COMPATIBILITY BETWEEN THEORY PREDICTIONS AT NNLO QCD ACCURACY AND EXPERIMENTAL DATA FOR TOP-ANTITOP HADROPRODUCTION*

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We extract the top-quark mass value in the on-shell renormalization scheme from the comparison of theoretical predictions for $pp \rightarrow t\bar{t} + X$ at next-to-next-to-leading order QCD accuracy with the experimental data collected by the ATLAS and CMS collaborations for absolute total, normalized single- and double-differential cross sections. For the theory computations, we use the MATRIX framework, interfaced to PineAPPL for the generation of grids of predictions, which are efficiently used a posteriori during the fit, performed within xFitter. We take several state-of-the-art parton distribution functions (PDFs). The results of the fit using as input different PDF sets agree with each other within 1σ uncertainty, whereas some datasets related to $t\bar{t}$ decay in different channels point towards top-quark mass values in slight tension among each other, although still compatible within 2.5 σ accuracy. Our results are compatible with the PDG 2022 top-quark pole-mass value.

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1. Introduction

Top-quark measurements at the Large Hadron Collider (LHC) play a pivotal role in modern collider physics. They are crucial for precisely extracting key parameters of the Standard Model (SM). Furthermore, they provide critical insights into the electroweak symmetry breaking mechanism, shedding light on how particles acquire mass. Finally, top-quark studies are a vital component of searches for physics beyond the SM.

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In the present study, we determine the top-quark mass from a comparison of inclusive and differential cross-section data for $t\bar{t} + X$ production collected by the LHC experiments ATLAS and CMS with theoretical predictions, including higher-order corrections in quantum chromodynamics (QCD) and computed using as input top-quark mass values in the on-shell renormalization scheme, m_t^{pole} . We use a customized version of MATRIX [1], optimized for the $pp \rightarrow t\bar{t} + X$ process and interfaced to PineAPPL [2], for the computation of all NNLO QCD theory predictions with uncertainties (without utilizing K-factors or other approximations) at NNLO accuracy. These are the first fits of m_t^{pole} with exact NNLO accuracy that make use of LHC double-differential $t\bar{t} + X$ data, to the best of our knowledge.

2. Modified MATRIX + PineAPPL framework for theoretical calculations

A target precision of a few per mill accuracy requires the generation of various billions of $t\bar{t} + X$ NNLO events, which takes $\mathcal{O}(10^5)$ CPU hours. A general solution to this problem is to use interpolation grids, where partonic matrix elements are stored in such a way that they can be convoluted later with any PDF + $\alpha_{\rm s}(M_Z)$ set. We choose the PineAPPL library [2] which is capable of generating grids and dealing with them in an accurate way to any fixed order in the strong and electroweak couplings, and which supports variations of the renormalization and factorization scales, $\mu_{\rm R}$ and $\mu_{\rm F}$.

The MATRIX computer program [3] has been kept quite general and this allowed for the implementation of a number of different processes in a comprehensive framework. We use a customized version of MATRIX, tailored to the $t\bar{t} + X$ case [1] only and optimized for it. Furthermore, we have performed a number of optimizations in the program flow and execution, which include (1) recycling of parts of computations already performed, instead of recomputing multiple times identical contributions, (2) adaptation of the code in view of its execution on local multicore machines, (3) optimizations in distributing the computation on different machines/cores, in the job and job failure handling, (4) optimization in the input/output information exchange with the computer cluster during remote job execution, (5) reduction in the memory usage and in the size of the stored output, leading to an overall gain in the speed of the computation, in the memory consumption and in the space allocation, without compromising the final results. Further details can be found in [4].

In order to validate our implementation of the interface to PineAPPL, we compared the genuine theoretical predictions from MATRIX with those obtained using the PineAPPL interpolation grids and found them to agree within a few per mill. Also, we compared our theoretical predictions with

those from Ref. [5] and found them to agree within the uncertainties of the latter of $\approx 1\%$. Based on these validation studies, we assign a 1% uncorrelated uncertainty in each bin of the predictions.

