Measurements on top quark pairs in proton collisions recorded with the ATLAS detector
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Simulation and reconstruction of top quark pair events

As in nearly all particle physics research, we compare observable quantities in data to their theoretical predictions in order to be able to quantify the level of understanding of the observations. The predictions are obtained by detailed simulation of the collisions and detector response. For instance, to measure the production cross section of top-antitop quark pair ($t\bar{t}$) events, we compare the number of events observed in data to the number we expect according to the Standard Model predictions. Besides this overall rate, also differential distributions—for example, the angular distribution of hadronic jets—are compared between the predictions and observations.

We describe the simulation of collisions between protons at LHC energies in this chapter. The simulation of collision events in ATLAS consists of several steps, as indicated in Figure 3.1. At the first step, particle collisions are generated with Monte Carlo event generators. This encompasses the simulation of the hard scattering between partons in the protons, their decay products (including the emission of extra partons), the hadronization to evolve the partons to colorless physical particles, and the description of the behavior of the proton remnants. During a second step, the produced particles are fed to a simulation that mimics the response of the ATLAS detector. In this step the interactions and decays of the particles with the magnetic field and the detector elements are simulated. During the last step, the digitization, the electronic signals that result from the energy losses of particles in the detector geometry are described. In this way, the output format of the detector response matches the actual format of the data. Finally, a sets of algorithms is applied in order to reconstruct physics objects from the digitized output of both the data and the simulation chain.
In this chapter, we discuss the four steps of event simulation (event generation, detector simulation, digitization and reconstruction) in more detail. This includes a separate study on the emission of extra partons during the generation of $t\bar{t}$ events, and the effect this may have on our results in the analyses that are conducted later.

Section 3.1 treats the different phases of the generation of events. In Section 3.2 we discuss the simulation and response of the ATLAS detector. The simulated samples of signal and background that we use throughout the analyses are described in Section 3.3, followed by the reconstruction of the physics objects in Section 3.4. Finally, in Section 3.5, we present a more detailed analysis of the effect of initial and final state radiation in top quark pair events.

### 3.1 Event generation

The generation of a collision event is split up according to the factorization principles we described earlier in Section 1.3.1, and as depicted in Figure 3.2. The factorized event generation process distinguishes between the hard scattering of the partons in the protons, the parton showers, the hadronization of the partons, and the subsequent decays of hadrons and leptons. Each part corresponds to a process at a different energy scale and is treated as an independent step. In the following we discuss these steps, where we include the treatment of so-called ‘underlying events’ that occur in addition to the hard scattering as well.

**Figure 3.1** – Consecutive steps in the simulation of collision events.

**Figure 3.2** – Processes of the event generation.

#### 3.1.1 Hard scattering

The process in which two partons of the colliding protons interact, and outgoing partons emerge from the propagator, is described by the hard scattering. Quark-antiquark annihilation, forming a gluon that splits into a top-antitop quark pair is an example of a hard scattering, as discussed in Section 1.3.1. The energy scale connected to this part of the
collision process can be up to the order of several TeV. The partonic cross section of the physics process connected to this hard scattering consists of matrix elements and phase space factors. The matrix elements can be calculated with perturbative techniques, we discussed this in Section 1.3.1 in view of top quarks.

In an event generator, candidate events are obtained by pulling a random configuration of the partons from the possible positions in phase space. In this way, all incoming and outgoing partons obtain a defined four-momentum. The differential cross section of that candidate event, the weight, can then be calculated from the probability obtained with the PDFs, the value of the matrix element and the phase space factor. The weight then corresponds to the probability of the occurrence of this particular candidate event. To obtain a sample of events that is proportional to the total cross section and has physical observables, an accept-reject method is deployed. This results in simulated events with characteristics of real events, produced according to the probability for the events to occur as predicted by the Standard Model. The set of generated outgoing partons are subject to decay and parton showering.

### 3.1.2 Parton showering

Each colored and charged parton coming out of the hard scattering has a probability to emit quarks, gluons or photons. This process of radiation results in a shower of partons. In practice, this shower is not calculable beyond a limited number of tree level splittings and neither are virtual emission nor absorption. Therefore, this step of event generation is approximated with parton shower models.

A parton shower model treats the branching as a step-by-step evolution from the energy scale of the hard scattering, down to a low cutoff scale. The cutoff scale is arbitrary, but of order 1 GeV, usually, and corresponds to the energy scale at which the strong coupling constant approaches a value at which tree level approximation is no longer valid. At any time, a parton \( a \) has a probability of splitting into partons \( b \) and \( c \). The momentum of the initial parton \( a \), is divided over partons \( b \) and \( c \) that are assigned with momentum fraction \( z \) and \( (1-z) \), respectively. Subsequently, the partons \( b \) and \( c \) each have a probability to branch themselves as well.

We will make a distinction between initial state radiation (ISR) and final state radiation (FSR), which is only valid at leading order. Initial state radiation is formed by the gluons or quarks that are emitted from a parton that is involved in the hard scatter, before it undergoes the interaction. Final state radiation is radiation of the partons that are the result of the hard scattering, or of any other spectator partons not involved in it. This is depicted in Figure 3.3(a). The radiation is usually of electromagnetic or strong interaction nature. An example of evolution of the parton shower is given in Figure 3.3(b).

The splitting evolution is handled in terms of a ‘pseudo time’ variable \( t \) that depends on the momentum scale \( Q \), by \( t = \ln(Q^2/\Lambda^2) \) (\( \Lambda \) is the QCD scale, the scale at which the coupling constant of QCD becomes of order 1). In this picture, when going from a large value of \( Q^2 \), losing energy and running down to the cutoff scale is equivalent to \( t \) running
Chapter 3. Simulation and reconstruction of top quark pair events

Figure 3.3 – (a) Hard scattering ($t\bar{t}$ event) with initial and final state radiation. (b) Example of parton shower evolution.

from $t_{\text{max}}$ to a smaller value. This corresponds to FSR. ISR is treated the other way around and evolves starting from $t_0$ to the momentum scale of the hard scattering.

