar{t}$ data in PDF fit	χ^2/NDP (all data)	
		w/ PDF unc.	w/o PDF unc.
ABMP16	only total $\sigma(t\bar{t}+X)$	$56/78$	$61/78$
CT18	total and diff. $\sigma(t\bar{t}+X)$	$80/78$	$250/78$
MSHT20	total and diff. $\sigma(t\bar{t}+X)$	$92/78$	$196/78$
NNPDF4.0	total and diff. $\sigma(t\bar{t}+X)$	$104/78$	$139/78$

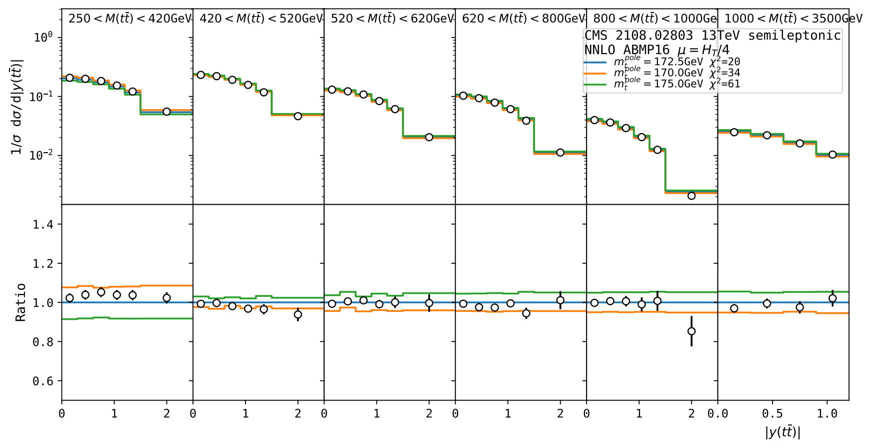
- No PDF fit include the datasets (1)-(4) that we considered
  - NNPDF4.0 include single-differential data from CMS studies [1803.08856, 1811.06625], using 2016 events, with partial overlap with the events used in the independent CMS Run 2 analyses that we considered. Additionally they include the double-differential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

CMS [arXiv:1904.05237] vs NNLO predictions using different m_t^{pole}



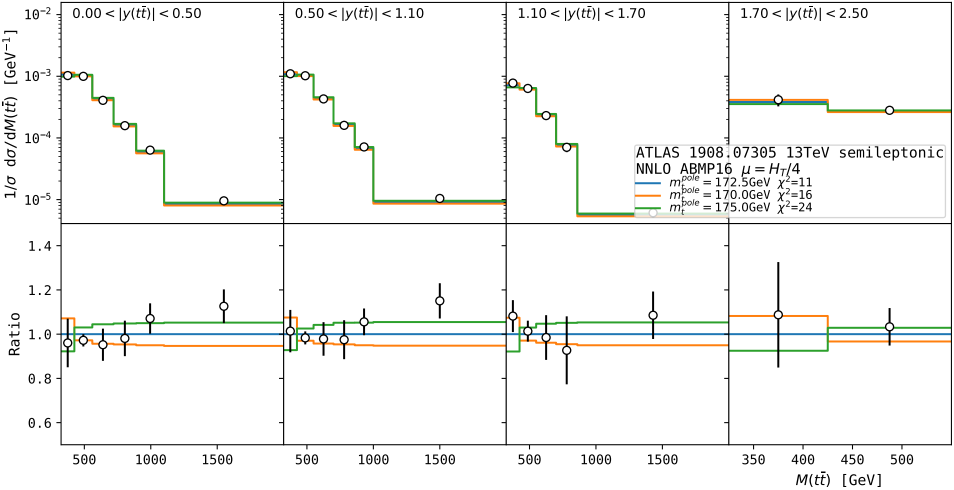
- Using ABMP16, $\mu_r = \mu_f = H_T/4$
- Reported χ^2 values with PDF uncertainties
- Large sensitivity to m_t^{pole} in the first $M(t\bar{t})$ bin (and due to cross-section normalisation, also in other $M(t\bar{t})$ bins)

