Higher Order QCD Corrections in Top–Antitop Production at the LHC

Tree Level Matrix Elements vs Parton Shower

MSc thesis

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Abstract

An important part of the physics analyses at the Large Hadron Collider (LHC) will concentrate on production and decay of heavy particles. To compare precision measurements with sufficiently detailed simulations, higher order QCD corrections must be included in the description of these processes. Higher orders modify the event kinematics of a lowest order approximation and lead to production of additional partons/jets.

QCD corrections in the production of top quark pairs are studied. Two methods are compared. The Monte Carlo event generator ALPGEN is used to calculate higher order matrix elements at tree level. This method is restricted to produce only hard (high energy), non-collinear (well separated) additional partons. In the second approach, the lowest order matrix element is convoluted with the virtuality ordered parton shower in PYTHIA 6. Parton shower results become unreliable when hard, non-collinear partons are generated.

First, results from ALPGEN, PYTHIA 6 and PYTHIA 8 are compared at lowest order for top–antitop (t\bar{t}) production. Differences between ALPGEN and PYTHIA are found in the treatment of spin correlations in the top and antitop decays. With default settings, there are some small differences in the hadronization process between the two versions of PYTHIA.

The matrix element and parton shower methods give comparable results for the kinematics of hard, non-collinear partons. The main difference is that the parton shower tends to overestimate the production of partons at high energy. Large differences are observed for other variables due to the lack of soft and collinear additional partons from matrix elements.

To obtain reliable results for both hard and soft parton emissions, the two approaches are combined by applying a merging scheme (the MLM matching procedure). Results show that higher order corrections to t\bar{t} production only modestly affect the top quarks and their decays. However, additional partons increase the observed jet multiplicity, which complicates analyses. The difference between the matrix element and parton shower approaches for hard, non-collinear partons affects the energy spectra of almost all partons and jets at high energy.
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Chapter 1

Introduction

1.1 The Top Quark

Common matter consists of protons, neutrons and electrons, all confined in atoms by the strong interaction and electromagnetism. We know that protons and neutrons are compositions of more elementary particles, called partons. Partons may be quarks or gluons. In the Standard Model of Particle Physics \cite{1, 2, 3} there are six different quarks, ordered in three generations. The proton and the neutron are composed of the members of the first generation, which are the down quark and the up quark. The second generation is formed by the strange and charm quarks and the third by the bottom and top quarks.

The heaviest of the six quarks is the top. Its mass is more than 170 times larger than the mass of the proton and the neutron, both of which consist of three lighter quarks. This makes the top quark heavier than a Tungsten atom, which consists of 74 protons and 110 neutrons. Top quarks do normally not exist in nature, but can be created in high energy particle collisions. This has been done for the first time in an experiment at the Tevatron proton–antiproton collider, which is located at Fermilab, near Chicago, in the USA. The top quark was discovered at the Tevatron in 1995 \cite{4} by the CDF \cite{5} and DØ \cite{6} experiments.

Several measurements of the top quark mass have been performed since this discovery. The latest combined result from CDF and DØ is $173.1 \pm 0.6 \text{ (stat.)} \pm 1.1 \text{ (syst.) GeV}/c^2$ \cite{7}. The first error in this result is a statistical error, which could be reduced by including a larger number of proton collisions in the analysis. The second error is systematic and caused by both theoretical and experimental uncertainties.

A new generation of experiments that will be able to observe top quarks are those at the Large Hadron Collider (LHC) \cite{8}. The LHC is located at CERN, near Geneva, Switzerland and started in 2009. In this machine protons collide with protons instead of protons with antiprotons. The ex-
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Experiments that will explore top quark physics at the LHC are ATLAS [9] and CMS [10].

The focus of the top quark research at the Tevatron experiments was on the discovery of the top quark and on measuring its properties. These results will be verified by ATLAS and CMS. In addition, the LHC experiments aim at a more precise measurement of the top quark properties. These measurements will reduce the experimental errors on for example the top quark mass and limits on rare decays of the top quark. This affects the main research interests at the LHC, which are searches for the Higgs boson and for physics beyond the Standard Model. Top quark properties are important parameters in this research.

Before any measurements can be performed at the LHC, detectors must be aligned and calibrated. Data from the first collisions are used mainly to understand the behaviour of the detectors. Because top quarks will be abundant at the LHC and their properties have been determined at the Tevatron, the signal from top quark production and decay can be used in this initial phase to understand early data.

When the underlying physics of top quark production at the LHC is understood in detail, this knowledge may be used in the analysis of other processes, in particular production of other heavy particles. One of the details associated with the description of processes in proton collisions is the inclusion of higher order QCD corrections. Higher order corrections in the production of top quark pairs are studied in this work. The remainder of this chapter gives an introduction to the production and decay of top quarks and to higher orders in these processes.

1.2 Top Quark Production and Decay

At both the LHC and the Tevatron, top quarks are created in collisions of protons and (anti)protons. In the dominant process for top quark production, the top quark is always accompanied by an antitop quark. This is depicted in Figure 1.1. The $t\bar{t}$ pair is produced in the hard scattering process, which is represented by part II of the figure.

