Modeling of $t$-channel single top-quark production at the LHC

Jun Gao$^{1,2}$ and Edmond L. Berger$^3$

$^1$INPAC, Shanghai Key Laboratory for Particle Physics and Cosmology, School of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai 200240, China
$^2$Center for High Energy Physics, Peking University, Beijing 100871, China
$^3$High Energy Physics Division, Argonne National Laboratory, Argonne, Illinois 60439, USA

We study the modeling of $t$-channel single top-quark production at Large Hadron Collider (LHC) energies. We compare predictions at next-to-next-to-leading order in a 5-flavor scheme to those of next-to-leading order in a 4-flavor scheme, finding the two schemes agree within a few percent in general for the shape of kinematic distributions of the top quark. The predictions in the 5-flavor scheme show strong stability for both normalization and distributions, and are superior to those of the 4-flavor scheme at comparable orders. We present comparisons of the predictions with LHC data. Our findings provide clear theoretical guidance for precision studies of single top-quark physics at the LHC.

Introduction. As the heaviest particle in the standard model (SM), the top quark ($t$) is thought to offer special opportunities to explore electroweak symmetry and possible new physics beyond the SM. Single top quark production at hadron colliders provides a great opportunity to directly probe the electroweak $Wtb$ vertex, including measurement of the Cabibbo-Kobayashi-Maskawa (CKM) matrix element $V_{tb}$. In addition, the data can be used to extract the top-quark mass $m_t$ and to constrain the ratio of $u$-quark to $d$-quark parton distributions $R_{ud}$. Single top-quark production is also sensitive to physics beyond the SM $\mathcal{G}$, including modified structure of the $Wtb$ vertex, new gauge bosons, new heavy quarks, and top-quark flavor-changing neutral currents.

The $t$-channel production of a single top quark has the largest rate among all single production channels at the Large Hadron Collider. It occurs via electroweak charged-current coupling with a bottom quark, where the bottom quark arises from gluon splittings. The production can be calculated either in a factorization scheme based on 4 flavors (4FS) in the initial state or in a factorization scheme that also treats the bottom quark as a massless parton in initial hadrons (5FS). Critical questions arise on the use and agreement of the two heavy-quark schemes in single top quark production, with initial efforts at understanding made in Refs. $[8,10]$. Large theoretical uncertainties in modeling of the signals and of various measured quantities at the LHC $[11,13]$ must be addressed in view of the unprecedented precision expected in upcoming high luminosity studies at the LHC. One issue is whether the 4FS provides a better description of kinematic distributions than the 5FS. In this manuscript we address these questions with a detailed comparison of the next-to-next-to-leading (NNLO) predictions in 5FS to those at next-to-leading order (NLO) in 4FS. Availability of the NNLO calculation in 5FS ensures a fair comparison since the 4FS calculation is effectively an order higher than that of 5FS. We observe excellent agreement between 5FS and 4FS for predictions of the shapes of kinematic distributions including the transverse momentum and rapidity of the top quark. Predictions in the 5FS further exhibit a better convergence and strong stability against choice of QCD scales, and are superior to predictions from the 4FS evaluated at comparable orders. The agreement of the two schemes provides important confidence in the reliability of higher order QCD predictions at the LHC.

Significant efforts have been made recently to improve the theoretical description of $t$-channel single top quark production. The NLO QCD corrections in the 5-flavor scheme are calculated in Refs. $[14,29]$. Further NNLO QCD corrections are reported in Refs. $[3,5,39]$. The NNLO calculation in the 4-flavor scheme is carried out in Ref. $[8]$. The 4FS electroweak corrections are also calculated $[31]$. Soft gluon resummation is considered in Refs. $[32,38]$. Matching of NLO calculations to parton showers is done in the framework of POWHEG and MC@NLO Refs. $[39,42]$. In the remaining paragraphs we present our numerical results on inclusive cross sections and kinematic distributions and comparisons with LHC data.