CMS [arXiv:2108.02803] vs NNLO predictions using different m_t^{pole}



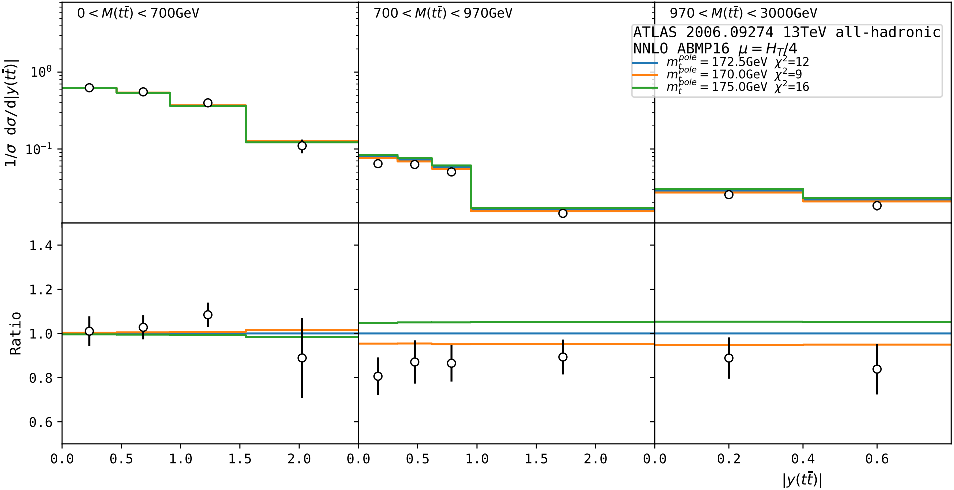
- Using ABMP16, $\mu_r = \mu_f = H_T/4$
- Reported χ^2 values with PDF uncertainties
- Large sensitivity to m_t^{pole} in the first $M(t\bar{t})$ bin (and due to x-section normalisation, also in other $M(t\bar{t})$ bins)
- Fluctuations of theory predictions are $\lesssim 1\%$ and covered by the assigned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

ATLAS [arXiv:1908.07305] vs NNLO predictions using different m_t^{pole}



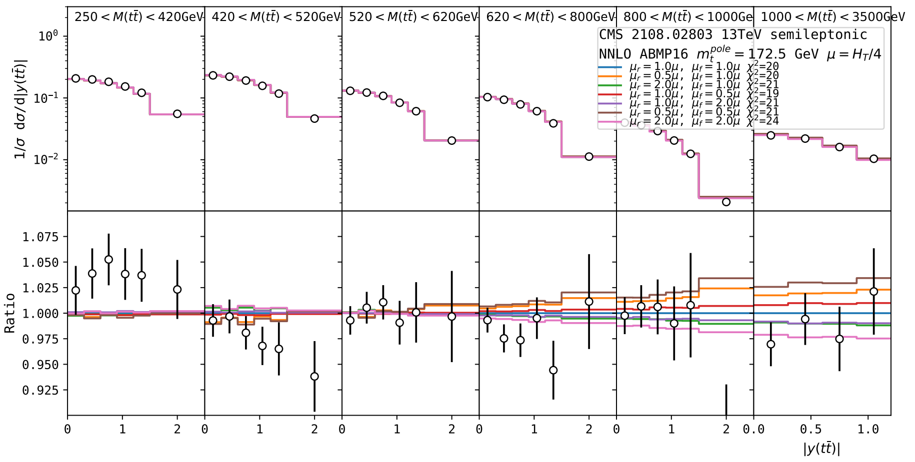
- Using ABMP16, $\mu_r = \mu_f = H_T/4$
- Reported χ^2 values with PDF uncertainties
- Large sensitivity to m_t^{pole} in the first $M(t\bar{t})$ bin (and due to x-section normalisation, also in other $M(t\bar{t})$ bins)

