Signal modeling uncertainties in top quark production

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The modeling of top quark production with Monte Carlo generators is discussed. The treatment of systematic uncertainties on the modeling of top quark pairs as well as single top quark production is presented for the four experiments ATLAS, CDF, CMS, and D0.

1 Introduction

The signal modeling with modern Monte Carlo generators is an important ingredient for precise measurements in top quark physics. In proton-proton collisions at the LHC, roughly about 10^7 top quarks have been produced in collision runs between 2010 and end of 2012. Various measurements of top quark quantities have been performed by the ATLAS [1] and CMS [2] collaborations, but also analyses from the Tevatron experiments, CDF [3] and D0 [4], are competitive in their precision. Many of these analyses are limited by the knowledge of the signal process modeled with Monte Carlo event generators. Therefore, the understanding of uncertainties arising from the choice of model parameters in the simulation is a prerequisite for a precise understanding of top quark physics.

The signal modeling of top quark production in hadron collisions comprises several steps. First of all, top quarks can be either produced in pairs via processes of the strong interaction or as single top quarks mediated by the electroweak force. The hard interaction of top quark production is usually simulated with matrix element generators. Matrix element generators evaluate Feynman diagrams for a specific process and randomly generate events according to the transition amplitudes. The matrix element simulation starts from initial state partons (quarks or gluons), includes the production of top quarks, and can include the decay of the top quarks into leptons and light quarks. Depending on the generator, the matrix element calculation includes only leading order (LO) or also next-to-leading order (NLO) diagrams. Additional parton radiation can be included in multi-parton generators.

The remaining low-energetic processes that take place in hadron collisions have to be generated with tools partially based on non-pertubative techniques. This includes the evaluation of parton density functions (PDF) for the initial state partons, showering including initial and final state radiation (ISR/FSR), hadronization, the simulation of the underlying event (UE), and the modeling of pile-up interactions.

All steps of the simulation include free parameters that have to be adjusted properly. Uncertainties on these modeling parameters have to be propagated into final results of top quark measurements.

2 Default $t\bar{t}$ Monte Carlo Samples

The four experiments follow different approaches on the modeling of top quark pair events. The list of most commonly used generator settings is summarized for the ATLAS experiment in Table 1, for the CMS collaboration in Table 2, for CDF in Table 3, and for D0 in Table 4. In the matrix element generators, the top quark mass has been set to 172.5 GeV in most samples. The choice of which sample is used as default depends on the needs of a particular analysis. Multi-parton generators like MadGraph [5] or Alpgen [6] may be best suited for an analysis relying on the correct modeling of additional jets. NLO generators like MC@NLO [7, 8] or Powheg [9, 10, 11] are expected to give most precise results in analyses depending on the correct description of higher-order effects.

Matrix element	Shower and hadronization	PDF	UE tune
MC@NLO v4.0	Herwig 6.5 + Jimmy 4.31 [12]	cteq66 [13] or CT10 [15]	AUET1/2 [14]
Powheg-hvq v1.0 [17], POWHEG-BOX v1.0	Pythia 6.4 [16]	cteq66 (7 TeV) CT10 (8 TeV)	Perugia 2011 C [18]
Alpgen 2.13	Herwig 6.5 + Jimmy 4.31	cteq6ll [19]	AUET2

Table 1: Default Monte Carlo samples used for top quark pair production at ATLAS.

Matrix element	Shower and hadronization	PDF	UE tune
MadGraph v5	Pythia 6.4	cteq6l [19]	Z2 [20] (7 TeV) Z2* [20] (8 TeV)
Powheg-hvq v1.0, POWHEG-BOX v1.0	Pythia 6.4	cteq6m [19] (7 TeV) CT10 (8 TeV)	Z2 (7 TeV) Z2* (8 TeV)
MC@NLO v3.4	Herwig 6 + Jimmy	cteq6m	default tune

Table 2: Default Monte Carlo samples used for top quark pair production at CMS.