The hard scattering is governed by the strong interaction, which is described by quantum chromodynamics (QCD). The QCD equivalent of electric charge is colour charge. Colour is carried by partons.

The partons that initiate the hard scattering process emerge from the incoming protons. The main constituents of the proton are up quarks, down quarks and gluons. Quarks may radiate more gluons and gluons will split into a quark–antiquark pair or two other gluons. Finally, one of these partons takes part in the hard scattering. The incoming protons and the parton splitting process are represented by part I of the figure.

Figure 1.1 shows the LHC case, with two incoming protons. For the Teva-
1.2. TOP QUARK PRODUCTION AND DECAY

Figure 1.1: t¯t production and decay: Parton interactions inside an incoming proton (I) result in a parton that participates in the hard scattering process (II), which produces a t¯t pair. Top quarks have a short lifetime and decay into other quarks or leptons (III). Partons that emerge from the t¯t production and decay processes are converted into hadrons in a hadronization process (IV).

Top quarks are not be observed directly, because they immediately decay (Figure 1.1-III). Decay products may be both (lighter) quarks and leptons (see Section 1.4).

Quarks carry colour charge and therefore the strong interaction still prohibits their direct observation. This phenomenon is known as confinement. Quarks from the top decays are converted into colourless hadrons in a hadronization process (Figure 1.1-IV). Any additional partons produced in the t¯t production and decay processes (see Sections 1.3 and 1.4) hadronize as well. Most of the resulting hadrons are unstable and decay into other, more stable hadrons, photons and leptons, which can finally be observed by a detector.

A multitude of particles is created in the hadronization process. These particles emerge from the point in which the top quark pair was created (the interaction point) with velocities close to the speed of light. Bundles of particles travelling in approximately the same direction are observed. These collimated bundles are called jets. Roughly speaking, each quark from the t¯t decay initiates a separate jet. The kinematic properties of a jet can be related to those of the partons, and therefore indirectly to the kinematics of the top quarks.

Besides the decay of a t¯t pair, there are other processes in proton collisions that produce jets. In fact, the probability to produce jets via other strong interactions is much larger than the probability to produce a (heavy) t¯t pair. In an experiment, it is often hard to distinguish the signature of
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this background signal from the t¯t signal. A thorough understanding of the produced jets is required to separate signal from background.

1.3 Top Quark Pair Production

The QCD process that results in a t¯t pair is represented by the Feynman diagrams in Figure 1.2. These diagrams are read from the left to the right. In Figure 1.2a, two incoming gluons fuse to produce the t¯t pair. The annihilation of a quark and an antiquark is represented by the diagram in Figure 1.2b. Note that antiquarks are represented by quarks “travelling backwards in time” in these diagrams. That is, the quarks and antiquarks are not distinguished by their labels, but by the direction of the arrow on their lines.

Figure 1.2: t¯t production: (a) gluon fusion (dominant mechanism at the LHC) and (b) quark–antiquark annihilation (dominant mechanism at the Tevatron).

Each of the diagrams in Figure 1.2 represents a term in the expression for the amplitude, or matrix element, for t¯t production. The matrix element is the basic ingredient in the calculation of the probability for the interaction to occur in a particle collision.

This probability is represented by the cross section (σ) for the process, which is obtained by squaring the matrix element and integrating over the phase space. The phase space is the set of variables that determines the momenta of the outgoing partons, in this case the top quarks. One may think of the cross section as the effective cross-sectional area represented by the incoming particles. Since this area is small, it is usually expressed in barn (1 b = 10^{-28} m^2).

The magnitude of the contribution from a given diagram not only depends on the diagram itself, but also on the probability to find the incoming partons in the (anti)protons. These probabilities are different for the LHC and the Tevatron, which results in different cross sections and relative contributions from gluon fusion and quark–antiquark annihilation. At the LHC, approximately 90% of the top quark pairs is produced through gluon fusion.
and 10% through quark–antiquark annihilation [11]. At the Tevatron it is almost the other way around: 15% and 85%, respectively.

The diagrams in Figure 1.2 all have two points where either three gluons or a gluon and two (anti)quarks are connected. These points are called vertices. At least two vertices are required for t¯t production, but diagrams with three or more vertices also contribute.

Each vertex introduces a factor proportional to the strong coupling constant \( g_s \propto \sqrt{\alpha_s} \). The matrix element is squared to obtain the probability, so this gives a term proportional to \( \alpha_s^n \) for a diagram with \( n \) vertices.

Because the value of the strong coupling constant in the hard scattering is well below one (\( \alpha_s \approx 0.1 \)), the contribution of order \( \alpha_s^n \) diagrams usually decreases for increasing \( n \). This makes it possible to apply perturbation theory. A process is approximated by including only diagrams of a fixed order \( n \) or less. The \( \mathcal{O}(\alpha_s^2) \) diagrams in Figure 1.2 represent the lowest order approximation. Because the lowest order gives the largest contribution to the full t¯t production process, this is also the leading order. Diagrams with more vertices represent higher order corrections, which improve the accuracy of the calculation.

