Improvements in $t\bar{t}$ modelling using NLO+PS Monte Carlo generators for Run 2

The ATLAS Collaboration

Monte Carlo generators at next-to-leading order (NLO) precision in QCD matched to a parton shower (PS) have been extensively used by ATLAS to model top-quark pair production. During Run 2 these NLO+PS configurations have been updated to provide improved modelling and reduced systematic uncertainties. This note provides a summary of these improvements. The studies are performed using published unfolded data at a centre-of-mass energy of 13 TeV.
1 Introduction

Reliable predictions for the production of a top-quark pair ($t\bar{t}$) are crucial for the study of the kinematic properties of the top quark as well as many new-physics searches at the Large Hadron Collider (LHC), where the sensitivity can depend critically on the $t\bar{t}$ modelling. The ATLAS Collaboration has previously documented its choice of Monte Carlo (MC) generator parameters and the testing of new MC setups in order to improve the description of top-quark kinematics in Refs. [1–5]. The aim of this note is to discuss the improvements of top-quark pair modelling for both the nominal MC generator setups and for the corresponding systematic uncertainty model in comparison to the setup used for the early Run 2 analyses. Only MC generator setups at next-to-leading order (NLO) in QCD interfaced to a parton shower (PS) are considered. The comparisons are done using published unfolded $t\bar{t}$ data at $\sqrt{s} = 13$ TeV. The different MC generator setups that have been studied are discussed in Section 2 and a brief overview of the Rivet [6] analyses used to compare to the unfolded data distributions are provided in Section 3. A side-by-side comparison between the early Run 2 setup and the improved Run 2 setup is given in Section 4 and a comparison of the combined systematic uncertainty is shown in Section 5. Finally, conclusions are given in Section 6.

2 MC Generator settings

In the following, a description of the inclusive $t\bar{t}$ samples used for the 13 TeV data analyses in Run 2 is given. The NLO $t\bar{t}$ inclusive production cross section is corrected to the theory prediction at next-to-next-to-leading order (NNLO) including the resummation of next-to-next-to-leading logarithmic (NNLL) soft-gluon terms calculated using Top++2.0 [7–13]. For proton–proton collisions at a centre-of-mass energy of $\sqrt{s} = 13$ TeV, this cross section corresponds to $\sigma(t\bar{t})_{\text{NNLO+NNLL}} = 832 \pm 51$ fb using a top-quark mass of $m_{\text{top}} = 172.5$ GeV.

2.1 Setups for early Run 2 analyses

The nominal $t\bar{t}$ sample used in early Run 2 data analyses was generated using Powheg [14, 15] v2 interfaced to Pythia6 [16] with the Perugia 2012 set of tuned parameters [17]. In this sample, the PDF used in the matrix element (ME) calculation is CT10 [18] and the PDF in the PS is CTEQ6L1 [19]. The functional form used for renormalisation and factorisation scales ($\mu_R, \mu_F$) is

$$\mu = \sqrt{m_{\text{top}}^2 + p_T^2},$$

which is calculated from the top quark mass, $m_{\text{top}}$, and the transverse momentum before radiation.

Two supplementary Powheg+Pythia6 samples were produced to assess the impact of more or less additional radiation. The parameters for these samples are as follows:

- The factorisation and renormalisation scales are coherently varied by a factor of 0.5, the $h_{\text{damp}}$ value is increased to 2.0 $m_{\text{top}}$ and the “radHi” variation from the P2012 tune is used.

$^1$ NLO electroweak corrections are not taken into account in the studies presented in this note.
The factorisation and renormalisation scales are coherently varied by a factor of 2.0, the $h_{\text{damp}}$ value stays at $m_{\text{top}}$ and the “radLo” variation from the P2012 tune is used. The envelope of these two samples is used to evaluate the uncertainty due to more or less additional radiation. To evaluate the impact of the model for parton showering and hadronisation, the Powheg sample is interfaced with Herwig++ [20–22]. To assess the uncertainty due to the choice of matching scheme, a MadGraph5_aMC@NLO [23, 24] sample is produced and interfaced with Herwig++. Further details can be found in Tab. 1.

