Calibration of the Top-Quark Monte Carlo Mass

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We present a method to establish, experimentally, the relation between the top-quark mass m_t^{MC} as implemented in Monte Carlo generators and the Lagrangian mass parameter m_t in a theoretically well-defined renormalization scheme. We propose a simultaneous fit of m_t^{MC} and an observable sensitive to m_t, which does not rely on any prior assumptions about the relation between m_t and m_t^{MC}. The measured observable is independent of m_t^{MC} and can be used subsequently for a determination of m_t. The analysis strategy is illustrated with examples for the extraction of m_t from inclusive and differential cross sections for hadroproduction of top quarks.

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Introduction.—The top-quark mass is one of the fundamental parameters of the standard model (SM). Its value significantly affects predictions for many observables either directly or via radiative corrections. As a consequence, the measured top-quark mass is one of the crucial inputs to electroweak precision fits, which enable comparisons between experimental results and predictions within and beyond the SM [1]. Furthermore, together with the Higgs-boson mass, it has critical implications on the stability of the electroweak vacuum [2–4].

In fixed-order and analytically resummed predictions, the top-quark mass appears as a parameter of the Lagrangian and, therefore, depends on the choice of the renormalization scheme once corrections beyond leading order (LO) are consistently included. The conventional scheme choice in many applications of quantum chromodynamics (QCD) is the pole mass m_t^p, while alternative definitions based on the (modified) minimal subtraction realize the concept of a running mass $\bar{m}_t(\mu)$ at a renormalization scale μ as a particular example of so-called short-distance masses. On the other hand, Monte Carlo (MC) simulations generally contain not only hard-interaction calculations at LO or next-to leading order (NLO), with the fixed-order matrix elements as functions of the top-quark's pole mass m_t^p, but also contributions from initial and final state radiation, hadronization, as well as underlying-event interactions, modeled by parton shower programs based on leading-logarithm approximations and heuristic models. All these effects can lead to systematic shifts in the value of the top-quark mass [5]. Therefore, MC simulations presently do not allow for a precise definition of the quark mass renormalization scheme.

The top-quark mass has been determined with remarkable precision: the current world average quoted as 173.34 ± 0.76 GeV is obtained by combining results from the Tevatron and the LHC [6]. However, these measurements rely on the relation between the top-quark mass and the respective experimental observable, e.g., the reconstructed invariant mass of the top-quark decay products. This relation is derived by using MC simulations, so that these measurements determine the top-quark mass parameter implemented in these simulations. Therefore, the determined parameter is the so-called Monte Carlo mass m_t^{MC}, which appears most appropriate to describe experimental data [1,6,7].

The unambiguous interpretation of the experimental results for m_t^{MC} in terms of a Lagrangian top-quark mass (m_t) in a specific renormalization scheme employed in the SM has been a longstanding and increasingly urgent problem, given the importance of the value of the top-quark mass for SM physics analysis and the small uncertainty in the experimental measurement of m_t^{MC} [6]. At present, the translation from m_t^{MC} to a theoretically well-defined mass definition in a short-distance scheme at a low scale can only be estimated to be $\mathcal{O}(1)$ GeV, see, e.g., Refs. [8,9].

In consequence, a measurement of m_t is preferable and can be performed by confronting a measured observable sensitive to m_t with its prediction, calculated at NLO in QCD or beyond in a well-defined renormalization scheme for the top-quark mass. For this purpose, the inclusive cross section (σ) and the normalized differential cross sections for top-quark pair ($t\bar{t}$) production have been employed to determine the pole mass [10–12]. For these measurements of m_t^p, detector and process modeling effects are evaluated using MC simulations, so that the measured observable typically depends on m_t^{MC}. Even though the extracted value of m_t^p does not depend on a specific m_t^{MC} hypothesis, it relies on the relation between both parameters, the exact difference ($\Delta_m^p = m_t^p - m_t^{\mathrm{MC}}$) being unknown. However, it is often assumed to be up to 1 GeV, leading to a systematic uncertainty on the measurement [10–12], which might be under- or overestimated. This uncertainty can be small when only the shape of a particular observable defined within the detectors fiducial volume is considered [12], since the dependence on m_t^{MC} mainly enters through detector-acceptance effects. However, the sensitivity to m_t increases when the total $t\bar{t}$ production rate is also taken into account.