Higher order diagrams are either loop diagrams (Figure 1.3) or tree level diagrams (Figure 1.4). In tree level diagrams, each additional vertex adds a parton to the final state. The additional partons in loop diagrams are virtual and do not change the final state. Therefore, loop diagrams interfere with tree level diagrams of lower order.

An important part of the contribution from loop diagrams is taken into account by redefining the strong coupling constant in calculations at tree level. This procedure is called renormalization. The resulting effective \( \alpha_s \) is a running coupling constant, which depends on the energy scale \( \mu \) of the hard scattering. This scale is a Lorentz invariant variable, which represents the magnitude of energy and momentum variables. In the approximation which includes only diagrams with one loop, the relation between \( \alpha_s \) and \( \mu \) is given by:

\[
\alpha_s^{(1)} = \frac{12\pi}{33 - 2n_f} \ln^{-1}\left(\frac{\mu^2}{\Lambda_{n_f}^{(1)\ 2}}\right)
\]

(1.1)

with \( n_f \) the number of quarks with a mass smaller than \( \mu \) and \( \Lambda_{n_f}^{(1)} \approx 0.2 \text{ GeV}/c \) the QCD scale parameter.

Note that the strong coupling increases with a decreasing energy scale. The scale of the hard scattering is much larger than \( \Lambda \), which results in an \( \alpha_s \) of order 0.1. For processes with \( \mu \) of the order of \( \Lambda \), \( \alpha_s \) is larger than one and the perturbative description (including Equation 1.1) breaks down.

The two examples of tree level diagrams in Figure 1.4 add one parton to the final state. This may either be a gluon (1.4a) or an (anti)quark (1.4b). Additional partons will participate in the hadronization process as
well. They may initiate additional jets and/or affect the properties of the jets from the top quark decays.

Figure 1.4b demonstrates another feature of higher order $t\bar{t}$ production. In diagrams of $\mathcal{O}(\alpha_s^3)$ and higher it is possible to produce a $t\bar{t}$ pair with a gluon and an (anti)quark in the initial state. Since these diagrams only appear at higher order, their contribution to the full production process is small.

The absence of higher order diagrams leads to an error in the prediction of parton level probability distributions. In an ideal situation, one would calculate as many orders as are needed to reduce the errors to the level of experimental errors or smaller. However, the number of diagrams grows rapidly with increasing order. This makes it harder to perform full higher order calculations beyond $\mathcal{O}(\alpha_s^3)$ (next-to-leading order).

To describe the abundant production of $t\bar{t}$ pairs at the LHC with the required precision, higher orders beyond $\mathcal{O}(\alpha_s^3)$ should be considered. Therefore, other techniques must be applied to approximate an exact calculation. A discussion of alternative methods to include higher orders can be found in Chapter 2.
The $t\bar{t}$ cross section that contains $O(\alpha_3^2)$ terms (next-to-leading order) and an approximation of $O(\alpha_4^2)$ terms (next-to-next-to-leading order) is calculated in reference [11]. Cross sections of $852 \pm 47$ pb at the LHC and $7.4 \pm 0.6$ pb at the Tevatron were found. A top quark mass of 173 GeV/c$^2$ was assumed in this calculation.

1.4 Top Quark Decay

The decay of the top quark is governed by the weak interaction. Figure 1.5 shows the lowest order Feynman diagram for the decay process. The top is an up-type quark and converts into a down-type quark (down, strange or bottom) at the first vertex. The process is mediated by a W boson.

At the second vertex, either quarks or leptons are produced. When the decay products are quarks, the decay is called hadronic. This channel will be studied in this work. In a hadronic decay, a lighter up-type quark (up or charm) and a down-type antiquark are created. The quarks and W boson are replaced by their charge conjugates in the antitop decay.

\[
\begin{align*}
&\text{Figure 1.5: Top quark decay into three lighter quarks.}
\end{align*}
\]

The probability for the coupling of up-type quark $i$ and down-type quark $j$ in weak vertices is proportional to $|V_{ij}|^2$, where $V$ is the CKM mixing matrix [12]. In a lowest order approximation of the CKM matrix elements, $V$ is equal to the identity matrix. This means that the up-type quarks always couple to the down-type quark of the same generation in this lowest order description (up and down, charm and strange, top and bottom).

In a higher order approximation of the CKM matrix, there is also a small probability for the coupling of up-type and down-type quarks from different generations. However, the top–bottom CKM element is so close to one ($|V_{tb}| = 0.999133^{+0.000044}_{-0.000043}$ [13]) that top quark decays into down or strange quarks can be neglected for most purposes. In this work, it will be assumed that the top quark decays exclusively into a bottom quark and a W boson.

The W boson is a virtual particle, so its invariant mass is not necessarily equal to the W resonance mass (80.4 GeV/c$^2$ [13]). Nevertheless, it is kinematically allowed to produce a W boson at its resonance mass and the probability distribution for the W mass peaks at this value. The width of this peak (2.1 GeV/c$^2$) is small compared to the top and W masses. Therefore,
the decay process can be approximated by assuming the W always reaches its resonance mass (it is always on shell).