2.2 Improved generator setups

After detailed studies presented in Refs. [2, 4], a new nominal $t\bar{t}$ sample was defined, using Powheg v2 interfaced with Pythia8 [25] and the A14 set of tuned parameters [26] using the NNPDF23LO PDF. Again, the functional form of the renormalisation and factorisation scale was set to the default scale defined in Eq. 1.

It was found that the choice of $h_{\text{damp}}$ set to 1.5 $m_{\text{top}}$ gives the best description of the data distributions [3]. The impact of varying the amount of additional radiation is assessed using two samples with the following settings:

- The factorisation and renormalisation scales are both varied by a factor of 0.5, the $h_{\text{damp}}$ value is increased to 3.0 $m_{\text{top}}$ and the Var3c up variation from the A14 tune is used.

- The factorisation and renormalisation scales are both varied by a factor of 2.0, the $h_{\text{damp}}$ value stays at 1.5 $m_{\text{top}}$ and the Var3c down variation from the A14 tune is used.

The Var3c A14 tune variation [26] corresponds to the variation of $\alpha_s$ for initial state radiation (ISR) in the A14 tune.

The impact of the PS and hadronisation model is evaluated by comparing the nominal generator setup with a Powheg sample interfaced to Herwig7 [21, 27], using the H7UE set of tuned parameters [27]. To assess the uncertainty due to the choice of the matching scheme, a new MadGraph5_aMC@NLO+Pythia8 setup was employed, which uses $\mu_q = H_T/2$ for the functional form of the shower starting scale. $H_T$ is defined here as the scalar sum of the $p_T$ of all outgoing partons. The renormalisation and factorisation scale choice is the same as for the Powheg setup.

A summary of these configurations can be found in Tab. 2.
Table 1: ME and PS/UE generator settings for each of the MC samples used for the early Run 2 analyses. The generator versions, the PDFs used for the ME and in the PS and the matching scheme are shown alongside the tune.

<table>
<thead>
<tr>
<th>ME Gen.</th>
<th>PS/UE Gen.</th>
<th>ME PS/UE PDF</th>
<th>PS Tune</th>
<th>Matching</th>
</tr>
</thead>
<tbody>
<tr>
<td>Powheg-Box</td>
<td>Pythia</td>
<td>CT10</td>
<td>P2012</td>
<td>Powheg</td>
</tr>
<tr>
<td>r3026 (v2)</td>
<td>6.427</td>
<td>CTEQ6L1</td>
<td></td>
<td>($h_{\text{damp}} = m_{\text{top}}$)</td>
</tr>
<tr>
<td>Powheg-Box</td>
<td>Pythia</td>
<td>CT10</td>
<td>P2012 (radHi)</td>
<td>Powheg</td>
</tr>
<tr>
<td>r3026 (v2)</td>
<td>6.427</td>
<td>CTEQ6L1</td>
<td></td>
<td>($h_{\text{damp}} = 2 \cdot m_{\text{top}}, \mu_R, F = 0.5$)</td>
</tr>
<tr>
<td>Powheg-Box</td>
<td>Pythia</td>
<td>CT10</td>
<td>P2012 (radLo)</td>
<td>Powheg</td>
</tr>
<tr>
<td>r3026 (v2)</td>
<td>6.427</td>
<td>CTEQ6L1</td>
<td></td>
<td>($h_{\text{damp}} = m_{\text{top}}, \mu_R, F = 2.0$)</td>
</tr>
<tr>
<td>Powheg-Box</td>
<td>Herwig++</td>
<td>CT10</td>
<td>UE-EE-5</td>
<td>Powheg</td>
</tr>
<tr>
<td>r3026 (v2)</td>
<td>2.7.1</td>
<td>CTEQ6L1</td>
<td></td>
<td>($h_{\text{damp}} = m_{\text{top}}$)</td>
</tr>
<tr>
<td>MadGraph5_aMC@NLO</td>
<td>Herwig++</td>
<td>CT10</td>
<td>UE-EE-5</td>
<td>MC@NLO</td>
</tr>
<tr>
<td>2.2.1</td>
<td>2.7.1</td>
<td>CTEQ6L1</td>
<td></td>
<td>($\mu_q = \sqrt{s}$)</td>
</tr>
</tbody>
</table>

Table 2: ME and PS/UE generator settings for each of the MC samples with the most recent generator version and improved settings. The generator versions, the PDFs used for the ME and in the PS and the matching scheme are shown alongside the tune.