The pole mass scheme, which is inspired by the definition of the electron mass in quantum electrodynamics, has short-comings when applied to quarks in a confined theory [13,14]. Nonperturbative corrections to m_t^p due to the infrared renormalon lead to an intrinsic theoretical ambiguity of the order of Λ_{QCD} [13–15]. Alternatively, σ can be calculated using other mass schemes [16–19], such as the aforementioned running mass definition at a scale μ, $\bar{m}_t(\mu)$, the so-called $\overline{\mathrm{MS}}$ mass. By using $\bar{m}_t$ in the calculation of σ, the perturbative expansion in the strong coupling exhibits a significantly faster convergence [19].

This Letter describes a generic approach to measure an observable ξ sensitive to m_t in a particular renormalization scheme without any prior assumptions on m_t^{MC} or its relation to m_t. The method employs a simultaneous likelihood fit of m_t^{MC} and ξ, comparing an observed distribution in data to its MC prediction. For the latter, two categories of processes are taken into account. The first one corresponds to the signal process, i.e., top-quark pair production or single top-quark production, for which the cross section and event kinematics depend on m_t. The second category comprises background processes such as, e.g., the production of electroweak bosons and shows no significant dependence on m_t. Subsequently, a determination of m_t can be performed in a given renormalization scheme comparing data to theory predictions for $\xi(m_t)$ and, therefore, a calibration of m_t^{MC} by quantifying the difference $\Delta_m = m_t - m_t^{\mathrm{MC}}$ is possible. The method is first discussed for the special case with ξ being an inclusive signal production cross section and extended to differential cross sections in a second step.

Calibration with inclusive cross sections.—Assume, to measure the inclusive cross section σ, a number of *detected* events, N^d, is reconstructed and selected experimentally, with an *efficiency* ϵ estimated by using simulation. In total, N^p expected events are confronted with those observed in data. We propose to perform this comparison in bins of an observable sensitive to m_t^{MC}. The parameterization is chosen such that the shape of the distribution constrains m_t^{MC}, while its normalization determines σ. For this purpose, the fraction of predicted signal events n_i^p in bin i is considered and the total number of predicted events N_i^p in the same bin is written as

$$N_i^p = \mathcal{L} \cdot \epsilon(m_t^{\mathrm{MC}}, \vec{\lambda}) \cdot \sigma \cdot n_i^p(m_t^{\mathrm{MC}}, \vec{\lambda}) + N_i^{bg}(\vec{\lambda}), \qquad (1)$$

with N_i^{bg} being the contribution from background processes and $\mathcal{L}$ the integrated luminosity. Systematic uncertainties due to detector effects as well as signal and background process modeling are symbolized as parameters $\vec{\lambda}$ and affect the expected event yields. For each bin i, a Poisson likelihood P is derived from N_i^p and the number of observed events N_i^d. The values for σ and m_t^{MC} are determined from the maximum $L_{\max}$ of the global likelihood

$$L(\sigma, m_t^{\mathrm{MC}}, \vec{\lambda}) = \prod_i P\big(N_i^p(\sigma, m_t^{\mathrm{MC}}, \vec{\lambda}), N_i^d\big) \cdot \Xi(\vec{\lambda}). \qquad (2)$$

Here, $\Xi(\vec{\lambda})$ represents optional terms that can model prior knowledge on the systematic uncertainties specific to the experiment. Alternatively, the fit can be repeated for each individual systematic variation, leaving only m_t^{MC} and σ as free parameters.

Explicit correlations between σ and m_t^{MC} are introduced by the term $\epsilon(m_t^{\mathrm{MC}}, \vec{\lambda})$. Hence, the contribution of m_t^{MC} to the total uncertainty on σ can be minimized by reducing the dependence of ϵ on m_t^{MC} or by the strong constraints on m_t^{MC} through n_i^p.

The dependence of the resulting measured cross section on m_t^{MC} has been diminished and absorbed into the uncertainty, while the predicted cross section σ^p remains a function of m_t. Therefore, m_t is given by the value at which the predicted and measured cross sections coincide. For calculating the uncertainties on Δ_m, correlations between σ and m_t^{MC} need to be accounted for but are known precisely as a result of the simultaneous fit.

Precise measurements of the inclusive $t\bar{t}$ cross section are performed in the dileptonic decay channel by the ATLAS and CMS collaborations [10,11]. The uncertainties of these measurements are below 4% and the dependence on m_t^{MC} is small. In both analyses, m_t^p is extracted assuming $|\Delta_m| \lesssim 1$ GeV, and assigning a corresponding uncertainty. The resulting total precision of m_t^p is about 2 GeV [10]. Measurements of m_t^{MC} have been performed in the same $t\bar{t}$ decay channel using LHC data at a center-of-mass energy of $\sqrt{s} = 7$ or 8 TeV [20,21]. The value of m_t^{MC} is extracted from the normalized distribution of the lepton and b-jet invariant mass m_{lb}. The resulting precision is about 1.3 GeV and the dominant uncertainties of both measurements are mostly orthogonal. Therefore, combining these analyses, the correlation between the simultaneously determined σ and m_t^{MC} will become small.