ATLAS [arXiv:2006.09274] vs NNLO predictions using different m_t^{pole}



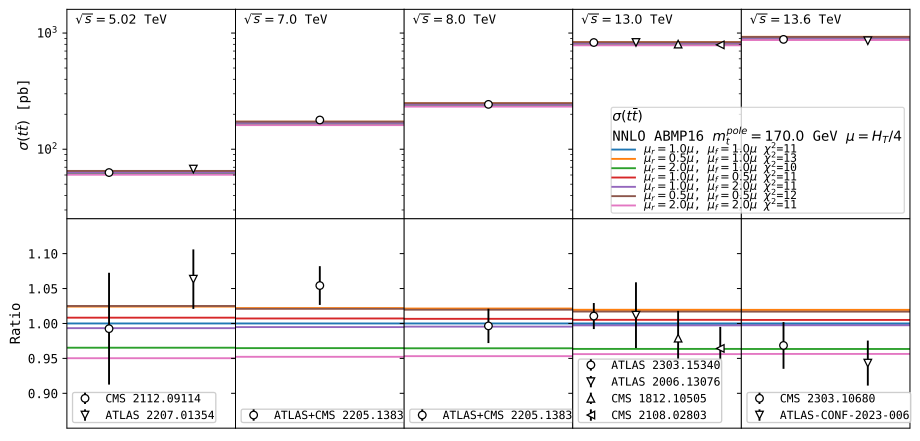
- Using ABMP16, $\mu_r = \mu_f = H_T/4$
- Reported χ^2 values with PDF uncertainties
- Limited sensitivity to m_t^{pole} in the $0 < M(t\bar{t}) < 700$ GeV bin, due to its wideness: this dataset is not used as standalone, but is still used in our global fits for m_t^{pole} extraction

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



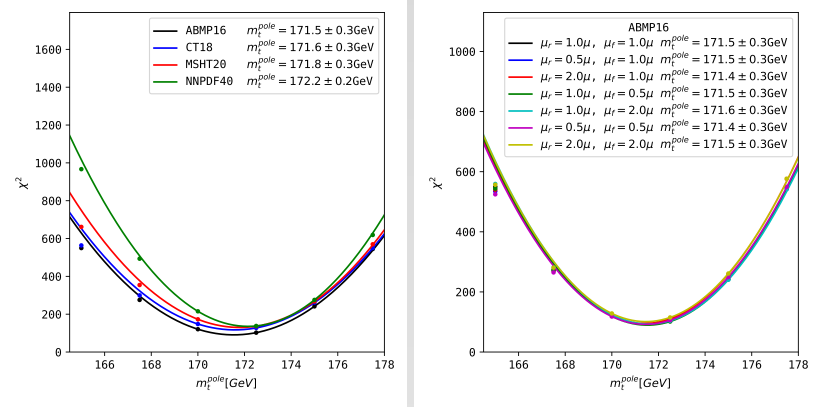
- Using ABMP16, $m_t^{\text{pole}} = 172.5$ GeV, $\mu = H_T/4$
- Reported χ^2 values with PDF uncertainties
- Effect of scale variations at NNLO $< 4\%$ (at low $M(t\bar{t}) < 1\%$), due to strong cancellations in the normalization) (analogous size of scale uncertainties are obtained for theory predictions compared to the ATLAS double-differential datasets).

Total inclusive σ vs NNLO predictions with scale variations



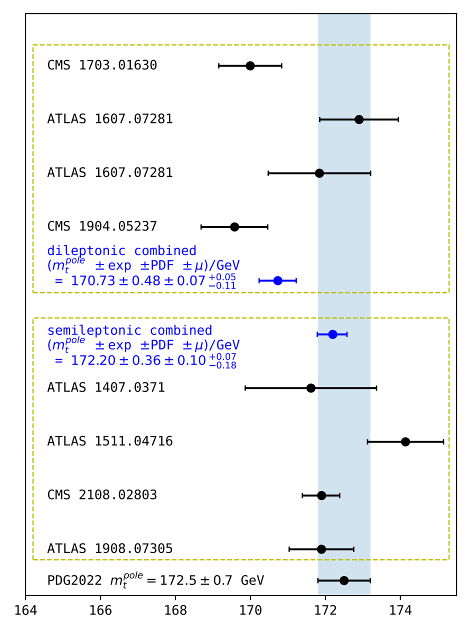
- Using ABMP16, $m_t^{\text{pole}} = 172.5$ GeV, $\mu = H_T/4$
- Reported χ^2 values with PDF uncertainties
- Effect of scale variations at NNLO $^{+3\%}_{-5\%}$ comparable or even larger than experimental uncertainty: $\Rightarrow$ this limits precision of m_t^{pole} extraction to $\gtrsim 1$ GeV
- Shall we go to aNNLO ? See talk by M. Guzzi