<table>
<thead>
<tr>
<th>ME Gen.</th>
<th>PS/UE Gen.</th>
<th>ME PS/UE PDF</th>
<th>PS Tune</th>
<th>Matching</th>
</tr>
</thead>
<tbody>
<tr>
<td>Powheg-Box</td>
<td>Pythia</td>
<td>NNPDF3.0NLO</td>
<td>A14</td>
<td>Powheg</td>
</tr>
<tr>
<td>r3026 (v2)</td>
<td>8.230</td>
<td>NNPDF2.3LO</td>
<td></td>
<td>($h_{\text{damp}} = 1.5 m_{\text{top}}$)</td>
</tr>
<tr>
<td>Powheg-Box</td>
<td>Pythia</td>
<td>NNPDF3.0NLO</td>
<td>A14 Var3c (Up)</td>
<td>Powheg</td>
</tr>
<tr>
<td>r3026 (v2)</td>
<td>8.230</td>
<td>NNPDF2.3LO</td>
<td></td>
<td>($h_{\text{damp}} = 3.0 m_{\text{top}}, \mu_E, F = 0.5$)</td>
</tr>
<tr>
<td>Powheg-Box</td>
<td>Pythia</td>
<td>NNPDF3.0NLO</td>
<td>A14 Var3c (Down)</td>
<td>Powheg</td>
</tr>
<tr>
<td>r3026 (v2)</td>
<td>8.230</td>
<td>NNPDF2.3LO</td>
<td></td>
<td>($h_{\text{damp}} = 1.5 m_{\text{top}}, \mu_E, F = 2.0$)</td>
</tr>
<tr>
<td>Powheg-Box</td>
<td>Herwig++</td>
<td>NNPDF3.0NLO</td>
<td>H7-UE-MMHT</td>
<td>Powheg</td>
</tr>
<tr>
<td>r3026 (v2)</td>
<td>7.0.4</td>
<td>MMHT2014lo68cl</td>
<td></td>
<td>($h_{\text{damp}} = m_{\text{top}}$)</td>
</tr>
<tr>
<td>MadGraph5_aMC@NLO</td>
<td>Pythia</td>
<td>NNPDF3.0NLO</td>
<td>A14</td>
<td>MC@NLO</td>
</tr>
<tr>
<td>2.6.0</td>
<td>8.230</td>
<td>NNPDF2.3LO</td>
<td></td>
<td>($\mu_q = H_T/2$)</td>
</tr>
</tbody>
</table>
3 Measurements of $t\bar{t}$ production

Predictions of various MC generators are compared to ATLAS data. Unfolded distributions from 13 TeV measurements are used. Measurements are unfolded to particle level in a fiducial phase-space. Particle-level objects are defined for simulated events in analogy to detector-level objects. Only stable final-state particles, i.e. particles with a mean lifetime $\tau > 30$ ps are considered. The results are corrected for all detector effects, in a fiducial volume as close as possible to the experimental acceptance. The studies shown in this document have been performed with Rivet v.2.5.4 [6] and the analyses used are listed below.

- Analysis A: Measurement of jet activity produced in top-quark events with an electron, a muon and two $b$-tagged jets in the final state in $pp$ collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector (ATLAS_2017_I1495243) [28]

  The cross-sections are measured at particle level as function of jet multiplicities and jet transverse momentum spectra, using $3.2 \text{ fb}^{-1}$ of $pp$ collision data. The events are selected in the dilepton channel, which is characterised by the presence of exactly one electron and one muon with opposite charge and at least two jets being identified to originate from a $b$-quark. Jets originating from $b$-quarks are defined using a $B$-hadron matching, requiring at least one $B$-hadron to be found within the jet using the ghost association technique [29–31]. The jets are reconstructed with the anti-$k_t$ jet algorithm with a radius parameter $R = 0.4$ [32]. Only jets and leptons with $p_T > 25$ GeV and $|\eta| < 2.5$ are considered in the analysis.