This approximation makes it possible to treat the W as a real (as opposed to virtual) particle. The decay process can now be divided into two independent parts. First the top quark decays into a bottom quark and a W boson and subsequently the W boson decays into a quark and an antiquark. This is the Narrow Width Approximation (see reference [14] for a discussion). Note that by separating $t\bar{t}$ production and the top quark decays, the Narrow Width Approximation is implicitly applied for the top and antitop quarks.

The decay rate is defined as the probability that a particle decays per unit time. This gives the familiar exponential distribution for a (top quark) decay as a function of time:

$$f(t) = \Gamma_t e^{-\Gamma_t t}$$

where $f(t)$ is the probability for a decay at time $t$ and $\Gamma_t$ is the top quark decay rate. The mean of this distribution is $1/\Gamma_t$, which is defined as the mean lifetime of the top quark.

Since the mass of the bottom quark is small compared to the top mass, terms of order $m_b^2/m_t^2$ are neglected. The lowest order decay rate (Figure 1.6) is then given by [15]:

$$\Gamma_t^{(0)} = \frac{G_F m_t^3 c^3}{8\pi\sqrt{2}\hbar^4} \left( 1 - \frac{M_W^2}{m_t^2} \right)^2 \left( 1 + 2 \frac{M_W^2}{m_t^2} \right)$$

(1.2)

with $G_F$ the Fermi coupling constant and $m_t, m_b$ and $M_W$ the masses of the top quark, bottom quark and W boson, respectively.

Although the top quark decay is a weak process, gluons couple to both the top and bottom quarks and give rise to QCD corrections. Two examples of $\mathcal{O}(\alpha_s)$ corrections are shown in Figure 1.7. When all $\mathcal{O}(\alpha_s)$ corrections are taken into account, but terms of order $\frac{\alpha_s}{\pi} M_W^2/m_t^2$ are neglected, Equation 1.2 becomes [15]:

$$\Gamma_t = \frac{G_F m_t^3 c^3}{8\pi\sqrt{2}\hbar^4} \left( 1 - \frac{M_W^2}{m_t^2} \right)^2 \left( 1 + 2 \frac{M_W^2}{m_t^2} \right) \left[ 1 - \frac{2\alpha_s}{3\pi} \left( \frac{2\pi^2}{3} - \frac{5}{2} \right) \right]$$

(1.3)
With $G_F = 1.17 \times 10^{-5} (hc)^3/\text{GeV}^2$, $M_W = 80.4 \text{ GeV}/c^2$, $m_t = 173 \text{ GeV}/c^2$ and $\alpha_s=0.11$, this results in a top quark decay rate of $1.4 \text{ GeV}/h$. This rate corresponds to a mean lifetime of $5 \times 10^{-25} \text{ s}$.

At small distance, the two top quarks essentially behave as free particles. However, when their separation becomes of the order of the QCD distance scale ($h/\Lambda_{\text{QCD}}$), their QCD interaction becomes too strong to neglect. This distance corresponds to a time scale $h/(c\Lambda_{\text{QCD}}) \approx h/(0.2 \text{ GeV}) \approx 10^{-24} \text{ s}$. As this is longer than the top quark lifetime, the top quark will decay before hadronization starts.

The difference in time scales is small, so hadronization effects will interfere with the weak top quark decay. However, it will be a good approximation to neglect this effect. This behaviour is quite different from that of other quarks, which have masses far below the W mass. This results in lifetimes much larger than the QCD time scale, so these lighter quarks enter the hadronization process and form hadrons before they decay.

In the Narrow Width Approximation, the decay of the W boson does not affect the total top quark decay rate. However, the W does not decay exclusively into quarks, as in Figure 1.5. It may also decay into leptons. Top–antitop decays are actually classified according to the W decay modes. When both W bosons decay into quarks, the process is called fully hadronic.

The probability for a decay channel is called the branching ratio. The W may decay into two generations of quarks, each with three different colours. This gives six different decay modes with approximately the same probability. There are three generations of leptons (without colour), which adds three possible modes. This gives an approximate branching ratio of two thirds for the W decay into quarks. Taking this branching ratio into account, the partial decay rate for the top quark into quarks is $\frac{2}{3} \Gamma_t = 0.9 \text{ GeV}/h$.

The naive branching ratio for fully hadronic $t\bar{t}$ decay is $\frac{2}{3} \cdot \frac{2}{3} \approx 0.44$. Higher order QCD corrections affect this value and lead to a branching ratio of 46% [13].
1.5 Parton Distributions

The energy scale of parton interactions within the proton is much lower than the scale of the hard scattering. This results in a value for $\alpha_s$ that is close to one or even larger than one. The perturbative formalism is useless in this regime, because higher order terms would be larger than the lowest order terms. Fortunately, it can be demonstrated that the total process can be approximated by separating the interactions inside the (anti)protons (Figure 1.1-I) and the hard interaction (Figure 1.1-II). This procedure is called factorization.