Matrix element	Shower and hadronization	PDF	UE tune
Pythia 6	Pythia 6	cteq5l [21]	Tune A [22] Tune A-pro
Powheg-hvq v1.0	Pythia 6	cteq66	Tune A-pro

Table 3: Default Monte Carlo samples used for top quark pair production at CDF.

Matrix element	Shower and hadronization	PDF	UE tune
Alpgen	Pythia 6	cteq6l	Modified Tune A
MC@NLO	Herwig 6	cteq66	Modified Tune A

Table 4: Default Monte Carlo samples used for top quark pair production at D0.

3 Modeling uncertainties on top quark pair production

To evaluate systematic uncertainties arising from the variation of different settings in the Monte Carlo event generation, several samples have been generated. In each of these samples, a specific parameter or setting is varied. The impact on the final result of an analysis is usually determined by exchanging the default Monte Carlo sample by the sample with systematically varied settings. In the following subsections, the common systematic uncertainties on top quark pair production modeling taken into account by measurements from the LHC and Tevatron experiments are summarized.

3.1 Matrix element variation

The choice of the matrix element generator used as default is more or less arbitrary because it is often not a priori clear which Monte Carlo event generator describes the specific features of an analysis best. To validate a systematic uncertainty on this choice, the usual approach is to exchange the default matrix element generator by another one and quote the difference on the final result of a measurement as systematic uncertainty. It is preferred to exchange the matrix element generator only and keep hadronization and shower models unaffected. Typical top quark analyses quote for instance the difference between Powheg and Alpgen or MadGraph and Powheg, i. e. the difference between LO and NLO generators.

3.2 Scale uncertainty

The renormalization and factorization scale Q^2 is a free parameter in the Monte Carlo event generation. It defines the scale at which the running coupling of the strong interaction and the PDF is evaluated. A usual choice of the scale parameter is $Q^2 = m_{\mathrm{top}}^2$ or $Q^2 = m_{\mathrm{top}}^2 + \sum_{\mathrm{partons}} p_{\mathrm{T}}^2$ in case additional partons are included in the matrix element. A variation of this scale leads to a change in the amount of additional partons being radiated. As systematic uncertainty, the scale parameter in the matrix element is varied up and down by a factor of two.

In CMS, the scale variation is done simultaneously in both the matrix element and the shower in case of MadGraph and Powheg interfaced to Pythia. With this approach, the uncertainty on the amount of ISR/FSR in the shower is assumed to be correlated with the scale variation in the matrix element. All other experiments quote an independent uncertainty on the amount of ISR/FSR by varying the ISR/FSR tuning parameters. The recent approach by ATLAS is to vary the renormalization scale in the Alpgen matrix element and in the Pythia ISR/FSR simultaneously [23].

3.3 Matching uncertainty

When using multi-parton generators like MadGraph or Alpgen, additional jets can be simulated by either the matrix element or the parton shower. The matrix element is expected to be best suited for the description of hard additional partons, the parton shower performs better in describing soft and collinear radiations. The transition between both approaches is handled with a matching algorithm to avoid a possible overlap. The MLM matching algorithm [24] is most often used in the simulation of hadron collisions. It comprises matching-specific free parameters. In CMS the *qcut*, defing the cut-off momentum scale for additional partons from the shower, is used to evaluate the matching uncertainty in MadGraph samples showered with Pythia. The optimal jet matching parameter is determined by inspecting differential jet rates for various values of *qcut* in the simulation. The differential jet rate distributions are required to be smooth in the transition region between additional jets generated in the matrix element and simulated with the parton shower. As systematic uncertainty, the value of *qcut* is varied up and down by a factor of two.

3.4 Hadronization

Similar to the variation of the matrix element, also the hadronization model can be exchanged to quote a systematic uncertainty. In the ATLAS collaboration, the result from Pythia that features the Lund string model is compared to the Herwig cluster model of hadronization. The difference between these samples is quoted as systematic uncertainty.