- Analysis B: Measurements of top-quark pair differential cross-sections in the lepton+jets channel in $pp$ collisions at $\sqrt{s} = 13$ TeV using the ATLAS detector (ATLAS_2017_I1614149) [33]

  The cross-sections are measured at particle level using $3.2 \text{ fb}^{-1}$ of $pp$ collision data. The observables are the transverse momentum and absolute rapidity of the hadronically decaying top quark as well as the the transverse momentum, absolute rapidity and invariant mass of the $t\bar{t}$-system. The events are selected in the lepton+jets channel, which is characterised by the presence of exactly one charged lepton (electron or muon) and at least four jets, with at least two jets being identified to originate from a $b$-quark using the same technique described in Analysis A. The jets are reconstructed with the anti-$k_t$ jet algorithm with a radius parameter $R = 0.4$ [32]. Only jets with $p_T > 25$ GeV and $|\eta| < 2.5$ are considered in the analysis.
4 Evaluation of systematic uncertainties

In the following, the MC predictions and their corresponding systematic variations for the early Run 2 and improved Run 2 setups are compared side-by-side. Only the uncertainty due to additional QCD radiation, the choice of NLO+PS matching scheme and the PS and hadronisation model are studied here. The figures are ordered such that the figures on the left always show the setups used for the early Run 2 analyses, while the right-hand figures show the improved setup. It has to be noted, however, that not all early Run 2 analyses used the setup as described here. Some analyses which were performed in more extreme regions of phase space strongly suffered from the large fraction of negative event weights in the MadGraph5_aMC@NLO setups, and have therefore chosen to assign the difference with respect to other alternative generator setups, such as Sherpa [34], as a conservative NLO+PS uncertainty. Furthermore, the studies presented here are performed at particle level in the phase space of published analyses and the size of the systematic effect might be different in the phase space probed by ongoing analyses. However, the studies give a good indication about the level of the agreement between data and MC and the overall size of uncertainties.

The sources of systematic uncertainties are summarised in Tab. 3 for the early Run 2 analyses, and in Tab. 4 for the improved setup.

Figures 1–5 show the impact of additional radiation on the jet multiplicity and kinematic distributions related either to the top quark or $t\bar{t}$ system. Fig. 1 and Fig. 3 exemplify the improvement in the nominal prediction and in particular the reduction of uncertainties for the new setup, which now provides a good bracket of the uncertainties in data. At the same time, other distributions like the ones in Fig. 2 and Figs. 4–5 are not significantly affected, and in some cases still display a bad description of data for all setups.

Figures 6–10 compare the different NLO+PS schemes and the effect of the PS and hadronisation model for the same observables as above. For Fig. 6(b), Figs. 7 and Fig. 10 the different setups agree now better with data within the corresponding uncertainties and the spread of the variations is reduced. The leading jet $p_T$ in Fig. 6(d) is not well modelled by the MadGraph5_aMC@NLO+Pythia8 prediction. In Fig. 8 the same effect can be seen, where the MadGraph5_aMC@NLO+Pythia8 prediction is shown to be incompatible with data for some of the veto regions, but the two other predictions agree now better with data than the ones from the early Run 2 setups. The discrepancy between predictions and data in the $p_T^{\text{top}}$ distributions in Fig. 9 is a long-standing issue [1, 4] and is still present in the new predictions. While the old setups with the extreme Powheg+Herwig++ variation showed somewhat better agreement with respect to data, the mismodelling is likely due to missing higher orders rather than due to a suboptimal generator setup.
Table 3: Systematic uncertainties for the $t\bar{t}$ process used for the early Run 2 analyses, with Powheg+Pythia6 as nominal sample. The symbol $\Delta$ denotes the difference of the predictions for the analysis observables between the two generators in the column ‘Samples’. The notation $\pm|\Delta|$ indicates that the full difference is symmetrised and applied to the nominal sample. Without the absolute value bars, $\Delta$ indicates that the signed difference with respect to the nominal for all variations is used to estimate the uncertainty.

