Higher-order computations for top-quark production at hadron colliders: implications for top-quark mass and PDF fits

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On the basis of [arXiv:2311.05509[hep-ph]], [arXiv:2407.00545[hep-ph]] and work in progress.

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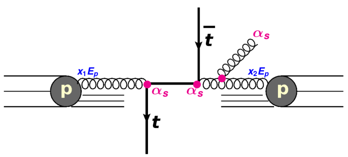
Heavy-quark pair hadroproduction in QCD

$$\sigma_{pp\to Q\bar{Q}+X} = \sum_{i,j} PDF(x_i,\mu) PDF(x_j,\mu) \otimes d\hat{\sigma}_{ij}(x_i P_i, x_j P_j, \mu, m_Q, \alpha_s(\mu))$$

- for charm and bottom quarks this is not enough, because they hadronize
- top quark: no complications due to hadronization, but it decays and then, in order to compare to predictions for top-production, it needs to be reconstructed (unfolding to the parton level)

Top-quark production has already been used for extracting m_t and x dependence of PDFs, also considering correlations with $\alpha_s(M_Z)$.

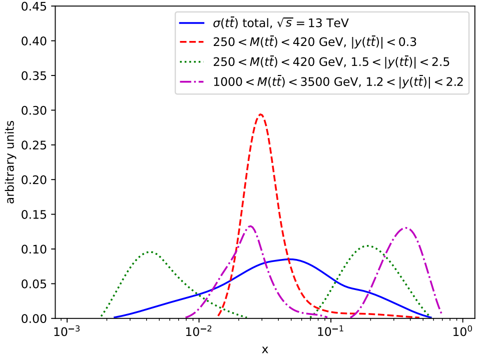


⇒ Novelty of this work: use of (normalized) double-differential distributions at NNLO QCD accuracy (no K-factors) and state-of-the-art LHC data in the NNLO fits of these quantities.

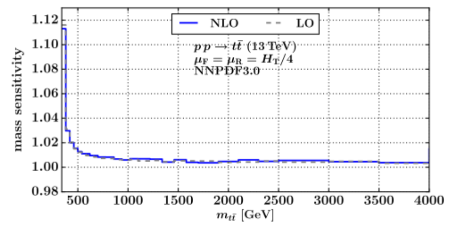
x intervals probed by $t\bar{t} + X$ hadroproduction

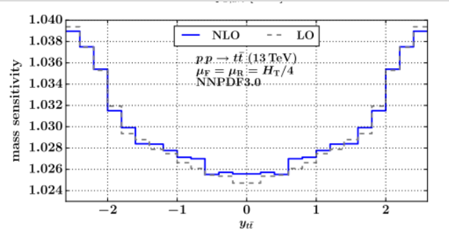
- $pp \to t\bar{t} + X$ @ 13 TeV probes $0.002 \lesssim x \lesssim 0.7$
  - gg contributes $\approx 90\%$
- double-differential data probe different x subintervals
- Scales m_H, M_W, M_Z and m_t are similar among each other
- Higgs production at the LHC probes $x \sim m_H/\sqrt{s} \sim 0.01$ which is well covered by differential $t\bar{t} + X$ data
- DY production at the LHC probes a similar region $x \sim m_{W,Z}/\sqrt{s}$
  - mostly sensitive to quark PDFs
  - helps with light flavor separation

LO: $x_{1,2} = (M(t\bar{t})/\sqrt{s}) \exp[\pm y(t\bar{t})]$



Sensitivity to m_t of $M_{t\bar{t}}$ and $y_{t\bar{t}}$ differential distributions





from M. Czakon et al., PRD 94 (2016) 114033

* Percentage shift of cross-sections for a 1 GeV change in m_t.
* The sensitivity to m_t is especially large for $m_{t\bar{t}}$ distribution close to threshold, but $y_{t\bar{t}}$ becomes also sensitive in case of forward rapidities.
* modified by the use of distributions normalized to σ_{tot}.

Theory predictions for $t\bar{t} + X$ hadroproduction

- 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. However, `HighTEA` database recently appeared.

- Master formula for $t\bar{t} + X$ hadroproduction in `MATRIX`:

$$d\sigma^{t\bar{t}}_{(N)NLO} = \mathcal{H}^{t\bar{t}}_{(N)NLO} \otimes d\sigma^{t\bar{t}}_{LO} + \left[d\sigma^{t\bar{t}+jet}_{(N)LO} - d\sigma^{t\bar{t},CT}_{(N)NLO} \right]$$

$*$ $\vec{q}_T = \vec{p}_{t,T} + \vec{p}_{\bar{t},T}$, the cross-section is splitted in a $q_T = 0$ and in a $q_T \neq 0$ parts. $q_T = 0$ at LO implies that for having the $q_T \neq 0$ part at NNLO one does not need to perform 2-loop calculations.