3.5 Underlying Event

The underlying event comprises multi-parton interactions, hadronization of beam remnants, hadron decays, and also ISR/FSR processes can be treated as part of the UE. The modeling of the UE depends on numerous parameters. The specific setting of these parameters is called tune. There exist various tunes derived from comparisons of collision data from several experiments (also including LEP) to simulations. The systematic impact of the UE tune is validated by comparing Monte-Carlo simulations with different tune settings. At the Tevatron experiments, this is often done in parallel with the hadronization uncertainty. When exchanging Pythia with Herwig, also the UE tune is changed from Tune A to the Jimmy tune. In ATLAS and CMS several comparisons of tunes are performed. For example, the Z2* tune is compared to Perugia 2011 C tune or the Perugia tune is compared to the Perugia 2011 mpiHi parametrization, a dedicated change in the Perugia tune with increased multi-parton interactions.

3.6 Color reconnection

In QCD processes like $\mathrm{t\bar{t}}$ production, initial and final state partons of the matrix element simulation are color charged particles. Due to color charge conservation and confinement the hadronization process has to include a color string connection between initial and final state. The UE tunes of Pythia include dedicated settings to handle color reconnection effects. To evaluate systematic uncertainties on this effect, UE tunes with and without the employment of color reconnections are compared.

3.7 Top quark mass

The top quark mass is set to 172.5 GeV in most of the default $\mathrm{t\bar{t}}$ simulations. For top quark mass measurements, additional samples with various mass values have been generated. In other analyses than top quark mass measurements, these samples can be used to evaluate the impact of variations in the top quark mass.

3.8 PDF

The uncertainty on the parton-distribution function is the only uncertainty that does not require the simulation of additional Monte Carlo samples. These uncertainties are obtained from re-weighting default simulations. The re-weighting is done for every generated event according to the probability to observe this event with certain initial state partons at specific momentum fractions x given another PDF set than the default PDF parametrization. Typical PDF sets used as default are cteq6 subsets or CT10. To determine the systematic uncertainty, the default samples are either weighted according to different PDF sets like CT10, NNPDF [25], or MSTW [26] or are re-weighted according to the cteq6 eigenvectors that parametrize the uncertainty of the cteq6 fit. In most analyses, the treatment of the PDF uncertainty follows these recommendations developed by the PDF4LHC working group [27].

3.9 Top quark p_{T}

Measurements of differential top quark pair production cross sections at CMS [28, 29] show a discrepancy in the top quark p_{T} distribution between data and simulation. The uncertainty on the modeling of the transverse momentum distribution in $\mathrm{t\bar{t}}$ events is only considered by the CMS experiment since no significant difference between data and simulation is observed in the corresponding ATLAS measurement [30]. To account for this difference seen by the CMS experiment, several analyses perform a re-weighting of simulated $\mathrm{t\bar{t}}$ events to correct the modeling of the top quark p_{T} distribution. The difference between un-weighted and twice weighted sample with respect to the nominally weighted sample is taken as systematic uncertainty in these analyses.

4 Validation of systematic uncertainties

To justify the variation of Monte Carlo models used to evaluate systematic uncertainties, several validation analyses are carried out. Many systematic variations are connected to changes in the strong coupling constant α_S, like modifications of the Q^2 scale, matching threshold, or the ISR/FSR parameters. Variations of α_S will lead to enhanced or reduced amount of parton radiation. A natural choice to evaluate these variations is the analysis of jet activity. Studies of additional jet activity in pure $\mathrm{t\bar{t}}$ events are carried out by the ATLAS [31, 32] and CMS [33] experiments. In these studies, additional jets that can not be assigned to the $\mathrm{t\bar{t}}$ system are selected. Beside the multiplicity of additional jets and basic kinematic observables like momentum and rapidity of these jets, the gap fraction of additional jets is measured. The gap fraction $f(Q)$ for leading additional jets is defined as