<table>
<thead>
<tr>
<th>Source of Uncertainty</th>
<th>Samples</th>
<th>Procedure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nominal</td>
<td>Powheg+Pythia6</td>
<td>N/A</td>
</tr>
<tr>
<td>NLO+PS matching</td>
<td>Powheg+Herwig++ vs.</td>
<td>$\pm</td>
</tr>
<tr>
<td></td>
<td>MadGraph5_aMC@NLO+Herwig++</td>
<td></td>
</tr>
<tr>
<td>Parton Shower and</td>
<td>Powheg+Pythia6 vs.</td>
<td>$\pm</td>
</tr>
<tr>
<td>Hadronization Model</td>
<td>Powheg+Herwig++</td>
<td></td>
</tr>
<tr>
<td>Additional Radiation</td>
<td>Powheg+Pythia6 P2012 (RadHi tune, $\mu_{R,F} = 0.5$, $h_{damp} = 1.5 , m_{top}$ vs. RadLo tune, $\mu_{R,F} = 2.0$, $h_{damp} = 1.0 , m_{top}$)</td>
<td>$\Delta$</td>
</tr>
</tbody>
</table>

Table 4: Systematic uncertainties for the $t\bar{t}$ process using Powheg+Pythia8 as nominal sample. The symbol $\Delta$ denotes the difference of the predictions for the analysis observables between the two generators in the column ‘Samples’. The notation $\pm|\Delta|$ indicates that the full difference is symmetrised and applied to the nominal sample. Without the absolute value bars, $\Delta$ indicates that the signed difference with respect to the nominal for all variations is used to estimate the uncertainty.