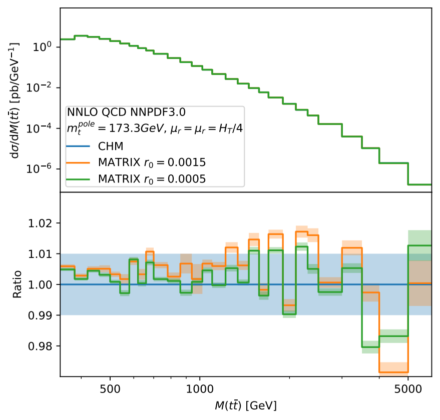
$*$ the two terms in parenthesis are separately IR divergent for $q_T \to 0$, but their difference is IR finite in the same limit. The counterterm compensating for the divergence is known from the fixed-order expansion of the resummation formula of the logarithmic contributions of the form $\alpha_s^{n+2}(1/q_T^2) ln^k(M^2_{t\bar{t}}/q_T^2)$ large in the limit $q_T \to 0$, affecting the q_T distribution.

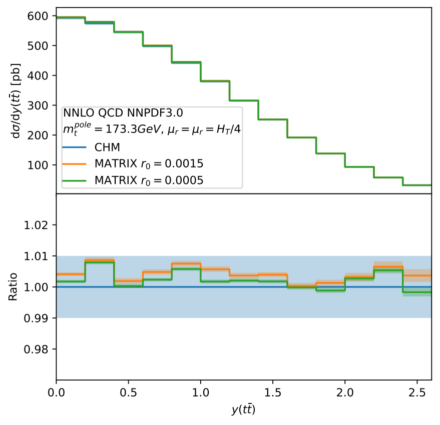
$*$ in practice the calculation is performed by introducing cuts in $r = q_T/M$. with $r_{cut} \in [0.01\%, r_{max}]$ with r_{max} varying between 0.5% and 1%.

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 $\Delta\sigma_{t\bar{t}} < 0.1\%$
  - 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 values with step of 2.5 GeV and $\Delta\sigma_{t\bar{t}} = 0.02\%$
  - $\approx$ 350000 CPU hours/run ($\sim$30 years on a single CPU)
  - for differential distributions, statistical uncertainties in bins are $\lesssim 0.5\%$
- 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)

Predictions for differential distributions with different r_{cut} values





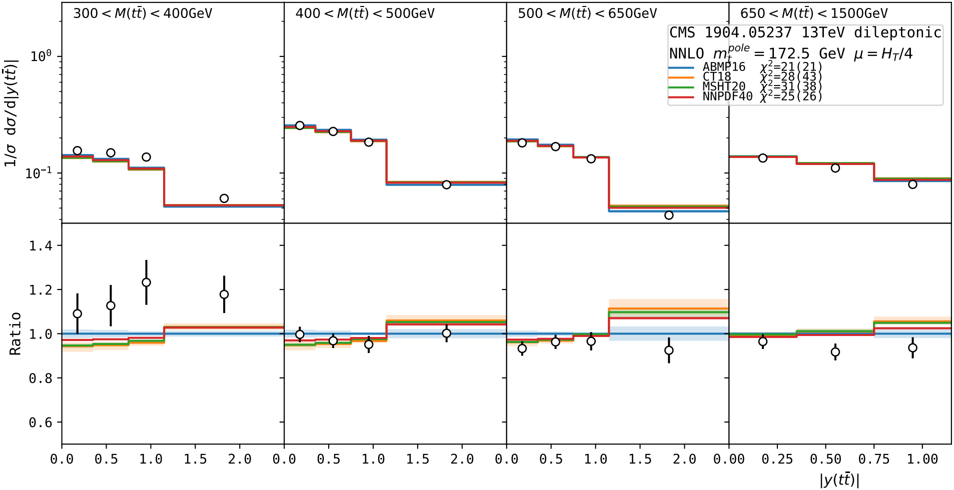
∗ In principle, the q_T-subtraction-based computation of (differential) cross-sections for finite r_{cut} introduces power corrections, which vanish in the limit $r_{cut} \to 0$.

∗ In practice, good agreement with the exact calculation (local) by Czakon et al. (at least considering their quoted 1% uncertainty).