For illustration, we use the $t\bar{t}$ production cross section, measured in Ref. [22] at $\sqrt{s} = 8$ TeV, $\sigma = 243.9 \pm 9.3$ pb to determine $\bar{m}_t$ and m_t^p for different orders of perturbative QCD. The LHC beam-energy uncertainty of 1.72% is assigned to the predicted cross section, evaluated with the program HATHOR [23] based on calculations of Refs. [19,24–27]. The cross section is calculated at LO, NLO, and next-to-next-to leading order (NNLO) accuracy with α_S at the Z-boson mass M_Z set to $\alpha_S(M_Z) = 0.118 \pm 0.001$ and is obtained using the parton distribution (PDF) set CT14 [28] evaluated at NNLO. Renormalization and

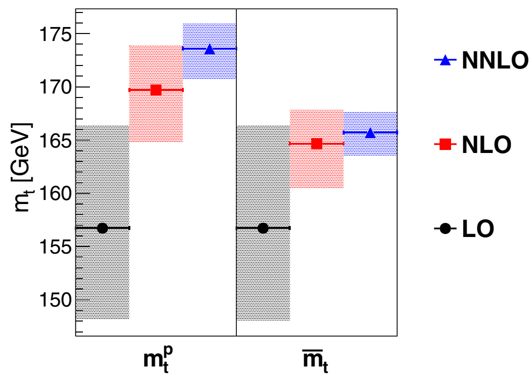

FIG. 1. Top-quark pole (m_t^p) and $\overline{\text{MS}}$ mass ($\bar{m}_t$) extracted from the inclusive $t\bar{t}$ production cross section by comparison with its prediction at different orders of perturbative QCD. The hatched areas indicate the total uncertainty on the measured mass values.

factorization scales are set to m_t^p or $\bar{m}_t$, respectively, and are varied independently by a factor of 2 up and down. The uncertainties due to variations of the CT14 PDF eigenvectors are scaled to 68% confidence level.

The extraction of m_t^p and $\bar{m}_t$ is performed by comparison of predicted and measured σ. Experimental and theoretical uncertainties are considered uncorrelated. The resulting top-quark mass values are illustrated in Fig. 1. The scheme choice does not play a role at LO. When higher orders are considered in the calculation of σ, $\bar{m}_t$ exhibits a more rapid convergence than m_t^p.

A detailed experimental analysis employing the method proposed here is documented in Ref. [22]: the fit of m_t^{MC} and σ is performed simultaneously at center-of-mass energies of 7 and 8 TeV. As illustrated in Fig. 2, the measured values are mostly uncorrelated.

The obtained cross sections are compared to calculations with NNLO accuracy to determine $\bar{m}_t$. For the extraction of m_t^p, next-to-next-to leading log (NNLL) contributions are also accounted for. The measured $\bar{m}_t$ is converted to the pole mass $m_t^{p,c}$ in perturbation theory with up to four-loop

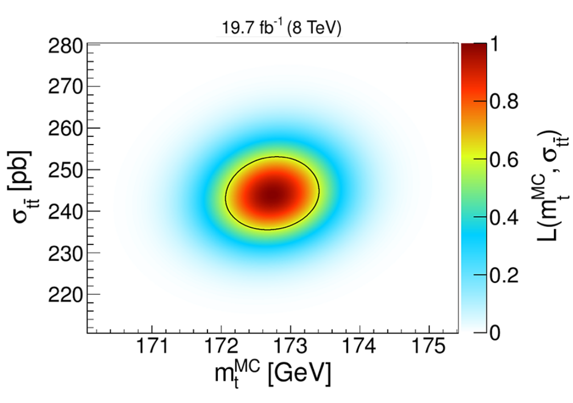

FIG. 2. Likelihood L for the measured MC mass (m_t^{MC}) and $t\bar{t}$ production cross section ($\sigma_{t\bar{t}}$) at a center-of-mass energy of 8 TeV. The black contour corresponds to the 1 sigma uncertainty [22].

TABLE I. Measured $\overline{\text{MS}}$ ($\bar{m}_t$), pole (m_t^p), and pole mass from conversion ($m_t^{p,c}$) for different PDF sets and values for the strong coupling constant, α_S, evaluated at the Z-boson mass, M_Z [22].