3. NNLO fits of the top-quark pole mass value

We use measurements of the absolute total and normalized differential inclusive $t\bar{t} + X$ cross sections. We collect all up-to-date ATLAS and CMS measurements of total $t\bar{t} + X$ cross sections [6–14] which appear on the summary plot of the total $t\bar{t} + X$ cross sections by the LHC Top Working Group as of June 2023 [15]. For differential measurements, we choose cross sections as a function of the invariant mass of the $t\bar{t}$ pair, or (if available) double-differential cross sections as a function of the invariant mass $M(t\bar{t})$ and rapidity $|y(t\bar{t})|$ of the $t\bar{t}$ pair [9, 16–22]. We use four state-of-the-art NNLO proton PDF sets as input of the theory computations: ABMP16 [23], CT18 [24], MSHT20 [25], and NNPDF4.0 [26].

In Fig. 1, we compare the absolute total $t\bar{t} + X$ cross sections at $\sqrt{s} =$ 5.02, 7, 8, 13, and 13.6 TeV from Refs. [6-14] with the theoretical predictions. The first row of plots shows predictions obtained with different $PDF + \alpha_s(M_Z)$ sets, at fixed $m_t^{pole} = 172.5$ GeV, the second row shows predictions for different m_t^{pole} mass values, and the third row shows predictions with ABMP16 for different scale choices. From the first row of plots, one can see that, within the PDF uncertainties, all considered PDF sets describe the data well. The smallest PDF uncertainties occur for the NNPDF4.0 PDF set, followed by ABMP16, MSHT20, and CT18 PDF sets. The sensitivity of the theoretical predictions to the PDF set increases with decreasing \sqrt{s} , since larger values of the partonic momentum fraction x are probed at lower \sqrt{s} , and the large-x region is characterized by a larger PDF uncertainty, especially for the gluon PDF. From the second row of plots, one can conclude that for the case of ABMP16, the value of m_t^{pole} which is preferred by the data is between 170 and 172.5 GeV, while the larger value $m_t^{\text{pole}} = 175 \text{ GeV}$ is clearly disfavoured. From the third row of plots, one can see that the scale uncertainties are asymmetric, amount roughly to $^{+3}_{-5}\%$ and slightly decrease with increasing \sqrt{s} . Thus, the NNLO scale variation uncertainties for the total $t\bar{t} + X$ cross section are larger than the most precise experimental measurements of this process.

As an example of data-to-theory comparison at the level of differential cross sections, in Fig. 2 the rapidity distribution of the $t\bar{t}$ -quark pair, $|y(t\bar{t})|$, is plotted in various $t\bar{t}$ invariant mass $M(t\bar{t})$ bins, corresponding to different panels, and compared to the experimental data of Ref. [9], a CMS analysis with $t\bar{t}$ -quark pairs decaying in the semileptonic channel. At present, this is the most precise LHC dataset in our study, on the basis of the phase



Fig. 1. Comparison of the experimental data on the total $t\bar{t} + X$ cross sections at different \sqrt{s} from Refs. [6–14] to the NNLO QCD predictions obtained using different PDF sets (upper), and, for the ABMP16 central PDF member, different m_t^{pole} values (middle) and different scales (lower).