The cross section for $t\bar{t}$ production is approximated by the product of the cross section for the hard interaction and the probability to find the required combination of partons in the (anti)protons. The probability density to find a particular parton with a given momentum is approximated by a Parton Distribution Function (PDF). These distributions have been determined experimentally and different parametrisations have been made.

To determine PDFs at different energy scales, distributions measured at a certain scale are extrapolated by applying perturbative QCD. Probabilities for a quark splitting into a quark and a gluon and for a gluon splitting into a quark-antiquark pair are used to derive QCD evolution equations (or DGLAP [16]). Evolution equations describe the rate of change of parton densities as a function of the energy scale at which the (anti)proton is “probed”. Expressions for the PDFs as a function of the energy scale are derived.

The total cross section is obtained by integration over parton momenta and summation of different combinations of incoming partons:

$$\sigma = \sum_{i,j} \int \int dx_i dx_j f_i(x_i, Q^2) f_j(x_j, Q^2) \hat{\sigma}_{i,j}(x_i, x_j, Q^2)$$

where $f_i(x_i, Q^2)$ is the density of partons of type $i$ as a function of the fraction of the (anti)proton momentum carried by an individual parton ($x$). $\hat{\sigma}_{i,j}$ is the partonic cross section for the hard interaction of incoming partons $i$ and $j$. The energy scale is denoted by $Q^2$.

For $t\bar{t}$ production, $Q^2$ is of the order of the square of the top quark mass, but several definitions exist. The following definition will be used in Chapters 3 through 5:

$$Q^2 = m_t^2 c^2 + \frac{1}{2} \left( p_{T_1}^2 + p_{T_2}^2 + \sum_{i} p_{T_i}^2 \right)$$

Where $m_t$ is the top quark mass and the $p_{T}$s are momenta in the direction perpendicular to the proton momenta. The sum runs over the partons that are produced in addition to the $t\bar{t}$ pair.
In this work, the CTEQ6L1 PDF parametrisations [17] will be used. These sets use the lowest order description of the parton splitting probabilities and the one-loop expression for \( \alpha_s \) (Equation 1.1 on page 11). The value of \( \Lambda^{(1)}_\chi \) in this parametrisation (0.165 GeV/c) should also be used for the hard interaction. This gives \( \alpha_s(M_Z^2) = 0.130 \) (with \( M_Z \) the mass of the Z boson) and \( \alpha_s(m_t^2) = 0.118 \).

Usually, the momentum density \( x f(x) \) is used instead of the number density \( f(x) \). This variable represents the total fraction of the (anti)proton momentum carried by partons with an individual momentum fraction between \( x \) and \( x + dx \). By definition, the sum over all types of partons is normalized to one: \( \sum_i \int_0^1 dx x f(x) = 1 \). Figure 1.8 shows the momentum density as a function of \( x \) according to the CTEQ6L1 PDFs at \( Q^2 = m_t^2 \).

Figure 1.8: Parton Distribution Functions for the proton at \( Q^2 = m_t^2 = (173.1 \text{ GeV/c})^2 \) according to the CTEQ6L1 parametrization [17]. The momentum density \( (x f(x)) \) is shown as a function of the momentum fraction \( (x) \) for different types of partons.

For the production of a \( t \bar{t} \) pair, an invariant mass of at least two times the top quark mass is required. If it is assumed that the incoming partons and (anti)protons have negligible mass and the two (anti)protons have equal energy, this invariant mass is given by \( 2\sqrt{x_1 x_2} E/c^2 \) for a proton energy \( E \). At the LHC, \( E \) is 7 TeV. With a top quark mass of 173 GeV/c\(^2\), this leads to a typical momentum fraction of order 0.02 for the hard scattering. The
Tevatron (anti)proton energy is 0.98 TeV, which implies a typical $x$ of order 0.2.

Figure 1.8 shows that gluons dominate the LHC protons at $x = 0.02$. At the typical Tevatron value $x = 0.2$, the (anti)up quark contribution dominates the (anti)proton and the (anti)down quark and gluon contributions are roughly equal. These PDF differences result in the different relative contributions from gluon fusion and quark–antiquark annihilation to the $t\bar{t}$ production process mentioned in Section 1.3. The large number of gluons in LHC protons gives the two orders of magnitude difference in cross section.

1.6 Hadronization

The strong interaction prohibits the existence of free colour charges, which confines partons to bound states. If the invariant mass of such a bound system is large enough, it is energetically favourable to divide it into sub-systems by creating new partons. The subsystems may be separated and are observed as hadrons. This is the hadronization process represented by part IV of Figure 1.1.

The energy scale of parton interactions in the hadronization process is small compared to the scale of the hard scattering. Therefore, this process cannot be described by perturbative QCD. Instead, phenomenological models have been developed. The probability for fragmentation of a given parton into a particular hadron is given by a fragmentation function.

A simple representation of the hadronization process is shown in Figure 1.9. A quark and an antiquark are imagined to be connected by a colour string (1.9a). The tension in the string increases as the initial quarks move apart. When the energy density in the string is large enough to create a new quark–antiquark pair, the string breaks. The system splits into two colourless parts: $q\bar{q}'$ and $q'\bar{q}$ (1.9b).