Total cross sections. The NNLO predictions for single top quark production in the 5-flavor scheme are calculated using phase-space slicing with the N-jettiness variable $[43,45]$ together with the method of “projection-to-Born” in Ref. $[47]$. Details for the NNLO calculation in the 5FS can be found in Ref. $[8]$. We use the program MCFM $[48,49]$ to calculate NLO predictions for single top quark production in the 4-flavor scheme. The original calculation was detailed in Ref. $[8]$. In both calculations, the QCD corrections can be further factored as from either fermion line with heavy quarks or light quarks neglecting certain color suppressed contributions $[50,51]$, which are irrelevant for the comparison.

Schematically the difference of 5FS and 4FS can be understood by taking cross sections at first comparable order, i.e., leading order (LO) in 4FS and NLO in 5FS as an example

$$
\sigma_{4F}^{LO} = \alpha_s(\mu)[a_1 \ln(m_t^2/m_b^2) + c_1 + d_1(m_b^2/m_t^2)],
$$
\[ \sigma_{5FS}^{NLO} = \alpha_s(\mu)[a_1 \ln(m_t^2/m_b^2) + c_1] \\
+ \alpha_s^2(\mu)[a_2 \ln^2(m_t^2/m_b^2) + a_3 \ln(m_t^2/m_b^2)] \\
+ \text{higher orders}, \tag{1} \]

where \( \mu \) is the factorization scale and \( \alpha_s(\mu) \) is the strong coupling constant; \( m_t \) and \( m_b \) are masses of the top quark and bottom quark respectively. Coefficients \( a_i \), \( c_i \), and \( d_i \) are independent of the bottom quark mass. Calculations in the 4FS are performed order by order in \( \alpha_s \) and include exact bottom quark mass dependence like power correction term \( d_i \) in Eq. (1) which is otherwise neglected in 5FS. We include only the leading power correction term for the purpose of this illustration. On another hand, calculations in the 5FS resum potential large logarithms of bottom quark mass due to gluon splitting into bottom quarks in the initial state through all orders in \( \alpha_s \), as in terms associated with \( a_i \). The NLO and NNLO predictions have a resummation accuracy of next-to-leading and next-to-next-to-leading logarithms.

We focus on results for top quark production at 13 TeV though results are similar for either top anti-quark or top quark production at 8 TeV. We use CT14 NNLO PDFs \([52]\) of corresponding flavor numbers throughout the comparison and a bottom quark mass of 4.75 GeV and a top quark mass of 172.5 GeV accordingly. We set the QCD renormalization scale and factorization scale to be the same and choose different values in the comparisons.

In Fig. 1 we plot the total inclusive cross sections for single top-quark production at 13 TeV as functions of QCD scales. In 5FS the choice of QCD scale \( \mu_{5F} \) determines size of the quasi-collinear logarithms that are resummed through the bottom quark parton distribution. Resummation leads to fast convergence of the cross sections and stability against scale choice at higher orders in 5FS. For instance the NNLO cross section varies between 134.3 pb to 136.4 pb for the range of scales considered. On another hand, predictions in 4FS exhibits larger scale dependence owing to missing higher order contributions, e.g., with a variation between 112.1 pb to 132.6 pb at NLO. We note a fair comparison of predictions from the two schemes should be NNLO(NLO) in 5FS to NLO(LO) in 4FS since contributions from gluon splitting at large angles are only included starting from NLO in 5FS. Predictions of the two schemes do approach each other at high orders as resummed contributions from even higher orders diminish. From Fig. 1 we conclude a preferable scale choice for the 5FS of either \( \mu_{5F} = m_t/4 \) or \( m_t/2 \) where the NNLO corrections are small and meanwhile the series show a good convergence, similar to the case of top quark pair production \([53]\). Indeed a lower value of the QCD scale in 5FS was suggested in Ref. \([9]\) which shows those quasi-collinear logarithms to be resummed are accompanied by a universal suppression from phase space integration. Unlike the case of 5FS we can not find a strong motivation for an optimal scale choice in 4FS though a lower value leads to better agreement with 5FS on the total cross sections. We use a nominal scale of \( \mu_{4F} = m_t \) in the following comparisons.