<table>
<thead>
<tr>
<th>Source of Uncertainty</th>
<th>Samples</th>
<th>Procedure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nominal</td>
<td>Powheg+Pythia8</td>
<td>N/A</td>
</tr>
<tr>
<td>NLO+PS matching</td>
<td>Powheg+Pythia8 vs.</td>
<td>$\pm</td>
</tr>
<tr>
<td></td>
<td>MadGraph5_aMC@NLO+Pythia8</td>
<td></td>
</tr>
<tr>
<td>Parton Shower and</td>
<td>Powheg+Pythia8 vs.</td>
<td>$\pm</td>
</tr>
<tr>
<td>Hadronization Model</td>
<td>Powheg+Herwig7</td>
<td></td>
</tr>
<tr>
<td>Additional Radiation</td>
<td>Powheg+Pythia8 A14 (Var. 3c up, $\mu_{R,F} = 0.5$, $h_{damp} = 3.0 , m_{top}$ vs. Var. 3c down, $\mu_{R,F} = 2.0$, $h_{damp} = 1.5 , m_{top}$)</td>
<td>$\Delta$</td>
</tr>
</tbody>
</table>
Figure 1: The impact of parameter variations that lead to additional radiation for the Powheg+Pythia6 generator (left) and the Powheg+Pythia8 generator (right) compared to data at \( \sqrt{s} = 13 \text{ TeV} \). The comparison is performed for (a,b) the number of additional jets and (c,d) the transverse momentum of the leading jet, using ATLAS data unfolded to particle level in Analysis A [28]. The expression \( h_d \) describes the \( h_{\text{damp}} \) parameter in multiplicities of \( m_{\text{top}} \). The data are represented as closed (black) circles with the total experimental uncertainty on the data (statistical and systematic) indicated by the error bars. The generator predictions are shown as coloured lines.
Figure 2: The impact of parameter variations that lead to additional radiation for the Powheg+Pythia6 generator (left) and the Powheg+Pythia8 generator (right) compared to data at $\sqrt{s} = 13$ TeV. The comparison is performed for (a,b) the transverse momentum of the leading and (c,d) the transverse momentum of the subleading $b$-jets, using ATLAS data unfolded to particle level in Analysis A [28]. The expression $h_d$ describes the $h_{damp}$ parameter in multiplicities of $m_{top}$. The data and generator predictions are presented the same way as in Fig. 1.
Figure 3: The impact of parameter variations that lead to additional radiation for the Powheg+Pythia6 generator (left) and the Powheg+Pythia8 generator (right) compared to data at $\sqrt{s} = 13$ TeV. The comparison is performed for the jet gap fraction in different rapidity veto regions: (a,b) for $0.8 < |y| < 1.5$ and (c,d) for $1.5 < |y| < 2.1$, using ATLAS data unfolded to particle level in Analysis A [28]. The expression $h_d$ describes the $h_{\text{damp}}$ parameter in multiplicities of $m_{\text{top}}$. The data and generator predictions are presented the same way as in Fig. 1.
Figure 4: The impact of parameter variations that lead to additional radiation for the Powheg+Pythia6 generator (left) and the Powheg+Pythia8 generator (right) compared to data at $\sqrt{s} = 13$ TeV. The comparison is performed for (a,b) the transverse momentum of the top quark and (c,d) the transverse momentum of the $t\bar{t}$ system, using ATLAS data unfolded to particle level in Analysis B [33]. The expression $h_d$ describes the $h_{\text{damp}}$ parameter in multiplicities of $m_{\text{top}}$. The data and generator predictions are presented the same way as in Fig. 1.
Figure 5: The impact of parameter variations that lead to additional radiation for the Powheg+Pythia6 generator (left) and the Powheg+Pythia8 generator (right) compared to data at $\sqrt{s} = 13$ TeV. The comparison is performed for the invariant mass of the $t\bar{t}$ system, using ATLAS data unfolded to particle level in Analysis B [33]. The expression $h_d$ describes the $h_{\text{amp}}$ parameter in multiplicities of $m_{\text{top}}$. The data and generator predictions are presented the same way as in Fig. 1.
Figure 6: Comparison of different generator setups used to assess the NLO+PS matching as well as the PS and hadronisation uncertainty as defined for early Run 2 analyses (left) and after optimisation (right), compared to data at $\sqrt{s} = 13\text{ TeV}$. The comparison is performed for (a,b) the number of additional jets and (c,d) the transverse momentum of the leading jet, using ATLAS data unfolded to particle level in Analysis A [28]. The expression $h_d$ describes the $h_{\text{damp}}$ parameter in multiplicities of $m_{\text{top}}$. The data are represented as closed (black) circles with the total experimental uncertainty on the data (statistical and systematic) indicated by the error bars. The generator predictions are shown as coloured lines.
Figure 7: Comparison of different generator setups used to assess the NLO+PS matching as well as the PS and hadronisation uncertainty as defined for early Run 2 analyses (left) and after optimisation (right), compared to data at √s = 13 TeV. The comparison is performed for (a,b) the transverse momentum of the leading and (c,d) the transverse momentum of the subleading b-jets, using ATLAS data unfolded to particle level in Analysis A [28]. The expression $h_d$ describes the $h_{\text{damp}}$ parameter in multiplicities of $m_\text{top}$. The data and generator predictions are presented the same way as in Fig. 1.
Figure 8: Comparison of different generator setups used to assess the NLO+PS matching as well as the PS and hadronisation uncertainty as defined for early Run 2 analyses (left) and after optimisation (right), compared to data at $\sqrt{s} = 13$ TeV. The comparison is performed for the jet gap fraction in different rapidity veto regions: (a,b) for $0.8 < |y| < 1.5$ and (c,d) for $1.5 < |y| < 2.1$, using ATLAS data unfolded to particle level in Analysis A [28]. The expression $h_d$ describes the $h_{\text{damp}}$ parameter in multiplicities of $m_{\text{top}}$. The data and generator predictions are presented the same way as in Fig. 1.
Figure 9: Comparison of different generator setups used to assess the NLO+PS matching as well as the PS and hadronisation uncertainty as defined for early Run 2 analyses (left) and after optimisation (right), compared to data at $\sqrt{s} = 13$ TeV. The comparison is performed for (a,b) the transverse momentum of the top quark and (c,d) the transverse momentum of the $t\bar{t}$ system, using ATLAS data unfolded to particle level in Analysis B [33]. The expression $h_d$ describes the $h_{\text{damp}}$ parameter in multiplicities of $m_{\text{top}}$. The data and generator predictions are presented the same way as in Fig. 1.
Figure 10: Comparison of different generator setups used to assess the NLO+PS matching as well as the PS and hadronisation uncertainty as defined for early Run 2 analyses (left) and after optimisation (right), compared to data at $\sqrt{s} = 13$ TeV. The comparison is performed for the invariant mass of the $t\bar{t}$ system, using ATLAS data unfolded to particle level in Analysis B [33]. The expression $h_d$ describes the $h_{\text{damp}}$ parameter in multiplicities of $m_{\text{top}}$. The data and generator predictions are presented the same way as in Fig. 1.
5 Improvement in $t\bar{t}$ modelling