The differential probability of a branching of type $a \rightarrow bc$ is given by

$$dP_a = \sum_{b,c} \frac{\alpha_{abc}}{2\pi} P_{a\rightarrow bc}(z) \, dt \, dz,$$

where $P_{a\rightarrow bc}$ are the splitting kernels, depending on the type of parton. This splitting kernels are $g \rightarrow gg$, $g \rightarrow q\bar{q}$, $q \rightarrow gg$, $q \rightarrow q\lambda$ and $l \rightarrow l\lambda$, where the latter two are non-QCD (lepton and photons). For QCD splittings $\alpha_{abc} = \alpha_s$, for QED $\alpha_{abc} = \alpha_{EM}$.

The integral of the probability of a parton to branch to a specific $b$ and $c$ for a given $t$, is then expressed as

$$I_{a\rightarrow bc}(t) = \int_{z^{-}(t)}^{z^{+}(t)} \frac{\alpha_{abc}}{2\pi} P_{a\rightarrow bc}(z) \, dz.$$

Hence, $I$ runs over the range of possible $z$ values. The probability for the parton to branch to any $b$ and $c$, during a time $dt$, is the sum of $I$ over all final states. Finally, the probability of parton $a$ to branch at time $t$ is composed of the sum of all integrals $I$ multiplied with an exponential suppression factor:

$$\frac{dP_a}{dt} = \left( \sum_{b,c} I_{a\rightarrow bc}(t) \right) \cdot e^{-\int_{t_0}^{t} \sum_{b,c} I_{a\rightarrow bc}(t') \, dt'}.$$

The suppression factor, the exponent, is known as the Sudakov form factor and represents the probability that parton $a$ did not branch in the given time interval. The equation looks slightly different for FSR, as the integral will run from $t$ to $t_{\text{max}}$ whilst the Sudakov factor is defined from the lower cutoff $t_0$. 

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The choice of shower parameters is important for our studies. Different settings of the event generators—of the value of the momentum cutoff scale, for example—may alter the energy that is contained in the jet (more final state showering), the parton-jet mapping (extra jets) and therefore the jet multiplicity. This affects the top quark reconstruction and as a consequence, the cross section measurement. We study these effects in simulation, in Section 3.5.

### 3.1.3 Hadronization

After the parton shower, ‘colored’ partons remain that undergo a transition to ‘colorless’ hadronic particles. The hadrons, or decay products of hadrons are the observable particles in the detector. The transition from quarks and gluons to colored hadrons is the hadronization (or fragmentation) step. Hadronization is a non-perturbative process ($\alpha_s$ is large), and therefore has to be modeled. Different models exist that describe hadronization, of which ‘cluster fragmentation’ [54] and ‘Lund string fragmentation’ [55] are the most used.

In cluster fragmentation, the shower has ended with the creation of quark-antiquark (color-anticolor) pairs. Color neutral clusters are formed from neighboring sets of quarks. The clusters, in turn, decay into hadrons that can be observed.

In string fragmentation, a color ‘string’ is formed between the quark and antiquark that belong to a pair. The string represents a color field that increases in potential energy when the quarks move apart. The string can break when enough energy is contained, producing new $q\bar{q}$ pairs.

The energy regime at which hadronization starts is at the cutoff scale for parton showers, $\sim 1$ GeV. A higher cutoff value, and thus an earlier terminated shower, would result in less partons, that each have higher virtuality. This has an effect on the number of hadrons and in this way on the number of jets that are found in the simulated event. The hadronization phase of the event is tuned to match data collected by previous experiments. The potential decay of the resulting hadrons follows the Standard Model theory, yet the relative branching fractions are obtained empirically.

### 3.1.4 Underlying event

The proton remnants, i.e., the quarks and gluons that are not involved in the hard scattering, can also interact with each other. This is called the underlying event. Partons in the proton that are not involved in the hard scattering can produce secondary interactions of any type. Generally, a $2 \rightarrow 2$ QCD process is assumed to occur, as this has by far the largest cross section. The secondary interactions can be of high transverse momenta in some cases, but most of the time they only produce soft interactions. But, theoretically all processes in the Standard Model contribute to the underlying event. The treatment of the underlying event is tuned to pre-LHC data.

Outgoing partons of the underlying event are subject to the parton showering and hadroniza-
tion steps as well. Underlying events can affect the particle multiplicity in an event, especially in jet-rich events, but it is relatively unlikely to affect rare high-$p_T$ processes like top quark production.

### 3.2 Detector simulation and response

The energy deposits of the generated particles in the ATLAS detector are mimicked with the GEANT4 toolkit [56]. With this software, a complete simulation of all geometrical and material properties of the ATLAS detector is constructed. This makes it possible to model the interaction of particles with the detector parts within the magnetic field that is present in the ATLAS detector. The modeling includes potential decays of the particles. Each particle of the generated event will lose energy according to the particle’s characteristics and the properties and layout of the material it traverses.

The behavior of the detection material responses to the particle are modeled too, in the process of ‘digitization’. When a particle hits a sensitive area, the energy that it deposits is translated to an electronic signal. In this way, any generated particle produces hits and signals, equivalent to the data output. By the step of digitization, the generated events are transformed into the format that is identical to the output of the ATLAS detector when recording data. Subsequent reconstruction of physics objects is performed equivalently for data and simulation.

Figure 3.4 shows an example of a reconstructed event, in a cutaway view of the simulated ATLAS geometry. It displays the support structure of ATLAS, including the magnet system, in gray colors. The MDT chambers are shown in blue. The event contains tracks in the inner detector, and energy deposits in the electromagnetic and hadronic calorimeter. A reconstructed muon and the total transverse energy imbalance ($E_T$, discussed later in this chapter) in the event are shown with a solid and dashed line, respectively.

### 3.3 Event samples for analysis

In this thesis we make use of several event generators to model signal ($t\bar{t}$) and background events.