$$f(Q) = \frac{N(p_{\mathrm{T}} < Q)}{N_{total}} \tag{1}$$

where N_{total} is the total number of selected events and $N(p_{\mathrm{T}} < Q)$ the number of events that does not contain any jet (apart from jets assigned to the $\mathrm{t\bar{t}}$ system) with transverse momentum p_{T} larger than the threshold parameter Q. Alternatively, the gap fraction can be defined as

$$f(Q) = \frac{N(H_{\mathrm{T}} < Q)}{N_{total}} \tag{2}$$

where $N(H_{\mathrm{T}} < Q)$ is the number of events where the summed transverse momentum H_{T} of all additional jets does not exceed Q. Examples of gap fraction distributions compared to different variations of Monte Carlo samples are presented in Figure 1. In the CMS measurement, it can be seen that the variations of Q^2 scale and matching parameters well cover the fluctuation

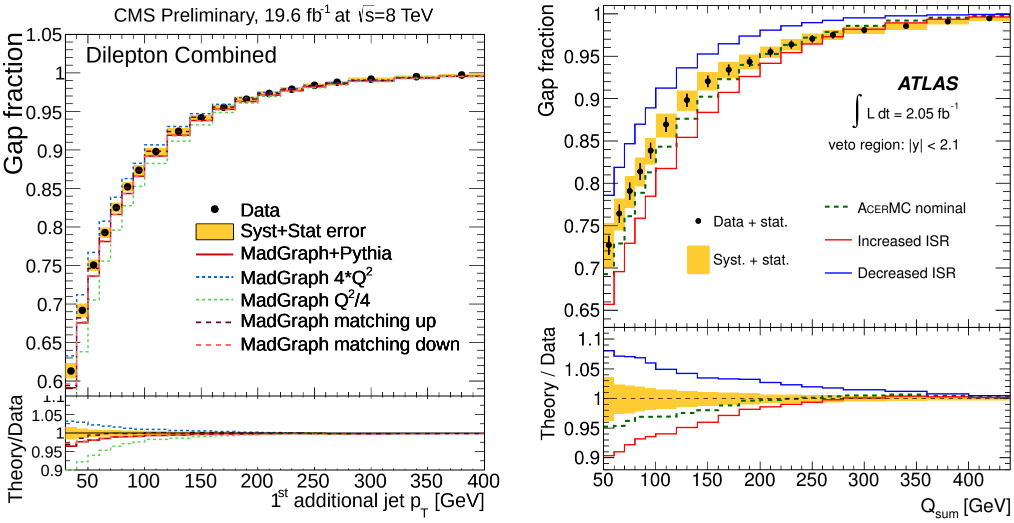

Figure 1: Examples of gap fraction measurements of CMS [33] (left) and ATLAS [32] (right) compared to different variations of $t\bar{t}$ simulations.

observed in data. From the gap fraction measurement in ATLAS it has been concluded that the variation of the ISR parameter in the AcerMC [34] simulation overestimates the uncertainty consistent with the observed data.

A validation of the different available UE tunes has been performed in an analysis by ATLAS [35] using jet shape variables. The internal structure of a jet gives rise to the evolution of the parton shower around a hard quark or gluon emission. In this analysis, jet shape variables are analyzed separately for light and b-quark jets in $t\bar{t}$ events. As exemplary variable, the integrated jet shape $\Psi(r)$ in a cone of radius r smaller than the jet radius R around the jet axis is defined as

$$\Psi(r) = \frac{p_\mathrm{T}(0,r)}{p_\mathrm{T}(0,R)} \tag{3}$$

where $p_\mathrm{T}(r_1, r_2)$ is the scalar sum of the p_T of the jet constituents within a slice of radii r_1 and r_2. The comparison of the integrated jet shape in data to various hadronization and UE models is shown in Figure 2. Most simulations describe the data very well, only the Pythia tune A pro without special treatment of color reconnection effects is found to show some deviations from data.