Extraction of m_t^{pole}: global analysis



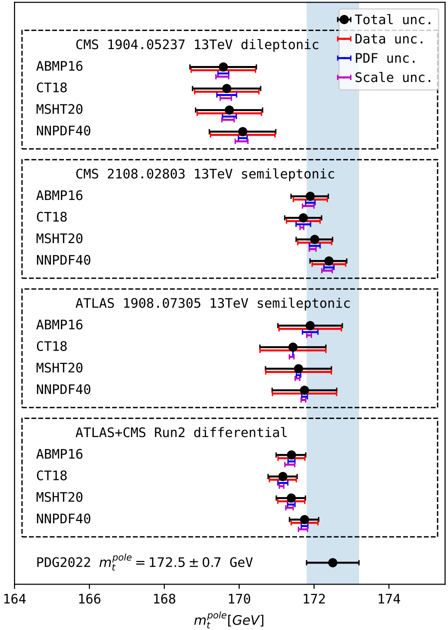
- χ^2 minimum is determined using parabolic interpolation of 3 points with lowest χ^2 values
- Both experimental, theory numerical, and PDF uncertainties included in χ^2
- Δm_t^{pole} uncertainty $\sim \pm 0.3$ GeV quoted in the plots takes into account all uncertainties included in the covariance matrix ($\Delta\chi^2 = 1$).
- Scale variations are not included in χ^2 (the uncertainties do not follow a gaussian distribution) but they are done explicitly (offset method) (span an interval of ~ 0.2 GeV)

Extraction of m_t^{pole}: slight tension ATLAS/CMS datasets



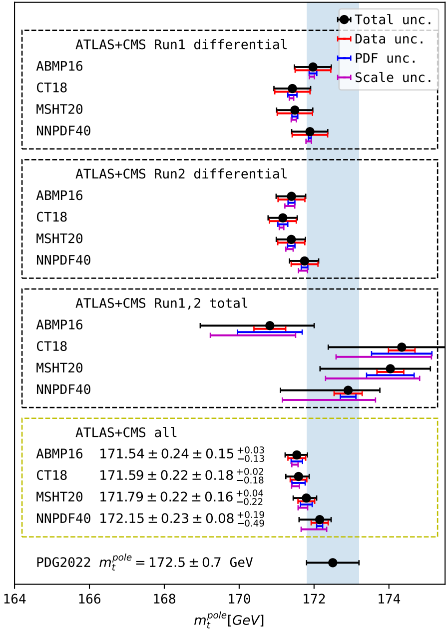
- compatibility between m_t^{pole} from the analysis of semileptonic and dileptonic data only within 2.5σ, driven by the fact that CMS dileptonic analyses seem to prefer smaller m_t^{pole} values than all others.
- it becomes fundamental to consider new analyses with full Run-2 statistics (ATLAS and CMS, dileptonic channel, full Run-2 integrated luminosity).

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



- Global Run-2 fit
- For the fit to the CMS [arXiv:1904.05237] 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 $\sim \mathcal{O}(1\text{ GeV})$ 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
  - these corrections will make possible m_t^{pole} extraction with reduced uncertainty.

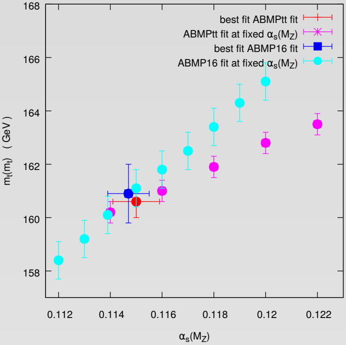
Extraction of m_t^{pole}: summary from Run-1+Run-2



- 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 $\sim 0.2 - 0.3$ GeV
  - PDF uncertainty $\sim 0.1 - 0.2$ GeV
  - NNLO scale uncertainty $\sim 0.1 - 0.2$ GeV
- in case of total cross-sections only, m_t^{pole} uncertainties dominated by scale variation effects
- for each PDF set, compatibility within uncertainties between m_t^{pole} extracted using Run-1 or Run-2 differential data
- compatibility within uncertainties among m_t^{pole} extracted using as input different (PDF+$\alpha_s(M_z)$) sets
- Significant dependence of the central m_t^{pole} value on PDFs (~ 0.6 GeV):
  - different m_t^{pole} used in different PDFs
  - PDFs, m_t^{pole} (and α_s (M_Z)) should be determined simultaneously