#### 3.3.1 Signal samples: top quark pairs

There is a multitude of event generators that attempts to describe the production of $t\bar{t}$ events. Most differences among them originate from the amount of extra radiation that are included in the matrix element calculation and the interface to the parton showering stage. In this thesis, the nominal sample of use is a combination of MC@NLO, HERWIG, and JIMMY for the underlying event. The matrix elements are calculated with MC@NLO, a next-to-leading order (NLO) generator [57]. The generated partons are input to the parton showering and hadronization schemes in HERWIG [58]. JIMMY simulates the underlying event. Alternatively we use POWHEG [59] (also NLO) as a matrix element generator that
3.3. Event samples for analysis

Figure 3.4 – Event display of event 2456382 of run 183602 in 2011. It shows hits and tracks in the inner detector, energy clusters in the calorimeters corresponding to hadronic jets and a reconstructed muon in white (going upwards). The reconstructed $E_T$ is depicted with the dashed line.

can be used in combination with HERWIG, but also with PYTHIA [60]. Finally, we use ACERMC [61], a leading order generator, for some systematic uncertainty evaluations at lowest order. The yields of the different generated samples are normalized to the calculated NNLO value of the inclusive cross section. This is done by applying a ‘K-factor’. The samples are summarized in Table 3.1. The top mass is taken to be 172.5 GeV in these simulations.

3.3.2 Background samples

The decay mode of $t\bar{t}$ we are interested in, is the single-lepton decay channel: $t\bar{t} \rightarrow W^+b + W^-\bar{b} \rightarrow q\bar{q}b + l^-\bar{\nu}b$ (or the charge conjugated version). A schematic view of this mode is shown in Section 1.3.3. The decay products are two $b$-quarks and two lighter quarks, together resulting in four hadronic jets, and a lepton, all with substantial transverse momentum. Additionally, the neutrino that is invisible to the detector produces an energy imbalance in the transverse plane, the missing transverse energy.
Table 3.1 – Generators for $t\bar{t}$ simulation. The cross section represents only the fraction of $t\bar{t}$ events in which one or more $W$ bosons decay leptonically.

<table>
<thead>
<tr>
<th>Generator</th>
<th>$\sigma$(7 TeV)</th>
<th>K-factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>MC@NLO+Herwig</td>
<td>80.20 pb</td>
<td>1.11</td>
</tr>
<tr>
<td>PowHeg+Herwig</td>
<td>79.12 pb</td>
<td>1.13</td>
</tr>
<tr>
<td>PowHeg+Pythia</td>
<td>79.12 pb</td>
<td>1.13</td>
</tr>
<tr>
<td>AcerMC+Pythia</td>
<td>58.23 pb</td>
<td>1.53</td>
</tr>
</tbody>
</table>

The backgrounds to $t\bar{t}$ processes come from processes that have similar signatures. This encompasses $W$ and $Z$ boson production with associated extra jets, the production of single top quark events and plain multijet production. We discuss the background samples below, and summarize the numbers in Table 3.2.

- **W+jets.** Production of a single $W$ boson that decays into a lepton-neutrino pair, see an example in Figure 3.5(a). Extra jets can result from radiation of the partons, and especially relevant is the splitting to a $b\bar{b}$-pair that can occur. In this case the signature is very similar to top quark decay. The cross section of $W$ boson production in combination with a leptonic decay at a CM-energy of 7 TeV ranges from 20.6 nb for $W + 0$ jets (exclusive) to 21 pb (three or more orders of magnitude) for $W+5$ jets (inclusive). ALPGEN (leading order, no virtual corrections) describes a fixed number of jets above a $p−T$ threshold in the hard scattering with the matrix element and is interfaced to either PYTHIA or HERWIG for additional showering and hadronization process. It is used as the default generator for $W+$ jets events. The events with high jet multiplicity form the major background to the analyses described in this thesis.

The normalization of $W+$ jets events is subject to a large uncertainty, in events with four or more jets this is estimated to reach 48% [62]. In addition, the amount of $b$ and $c$ quarks produced in association with the $W$ boson is theoretically uncertain. In Chapter 4 we discuss the methods we implemented to reduce the dependence on simulation. For example, for the charge asymmetry analysis we use a data-driven method to obtain the normalization, whilst taking the shapes of the observable distributions from the simulated samples.

- **Z+jets.** Production of a single $Z$ boson that decays into a charged-lepton pair, with extra jets, as in Figure 3.5(b). The cross section (times branching ratio to a charged-lepton pair) is an order of magnitude smaller than $W$ bosons decaying to lepton-neutrino pairs. This type of background can be reduced strongly when a second lepton is vetoed during event selection. It is described in ALPGEN, similar to $W+$ jets.

- **Single top.** Production of a single top or antitop quark. This process occurs
through the weak force and produces a top quark in combination with a light quark, a $b$-quark or a $W$ boson, and possibly with extra jets, making it a background difficult to reduce. The cross section is sufficiently low, however. The total cross section, combining the three production channels, is below 40 pb. The largest channel, the $t$-channel (as in Figure 3.5(d)) producing a top quark in conjunction with a $b$-quark has a cross section of 24 pb (taking only the events in which the $W$ boson decays into a lepton-neutrino pair). Single top production is described with MC@NLO + HERWIG and ACERMC + PYTHIA. The K-factors can take values below 1, in case of the $t$-channel [63].

- **Diboson.** Production of a $WW$, $ZZ$ or $WZ$ pair, all of which can result in leptons, jets and missing transverse energy. The first is depicted in 3.5(c). The cross section is low, compared to all other processes, 15.9 pb in total, at a CM-energy of 7 TeV. The generator we use for this type of processes is MC@NLO + HERWIG.