ATLAS and CMS data used in this work

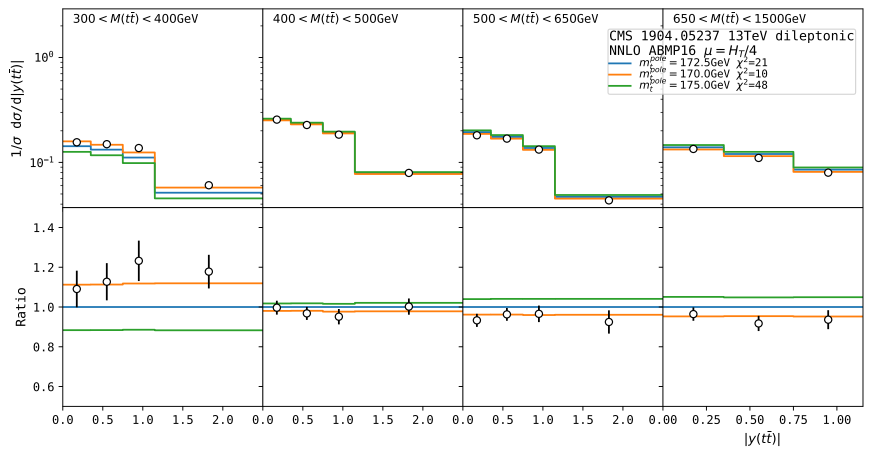
- We focus especially on measurements at 13 TeV where double-differential $M(t\bar{t})$, $y(t\bar{t})$ cross sections at parton level are available
  - **(1)** CMS EPJ C80 (2020) 658 [1904.05237, TOP-18-004]:
    2D cross sections in dileptonic channel, $L = 35.9$ pb^{-1}
    - for 3D $M(t\bar{t})$, $y(t\bar{t})$, $N_{\rm jet}$ 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, $L = 137$ pb^{-1}
  - **(3)** ATLAS EPJ C79 (2019) 1028 [1908.07305]:
    2D cross sections in l+jets channel, $L = 36$ pb^{-1}
  - **(4)** ATLAS JHEP 01 (2021) 033 [2006.09274]:
    2D cross sections in all-hadronic channel, $L = 36.1$ pb^{-1}
- For all measurements, we use normalised cross 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 cross sections)
- it would be nice to also use LHCb data (sensitivity to larger x and to m_t), but they are not yet available in the format of normalized differential cross sections.
- Additionally, we use total inclusive $t\bar{t} + X$ and single-top cross-section data

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



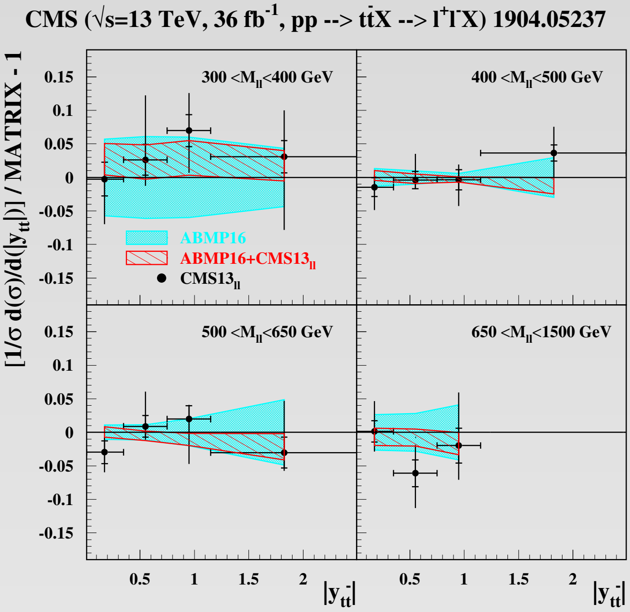
- Fixed $m_t^{\text{pole}} = 172.5$ GeV, $\mu_r = \mu_f = H_T/4$
- Reported χ^2 values with (and without) PDF uncertainties
- All PDF sets describe data reasonably well, with best description by ABMP16

CMS TOP-18-004 vs NNLO predictions with ABMP16 PDFs and different m_t^{pole}



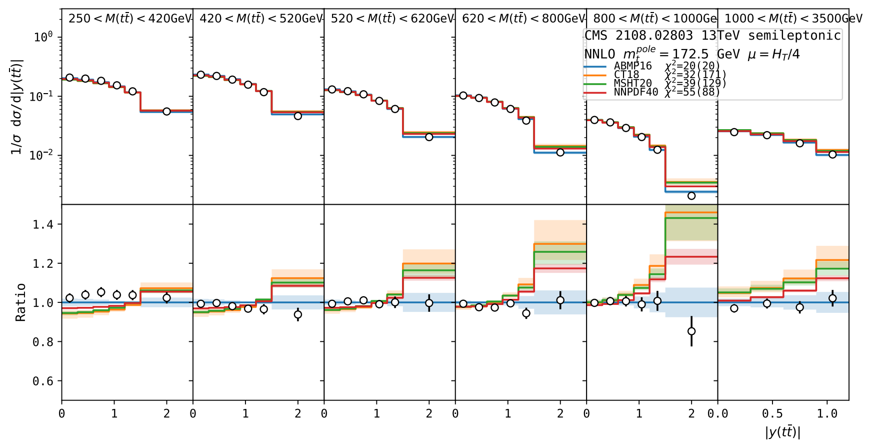
- Using ABMP16, $\mu_r = \mu_f = H_T/4$
- Reported χ^2 values with PDF uncertainties
- Large sensitivity to m_t^{pole} in the first $M(t\bar{t})$ bin (and due to cross section normalisation, also in other $M(t\bar{t})$ bins)

