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Testing parton distribution functions with t-channel single-top-quark production

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The production of single top-quarks in the t-channel at hadron colliders imposes strong analytic constraints on parton distribution functions (PDFs) through its double deeply inelastic scattering (DDIS) form. We exploit this to provide novel consistency checks between LO, NLO and NNLO PDF fits and propose to include it as a constraint in future PDF fits. Furthermore, while it is well-known that the b-quark PDF is highly sensitive to the b-quark mass, we show that the treatment of this systematic uncertainty is still incomplete, fragmented or outright missing at the moment. Consequently, we conclude that the b-quark mass uncertainty is the dominant but so far broadly neglected theory uncertainty for this process.

INTRODUCTION

Parton distribution functions (PDFs) are an integral part of high-energy collider predictions. With increasing proficiency in multi-loop predictions for perturbative hard scattering cross-sections, PDFs are now one of the largest sources of uncertainty in theory predictions. Some processes are initiated by heavy-quarks with masses large enough to be in the perturbative regime. The construction of associated heavy-quark PDFs requires an understanding of quark masses, mass-threshold and mass-scheme effects, all of which contribute to additional systematic PDF uncertainties. These are typically not covered by uncertainty prescriptions of individual PDF groups yet [1], but have become relevant with small percent-level perturbative truncation and PDF fit uncertainties. Through PDF sum-rules such heavy-quark effects even propagate to other processes.

One of the most precisely measured heavy-quark initiated processes is t-channel single-top-quark production, see fig. 1. As we elaborate below, t-channel production plays a pivotal role in the development and understanding of improved perturbation theory and heavy quark PDFs. It has been measured inclusively at the Tevatron [2, 3], and also more differentially at the LHC operating at 7 TeV [4–7], 8 TeV [8, 9] and 13 TeV [10–12]. The precision of the cross-section measurement is at the level of 13% for the Tevatron [13] and 7% for the LHC 8 TeV ATLAS and CMS combination [14].

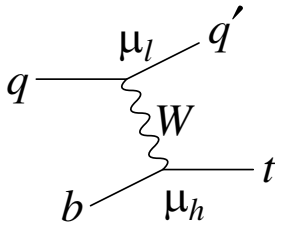

FIG. 1: Leading order Feynman diagram for t-channel single-top-quark production. The light-quark and heavy-quark parts of the diagram factorize with independent renormalization- and factorization-scales $\mu_l = \sqrt{Q^2}$ and $\mu_h = \sqrt{Q^2 + m_t^2}$, respectively, where Q^2 is the virtuality of the W boson.

The analytic connection between t-channel single-top and deeply inelastic scattering (DIS) puts significant constraints on higher order corrections and can be used as an order-consistency check of PDF fits. In this letter we use this connection to test the consistency of recent PDF fits and propose its use in future PDF fits. We also identify and discuss the b-quark mass as a systematic uncertainty in the PDFs that leads to differences of more than five times the PDF fit uncertainty. It is a systematic effect that has been broadly neglected so far but that has now become dominant.

The novel consistency checks provided by this process are a result of the fact that, in PDFs, bottom quarks are typically not included by fitting to data but instead described perturbatively by splitting of the gluon PDF. In this "five-flavor scheme" the b-quark is an intrinsic part of the proton structure. Logarithms of the form $\alpha_s \log\left((Q^2 + m_t^2)/m_b^2\right)$, that appear at each order of perturbation theory in t-channel single-top-quark production (where Q^2 is a typical hard process scale and m_b is the b-quark mass) are resummed through evolution equations [15–18], see eq. (1). Successfully predicting cross-sections in the five-flavor scheme is therefore a strong test of our understanding of heavy quark PDFs and the associated

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framework of improved perturbation theory.

$$b(x,\mu^2) = \frac{\alpha_s(\mu^2)}{2\pi} \ln\left(\frac{\mu^2}{m_b^2}\right) \int_x^1 \frac{dz}{z} P_{bg}(z) g\left(\frac{x}{z},\mu^2\right) . \tag{1}$$

A distinct property of this process is due to its structure: the LO Feynman diagram (shown in fig. 1) implies that the W-boson exchange factorizes the process into two copies of DIS. This factorization is robust under QCD radiation for an on-shell top-quark, up to (small) interference corrections at NNLO [45] so that higher-order effects can be described by independent vertex corrections on the light-quark and heavy-quark lines. Consequently, this leads to an exact analytic correspondence between the DIS processes used to extract PDFs from data and the t-channel calculation.