The resulting quark–antiquark systems may split again (1.9c) or form mesons (1.9d). When a string breaks into a $q\bar{q}'$–$q'\bar{q}$ pair instead of a $q$–$q'$ pair, the resulting hadrons are baryons.

Also gluons and the coloured proton fragments that remain after the hard interaction (beam remnants) participate in the hadronization process. A similar mechanism that includes these objects can be constructed.

The majority of the produced hadrons has a short mean lifetime and decay close to the interaction point. Decay products that are stable enough to reach a detector are mainly light hadrons (pions and kaons) and photons.

Directions of these particles and the initial partons are strongly correlated. In general, a particle jet originates from one parton or a few partons with collinear directions. Therefore, a jet is defined at parton level before hadronization, at hadron level after hadronization and at particle level after hadrons decay.
1.7 From Tevatron to LHC

The (anti)protons of the LHC and the Tevatron are accelerated and stored in large rings. The particles circle around these rings at almost the speed of light. Magnets are used to bend their paths.

The (anti)protons are distributed over the ring and form two beams, circling in opposite directions. The beams consist of bunches, separated by at least 396 ns at the Tevatron and 25 ns at the LHC. The number of protons per bunch is of the order of $10^{11}$ and the number of Tevatron antiprotons is of the order of $10^{10}$. The energy of both the protons and antiprotons at the Tevatron is 0.98 TeV. The design energy for the LHC is 7 TeV.

When all particles have reached this energy and the beams are stable, they are focussed at the interaction points. At these points, the beams intersect and bunches cross. Proton–(anti)proton interactions and the particles that are produced in a bunch crossing form an event.

The mean number of events for a particular interaction per unit time is given by the product of the cross section for the process and the luminosity of the beams. The luminosity is the mean number of crossing (anti)protons per unit area, per unit time. At the Tevatron, the luminosity is of the order of $10^{32} \text{ cm}^{-2} \text{s}^{-1}$. The design luminosity for the LHC is of the order of $10^{34} \text{ cm}^{-2} \text{s}^{-1}$.

With the cross sections from Section 1.5, the expected rates for $\bar{t}t$ production are about $10^{-3}$ Hz for the Tevatron and 10 Hz for the LHC at its design performance. The difference is the result of a factor $\approx 100$ between the luminosities and a factor $\approx 100$ between the $\bar{t}t$ cross sections at the Tevatron and LHC energies.

Unfortunately, $\bar{t}t$ production adds only a small fraction to the total proton–proton cross section. The total cross section at the LHC is of the
order of 0.1 fb [18], which is roughly a factor $10^8$ larger than the $t\bar{t}$ cross section. This results in a collision rate of 1 GHz. The experiments use a trigger system based on the signature of the created particles to select interesting events.

Detectors are built at the interaction points to observe the particles that emerge from collisions. The ATLAS, CMS, CDF and DØ detectors almost completely enclose the interaction points. Figure 1.10 shows a cross section of the ATLAS detector. The ATLAS interaction point is located at the centre.

Two types of measurements are performed on the particles that reach the detector. Their energy is measured in the calorimeters and the tracks of charged particles in the tracking systems. Both measurements are based on the electromagnetic interaction of charged particles with materials in the detector.

High energy particles ionize atoms when they are passing through a material. The ionization is converted into an electric signal, which is measured by electronics. In the calorimeters, the signal is used to determine the loss of energy due to ionization in the calorimeter. In the tracking system, it is used to determine the position of the particle.

With the solenoid and toroid magnets, indicated in Figure 1.10, a magnetic field is applied in the entire detector. Therefore, the tracks of charged particles are curved. The radius of this curvature is used to determine the momentum of the particle.
The analysis of jets is based on the measurement of electron, muon, photon and hadron energy depositions in the calorimeter system. Contrary to the trackers, the calorimeters are designed to stop these particles (except for the muon). The particles lose all their energy in the calorimeters and a full energy measurement can be performed.

A cutaway view of the Atlas calorimeter system is shown in Figure 1.11. The system is divided into a barrel part and an end-cap part. The barrel covers a cylinder around the centre of the detector. The end-caps cover both sides of this cylinder. Both in the barrel and the end-caps, the particles first traverse an electromagnetic calorimeter and then a hadronic calorimeter.

In the electromagnetic calorimeters, electrons and photons are absorbed. At energies well above $\approx 50$ MeV, the dominant mechanism for energy loss of electrons is the radiation of a photon in the interaction with atomic nuclei ($\text{bremstrahlung}$). The dominant mechanism for energy loss of a high energy photon in interactions with nuclei is the creation of an electron–positron pair. This leads to a cascade of electrons and photons, which is called an electromagnetic shower. The shower continues until electron and positron energies approach a critical energy, below which other processes dominate the energy loss.