Pulls of CMS TOP-18-004 data with respect to ABMP predictions



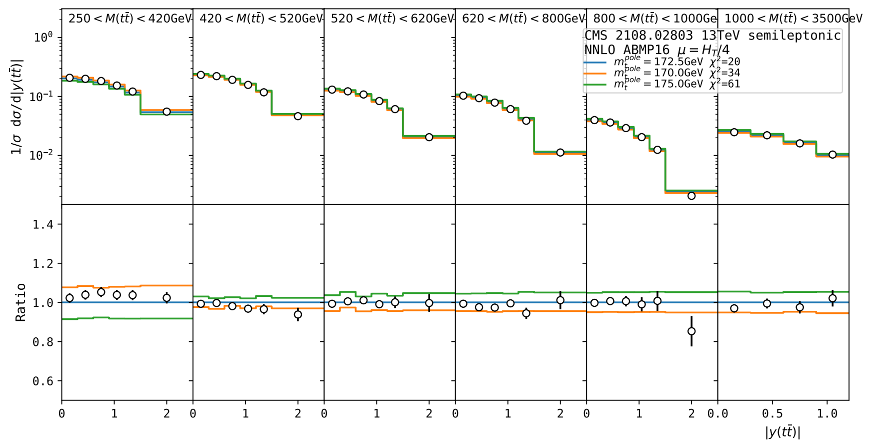
- ABMP PDF fit variant incorporating this specific dataset, w.r.t. already available ABMP16 PDF fit without it

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



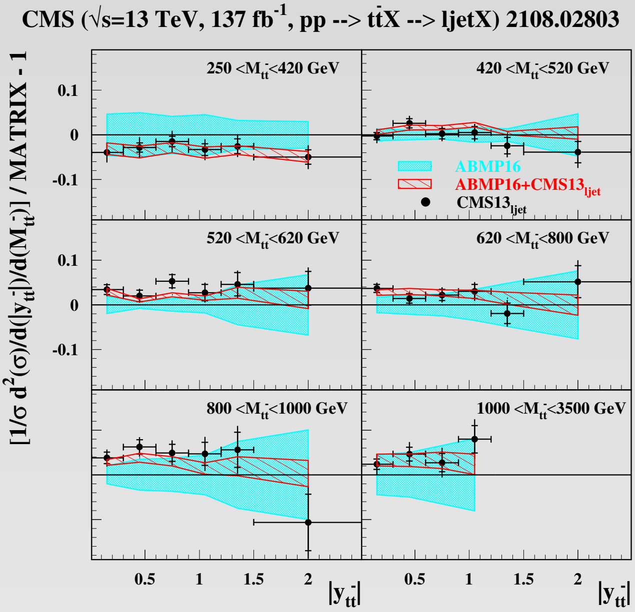
- Fixed $m_t^{\text{pole}} = 172.5$ GeV, $\mu_r = \mu_f = H_T/4$
- Reported χ^2 values with (and without) PDF uncertainties
- All PDF sets describe data reasonably well, with best description by ABMP16
  - CT18, MSHT20 and NNPDF40 show clear trend w.r.t data at high $y(t\bar{t})$ (large x)
- This is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

CMS TOP-20-001 vs NNLO predictions with ABMP16 and different m_t^{pole}



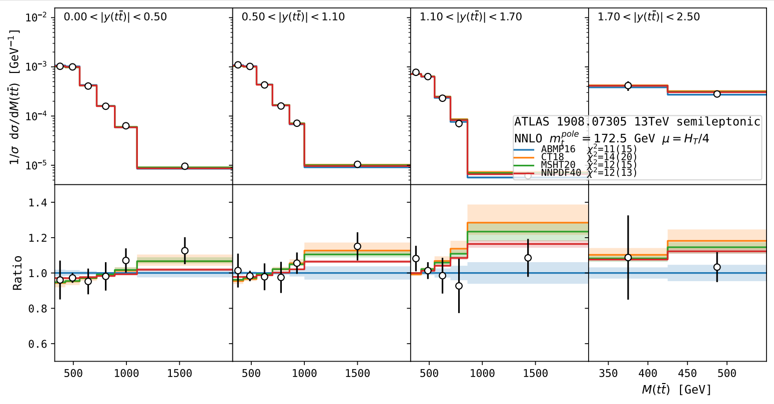
- Using ABMP16, $\mu_r = \mu_f = H_T/4$
- Reported χ^2 values with PDF uncertainties
- Large sensitivity to m_t^{pole} in the first $M(t\bar{t})$ bin (and due to cross section normalisation, also in other $M(t\bar{t})$ bins)
- Fluctuations of theory predictions are $\lesssim$ 1% and covered by the assigned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