When using DIS data to extract PDFs, the renormalization and factorization scales $\mu^2 = Q^2$ are used, where Q^2 is the virtuality of the W boson. Using any other scale choice does not necessarily reproduce the input data when PDFs and matrix elements are combined (though the difference diminishes with increasing perturbative order). This fixes the scales for t-channel single-top to be $\mu_l = Q^2$ on the light-quark line and $\mu_h = Q^2 + m_t^2$ on the heavy-quark line, which constitute the double-DIS (DDIS) scales. It is exactly this particular choice of scales that effectively undoes PDF fits and constrains total inclusive perturbative predictions to be the same at LO, NLO and NNLO, up to the aforementioned interference and off-shell effects and provided that PDFs are primarily fitted using DIS data.

Taken together, precise predictions of this process in the five-flavor scheme therefore allow for a precision test of the heavy b-quark PDF framework. A previous study found that LO and NLO predictions for the Tevatron using various PDF fits disagree by up to five times the PDF fit uncertainty [19]. It was suggested that such discrepancies might just be an artifact of LO fits that have not received the same continuous attention as their higher-order counterparts. To follow up on this hypothesis, we use our recent NNLO calculation [46] that allows the use of DDIS factorization and renormalization scales [20] to scrutinize the consistency of LO, NLO and NNLO fits of different PDF groups. Small mistakes in either the PDF calculation or input (e.g., through faulty evolution or poor fits) can reintroduce potentially large logarithms in the calculation. As a result, formerly delicate cancellations – that occur to enforce the equality of the inclusive cross-sections between orders – are broken, leading to large measurable deviations.

In the rest of this letter we use the framework described above as follows: We first check the order consistency of PDF fits using DDIS scales. Focusing on NLO and NNLO here, we find that the commonly used modern PDF fits are consistent between NLO and NNLO. We then turn to the effect of the b-quark mass parameter and find that its uncertainty has been broadly neglected in PDF fits. This leads to large systematic differences in t-channel single-top-quark predictions between some commonly used PDF fits. NNLO predictions only agree within fit uncertainties once the systematic differences in b-quark masses are taken into account. Since the momentum sum-rule connects heavy-quark PDFs to other PDFs, especially the gluon PDF, it can also affect a range of other processes, albeit only at the subleading level. We argue that on the path towards the proton structure at one-percent accuracy [21] this systematic effect becomes relevant for LHC phenomenology in general. In fact, for t-channel single-top-quark production it is now the dominant theoretical uncertainty.

ORDER-CONSISTENCY OF MODERN PDFS

Using DDIS scales we expect that total inclusive cross-sections are equal at LO, NLO and NNLO, up to small interference effects at NNLO and up to non-DIS data used in PDF fits. We perform our tests for Tevatron ($\sqrt{s} = 1.96\,\text{GeV}$) $p\bar{p}$ collisions to have the highest sensitivity with respect to the DDIS property. This is because for higher center of mass energies the differences between LO, NLO and NNLO cross-sections shrink, regardless of the scales used, due to cancellations originating from the different parton density regimes. For example, in ref. [19] agreement to better than one percent between LO and NLO was found when using DDIS scales and the CTEQ6 PDF set. At the Tevatron the difference grows to $\sim 10\%$ when using fixed m_t scales instead, which allows for a stringent check. If the LHC was run at $\sqrt{s} = 1.96\,\text{GeV}$ this difference would still be 9%, but an increase to $\sqrt{s} = 8\,\text{TeV}$ or $\sqrt{s} = 13\,\text{TeV}$ reduces the sensitivity to 6% for a top-quark and to 3% for an anti-top-quark. To be maximally sensitive to the order consistency we therefore study Tevatron $p\bar{p}$ cross-sections at $\sqrt{s} = 1.96\,\text{GeV}$. This also allows for a comparison with the measurements, in principle, although we do not pursue that here.

In fig. 2 we show total inclusive t-channel cross-sections up to NNLO using DDIS scales with 1σ uncertainties as reported by LHAPDF [22] for various recent PDF fits [23–30]. Note that only a few groups provide LO fits with uncertainties and, with the exception of NNPDF3.0 and NNPDF3.1, there is no overlap between the uncertainties at LO and higher orders. We observe broad agreement between NLO and NNLO cross-sections. For the ABMP fits the NLO [23] and NNLO [24] fits show a better consistency when using a fixed value of $\alpha_s(m_Z) = 0.118$ ("ABMP16als118"). The regular fit ("ABMP16") includes a fitted $\alpha_s(m_Z) \simeq 0.119$ at NLO and $\alpha_s(m_Z) \simeq 0.115$ at NNLO. A fixed $\alpha_s(m_Z)$

must typically be treated as an additional systematic uncertainty and other groups commonly use the same value, at least at NLO and NNLO.