Simultaneous fit of top-quark mass, PDFs, $\alpha_s(M_Z)$

in the ABMP framework, using most of the data listed before + single-top, is in progress: FIRST PRELIMINARY RESULTS



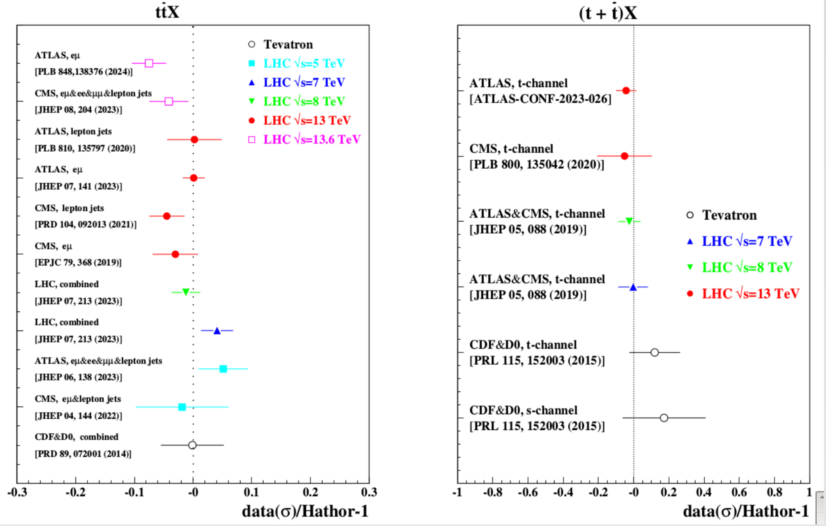
$\alpha_s(M_Z, N_f = 5)$		$m_t(m_t)$ (GeV)
Fitted	0.1150(9)	160.6(6)
$\alpha_s(M_z)$ fixed	0.114	160.2(4)
	0.116	161.0(4)
	0.118	161.9(4)
	0.120	162.8(4)
	0.122	163.5(4)

Table: The values of $m_t(m_t)$ obtained with different values of α_s in the ABMPtt fit.

- Correlations between PDF $g(x)$, $\alpha_s(M_Z)$ and $m_t(m_t)$ follows from the factorization theorem.
- Fit of $m_t(m_t)$ at fixed $\alpha_s(M_Z)$ shows positive correlation between $\alpha_s(M_Z)$ value and $m_t(m_t)$.
- When including the $t\bar{t} + X$ differential data, the correlation coefficient decreases w.r.t. to the ABMP16 analysis, whereas the best-fit $\alpha_s(M_z)$ value remains approximately the same.
- Open question: compatibility with $\alpha_s(M_Z)$ from lattice QCD (see talk by L. Del Debbio)

Simultaneous fit of top-quark mass, PDFs, $\alpha_s(M_Z)$: agreement with total cross-section data

FIRST PRELIMINARY RESULTS



Summary and outlook

- Compared very recent 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 when considering only the central set neglecting PDF uncertainties
  - including these data in PDF fits make it possible to further reduce gluon PDF uncertainties at large x
- $(1/\sigma)d\sigma/dM(t\bar{t})$ and $(1/\sigma)d^2\sigma/(dM(t\bar{t})dy(t\bar{t}))$ provide great sensitivity to $m_t^{\rm pole}$
  - extracted $m_t^{\rm pole}$ values with precision ± 0.3 GeV and consistent with PDG value: e.g. using ABMP16 $m_t^{pole} = 171.54 \pm 0.24(\,\mathrm{exp}) \pm 0.15(\,\mathrm{PDF})^{+0.03}_{-0.13}(\,\mu)$ 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 + $m_t^{\rm pole}$ + $\alpha_s\,(M_Z)$ fit (in progress)
  - residual dependence on m_t^{MC} (related to the unfolding) still needs to be estimated (important when m_t^{pole} uncertainties become small).
- 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.