Pulls of CMS TOP-20-001 data with respect to ABMP predictions



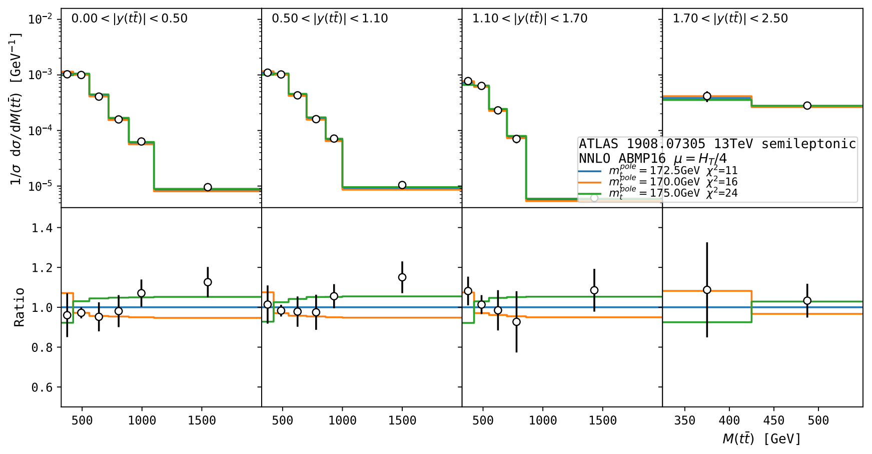
- ABMP PDF fit variant incorporating this specific dataset, w.r.t. already available ABMP16 PDF fit without it

ATLAS 1908.07305 vs NNLO predictions using different PDFs



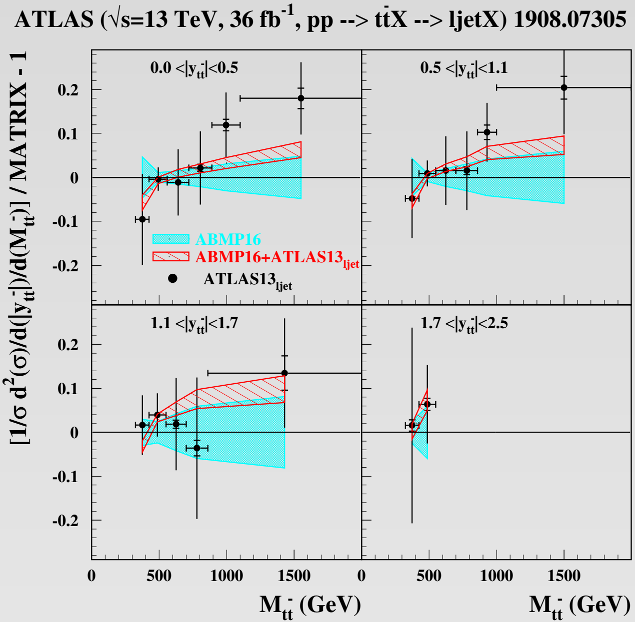
- Fixed $m_t^{\text{pole}} = 172.5$ GeV, $\mu_r = \mu_f = H_T/4$
- Reported χ^2 values with (and without) PDF uncertainties
- All PDF sets describe data equally well
- $\chi^2/\text{dof} < 1$ indicating possible overestimate of experimental uncertainties (additionally, the data covariance matrix is not 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 1908.07305 vs NNLO predictions with ABMP16 PDFs and 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)

Pulls of ATLAS 1908.07305 data with respect to ABMP predictions



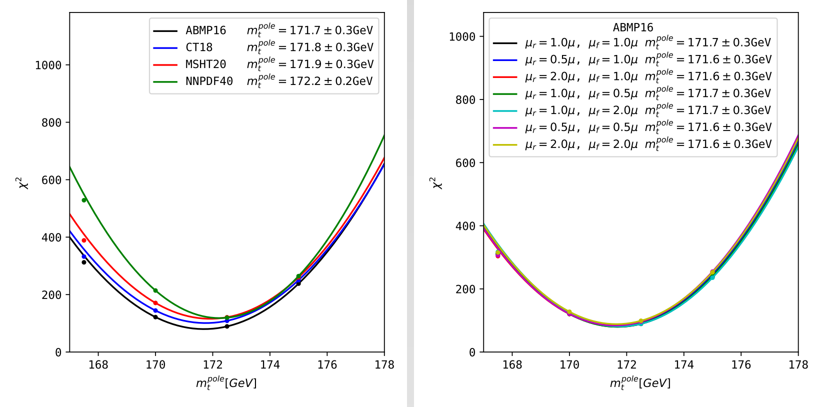
- ABMP PDF fit variant incorporating this specific dataset, w.r.t. already available ABMP16 PDF fit without it.
- ATLAS $\ell + j$ data tend to be larger than central theory predictions at large $M(t\bar{t}) \sim 1500$ GeV. But the data uncertainties are still large.
- ATLAS $\ell + j$ analysis with better statistics wanted.