The Atlas electromagnetic calorimeters use liquid argon (LAr) to measure the energy loss. Layers of LAr are interspersed with lead absorber plates, which have a high density and reduce the size of the calorimeter. Be-
cause ionization in the absorbers is not measured, this part of the particle energy must be calculated from the energy loss in the liquid argon to obtain the total energy.

Hadrons lose energy in the electromagnetic calorimeters, but in general they are not stopped. They will enter the hadronic calorimeter, where they start a **hadronic shower**. In the interactions of hadrons with atomic nuclei, other hadrons, electrons and photons are produced. The secondary hadrons continue the hadronic shower, while electrons and photons may start an electromagnetic component.

Hadronic showers are longer and wider than their electromagnetic counterparts. More material is needed to contain a hadronic shower, so the hadronic calorimeters are larger than the electromagnetic calorimeters and contain relatively more absorber material.

The hadronic **Tile Calorimeters** use plastic scintillators instead of liquid argon. In a scintillator, electrons that were freed by ionization can excite atoms. When the excited states decay, photons are emitted. These photons are converted into an electrical signal by **photomultipliers**. The absorber material used in the Tile Calorimeters is steel.

In the **Hadronic End-Cap and Forward Calorimeters** liquid argon is used again. The absorber material in the Hadronic End-Cap is copper. The Forward Calorimeters are divided into a copper electromagnetic part and a tungsten hadronic part.

Calorimeters consist of several layers in the direction perpendicular to the proton beams. A layer consists of many independent cells. This segmentation makes it possible to measure not only the energy loss, but also the position of the energy deposition.

For the reconstruction of a jet, energy depositions from the particles in the jet are combined. The energies of all cells that are part of the jet are summed to obtain the jet energy. The direction of the jet is given by the direction from the interaction point to the energy depositions.

### 1.8 Simulation of Proton Collisions

Experimental results are compared to the model described in Sections 1.2 through 1.6 by examining probability distributions for relevant variables. Examples of these variables are momenta and multiplicities of particles and jets. Due to the complexity of proton collisions and high particle multiplicities, the distributions cannot be obtained analytically. Therefore, events are simulated by applying Monte Carlo techniques.

Partons and particles in the simulation are created by an **event generator**. Probability distributions for variables at parton, hadron or particle level are approximated by histograms for a sufficiently large number of events. When also the response of a detector is required, the particles from the
1.8. SIMULATION OF PROTON COLLISIONS

Figure 1.12: Event generation: (a) lowest order matrix element with parton shower, (b) merging of higher order tree level matrix elements and parton shower.
event generator are input to a detailed detector specific simulation.

Generation of an event is represented by the diagram in Figure 1.12. The inputs for the event generator are a number of parameters (at the top of the figure). Incoming particles and their energies, selected processes for the hard scattering and parameters like particle masses are specified.

Kinematic properties of the generated partons and particles and the weight of the event \(W\) are output (at the bottom of the figure). The weight is the relative probability for the event to occur. It is used to estimate the cross section for the generated process (see below).

Figure 1.12 shows two different paths, which both lead to the simulation of an event at particle level. The simulation process starts with the random selection of the event variables from uniform distributions. A combination of incoming and outgoing partons and their momenta are selected. In path (a), only the lowest order Feynman diagrams are used. Path (b) includes higher order diagrams, but only at tree level. Additional input parameters and variables are required to describe the additional tree level partons in path (b).

Evaluation of matrix elements and PDFs leads to the differential cross sections for both paths. The weight of an event is the product of the differential cross section and the available phase space volume. This gives an estimate of the phase space integral. The average weight of all events (of all selected phase space points) is an approximation of the lowest order cross section for path (a) and the tree level higher order cross section for path (b).

The lowest order approximation in path (a) is improved by allowing partons to split into two other partons. The result is the tree-like structure of partons from higher order diagrams at tree level. This procedure is implemented in a parton shower algorithm, which is based on parton splitting probabilities. These probabilities are the same as in the derivation of the QCD evolution equations (Section 1.5).

The parton shower approximates higher order corrections to all orders in \(\alpha_s\). A disadvantage is that it neglects interference between different parton branches. This is a good approximation, provided that the additional partons are either soft (small energy) or collinear with each other or with the incoming partons (small opening angles). The reliability of the parton shower decreases when hard, non-collinear partons are generated.

Combination of the lowest order approximation and the splitting probabilities gives an approximation of the full higher order matrix element. Because the weight is not affected by the parton shower, the cross section is still calculated at lowest order. See Chapter 2, Section 2.2 for a more detailed description of the parton shower.

Although the tree level matrix elements in path (b) represent the generated process at higher order in \(\alpha_s\), only the lowest order matrix element for the process with \(n\) additional partons is calculated. The advantage of this method is that interference is included. However, the lowest order approxi-
imulation becomes unreliable when additional partons become soft and/or collinear. Due to these *divergences*, cuts on parton momenta are needed. The available phase space is limited to hard and non-collinear additional partons. The tree level matrix element approximation is discussed in Section 2.1.

The parton shower and tree level matrix element approaches may be combined to exploit the best properties of both. This is shown in path (b), where a *merging scheme* is applied on events with hard, non-collinear additional partons from the matrix element calculation. Soft and collinear partons are added with the parton shower algorithm.