**Kinematic distributions.** Comparison of the predictions of the two schemes for various kinematic distributions of the top quark can be enlightening, in part since there have been recommendations in the literature that the 4FS provides better modeling at the exclusive level \([9]\). We examine first the transverse momentum of the top quark at 13 TeV. In Fig. 2 (a) we show absolute cross sections at various orders with nominal scale choices for both schemes, i.e. \( \mu_{5F} = m_t/4 \) and \( \mu_{4F} = m_t \). In the 5FS the LO prediction (not shown in the figure) tends to have soft spectrum for the transverse momentum of the top quark. Gluon splitting at large angles can boost the top quark in the transverse direction. Those contributions are included at LO in the 4FS but only starting at NLO in the 5FS. In the 5FS, we see only a modest change in shape and normalization of the distribution in going from NLO to NNLO. In Fig. 2 (b) and (c) we show results for the 5FS and 4FS respectively. The ratio is shown of NNLO cross section to the NLO predictions in Fig. 2 (b) for different choices of the scale \( \mu_{5F} \). In Fig. 2 (c), the ratio is presented of the NLO and LO cross sections, for various choices of \( \mu_{4F} \). We again find that \( \mu_{5F} = m_t/4 \) or \( m_t/2 \) are the optimal choices that provide fastest convergence in general for the transverse momentum distribution. Larger scales lead to enhancement of the quasi-collinear contributions thus a softer spectrum at NLO until they are replaced by the full NNLO cor-
ctions and vice versa. An alternative choice could be a
dynamic scale of $\mu_{5F} = H_T/4$ with the transverse mass
$H_T = (m_t^2 + p_{T,\text{top}}^2)^{1/2}$, that interpolates in between. De-
pendence of the ratios on scale choice in 4FS is seen most
significantly for the overall normalizations similar to that
in Fig. [1] NLO corrections in the 4FS have less impact on
the shape of the distributions especially with the choice
of larger scales.

![Graphs showing differential distribution in transverse momentum (a) and comparison of ratios (b) for various scale choices.](image)

**FIG. 2.** Differential distribution in transverse momentum of a top quark at 13 TeV. (a): absolute cross sections with the nominal scale choices for both schemes; (b) and (c): ratio of NNLO(NLO) to the respective NLO(LO) predictions with various scale choices in 5FS(4FS).

We turn next to a direct comparison of predictions of kinematic distributions at the highest order of each scheme. The normalized distribution on the transverse momentum of the top quark is shown in Fig. [3](a). We normalize the distribution to the individual total cross sections in order to concentrate on the shape of the distribution. For each distribution we plot ratios of the NNLO predictions in 5FS and NLO predictions in 4FS to a common reference of NNLO prediction in 5FS with the nominal scale choice $\mu_{5F} = m_t/4$. We find remarkable agreement in shapes between the two schemes at a level of a few percent for the kinematic region in transverse momentum considered. The principal differences are seen close to the boundary of phase space, e.g., at the smallest and highest transverse momenta. The prediction of the two schemes differ by at most 2% for the nominal scale choices. The spread of all predictions is within 5% even if alternative scale choices of $\mu_{5F} = m_t/2$ and $\mu_{4F} = m_t/2$ are chosen.

A similar comparison for the absolute distributions and for an extended $p_T$ range is shown in Fig. [3](b). It is interesting that the two schemes converge in the tail region of large transverse momentum, and that the normalization of the 4FS is off exactly in the region sensitive to resummed contributions from higher orders. For the rapidity distribution, the spread of all predictions is at the permille level up to a rapidity value of 2.4, and increases to at most 2% for larger values. This occurs because at high rapidities NNLO corrections from the light quark line become significant and are only included in the 5FS calculations.

![Graphs showing comparisons of the transverse momentum of the top quark (a) and ratio of NNLO(NLO) to NLO(4FS) predictions (b).](image)

**FIG. 3.** Comparisons of the transverse momentum of the top quark at 13 TeV for NNLO(NLO) predictions in 5FS(4FS), presented as ratios to a common reference, for normalized and absolute distributions in (a) and (b) respectively.