- **Multijet.** Processes producing only quarks and gluons and hence a number of observable hadronic jets. Multijet production is the most common result of an inelastic proton-proton collision. Estimates for the cross section (depending on the number of jets produced) can be of order $10^7$, but are affected by large uncertainties. The production rate is huge, but the signature itself is quite different from the single-lepton top quark decay. Still, when a jet is misidentified as a lepton, or a real lepton is present in a jet, multijet events can contaminate the selection. Since the uncertainty of the cross section of the production of $n$ jets is large, we do not rely on simulated samples for this process. Instead, we use data-driven techniques to assess this background, as will be discussed in Chapter 4.

### Table 3.2 – Generators for background simulation. The cross sections only represent the events in which at least one of the bosons decays leptonically. The K-factors indicate the correction to obtain a value at NNLO-level.

<table>
<thead>
<tr>
<th>Type</th>
<th>Generator</th>
<th>$\sigma$ (7 TeV)</th>
<th>K-factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>$W$+ jets</td>
<td>ALPGEN+HERWIG</td>
<td>26182 pb</td>
<td>1.22</td>
</tr>
<tr>
<td>$Z$+ jets</td>
<td>ALPGEN+HERWIG</td>
<td>2541 pb</td>
<td>1.22</td>
</tr>
<tr>
<td>Single top ($Wt$, $s$-channel)</td>
<td>MC@NLO+HERWIG</td>
<td>16.0 pb</td>
<td>1-1.1</td>
</tr>
<tr>
<td>Single top ($t$-channel)</td>
<td>ACERMC+PYTHIA</td>
<td>24.2 pb</td>
<td>0.9</td>
</tr>
<tr>
<td>Diboson</td>
<td>MC@NLO+HERWIG</td>
<td>15.94 pb</td>
<td>1.30-1.60</td>
</tr>
</tbody>
</table>

### 3.4 Object reconstruction

After the detector simulation and digitization steps, the output format of simulated events is identical to data. From then on, data and simulation are subject to the same set of algo-
Chapter 3. Simulation and reconstruction of top quark pair events

Figure 3.5 – Example diagrams of physics background: (a) W+ jets (2 extra jets), (b) Z+ jets (2 extra jets), (c), diboson (WW), and (d) single top (t-channel).

3.4.1 Electron reconstruction

Energy deposits (clusters) in the electromagnetic calorimeter that can be matched with a charged particle track form electron candidates in our offline selection. A match between the cluster and the track is established if the extrapolated inner detector track is within a window of $\eta \times \phi = 0.05 \times 0.1$ around the energy cluster in the calorimeter. A threshold of 2.5 GeV is imposed on the cluster energy. The electron candidate has to pass a number of quality cuts, to eliminate noise from photon conversions and jets that fake an electron. Among them are a minimum number of hits in the pixel and SCT detectors and a constraint on the width of the electromagnetic shower. The transverse energy of an electron is defined as $E_T = E_{clus} / \cosh(\eta_{track})$, using the total energy of the cluster and the direction of the matched track. The cluster energy is corrected for energy losses before the calorimeter, and for lateral and longitudinal leakage.

The efficiency of measuring electrons and muons is usually split up in a trigger component, a reconstruction component, and an identification component. Each efficiency represents one step in the process from going from a loosely defined inner detector track, to a well-defined ‘tight’ lepton that passes trigger, lepton quality requirements and the analysis-specific lepton selection (‘identification’). The latter is analysis-specific, since for example
top quark analyses use different isolation criteria than others. To some extent, the trigger efficiency is analysis-dependent as well, since the choice of the trigger and its momentum threshold depend on the typical transverse momentum or energy range of the lepton in the physics analysis. All three efficiencies are measured independently in data using so-called tag-and-probe methods and compared to simulated values. Scale factors are introduced to scale the simulation to match the data efficiencies, as a function of $\eta$, $p_T$ or $E_T$. These scale factors are supplied by the ATLAS performance subgroups.

**Trigger efficiency**

The trigger efficiency for electrons in the 2010 data set is shown in Figure 3.6(a) as a function of the transverse energy of the electron. The efficiency is obtained from a tag-and-probe method in a $W \rightarrow e + \nu$ sample. Events are triggered with a trigger orthogonal to the lepton trigger, the $E_T$ trigger, after which a selection aimed to isolate the signal events is applied. After subtracting the residual background events, a pure sample of $W \rightarrow e + \nu$ events remains. The electron then forms the probe, and the electron trigger efficiency is the ratio of events where an offline electron was found, with respect to all selected events. After the turn-on curve in the low-$p_T$ range, the efficiency forms a plateau where it reaches an efficiency of about 99%. The difference between simulation and data is small, but any difference in data and simulation efficiencies is corrected for with a scale factor in the later analyses.

**Reconstruction efficiency**

The efficiency of reconstructing electrons, the step from a loosely defined inner detector track to a ‘tight’ electron is also obtained from tag-and-probe studies. A pure sample of electron probes is defined from $Z \rightarrow e + e$ events where the ‘tag’ is one of the two electrons. The reconstruction efficiency obtained from the latter is shown in Figure 3.6(b). It is given in bins of $\eta$ and is 95% in the region $|\eta| < 1$ and 90% beyond this region. This is due to the requirement on the number of hits in the silicon detector [64].

The resolution of reconstructed electrons is obtained from the same type of $Z$ boson events. The reconstructed mass of the $Z$ boson in data is compared to simulation. For example, events in 2010 data with electrons in the range $|\eta| < 2.47$ show a width of $1.88 \pm 0.08$, whereas in simulation this is $1.60 \pm 0.02$ [64]. Electrons in simulation are corrected for the measured energy resolution.

### 3.4.2 Muon reconstruction

Muons are reconstructed from inner detector and muon spectrometer information. In the muon spectrometer, series of hits in a muon chamber (two multilayers) are combined and a straight track is fitted through. The hit position follows from the drift circles in each tube: a large drift circle, constructed from the time spectrum of the signal, indicates that the muon has passed through close to the borders of the tube. Vice versa, a small drift circle means the muon passed through the center. The fit through a series of hits in a
chamber form a segment. Multiple of such segments, or partial tracks, are combined. If this track can be combined with an inner detector track (if their position matches) it is considered a muon candidate. A refit to all hits in the track then defines the muon candidate and its parameters.