Data vs NNLO predictions using different PDFs at fixed m_t: 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. $\sigma(t\bar{t}+X)$	$80/78$	$252/78$
MSHT20	total and diff. $\sigma(t\bar{t}+X)$	$92/78$	$196/78$
NNPDF4.0	total and diff. $\sigma(t\bar{t}+X)$	$104/78$	$139/78$

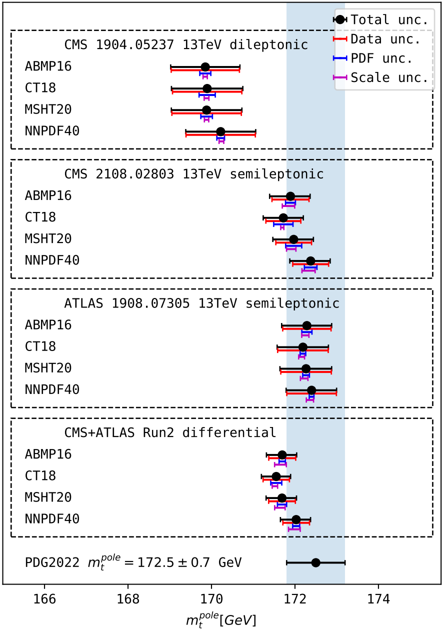
- No PDF fit so far includes the datasets (1)-(4) that we considered
  - NNPDF4.0 include single-differential data from CMS studies [1803.08856, 1811.06625], using 2016 events, with partial overlap with the events used in the independent CMS Run 2 analyses that we considered. Additionally they include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

Extraction of m_t^{pole}: global analysis



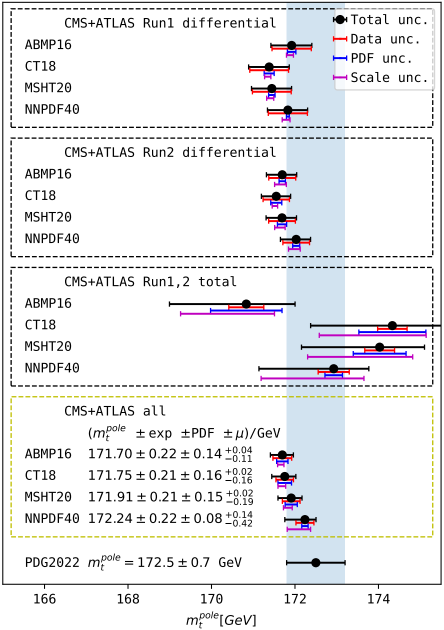
- χ^2 minimum is determined using parabolic interpolation of 3 points with lowest χ^2 values
- Both experimental, theory numerical, and PDF uncertainties included in χ^2
- Δm_t^{pole} uncertainty $\sim \pm$ 0.3 GeV quoted in the plots takes into account all uncertainties included in the covariance matrix ($\Delta\chi^2 = 1$).
- 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 $\sim$ 0.2 GeV)

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



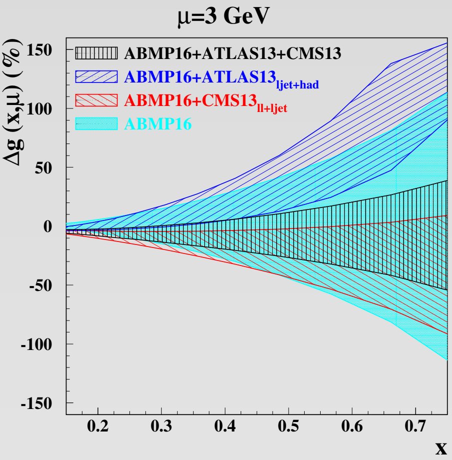
- Global Run-2 fit
- For the fit to the CMS [arXiv:1904.05237] dataset, our NNLO results are consistent with the NLO ones published in the experimental paper itself.
  - $\sim 2\sigma$ difference w.r.t other LHC data (unfolding effect ?)
- Coulomb and soft-gluon resummation effects near the $t\bar{t}$ production threshold are neglected: expected correction $\sim \mathcal{O}(1$ 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

Extracted $g(x)$ in variants of the ABMP fit

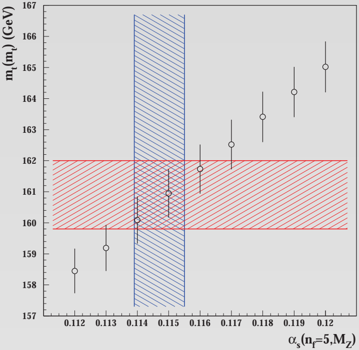


- $g(x)$ at the starting scale $\mu = 3$ GeV.