	$\alpha_S(M_Z)$	$\bar{m}_t$ [GeV]	m_t^p [GeV]	$m_t^{p,c}$ [GeV]
ABM12	0.113	$158.4\pm^{1.2}_{1.9}$	$166.6\pm^{1.6}_{1.9}$	$168.0\pm^{1.3}_{2.1}$
NNPDF3.0	0.118	$165.2\pm^{1.1}_{1.7}$	$174.0\pm^{1.4}_{1.7}$	$175.1\pm^{1.2}_{1.9}$
MMHT2014	0.118	$165.4\pm^{1.1}_{1.9}$	$174.3\pm^{1.4}_{1.8}$	$175.3\pm^{1.3}_{2.1}$
CT14	0.118	$165.5\pm^{1.5}_{2.0}$	$174.4\pm^{1.8}_{2.0}$	$175.4\pm^{1.7}_{2.2}$

accuracy in QCD [29]. It is well known that this leads to an additional positive shift of the value of m_t^p, the size of which indicates the residual theoretical uncertainty of m_t^p at yet higher orders. For example, using a fixed $\bar{m}_t$ as input, the value of m_t^p is approximately 0.5 GeV (0.2 GeV) larger if the conversion formula is applied at three(four)-loop instead of two(three)-loop accuracy, respectively.

The results obtained at $\sqrt{s} = 7$ and 8 TeV for $\bar{m}_t$, m_t^p, and $m_t^{p,c}$ are listed in Table I for different PDF sets [28,30–32]. A strong correlation between the strong coupling constant, α_S, and the measured top-quark mass can be observed. All extracted values for m_t are used to calibrate the m_t^{MC} parameter, which is nonuniversal and, in principle, depends on the subtleties of its implementation in the MC simulation. In Ref. [22], $\bar{\Delta}_m = \bar{m}_t - m_t^{\text{MC}}$, $\Delta_m^p = m_t^p - m_t^{\text{MC}}$, and $\Delta_m^{p,c} = m_t^{p,c} - m_t^{\text{MC}}$ are calculated for m_t^{MC} as implemented in MadGraph5 [33] interfaced with Pythia6 [34] using the tune Z2* [35] and top-quark decays simulated with MadSpin2 [36]. The results are listed in Table II. A precision of about 2 GeV is achieved.

Calibration with differential cross sections.—An extension of the method to differential cross sections used for the determination of m_t can provide a larger sensitivity and, possibly, a further reduction of systematic uncertainties. In the following, a differential production cross section for the signal process as a function of an observable x is considered and employed to determine m_t. The approach used for σ is applied to each bin of this differential cross section. For this purpose, the efficiency ϵ is replaced by a matrix M describing the detector response to the predicted cross section σ_k^{MC} in bin k of the distribution in terms of x, defined by

TABLE II. Difference between the top quark mass in well-defined schemes and the top-quark MC mass for different PDF sets. The MC mass is compared to the $\overline{\text{MS}}$ mass ($\bar{\Delta}_m$), pole mass (Δ_m^p), and the pole mass from conversion ($\Delta_m^{p,c}$) [22].

	$\bar{\Delta}_m$ [GeV]	Δ_m^p [GeV]	$\Delta_m^{p,c}$ [GeV]
ABM12	$-14.3\pm^{1.4}_{2.0}$	$-6.1\pm^{1.7}_{2.0}$	$-4.7\pm^{1.5}_{2.2}$
NNPDF3.0	$-7.6\pm^{1.3}_{1.9}$	$1.3\pm^{1.6}_{1.9}$	$2.4\pm^{1.5}_{2.0}$
MMHT2014	$-7.3\pm^{1.3}_{2.1}$	$1.5\pm^{1.6}_{2.0}$	$2.6\pm^{1.5}_{2.2}$
CT14	$-7.2\pm^{1.7}_{2.1}$	$1.6\pm^{1.9}_{2.1}$	$2.7\pm^{1.8}_{2.3}$

$$N_j^{ps} = \mathcal{L}\sum_k M_{jk}\sigma_k^{\mathrm{MC}}, \tag{3}$$

with N_j^{ps} being the predicted number of reconstructed and selected signal events in bin j of the reconstructed distribution. The response matrix is derived from MC simulation and therefore depends on $\vec{\lambda}$ as well as on m_t^{MC} [37].

Each bin j of the reconstructed distribution is considered as a category. In each category, a second observable y is defined, sensitive to m_t^{MC}. The shape of this observable is used to constrain m_t^{MC}, while the total number of signal events in each category corresponds to N_j^{ps}, and hence can be used to derive the differential cross section. The number of predicted events, N_{ij}^p, in bin i of the observable y is given as

$$N_{ij}^p = \mathcal{L}\sum_k M_{jk}(m_t^{\mathrm{MC}}, \vec{\lambda})\sigma_k^{\mathrm{MC}} \cdot n_{ij}^p(m_t^{\mathrm{MC}}, \vec{\lambda}) + N_{ij}^{bg}(\vec{\lambda}), \tag{4}$$

with n_{ij}^p being the fraction of predicted signal events in bin i with respect to N_j^{ps} and N_{ij}^{bg} the contribution from background processes.