Like electrons, muons are detected and reconstructed efficiently in the ATLAS detector, but nonetheless a small fraction is missed in the trigger, reconstruction and identification steps.

### Trigger efficiency

The trigger for muons changed during the data taking period. We used `EF_mu10_MSonly` (online only the muon spectrometer was used for reconstruction), `EF_mu13` and `EF_mu13_tight` for different time periods. For the naming convention, we refer back to Section 2.2.6. The reason for choosing different triggers is that some triggers are prescaled during the runs, meaning that only a fraction of the events is recorded, rather than all. We therefore always use the trigger with the lowest $p_T$ threshold that was not prescaled during that data taking period. For 2011, we switch to `EF_mu18` (muon) for the entire year. In all cases the offline $p_T$ threshold remains set to 20 GeV. The trigger efficiency for 2010 data is measured in tag-and-probe studies similar to what was done with electrons, and is shown as a function of $p_T$ in Figure 3.7(a). In $Z \rightarrow \mu\mu$ events, one of the two muons is used as the trigger tag, and the times the other muon is triggered as well are counted to calculate the efficiency. Starting from 20 GeV the trigger efficiency for muons is about 80%. The difference between data and simulation is accounted for by scale factors.

Similar to electrons, the muon momentum resolution is measured from the invariant mass distribution of $Z$ boson events and corrections are applied to the simulation where the values deviate from the measured distribution in data.
3.4. Object reconstruction

The reconstruction efficiency of muons is shown in Figure 3.7(b), also as function of the transverse momentum of the muon. An inner detector track that, together with a well reconstructed muon of opposite charge, forms an invariant mass within 10 GeV of the \( Z \) boson mass, is defined as the probe. The reconstruction efficiency is defined as the times this probe is reconstructed as a muon as well. This efficiency is about 95% over the measured range.

### 3.4.3 \( E_T \) reconstruction

The missing transverse energy, \( E_T \), is the momentum imbalance that is measured in the transverse plane. The \( z \)-components are not useful, since the hard scattering usually has nonzero longitudinal momentum. Conservation of momentum dictates that the total transverse momentum vector that is the sum of all outgoing objects should be equal to zero. Undetected particles that emerge from the collision, i.e., neutrinos, will result in missing transverse energy. A precise reconstruction of the missing transverse energy is valuable for top quark events, since it can point to the presence of neutrinos. Fake \( E_T \) can result from errors or miscalibrations in any of the ingredients of the total summed energy. The magnitude of \( E_T \) is the squared sum of the total \( x \)- and \( y \)-component of the energy deposited.

The value for \( E_T \) is obtained from the sum of all calorimeter deposits, but depend on the reconstructed particles in the event. The deposits associated to a jet are scaled to match the jet energy scale. Those deposits associated to an electron are corrected to the calibrated electron energy. All other deposits are included at electromagnetic scale. There is one exception: the contribution of the muons to the \( E_T \) calculation is computed from the track momentum. Subsequently, the calorimeter deposits that are associated to the
muon are subtracted.

Figure 3.8 shows the missing transverse energy in a sample aimed to select $W \rightarrow \mu \nu$ events. This is a frequently produced process, with a neutrino in the decay that creates an energy imbalance and is used for validation of the $E_T$ observable. The figure shows $E_T$ for several types of events that are expected to pass the selection, superimposed with the data set of 2010. The sum of the simulated samples match the data reasonably well.

![Figure 3.8 – Missing transverse energy in 2010 data, after selection aimed to isolate $W \rightarrow \mu \nu$ events.](image)

### 3.4.4 Hadronic jet reconstruction

Gluons and quarks shower and hadronize into multiple particles that form hadronic jets. A jet consists of particles that are assumed to have originated from a single parton, depositing energy in the hadronic calorimeters. The reconstruction of jets, assembling them from energy deposits that belong together, is not straightforward. Associating particles to their original partons is ambiguous, as there is overlap between jets in the detectors when there is a lot of activity in the events. Moreover, choices have to be made for the reconstruction and calibration of the four-momentum of a hadronic jet as well. The reconstruction of jets is important to top quark studies. We select events based on the multiplicity of events: in the single-lepton channel of the top quark pair decay at least four jets are expected. Besides counting jets, we need their kinematical properties, as this provides direct information on the decay products of the top quark.

Different jet algorithms exist, varying in performance and treatment of soft and collinear radiation. The input to the jet algorithms we use are clusters of calorimeter cells. They
are groups of calorimeter cells that are formed from individual seed cells. If a cell has a signal-to-noise ratio over 4, it is used as a seed to the cluster formation. The assumed noise is this ratio is estimated from other, random events. Cells neighboring the seed cell, in 3D, with signal-to-noise ratios over 2 are added iteratively. In this way a cluster of above-threshold cells is formed. Finally all adjacent cells surrounding the cluster are added as well. If the clusters have local maxima the formation is run from that maximum as well, to find finer clusters if they exist. The energy of the cluster is the sum of all included cells. The direction is obtained from the weighted average of the angular position of the hit cells, and the mass is set to zero. Alternatively to clusters, ‘towers’, squared areas of cells are used in some analyses. The clusters are input to the actual jet algorithms, the following sections discuss the ‘cone’ and ‘anti-
\[ k_T \]’ algorithms we make use of.

Figure 3.9 shows an example of a hadronic jet in one quadrant of the ATLAS detector. The figure contains the tracks the parton leaves behind in the inner detector, and the energy it deposits in the calorimeters. Ideally, a reconstructed jet contains all energy that is carried by the original parton.