On the other hand we observe significant large differences between the HERAPDF [26] predictions, indicating a serious consistency issue. While one might expect other sets to deviate more between orders since they include non-DIS data, this is not the case for HERAPDF. The difference between NLO and NNLO is more than five times the PDF fitting uncertainty. Note that at the LHC ($\sqrt{s} = 13\,\text{TeV}$) the differences between LO, NLO and NNLO completely disappear for HERAPDF.

While the sensitivity at higher center of mass energies might be reduced, we suggest that it will still be useful to include LHC single-top-quark data into fits with additional DDIS constraints.

b-QUARK MASSES IN PDF FITS.

We can also use fig. 2 to compare the NNLO predictions with each other. A striking feature is the difference, greater than five times the fit uncertainty, between NNPDF3.0 [29] and the newer version 3.1 [30]. The latter include new data and improved methodology, but a 5σ difference between successive iterations is an unexpected feature.

The reason for this large difference lies in the widely different b-quark masses used in the fits. This was also found in ref. [31] where the authors studied H and Z associated single-top-quark production at NLO. They find a cross-section difference that is several times larger than can be explained by the PDF uncertainties of NNPDF3.0 and NNPDF3.1, but state that the difference shrinks when using NNLO PDFs. In contrast, in our case the difference observed at NLO is maintained at NNLO.

t-channel single-top-quark production and other heavy-flavor processes are largely dependent on the b-quark PDF. Their sensitivity to the b-quark mass is well-known in the PDF community, with global analyses routinely emphasizing this feature [28, 32–34]. The overall finding is that the b-quark PDF is strongly anticorrelated with the b-mass, i.e. when the mass is increased the b-quark PDF is reduced. We show this strong b-mass dependence in fig. 3 for t-channel single-top-quark production. Varying the b-quark mass by 0.2 GeV results in a cross-section shift of about 2%. Another contributing systematic is the heavy-quark flavor scheme. It describes the matching of different calculations in the heavy-quark PDF above and below the mass threshold [35].

So while well-known in principle, we argue in the following that agreement on how to treat heavy-quark systematic effects are still incomplete and fragmented or outright missing at present. An important contribution to the heavy-quark mass-induced uncertainties is the mass scheme used to encode it. While the $\overline{\text{MS}}$ heavy-quark masses can be, and are, precisely determined [36] the pole masses are unphysical. Furthermore, the matching series to schemes like the $\overline{\text{MS}}$ scheme diverges [37, 38]. Due to this issue, typically a renormalon ambiguity of 0.1 GeV to 0.2 GeV is assumed [34, 39]. This means that every PDF fit working in the pole-mass scheme has an irreducible mass uncertainty that translates to an additional systematic uncertainty of about 2% in t-channel single-top-quark cross-sections. This is equal to or larger than the PDF fit uncertainty of the most recent generation of PDFs and larger than residual perturbative truncation uncertainties at NNLO.

The theoretical framework for virtually all PDF groups is based on the pole-mass scheme, and this is the limiting factor in the precision of current predictions of t-channel single-top-quark production. An exception to this is the ABMP group – the ABMP16 fit is consistently performed in the $\overline{\text{MS}}$ scheme [24]. It furthermore directly includes the heavy-quark mass uncertainty by simultaneously fitting the heavy-quark masses.

All other PDF groups fix the quark-mass in the fits. While that is a legitimate choice that can be made, unfortunately not all PDF groups provide sets to vary the b-quark mass or give prescriptions to include heavy-quark mass uncertainties. For example the commonly used CTEQ fits provide no variation sets and this systematic uncertainty is broadly neglected. The iterations of NNPDF fits used recommended values from the literature with widely different values in different schemes. For example for NNPDF3.0 it was argued [29] that, since scheme differences in their expressions are small, using a more precisely determined $\overline{\text{MS}}$ mass in place of a pole mass seemed appropriate.