A similar analysis of the UE has been carried out by CMS [36]. This analysis features the particle flow (PF) algorithm [37] that allows for reconstructing individual particles from the combination of measurements in various detector components. In highly pure $t\bar{t}$ events, the number of charged PF candidates, the total momentum flux in the transverse plane of all charged PF candidates, and their average transverse momentum are measured in different regions with respect to the momentum of the reconstructed $t\bar{t}$ system. Results of this analysis are shown in Figure 3. The difference observed between data and simulation is almost covered by the considered UE tune variations. Especially the tune without color reconnection (labeled No CR) over-estimates the observed variation in data.

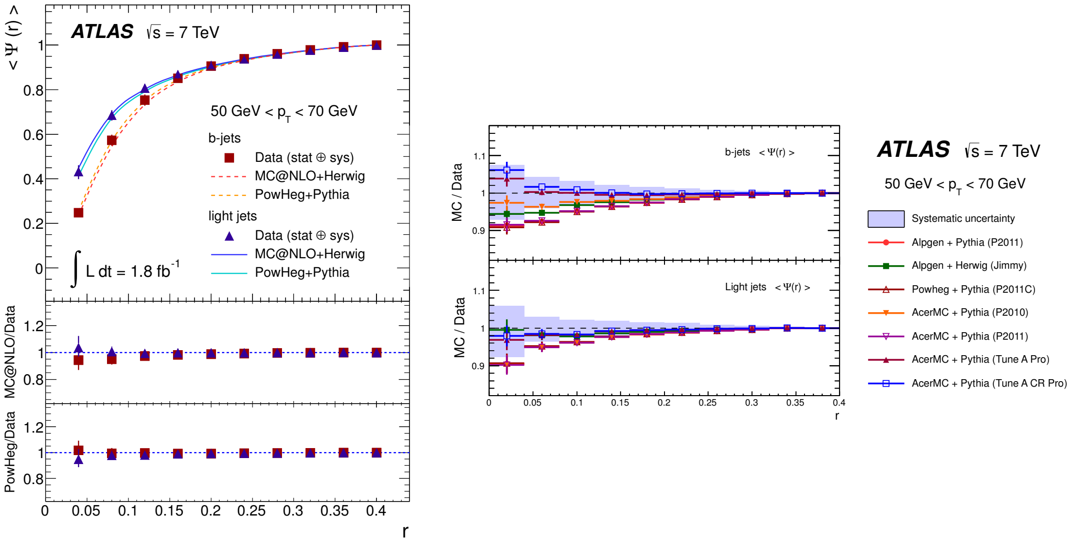

Figure 2: Integrated jet shape measurement [35] for jets with p_{T} between 50 and 70 GeV. A comparison to Monte Carlo simulations with different hadronization models (left) and ratios between measured and simulated integrated jet shapes for different UE tunes (right) are shown.

A second aspect of this analysis is the study of b-quark fragmentation in $\mathrm{t\bar{t}}$ events. Events with an additional muon pair inside a b-tagged jet are selected. This is a clear signature for a decay of a b quark into J/ψ with J/ψ further decaying into $\mu^+\mu^-$. The reconstructed J/ψ mass peak is shown in Figure 4. A good agreement between data and $\mathrm{t\bar{t}}$ simulation is observed, also for other kinematic properties of the J/ψ meson.