- $g(x)$ in the new ABMP fit variants compatible with ABMP16 previous fit.
- uncertainties on $g(x)$ decreased by a factor ~ 2 w.r.t. ABMP16 previous fit.
- ATLAS and CMS data points towards opposite trends of $g(x)$ at large x. ATLAS prefers a larger $g(x)$, related to the fact that ATLAS ($\ell + j$) data tend to be larger than theory predictions at large $M(t\bar{t}) \sim 1500$ GeV. Note that this trend is not visible for ATLAS hadronic data.
- fit including both ATLAS and CMS data dominated by the CMS $\ell + j$ differential data.
- Observe that new $m_t(m_t)$ and $\alpha_s(M_Z)$ values are extracted simultaneously. In particular, the smaller $g(x)$ of the “global” fit is accompanied by a smaller $m_t(m_t)$ value (see next slides).

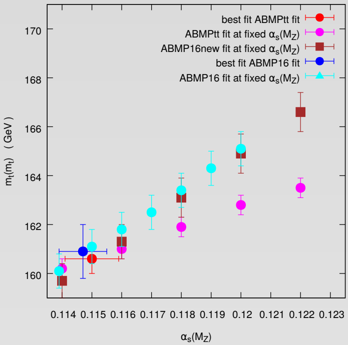
Correlation between $m_t(m_t)$ and $\alpha_s(M_Z)$ in the old ABMP16 fit

from ABMP16 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 $m_t(m_t)$.

Correlation between $m_t(m_t)$ and $\alpha_s(M_Z)$ in the new ABMP fit (vs. old ABMP16)



$\alpha_s(M_Z, N_f = 5)$		$m_t(m_t)$ (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 new ABMP 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.
- With improved precision of data on single-top production in the t-channel, the impact of $\alpha_s(M_Z)$ on the m_t determination can be further leveled.

Higgs cross section with ABMPtt (in collaboration with Goutam Das)

PDF Name	N2LO	N3LO	N4LOsv
ABMP16	$(45.4\pm4.6)^{+0.7}_{-0.7}$	$(49.6\pm2.6)^{+0.8}_{-0.8}$	$(50.8\pm1.9)^{+0.9}_{-0.9}$
ABMPtt	$(45.0\pm4.6)^{+0.6}_{-0.6}$	$(49.2\pm2.6)^{+0.7}_{-0.7}$	$(50.4\pm1.9)^{+0.8}_{-0.8}$
CT18NNLO	$(47.4\pm5.1)^{+1.3}_{-1.7}$	$(52.0\pm2.9)^{+1.4}_{-1.9}$	$(53.4\pm2.1)^{+1.5}_{-1.9}$
MMHT2014nnlo68cl	$(47.7\pm5.1)^{+0.6}_{-0.8}$	$(52.3\pm2.9)^{+0.7}_{-1.0}$	$(53.8\pm2.2)^{+0.7}_{-1.0}$
MSHT20nnlo_as118	$(47.4\pm5.1)^{+0.5}_{-0.6}$	$(52.0\pm2.9)^{+0.6}_{-0.6}$	$(53.4\pm2.1)^{+0.6}_{-0.6}$
NNPDF40_nnlo_as_01180	$(47.8\pm5.1)^{+0.3}_{-0.3}$	$(52.4\pm2.9)^{+0.3}_{-0.3}$	$(53.8\pm2.2)^{+0.3}_{-0.3}$
PDF4LHC21_40	$(47.6\pm5.1)^{+0.8}_{-0.8}$	$(52.3\pm2.9)^{+0.9}_{-0.9}$	$(53.7\pm2.2)^{+0.9}_{-0.9}$
MSHT20an3lo_as118	$(45.0\pm4.8)^{+0.8}_{-0.7}$	$(49.4\pm2.8)^{+0.9}_{-0.8}$	$(50.7\pm2.0)^{+0.9}_{-0.8}$

Table 1: Higgs cross-section along with the absolute error obtained from seven-point scale variation around $(\mu_R{}^c, \mu_F{}^c) = (1,1)m_H$ as well as intrinsic PDF uncertainty using LHAPDF. $\sqrt{S} = 14$ TeV, α_S from LHAPDF (NNLO value).