By comparison with the number of observed events N_{ij}^d in each category j and bin i, and considering $\sigma_k^{\mathrm{MC}} \to \sigma_k$ as free parameters, a fit can be performed maximizing the likelihood:

$$L(\sigma_0, \ldots, \sigma_k, m_t^{\mathrm{MC}}, \vec{\lambda}) = \prod_i \prod_j P(N_{ij}^p, N_{ij}^d) \cdot \Xi(\vec{\lambda}). \tag{5}$$

This unfolding problem can be ill-posed and regularization techniques might need to be applied. A well-suited regularization condition is provided, for instance, by the aim to determine m_t by comparison of σ_k with its prediction $\sigma_k^p(m_t)$ as a function of m_t. Replacing σ_k with this prediction corresponds to the folding approach used in Ref. [20] and reduces the number of free parameters significantly, such that the likelihood becomes

$$L(m_t, m_t^{\mathrm{MC}}, \vec{\lambda}, \vec{\kappa}) = \prod_i \prod_j P(N_{ij}^p, N_{ij}^d) \cdot \Xi(\vec{\lambda}, \vec{\kappa}), \tag{6}$$

with $\Xi(\vec{\lambda}, \vec{\kappa})$ representing optional nuisance terms and $\vec{\kappa}$ being theoretical uncertainties on the predicted $\sigma_k^p(m_t)$. Both, $\vec{\lambda}$ and $\vec{\kappa}$ can be incorporated as nuisance terms in Ξ or can be evaluated individually. In the latter case, L depends on m_t and m_t^{MC}, only. A maximization of L directly returns the relation between these parameters as well as their correlations. The correlations are mainly incorporated through the response matrix M. Therefore, the event selection and the observable x should be chosen such, that the dependence of M on m_t^{MC} is minimized and the sensitivity of y on m_t^{MC} becomes maximal.

For the optimization of the result, also the correlation between the observables x and y should be small. A possible choice for x would be the differential $t\bar{t}$ production cross section as a function of the top-quark transverse momentum predicted up to NNLO accuracy [38]. The dependence of this observable on m_t^p and $\bar{m}_t$ can be studied at approximate NNLO with programs publicly available [39]. This distribution, describing the production dynamics, can be combined with an observable based on the kinematics of the decay products such as m_{lb} in the dileptonic decay channel or the invariant mass of the 3 jets that originate from the top-quark decay $t \to Wb \to bq\bar{q}$ in the semileptonic channel.

The additional sensitivity of the differential cross sections to m_t can result in uncertainties below 2 GeV on the extracted m_t and Δ_m, starting to challenge the measurements of m_t^{MC} in precision and improving the understanding of this parameter. Moreover, determinations of the running of $\bar{m}_t(\mu)$ at varying scales μ as well as simultaneous extractions of the strong coupling α_S and m_t become possible.

Conclusion.—The simultaneous determination of m_t^{MC} and of differential or inclusive production cross sections of processes sensitive to the top-quark mass m_t allows for subsequent extraction of m_t in a well-defined renormalization scheme. This method solves the longstanding problem of the calibration of the top-quark Monte Carlo mass m_t^{MC} and, in addition, allows for a consistent quantification of the difference $\Delta_m = m_t - m_t^{\mathrm{MC}}$ for the particular MC tools used in the analysis and within the uncertainties of the measurement.

The extraction of m_t is preferably performed in a scheme, where the perturbative expansion of the theory prediction for the respective cross section displays fast apparent convergence. For the inclusive cross section, this applies to short-distance masses and favors an experimental determination of a running top-quark mass $\bar{m}_t$ over the pole mass m_t^p. The extracted $\bar{m}_t$ is more precise than m_t^p obtained at the same order of perturbation theory and additional higher-order corrections result in smaller corrections to $\bar{m}_t$ than m_t^p. The latter can always be obtained up to four-loop accuracy in QCD.

With the current precision of the inclusive top-quark cross section and mass measurements an uncertainty on Δ_m of approximately 2 GeV can be achieved. Dedicated analyses based on differential cross sections seem to be a promising approach to further decrease this uncertainty and to measure theoretically well-defined mass parameters independently of the interpretation of the top-quark MC mass to a high precision.

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