5 Impact of modeling uncertainties on selected results

Many analyses of top quark pair production have reached a relatively high level of precision. First of all, the inclusive $\mathrm{t\bar{t}}$ cross section measurements at LHC but also at Tevatron are systematically dominated. For example, the latest inclusive cross section combination of both Tevatron experiments yields $\sigma_{\mathrm{t\bar{t}}}(1.96\ \mathrm{TeV}) = 7.65 \pm 0.20(\mathrm{stat.}) \pm 0.29(\mathrm{syst.}) \pm 0.22(\mathrm{lumi})$ pb [38]. The systematic uncertainty on the total measurement includes uncertainties on the signal modeling of 0.22 pb for the CDF measurement and 0.13 pb on the D0 result. Also one of the latest single measurements performed by ATLAS that yields $\sigma_{\mathrm{t\bar{t}}}(8\ \mathrm{TeV}) = 237.7 \pm 1.7(\mathrm{stat.}) \pm 7.4(\mathrm{syst.}) \pm 7.4(\mathrm{lumi}) \pm 4.0(\mathrm{beamenergy})$ pb [39] has a dominant uncertainty of 1.52% on the total cross section due to modeling uncertainties on the $\mathrm{t\bar{t}}$ signal.

The mass measurements are perhaps the most precise measurements in the top quark sector. An accurate modeling of the $\mathrm{t\bar{t}}$ signal process is a crucial ingredient to these measurements. Mass determinations are nearly the only analyses considering all uncertainties on the Monte Carlo modeling described above. The Tevatron combination results in $m_{\mathrm{t}} = 173.20 \pm 0.87$ GeV [40]. The uncertainty on the measured mass value is dominated by $\mathrm{t\bar{t}}$ modeling uncertainties which sum up to $\Delta m_{\mathrm{t}} = 0.52$ GeV. Also the latest mass combination of the LHC experi-

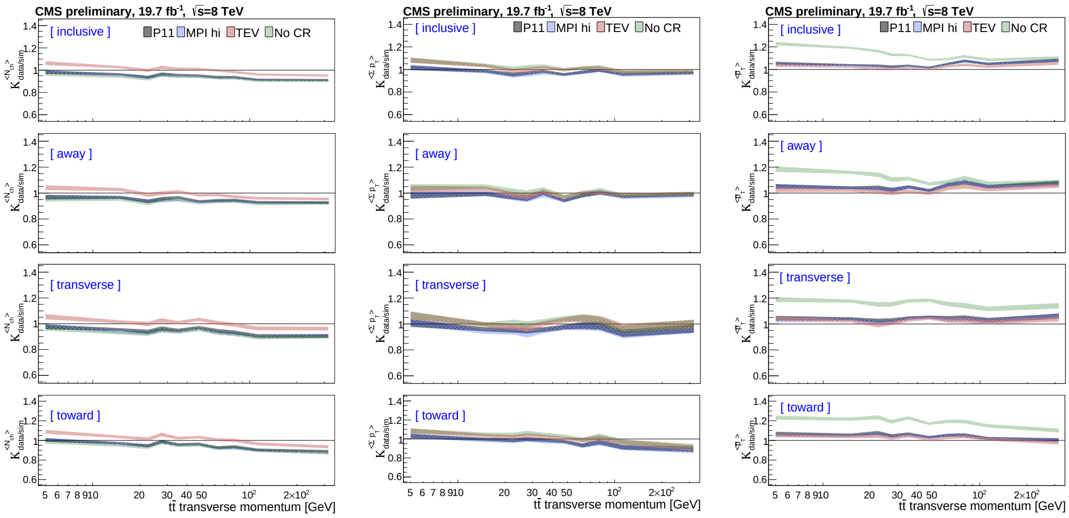

Figure 3: Data to Monte Carlo ratio distributions from the CMS UE measurement [36] for the average number of charged particles (left), total transverse momentum (center), and average particle momentum (right) as function of the p_T of the $\mathrm{t\bar{t}}$ system in different orientations with respect to the $p_\mathrm{T}(\mathrm{t\bar{t}})$ direction.