In the following, the early Run 2 setup is compared to the improved setup, combining the uncertainties due to additional radiation, the NLO+PS matching and the parton shower and hadronisation model in one uncertainty band. The difference between the nominal distribution and the variation is calculated in each bin, and are added in quadrature for the three systematic effects. For the NLO+PS matching as well as the parton shower and hadronisation uncertainty, the effect is symmetrised around the nominal, while for the additional radiation systematic the up and down shifts are taken into account separately. The nominal prediction along with its corresponding uncertainty band is shown in red for the early Run 2 setup, and in blue for the improved setup. The uncertainty on the data includes the full experimental uncertainty (statistical and systematic) and is indicated by the error bars.

For the Figures 11 (a,c) 12 and 13 (a,c), an overall reduction in the uncertainty band for the improved setup is observed, such that in most bins the reduced uncertainty band is no longer significantly larger than the measurement uncertainty, indicated by the error bars.

The nominal predictions are found to better reproduce the data in terms of jet multiplicity, jet gap fraction and, marginally, the $p_T$ of the hadronic system, whilst a similar agreement is found for the remaining distributions.
Figure 11: Comparison of the generator setup defined for early Run 2 analyses (red) with the improved Run 2 setup (blue), compared to data at $\sqrt{s} = 13$ TeV. The comparison is performed for (a) the number of additional jets, (b) the transverse momentum of the leading additional jet, (c) the transverse momentum of the leading $b$-jet as well as (d) the transverse momentum of the subleading $b$-jet, using ATLAS data unfolded to particle level in Analysis A [28]. The data are represented as closed (black) circles with the total experimental uncertainty on the data (statistical and systematic) indicated by the error bars.
Figure 12: Comparison of the generator setup defined for early Run 2 analyses (red) with the improved Run 2 setup (blue), compared to data at $\sqrt{s} = 13$ TeV. The comparison is performed for the jet gap fraction in different rapidity veto regions: (a) $0.8 < |y| < 1.5$ and (b) $1.5 < |y| < 2.1$, using data unfolded to particle level in Analysis A [28]. The data are represented as closed (black) circles with the total experimental uncertainty on the data (statistical and systematic) indicated by the error bars.
Figure 13: Comparison of the generator setup defined for early Run 2 analyses (red) with the improved setup (blue), compared to data at $\sqrt{s} = 13$ TeV. The comparison is performed for (a) the transverse momentum of the hadronic top quark, (b) the transverse momentum of the $t\bar{t}$ system, and (c) the invariant mass of the $t\bar{t}$ system, using ATLAS data unfolded to particle level in Analysis B [33]. The data are represented as closed (black) circles with the total experimental uncertainty on the data (statistical and systematic) indicated by the error bars.
6 Conclusion

Studies of Monte Carlo generator setups for the top-quark pair production in $pp$ collisions at a centre-of-mass energy of 13 TeV have been presented. Two different setups have been compared: the first one being the generator setup used for the early Run 2 data analyses with Powheg+Pythia6 as the nominal MC generator, as well as Powheg+Herwig++ and MadGraph5_aMC@NLO+Herwig++ to evaluate systematic uncertainties. The second setup uses newer generators and improved settings, with Powheg+Pythia8 as the nominal as well as Powheg+Herwig7 and MadGraph5_aMC@NLO+Pythia8 to evaluate systematic uncertainties. The studies were performed in the lepton+jets and dilepton channels and show a clear improvement for the updated setup, both for the nominal MC generator and for the combined systematic uncertainty. Although not explicitly discussed in this note, significant work is ongoing on the theory side to improve the modelling further [35–38].
References