![Figure 3.9 – Quadrant of the ATLAS detector, with tracks in the inner detector and energy deposits in the electromagnetic and hadronic calorimeter, surrounded by a cone-shaped jet.](image)

**Fixed-cone jet algorithm**

The fixed-cone algorithm is based on the principle of constructing symmetric cones around energy deposits, accumulating the energy that is deposited within it. The algorithm starts from the calorimeter cluster with the highest transverse momentum, the seed, and checks whether it is above a certain threshold, for example 1 GeV. A cone of radius \( \Delta R = 0.4, 0.7 \) is formed around the seed and all objects contained in that cone are combined. A new, combined four-momentum can be composed of the combined objects. The cone rotates to the new center that is thus based on the relative energy contributions and direction of the objects contained before. All objects contained in this cone are used for a new
combination. This process iterates until the cone does not move anymore and is considered a stable jet. Starting from the second seed in line, multiple jets can be formed in a similar way. Spatial overlap between different jets can occur. In this case a split-merge technique is applied. When the overlapping fraction of energy is above a threshold, the jets are merged. Otherwise they are split, each assigned with a fraction of the attributed energy.

This jet algorithm is not infrared safe, meaning that a little extra radiation can potentially lead to different jet topology, even after having applied the split-merge technique. In Section 3.5 we study the effect of tuning the radiation parameters in simulation, using particle jets obtained with the cone algorithm. In ATLAS, the cone algorithm has been default for years, but is replaced by better performing jet finders since collisions started at the LHC.

**Anti-$$k_t$$ jet algorithm**

The anti-$$k_t$$ jet clustering algorithm [67] is the current default jet algorithm in ATLAS. It follows a sequential recombination scheme based on the ‘distance between entities’. An entity can be a particle or candidate jet or cluster. The distance $$d_{ij}$$ between entities $$i$$ and $$j$$ and the distance $$d_{iB}$$ between $$i$$ and the beam are defined as

$$d_{ij} = \min\left(1/k_t^2, 1/k_{t,ij}^3\right) \frac{\Delta R_{ij}^2}{R^2}, \quad d_{iB} = k_t^2,$$

(3.1)

where $$k_{t,i}$$ is the transverse momentum of the entity $$i$$. The geometrical distance is $$R_{ij}^2 = (y_i - y_j)^2 + (\phi_i - \phi_j)^2$$, and $$R$$ is the free radius parameter, usually of value 0.4. The calorimeter clusters, with well-defined four-momenta, are the entities that are input to the distance comparison. The minimum distance that exists between them, $$d_{ij}$$, and the minimum distance of any cluster to the beam, $$d_{iB}$$, are compared. When $$\min(d_{ij}) < \min(d_{iB})$$, the two entities are combined, forming a single new entity. Else, the entity $$i$$ is considered a jet and taken out of the iteration. The procedure is repeated until all clusters are either part of a jet, or a jet itself.

The result of this approach is that soft clusters are preferably combined with a hard cluster, before clustering among themselves. It is a direct consequence of the inverse of the momentum squared in the definition of $$d_{ij}$$, and distinguishes the anti-$$k_t$$ from other algorithms. Soft and collinear radiation do not alter the jet assignment, contrary to the cone algorithm. Another positive effect is that the jets have a cone shape as consequence of this algorithm (unless there is overlap between two jets, in that case only the hardest jet remains conical), rather than more exotically shaped jets that can result from other infrared and collinear safe algorithms that we will not discuss here.

The output of the jet algorithm is a number of well-defined jets.
### 3.4. Object reconstruction

#### Jet calibration

The clusters, and subsequently the reconstructed jets, are initially calibrated to the electromagnetic scale, which is appropriate for electrons and photons. But, the reconstructed jets contain all kinds of hadrons. Besides that, not all energy is detected and noise affects the measured energy as well. Therefore corrections have to be applied to the jet energy. This is done following the EM+JES calibration scheme. This scheme uses ‘truth jets’ for comparison. Truth jets are constructed by running the anti-$k_t$ algorithm over truth particles: truth particles are simulated particles after the hadronization phase that are stable (i.e., have sufficient lifetime). The truth particles skip the detector simulation and are directly inserted to the jet algorithm. The jets resulting from the generated particles are compared to the jets that are reconstructed from energy clusters after detector simulation, to obtain knowledge on the response.

A reconstructed jet is matched to a truth jet if their relative distance is small enough, $\Delta R < 0.3$. Both jets have to be isolated: no jet of $p_T > 7$ GeV can be in the area of $\Delta R < 1$. The response

$$ R_{\text{jet}}^{\text{EM}} = \frac{E_{\text{jet}}^{\text{EM}}}{E_{\text{truth}}^{\text{jet}}}, $$

is computed in bins of transverse energy and rapidity. Calibration functions $F_i$ are fitted to the response, in each $\eta$-bin. The measured electromagnetic energy of each jet is corrected with this calibration function to obtain the energy at the hadronic scale, by

$$ E_{\text{jet}}^{\text{EM+JES}} = \frac{E_{\text{jet}}^{\text{EM}}}{F(E_{\text{EM}}^{\text{jet}})|\eta}, $$

where the calibration functions $F$ are binned in $\eta$. Figure 3.10 shows the average correction that is obtained as a function of the transverse momentum of the jet, for three regions of pseudorapidity. The corrections are larger in the central region. For instance, for a 20 GeV jet in $0.3 \leq |\eta| \leq 0.8$, the correction factor is 2, while more forward jets require smaller corrections. Jets with a radius parameter $R$ of 0.6 are used in this plot, but the $R = 0.4$ shows similar behavior.

Besides the jet energy, the direction is also modified. The origin of the jet is replaced from the origin of the detector (0, 0, 0) to the vertex it belongs to. Furthermore, some calorimeter regions are better in reconstructing the energy, or more sensitive. The direction of the jet is corrected for this effect as well. The size of the correction is of order 0.01 in most regions, but in the transition regions of the detector it can run up to 0.06. In our analysis we use the pseudorapidity before origin correction to accept events, but the corrected value as input to the top quark reconstruction.

The treatment of the calibration of the jet energy induces a systematic uncertainty. But, apart from that, the uncertainty on the energy of jets is also influenced by uncertainties on the detector, the detector simulation, the event simulation uncertainty and pile-up. All
these effects add to the systematic uncertainty on the jet energy scale that we evaluate later on in the analyses.