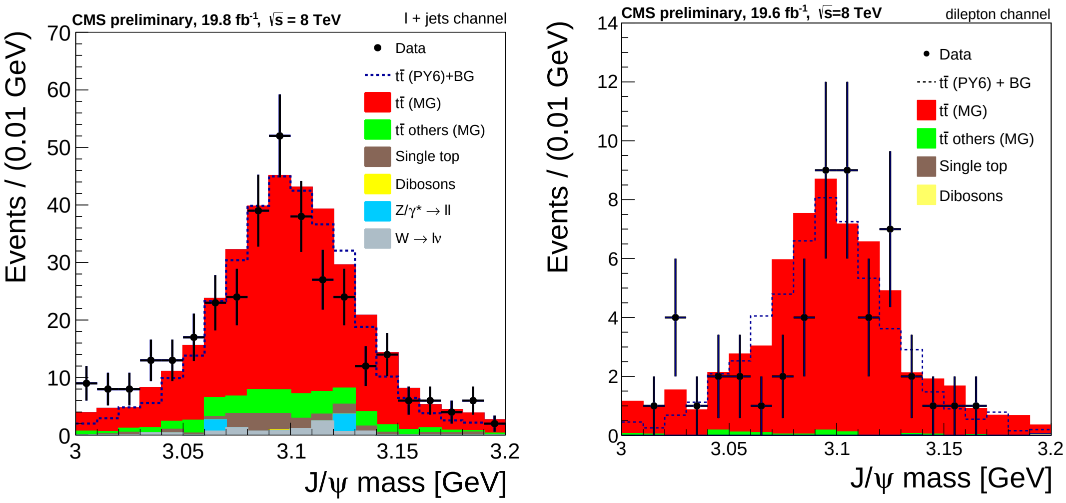

Figure 4: Data to simulation comparison of reconstructed J/ψ mass from muon pairs selected in b-tagged jets in $\mathrm{t\bar{t}}$ events selected in the lepton+jets channel (left) and the di-lepton channel (right) [36].

ments [41] is dominated by uncertainties on the signal model. Beside the uncertainty on the b-jet energy scale, the total uncertainty on the result of $m_\mathrm{t} = 173.29 \pm 0.23(\mathrm{stat.}) \pm 0.92(\mathrm{syst.})$ GeV is dominated by uncertainties on color reconnection ($\Delta m_\mathrm{t} = 0.43$ GeV) and radiation modeling ($\Delta m_\mathrm{t} = 0.32$ GeV).

Also in several measurements of top quark properties, the modeling of the $\mathrm{t\bar{t}}$ signal has often the largest impact on the total systematic uncertainty. As an example, the charge asymmetry measurement by CMS [42] has reached a high precision using the total data sample from the 2012 run. Although the systematic uncertainty on the inclusive charge asymmetry of $A_C = 0.005 \pm 0.007(\mathrm{stat.}) \pm 0.006(\mathrm{syst.})$ is rather small, the uncertainties become larger when measuring the charge asymmetry differentially as function of kinematic observables. In this case, the uncertainty rises to more than $\Delta A_c = 0.02$ in certain bins of the measurement, dominated by uncertainties on hadronization and matrix element generation. Also other properties measurements like the W helicity combination from ATLAS and CMS [43] heavily rely on the correct modeling of differential distributions of the $\mathrm{t\bar{t}}$ process in simulation. Approximately half of the systematic uncertainties on the measured helicity fractions $F_0 = 0.6262 \pm 0.034(\mathrm{stat.}) \pm 0.048(\mathrm{syst.})$ and $F_L = 0.3592 \pm 0.021(\mathrm{stat.}) \pm 0.028(\mathrm{syst.})$ are driven by uncertainties on the signal model.