Returning to the large difference found between NNPDF3.0 and NNPDF3.1, it is straightforward to check whether this difference can be explained by the choice of m_b. To do this, and also include all the other predictions on an equal footing, we have rescaled the NNLO predictions by $\log(m_b)/\log(4.7\,\text{GeV})$ in fig. 4, where m_b is the pole mass used in the individual PDF fits.[47] At LO this rescaling corresponds to an exact translation to a b-quark mass of 4.7 GeV since the process is purely b-quark initiated on the heavy-quark line, c.f. eq. (1), and we expect this to be a good approximation at higher orders too [18]. The value of 4.7 GeV is chosen as an average of recently-used b-quark pole masses in PDF fits between 4.5 GeV and 4.9 GeV. This rescaling indeed resolves the large 12% discrepancy we found between using NNPDF3.0 and NNPDF3.1, where fixed (pole mass) values of $m_b = 4.18\,\text{GeV}$ and $m_b = 4.92\,\text{GeV}$ have been used, respectively. For reference, the NNPDF3.0 fit uncertainty is 2%, while in NNPDF3.1 it decreases to 1.1%. Moreover, after rescaling, all the predictions considered here are compatible within $\sim 1\sigma$

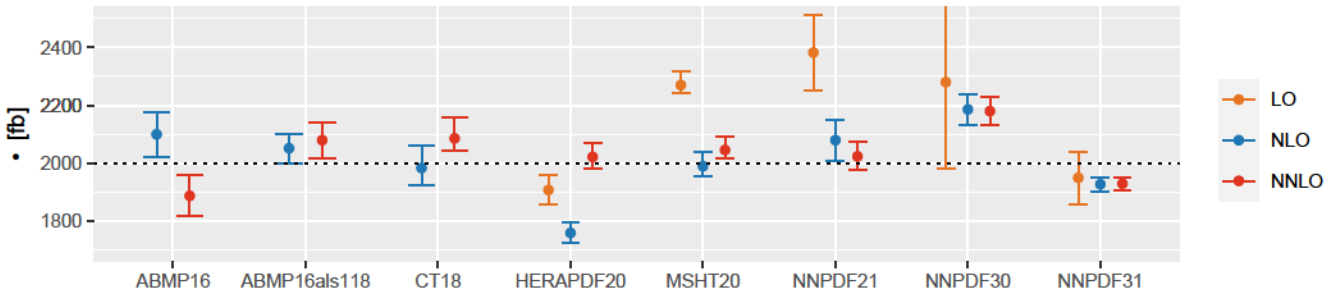

FIG. 2: Inclusive Tevatron cross-sections for different PDF sets at LO, NLO and NNLO with nominal m_b as used by each group. The solid error bars show 1σ PDF fitting uncertainties.

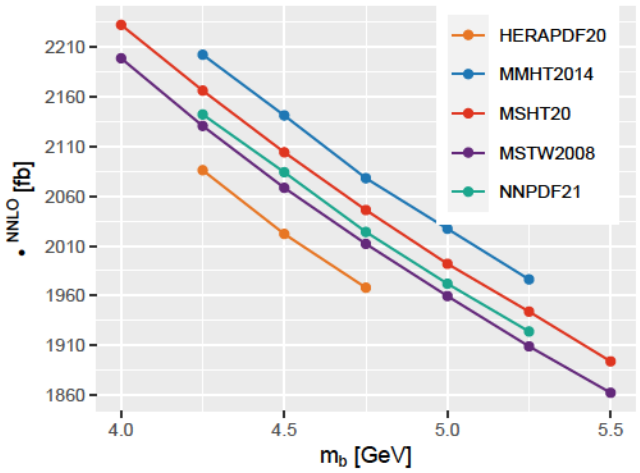

FIG. 3: b-quark mass dependence of inclusive cross-section for different NNLO PDF sets.

fit uncertainties.

Given the large b-quark mass sensitivity, one would hope to use single-top-quark production to provide a measurement of the b-mass. Current uncertainties of b-quark masses obtained in PDF fits are at the level of 2–3% [24] and matching this precision would require a large amount of statistics at the LHC. However, it would also require the elimination of systematic uncertainties such as the luminosity uncertainty. This would likely require the construction of a cross-section ratio, or normalized distribution, for which the b-mass dependence itself would either be eliminated or strongly reduced. So, while t-channel single-top-quark production will help to constrain the b-quark mass in global PDF fits, we do not anticipate its use as a measurement channel on its own.