Reconstruction efficiency

The jet reconstruction efficiency is measured in data by the ATLAS performance subgroup, from so-called ‘track-jets’. These are jets made up of sets of tracks in the inner detector that originate from the same vertex. In minimum bias events where two back-to-back track-jets are found, the one with the highest momentum is considered the tag if it can be matched to a calorimeter jet. The other track-jet is used to probe the efficiency. The efficiency is defined as the ratio of events where the track-jet can be matched to a calorimeter jet. The reconstruction efficiency is shown in Figure 3.11, as a function of the transverse energy of the jet. The efficiency reaches a plateau of 100% around \( p_T = 25 \) GeV. Due to the use of the inner detector, this efficiency measurement is only valid up to \( \eta = 2.5 \).

3.5 Initial and final state radiation in top quark events

We discussed the treatment of parton showering in the process of event simulation. In this section we examine the effect that extra emittance of partons has on top quark events.

Initial and final state radiation (ISR, FSR) are responsible for extra particle jets in the event, on top of the jets that result from the partons coming from the hard scattering process itself. ISR can have large transverse momenta and produce jets of the same order of momentum of the top quark decay products. FSR parton momenta are lower, but those partons contain energy that originates from the hard scatter and hence contain
3.5. Initial and final state radiation in top quark events

Figure 3.11 – Jet reconstruction efficiency from track-jets, as a function of the transverse momentum [68].

information on the process that produced the top quarks. As a result, the effect of ISR and FSR on the top quark acceptance and reconstruction is different.

Tuning the initial and final state radiation energy scale parameters in the event generator results directly in differences in the final jet multiplicity. In this way the treatment of ISR and FSR introduces a systematic uncertainty in any top quark study. We study the behavior of \( t\bar{t} \) events in samples of events generated with AcerMC, together with Pythia. As mentioned before, AcerMC is an LO event generator, which means that all radiation effects are treated by Pythia and tuning parameters in the latter is unambiguous. The CM-energy of the studied samples is 14 TeV, the LHC design value.

3.5.1 Parameters

There are several parameters involved in the treatment of ISR and FSR in Pythia, but we investigate two parameters in particular:

- \( \Lambda_{QCD} \). This parameter represents the energy scale at which the (running) strong coupling constant \( \alpha_s \) becomes of order 1. This parameter is of order 200 MeV (depending on the exact definition), in Pythia it is nominally set to 192 MeV. A larger value of \( \Lambda_{QCD} \) results in a stronger coupling, and thereby in more radiation.

- \( Q_0 \). This is the cutoff value of the virtuality at which the partons are no longer evaluated, incorporated in the integral over pseudo-time that was introduced before. Nominally, \( Q_0 \) takes a value of 1 GeV, a higher value stops showering early and results in less partons.

Both parameters are separately tunable for ISR and FSR, even though this can result in unphysical situations. The samples we utilized are obtained from varying one of the four \((2 \times 2)\) parameters, conserving the values of all other parameters. The generated events do
not pass through the full reconstruction scheme of ATLAS, but use the ‘fast reconstruction algorithm’, ATLASFAST, where the generated particle momenta and direction are smeared according to measured resolution that is obtained in the full simulation scheme. Hence, the detector simulation and the reconstruction step are replaced with a procedure to translate the generated list of particles to a set of physics objects. The output is a collection of reconstructed physics objects.

3.5.2 Effect of $\Lambda_{QCD}$ and $Q_0$ on jet multiplicity

Whether an event is selected in the top quark analysis depends among other things on the number of high-$p_T$ jets. We examined the influence of ISR and FSR on the number of jets in the event. The parameter $\Lambda_{QCD}$ is varied in a systematic way by a factor of two with respect to the nominal value, producing samples for $\Lambda_{QCD} = 0.096$ and $0.384$ GeV, in addition to the nominal $0.192$ GeV.

The effect on the number of ‘good’ jets in top quark events, before any event selection, is shown in Figure 3.12. A jet is considered good if its transverse momentum is above 20 GeV and the pseudorapidity is $|\eta| < 2.5$. The sample with a higher value of $\Lambda_{QCD}$ (`ISR >' and `FSR >'), is depicted with a dotted line, the lower value (`ISR <' and `FSR <') with a dash-dotted line. In the left plot, displaying the effect of tuning ISR only, it shows that there indeed are more jets when $\Lambda_{QCD} = 0.384$ GeV. Events with 6 or 7 jets occur up to 10% more often, with respect to the nominal. And vice versa, a low value for $\Lambda_{QCD}$ has a significant negative effect on the number of jets above 20 GeV in the event. Two elements are added for comparison. The green areas reflect the uncertainty resulting from a 2% variation of the jet energy scale, applied to the Pythia samples. And $t\bar{t}$ events generated with MC@NLO are shown (blue dots). The effect of the variation of $\Lambda_{QCD}$, with respect to the number of jets, is of the same order as changing to a different generator.

For FSR, the effect is opposite, although less pronounced. A higher value of $\Lambda_{QCD}$ for FSR leads to slightly less high-$p_T$ jets. The reason is that FSR jets are softer, and extra splitting will lead to more soft jets, eventually failing to pass the 20 GeV momentum cut. The effect is much smaller than for ISR and also in comparison to the MC@NLO events.

The cutoff parameter $Q_0$ is varied with a factor two, namely to 0.5 and 2 GeV, for both ISR and FSR. The effect of varying $Q_0$ is negligible for the jet acceptance. The effect of $Q_0$ in the studied range on the jet acceptance is of order 1%. Due to the 20 GeV threshold, the radiation at cutoff threshold will barely influence the formation of the high-$p_T$ jets we are interested in.

Only ISR shows a measurable effect with respect to the jet multiplicity, whereas FSR does not affect it significantly. To assess the effect of FSR, we study the reconstructed top quark mass on the hadronic side of the decay, a purely hadronic observable.
3.5. Initial and final state radiation in top quark events

![Diagram](image-url)

**Figure 3.12** – Effect of varying $\Lambda_{QCD}$ in ISR (a) and FSR (b), for $t\bar{t}$ events with a CM-energy of 14 TeV. Statistical uncertainties are negligible.