Fig. 2. Comparison of the experimental data from Ref. [9] to the NNLO QCD predictions obtained using different PDF sets (upper), and for the ABMP16 central PDF member, different m_t^{pole} values (middle) and different (μ_{R} , μ_{F}) scales varied by a factor of two around the central value $\mu_{\text{R},0} = \mu_{\text{F},0} = H_T/4$ (lower).

space of the measurement, the number of measured data points, and their experimental uncertainties. From the first row of plots, it is clear that the best agreement between theoretical predictions and experimental data as for the shape of the distributions, that is probed when considering normalized cross sections, is achieved when using the ABMP16 set. Predictions with the CT18, MSHT20, and NNPDF4.0 sets show a similar trend among each other, but the shapes are systematically different from those of the experimental distributions at large $|y(t\bar{t})|$, overestimating the latter. The plots of the second row, all obtained with the ABMP16 set, show that, the largest is the m_t^{pole} value, varied in the range of 170 GeV $< m_t^{\text{pole}} < 175$ GeV, the smallest is the cross section for low $M(t\bar{t})$ close to the threshold, while the opposite is true for large $M_{t\bar{t}} > 420$ GeV due to the cross-section normalization. The plots of the third row show that the scale uncertainties increase at large $M(t\bar{t})$, reaching values up to $\pm 3\%$ in the largest $M(t\bar{t})$ bin, comparable to the data uncertainties in this kinematic region. Due to the cross-section normalization, the average size of the scale uncertainties for the normalized differential cross sections is a few times smaller than for the total cross section, with an impact on the fit results.

To extract m_t^{pole} , we use the xFitter framework [27], an open source QCD fit framework. In Fig. 3, the results for the m_t^{pole} extraction from various experimental datasets are shown. In the left panel, results related to Run 2 measurements of differential $t\bar{t} + X$ cross sections are shown separately. The right panel reports the results of the global fit, including Run 1 + Run 2data on both total and differential cross sections. We assign the maximum difference on the m_t^{pole} values from the $(\mu_{\rm R}, \mu_{\rm F})$ 7-point scale variation as a scale uncertainty. The results of the extraction using either differential or total cross sections agree with each other within $\approx 1\sigma$, for any PDF set. We consider the compatibility of the results obtained as a sign of their robustness. Data related to $t\bar{t}$ decays in the dileptonic channel (Refs. [16, 19]) point towards central m_t^{pole} values smaller than data from decays in the semileptonic channel (Refs. [9, 17]). The values extracted from all ATLAS and all CMS differential measurements are compatible within 2.5σ , and the same level of compatibility is observed for the results extracted from the measurements in the dileptonic or semileptonic $t\bar{t}$ decay channels. In both cases, the difference originates almost entirely from the two CMS measurements of Refs. [16, 19], which point to a lower value of m_t^{pole} than all other measurements.



Fig. 3. Summary of the m_t^{pole} values extracted from Run 2 differential (left), and Run 1 + Run 2 measurements of differential and total $t\bar{t} + X$ cross sections (right).

4. Conclusions

In summary, adding the differential data to the fit only including total cross sections plays a crucial role in decreasing the uncertainties on m_t^{pole} by a factor of ~ 3. The result of the most comprehensive fit has an uncertainty band ranging from 0.3 to 0.5 GeV, depending on the PDF set. This uncertainty is a factor 2.5 smaller than that affecting the most recent average $m_t^{\text{pole}} = 172.5 \pm 0.7$ GeV by the PDG [28]. Further uncertainties affecting m_t^{pole} are due to renormalon ambiguity. One should also observe that uncertainties related to the data used have a similar size to scale + PDF variation uncertainty at a fixed PDF set. We expect that forthcoming experimental data from Run 3 and Run 4 will challenge theoretical capabilities of reducing theory uncertainties to at least a similar level as well.

Our work provides a proof-of-principle that a simultaneous fit of m_t^{pole} , PDFs, and $\alpha_s(M_Z)$ at NNLO accuracy, considering the correlations among them and using state-of-the art total and multi-differential $t\bar{t}+X$ production data, is possible. We plan to perform such a fit in a next work, upgrading the precision and accuracy of the NLO fit results we presented in Ref. [29]. The work of M.V.G. and S.-O.M. has been supported in part by the Bundesministerium für Bildung und Forschung (BMBF), under contract 05H21GUCCA. The work of O.Z. has been supported by the *Philipp Schwartz Initiative* of the Alexander von Humboldt Foundation.

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