6 Modeling of single top quarks

Beside top quark pair production, top quarks are also being produced as single quarks in electroweak processes. Three processes contribute to single top quark production: t channel, s channel and tW channel. These three processes are generated separately by all collaborations. At the Tevatron, the contribution of the tW channel is negligible. Therefore, only s and t channel processes are simulated. CDF utilizes Powheg [44] interfaced to Pythia 6 for the shower with cteq66 as PDF for both single top quark production modes. D0 simulates single top quark events with the SINGLETOP generator [45] together with Pythia 6 for shower and hadronization and cteq6m as PDF. At the ATLAS experiment, different generators are used for all production modes. The t channel is simulated with AcerMC v3.7 [34] interfaced to Pythia 6 and PDF set cteq6ll. The s and tW channels are either being generated with MC@NLO 4 together with Herwig 6 and Jimmy and cteq66 PDF for samples with 7 TeV center-of-mass energy, or with Powheg [44, 46] interfaced to Pythia 6 and with the CT10 PDF in case of 8 TeV. CMS uses the same combination of Powheg and Pythia for all three single top quark production modes but with cteq6m as default PDF set.

Most systematic uncertainties on the modeling of single top quark production are handled in a similar way as the modeling uncertainties on $\mathrm{t\bar{t}}$ production described above. Since no analysis uses multi-parton generators like MadGraph for the simulation of single top quark events no parton matching uncertainty has to be considered. The precision of most single top quark measurements has not yet reached the same level of accuracy as some analyses of top quark pair production. Thus, uncertainties on color reconnection and UE tunes have not yet been considered for the simulations of single top quarks. Although statistical uncertainties are still larger compared to most $\mathrm{t\bar{t}}$ studies, the inclusive single top quark t channel cross section measurements are already limited by systematic uncertainties. In a recent ATLAS measurement, a cross section of $\sigma_\mathrm{t} = 95 \pm 18$ pb has been determined [47]. The statistical error is almost negligible and the systematic uncertainty is mainly driven by modeling uncertainties on ISR/FSR treatment and matrix element generators. In this particular analysis, the uncertainty on the matrix element generation is estimated by comparing the default AcerMC simulation to higher-order predictions from MCFM [48].

In the tW channel, a special systematic uncertainty on the modeling with Monte Carlo generators has to be considered. The tW process is not unambiguously distinguishable from $t\bar{t}$ at NLO because there are interfering Feynman diagrams from both processes. Two different approaches exist to remove the overlap between tW and $t\bar{t}$ processes, the diagram subtraction (DS) and the diagram removal (DR) methods. Both schemes are available in the MC@NLO and Powheg event generators. Samples for the tW process with both schemes have been generated and the difference between the DS and DR schemes is considered as additional systematic uncertainty. In the analysis of the tW channel by CMS [49] that yields a cross section of $\sigma_{\mathrm{tW}} = 23.4^{+5.5}_{-5.4}$ pb, a change on the result of 2% is observed when exchanging the simulations with DS and DR schemes.

7 Conclusion

The modeling of top quark production in hadron collisions with Monte Carlo event generators includes several technical steps that require dedicated tuning of parameters. Optimizing the event generation is a key ingredient for precise measurements in top quark physics. Uncertainties on the modeling of top quark production are limiting many analyses performed by the four experiments ATLAS, CDF, CMS, and D0. The choice of generator parameters and their variation that is done to determine systematic uncertainties are often not well justified. For example, scale and matching parameters are usually varied by an arbitrary factor of two.

Several studies have been performed to reduce the uncertainties on the modeling of $t\bar{t}$ events and to optimize the generator tuning. In jet activity and underlying event analyses, it has been shown that the considered systematic variations cover the observed fluctuations in data but some of these variations show significant discrepancies with respect to measured distributions. Especially variations of ISR and color reconnection effects clearly overestimate the uncertainties consistent with the observed data. In case of the ISR variations, a new treatment of the radiation uncertainty has been developed in the ATLAS collaboration based on the jet gap fraction measurement. Other systematic uncertainties have been validated but an optimization has not been propagated to the event generation yet. This will have to take place in the future to further improve the sensitivity of many analyses in top quark physics.

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