### 3.5.3 Effect of $\Lambda_{QCD}$ and $Q_0$ on reconstructed top quark mass

We study the effect on the reconstructed top quark mass using the same simulated samples containing variations of $\Lambda_{QCD}$ and $Q_0$. The mass of the (anti-)top quark that decays hadronically is reconstructed from three particle jets, after a selection aimed to increase the purity of $t\bar{t}$ (although for this study we disregard background samples).

#### Event selection

We expect at least four high-$p_T$ jets, a high-$p_T$ lepton and a neutrino, in top quark pair events. Based on earlier studies, we select an event when it contains:

- Exactly one muon or electron, with $|\eta| < 2.5$;
Chapter 3. Simulation and reconstruction of top quark pair events

- At least four jets within $|\eta| < 2.5$, with a transverse momentum above 20 GeV, of which at least three must have a momentum over 40 GeV;
- Missing transverse energy larger than 20 GeV.

All selected objects have an absolute value of pseudorapidity $|\eta| < 2.5$. For muons and electrons an isolation cone of 6 GeV is defined and jets that overlap with electrons within $\Delta R < 0.2$ are removed. Approximately 30% of the events pass the selection. The origin of the loss are events with two-lepton decays, or involving a tau lepton, and events where a jet or lepton is misreconstructed.

Reconstruction of the hadronic side of decay

The top on the hadronic side (i.e., the top quark that decays hadronically) is reconstructed using the so-called $\sum p_T$-algorithm, which is based on the following: of all jets with a transverse momentum above 20 GeV, in the selected events, we make all possible combinations of three jets. The resulting vectors are compared. The vector with the highest transverse momentum forms the candidate top quark. This method is based on the assumption that top quarks are produced with large transverse momentum. Additionally, we omit the candidate if none of the two-jet combinations within the three-jet combination have an invariant mass that is consistent with a $W$ boson mass of 80.4 GeV, quantified by a window of 20 GeV around this value (in later chapters we call this the $W$ boson mass constraint). It is a robust algorithm, resulting in a visible mass peak, but it leads to significant fraction of events where the wrong jet combination is picked, i.e., so-called combinatorial background. The $\sum p_T$ algorithm is used as a benchmark reconstruction algorithm, throughout ATLAS studies.

Results

The resulting distribution is plotted in 3.13(a), for the case of nominal radiation settings. The distribution peaks at a value close to the top quark mass. The distribution is fitted with a Gaussian on top of a polynomial background, the latter describing the background formed by combinatorial mistakes. The mean of the Gaussian distribution is at 157.4 GeV, which is lower than the input mass of 172 GeV. Radiation outside the cone of the jets and misreconstruction of background in jets are responsible for this deficit.

The variation of $\Lambda_{QCD}$ for FSR results in a shifted location of the peak: for $\Lambda_{QCD} = 0.384$ the distribution peaks at 154.3 GeV, with $\Lambda_{QCD} = 0.096$ it peaks at 159.9 GeV. This is a 2% effect. The comparison is shown in 3.13(b), for the subregion of 100-210 GeV, and overlayed to a ±2% uncertainty of the jet energy scale. The shift is of comparable size.

The event sample with events generated with MC@NLO (not shown in the plot) has a mass peak around 160.2 GeV. This shows that the radiation settings cause differences almost of the same order as obtained when switching between the LO and NLO generator. The explanation for the shift is that extra radiation will not be contained in the three jets that are used for reconstruction. The energy can either be outside the cone of the jet, or be contained in another jet in the event that is not used. In contrast, changing $\Lambda_{QCD}$ for ISR
shows no significant shift of the mass of the top quark, whereas its effect on acceptance showed be large. Also the cutoff parameter $Q_0$ does not influence the distribution, neither for ISR nor for FSR.

![Graph of reconstructed top quark mass](image1)

**Figure 3.13** – (a). Reconstructed top quark mass for nominal sample, with the fit function displayed on top. The background contribution in the fit is depicted with a dashed line. (b) Reconstructed top quark mass for values of $\Lambda_{QCD} = 0.092, 0.196, 0.384$ in FSR for $t\bar{t}$ events with a CM-energy of 14 TeV. The colored area represents a jet energy scale uncertainty of 2%.

Besides the shift in mass, the number of events in the peak area decreases for larger amounts of final state radiation. The number of events in the peak area of the mass distribution (see again 3.13(a)) can be used as a measure for the cross section. In Chapter 5 we indeed make similar, but more involved use of the top quark mass distribution to measure the cross section. In this way the amount of radiation will have an effect on the
measurement. The number of events in the peak decreases (increases) with 10.4% (8.2%) for $\Lambda_{QCD} = 0.384$ (= 0.096) in FSR. This partly due to the acceptance difference, but mostly due to the reconstruction that is affected. For ISR, the effect is smaller, of order 5%, because only the acceptance is majorly affected.

### 3.5.4 Conclusions on ISR and FSR

The value for the parameter $\Lambda_{QCD}$ for both ISR and FSR can have a significant effect on the selection and reconstruction of top quark events. The effects are different. A higher value of $\Lambda_{QCD}$ in ISR leads to more high-momentum jets and therefore a higher acceptance rate of events. Increased FSR distorts the information that is contained in the decay products of the top quark and affects the reconstructed mass. All effects are of order 5-10%, maximally, in the parameter range we evaluated. The effects are of comparable size to the jet energy scale uncertainty, and to the difference between the AcerMC + Pythia sample and the Herwig + MC@NLO sample. Since these are sizeable effects, we assign systematical uncertainties to this part of event simulation. For the measurement of the production cross section of top quark pairs in Chapter 5, we use AcerMC+Pythia samples with ISR and FSR minimized and maximized, similar to what we used here, to evaluate the relative effect on our measurement.