We conclude this section by noting that similar considerations also apply to the treatment of the charm-quark mass in PDF fits. Already in ref. [1, 24] it has been pointed out that fixing the charm-quark mass leads to the neglect of essential gluon PDF correlations. In addition, then, using the charm-quark mass in the pole-mass scheme with its large uncertainties leads to predictions with significant bias. For example the renormalon ambiguity in the charm-quark pole mass is about 10%, while the $\overline{\text{MS}}$-mass can be obtained in PDF fits to better than 2% [24]. For gluon fusion Higgs production at NNLO this systematic uncertainty in the charm-quark mass translates into a cross-section uncertainty of $\pm 3.5\%$, larger than the PDF uncertainties of one to two percent reported by recent individual PDF fits. Unless groups provide PDF variation sets to estimate this systematic bias or include its effects directly in the fit, this represents a significant neglected uncertainty.

CONCLUSIONS

t-channel single-top-quark production strongly constrains order-by-order consistency of PDF fits when using double-DIS scales, especially when fits are dominated by DIS data. Focusing on differences between NLO and NNLO, we have tested several recent PDF fits and find that most PDFs are consistent across orders. One exception is the HERAPDF fit, which shows a serious inconsistency between orders, indicating an issue. We propose to exploit the double-DIS connection for future PDF fits.

On the other hand, comparing NNLO cross-sections from different PDF groups, we find that they are only consistent within standard fitting uncertainties once differences in b-quark masses are taken into account. With that we have identified and highlighted one of the most important systematic biases, the choice of mass entering the equations used to construct the heavy-quark PDFs. So far such effects have been broadly neglected, as evident by predictions based on PDFs from the past ten years that lead to systematic differences of more than 10%, but with PDF fit uncertainties at the level of 1–2%. In fact for t-channel single-top-quark production we find that the b-quark mass uncertainty is currently the largest uncertainty overall. We further argued that to decrease

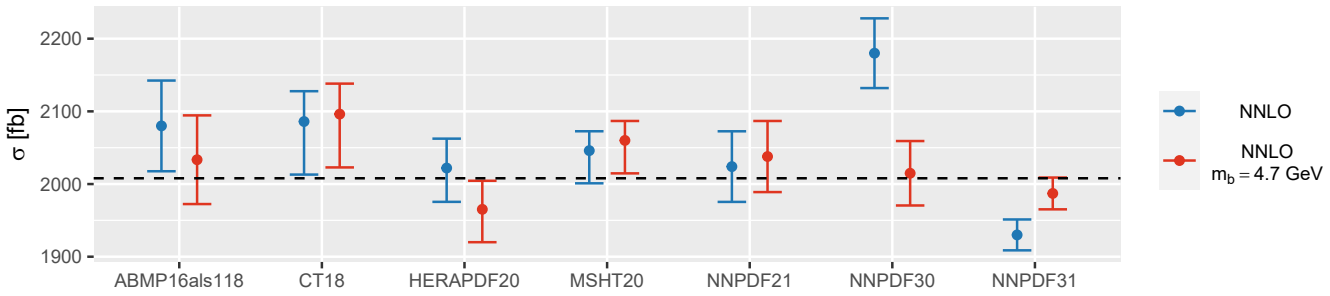

FIG. 4: Inclusive Tevatron cross-sections for different PDF sets at NNLO with nominal m_b as used by each group, and rescaled to $m_b = 4.7$ GeV. The solid error bars show 1σ PDF fitting uncertainties. The dashed horizontal line indicates a weighted average of the rescaled results (2007 fb). For the rescaling of the ABMP results which use the $\overline{\text{MS}}$ mass in the fit we use its value converted to the pole scheme (see text).

this systematic uncertainty of the cross-section, the pole-mass scheme with its irreducible renormalon ambiguity of 0.1 GeV to 0.2 GeV will have to be abandoned in PDF fits.

Heavy-quark mass effects are not just relevant for single-top quarks, but also for other measured processes like Zb and Zc, which enter the LHC jet energy scales, and Wbj, which is a large background to multiple channels at the LHC. We encourage PDF groups to update recommendations to include b-mass uncertainties and ideally avoid the pole mass ambiguity. Our findings therefore strengthen the conclusions of ref. [1], where the authors argue that generally differences in PDF sets are due to systematic effects.

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[45] See e.g. ref. [41] for recent work in that direction.
[46] A first NNLO calculation without top-quark decay has been presented in ref. [42]. Later the decay has been added [43, 44] and a discrepancy with the first calculation was found. Subsequently, our calculation [20] resolved this discrepancy and added the possibility to use different dynamic renormalization and factorization scales in both production pieces and the decay separately.
[47] Note that ABMP uses the $\overline{\text{MS}}$ mass in their fit, but to be able to compare with the other predictions we used their converted pole mass of 4.54 GeV to rescale.