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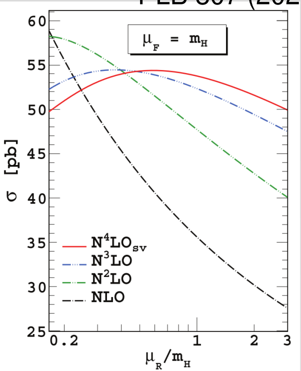


- Das, Moch, Vogt, Phys.Lett.B 807 (2020) 135546
  - N4LOsv: plus N^{4}LO soft+virtual corrections
  - N3LO: effective theory for $m_t \gg m_H$
  - N2LO: full theory for $m_H \lesssim m_t$
  - $\rightarrow$ apparent convergence of perturbative series
- N4LOsv estimates missing higher-order corrections: 2%
- Larger differences originate from (PDF+α_S) sets:

  7% (1995) $\rightarrow$ 12% (2020) $\rightarrow$ **7% (2024)**
- Expect smaller effect within single NNLO$\rightarrow$N3LO PDF sets

Conclusions - constraints from $t\bar{t}$

- 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 + $\alpha_s(M_Z)$.
- $M(t\bar{t})$ x-section near and far from the production threshold provides great sensitivity to m_t whereas $y(t\bar{t})$ x-section provide sensitivity to $g(x)$ (and some sensitivity to m_t).
- m_t^{pole} fitted value from differential distributions using as input different PDFs agree among each other within uncertainties.
- Double-differential $M(t\bar{t})$, $y(t\bar{t})$ cross sections included in the ABMPtt PDF + $\alpha_s(M_Z)\ +\ m_t(m_t)$ fit make it possible to reduce gluon PDF uncertainties at large x and $m_t(m_t)$ uncertainties by a factor ~ 2 with respect to ABMP16 fit, with no impact on the $\alpha_s(M_Z)$ value and uncertainty.
- correlations between $m_t(m_t)$ and $\alpha_s(M_Z)$ reduced by the inclusion of double-differential data in the fit w.r.t. to the case of total cross sections, where the effects of correlations are much larger.
- slight tension between CMS $(\ell + j)$ and $\ell^+\ell^-$ analyses, which tend to prefer different top-quark mass values, but compatible between 2σ.
- ATLAS $(\ell$ + j) data characterized by the worst theory description, in tension with all other data. A new ATLAS $(\ell$ + j) analysis with larger statistics is wanted.

Possible improvements and extensions

- Inclusion of NLO EW corrections to $pp \to t\bar{t} + X$: available, but expected to play a minor role, at least considering the PDF groups who already included them in their NNLO fit. However, NLO EW corrections become indispensable when going to higher-order fits.

- Inclusion of resummation effects related to soft-gluon emission and Coulomb-gluon exchange around threshold: partly available, expected to play a role, first of all on the extraction of m_t from bins close to threshold. This will become more relevant when small bin size will be reached in the experiments.

- Fit of 3-differential cross-sections in $M_{t\bar{t}}$, $y_{t\bar{t}}$, N_j: experimentally already available, relevant for better constraints on $\alpha_s(M_Z)$ and further decreasing correlations with the m_t value: NNLO theory predictions for $t\bar{t}j$ (still missing) are necessary!

- Use data at more differential level, e.g. information on leptons. This requires the implementation of $pp \to l^+ \nu b l^- \bar{\nu} \bar{b}$ at NNLO in publiclty available codes. Inclusion of top-decays is work in progress within the MATRIX collaboration.

- aN^{3}LO computations of single and double-differential distributions in aN^{3}LO PDF fits: theory work allowed already to obtain some of these distributions (in particular those differential in p_T and y) from fixed-order expansion of soft-gluon resummation formulas. The theory work needs to be extended to the consideration of other differential distributions.

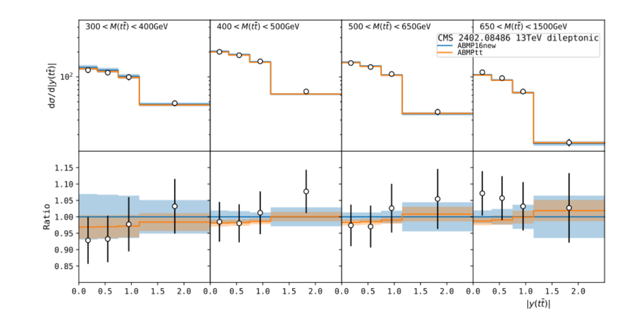
- Improved unfolding procedures

- More info on correlations between different datasets (experimental effort)

In the meanwhile....

ABMPtt PDFs available soon in the LHAPDF interface.

We plan to make public the grids of NNLO QCD predictions we obtained from the `MATRIX+PineAPPL` framework, to facilitate their public use, in particular by other PDF and m_t fitting groups, and by the experimental collaborations



comparison of ABMPtt predictions with most recent CMS recent $t\bar{t} + X$ data [arXiv:2402.08486], not yet included in the fit.

Thank you for your attention!