In the conventional 5FS for single top quark production we use matrix elements with massless bottom quarks, which is regarded as a zero-mass variable flavor number scheme. The power corrections from a finite bottom quark mass can be added back order by order with the so-called general-mass variable flavor number scheme [54]. We should not expect such power corrections to be significant in single top quark production since the top quark mass is so large [55]. We have verified this ex-
plicitly with a NLO calculation using a simplified ACOT scheme \cite{59, 64}. In the calculation we replace the gluon initiated matrix element in 5FS with the LO matrix element from 4FS. We find the finite mass corrections increase the total cross section by 0.1%. The impact on the shape of the transverse momentum distribution is negligible except for a region below 20 GeV that is shifted upward by less than 1%.

**Comparison with data.** The good general agreement of the theoretical predictions of the 5FS at NNLO and the 4FS at NLO show that uncertainties associated with scheme dependence are under control. There are also experimental modeling uncertainties since the top quark momentum must be reconstructed from the kinematics of its decay products, for example, from semileptonic decay with an electron or muon observed in single top quark production. These measurements are usually unfolded back to the parton level with stable top quarks for easy comparison to theories, e.g., for a global fit of PDFs \cite{6, 58}. Comparison can also be made at the level of decay products if a model of top quark decay is included in the calculations as in Ref. \cite{59, 69, 62}. We select two measurements, one from ATLAS at 8 TeV \cite{11} and the other from CMS at 13 TeV \cite{63}. We compare predictions from both the 5FS and the 4FS with their nominal scale choices to the measured distributions of the transverse momentum of top quark in Fig. 4 and of the rapidity of the top quark in Fig. 5. In each figure we show ratios of the predictions to the central value of data for both absolute cross sections and normalized distributions.

For predictions of normalized distributions we normalize the bin-by-bin cross section to the sum from all bins. Error bars represent total experimental errors by adding statistical and systematic errors in quadrature.

For the transverse momentum distributions shown in Fig. 4 (a) and (b), we find very good agreement with ATLAS data for the NNLO predictions in the 5FS, for both absolute and normalized distributions. The NLO predictions in 4FS are systematically lower than the central values of ATLAS data for the absolute distribution, an aspect that can be improved if a lower scale is used. Regarding the case of CMS, we find none of the theoretical curves describes the CMS data particularly well for the normalized distribution in Fig. 4 (c). The differences of the predictions in 5FS and 4FS are much smaller than the experimental errors for the normalized distribution. Interestingly the CMS data on the absolute distribution in Fig. 4 (d) seem to agree better with the NLO prediction in the 4FS for the overall normalization. This is opposite to the case of the total inclusive cross sections at 13 TeV \cite{12, 64, 65} which agree better with predictions in the 5FS.

For rapidity distributions shown in Fig. 5 all predictions agree quite well with the data on normalized distributions. The normalization of predictions in the 4FS are again lower than the ATLAS central data. We find the overall normalization of CMS data on the rapidity distribution is larger by 6% compared to data on the transverse momentum distribution. Comparing Fig. 4 (d) and Fig. 5 (d) we see that the predictions from 4FS are higher than the central values of data on average for transverse momentum and much lower than data for rapidity.

We are left puzzled by what may be inconsistencies within the CMS data set and refrain from drawing stronger conclusions.

**Summary.** We study the modeling of $t$-channel single top quark production at the LHC at the highest perturbative order available in both a 5-flavor and 4-flavor scheme. We find excellent agreement between the two schemes for predictions of the shape of kinematic distributions of the top quark. The 5FS further exhibits strong stability of predictions of the normalization and distributions, and are superior to predictions from 4FS when evaluated at comparable orders in perturbation theory. Our comparisons with current data on top quark distributions show good agreement with ATLAS measure-
ments but some discrepancies with CMS. The perturbative uncertainty reaches a few percent for both inclusive cross sections and distributions with NNLO predictions in 5FS. Our results point the way toward the precision study of single top quark production in future studies with LHC data.

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