The weight of the event is affected by the merging procedure. This becomes the lowest order weight, multiplied by the probability to produce $n$ additional partons. The merging procedure is described in Section 2.3.

When a simulation at particle level is required, generated partons from one of the parton level approximations are processed by a simulation of the hadronization process. There are various phenomenological hadronization schemes. Another phenomenological model is used for the subsequent decays of unstable hadrons into (more) stable hadrons, photons and leptons.

The focus of this work is on testing the matrix element method, the parton shower and the merging procedure. The possible advantage of using tree level matrix elements instead of a parton shower for hard, non-collinear partons is investigated.

The different approaches are discussed in more detail in Chapter 2. The remaining chapters are devoted to a discussion of the results of simulations. In Chapter 3, a lowest order simulation is presented. These lowest order results will be used as reference. The applied techniques for analysis of the simulation results are introduced in Chapter 3.

Results from higher order simulations are discussed in Chapter 4. Simulations with tree level matrix elements are compared with parton shower simulations. In Chapter 5, the two methods are merged. The merging results are compared with the results of the parton shower approach.
Chapter 2

Higher Order QCD Corrections

Two methods of simulating higher order QCD corrections were introduced in Section 1.8: calculation of tree level matrix elements and the parton shower algorithm. Results from simulations with these approaches will be compared in Chapters 4 and 5. This chapter gives an overview of both techniques.

2.1 Matrix Elements

An approximation of the $t\bar{t}$ production process with $n$ additional partons may be obtained by calculating only tree level diagrams. One of the event generators that can perform such a calculation is Alpgen [19]. In this work, ALPGEN 2.1.3 is used.

Figures 2.1 through 2.3 show the diagrams for $t\bar{t}$ production with one additional parton. Diagrams with the same initial and final states interfere. An advantage of the matrix element method over the parton shower is that it includes all these interference terms.

Matrix elements also generate additional partons that are not present in the parton shower. Since the latter only works on initial and final state partons, it omits configurations shown at the right hand side of Figures 2.1 through 2.3.

A problem with the matrix element method arises when no cuts are applied in the additional parton phase space. A cross section obtained from calculation of tree level matrix elements contains logarithms. The arguments of these logarithms may become very large, depending on the phase space cuts. In a full higher order calculation, the logarithmic terms are cancelled by contributions from loop diagrams. Such cancellations are not present when only tree level diagrams are calculated, which gives an unreliable result.
CHAPTER 2. HIGHER ORDER QCD CORRECTIONS

Figure 2.1: $t\bar{t}$ production through $\mathcal{O}(\alpha_s^3)$ gluon fusion diagrams.

Figure 2.2: $t\bar{t}$ production through $\mathcal{O}(\alpha_s^3)$ quark–antiquark annihilation diagrams.

Figure 2.3: $t\bar{t}$ production through $\mathcal{O}(\alpha_s^3)$ quark–gluon initiated processes.
There are three types of logarithms. The first contains the minimum energy of additional partons. This type causes an \textit{infrared divergence} when the minimum energy is lowered. The second type gives rise to a \textit{collinear divergence}. These logarithms contain the minimum opening angle of the directions of an additional and an incoming parton. The third type is introduced when two or more additional partons are generated. The minimum opening angle of these partons controls another collinear divergence.

A reliable lowest order approximation of the $t\bar{t} + n$-parton process may be obtained if the contribution of the logarithmic terms is small compared to other terms. This can be achieved by applying sufficient cuts on the additional parton momenta, which limits the available phase space to hard, non-collinear partons.

The number of possible diagrams for $t\bar{t} + n$ partons grows rapidly with increasing order in $\alpha_s$. An algorithm called \textsc{Alpha} has been developed to calculate the matrix element squared in Monte Carlo simulations without explicit calculation of the diagrams [20]. This reduces the growth of complexity to a power in the number of partons, instead of the factorial-like growth associated with the increasing number of diagrams. \textsc{Alpha} is implemented in \textsc{Alpgen}.

Even at this level of complexity, practical reasons like computing time still limit the maximum number of orders that can reasonably be calculated. The maximum number of additional partons for $t\bar{t}$ production in \textsc{Alpgen} is six.

\section*{2.2 Parton Shower}

Higher order corrections are implemented in the parton shower by allowing the splitting of partons produced at lowest order. The allowed parton branches are shown in Figure 2.4. A quark may radiate a gluon (2.4a) and a gluon may either split into two new gluons or into a quark–antiquark pair (2.4b). The produced partons may split again and a tree-like structure of partons emerges.

![Figure 2.4: Splitting of partons: (a) quark splitting and (b) gluon splitting.](image-url)
All branches occur at a different energy scale. There are several definitions of this scale. In this work, the default implementation of the parton shower algorithm in the event generator PYTHIA 6 [21] (version 6.4.19) is used. This implementation is virtuality-ordered, which means that the energy scale is equal to the invariant mass of the branching parton.

The parton shower starts at energy scale \( Q_{PS} \). All partons evolve until they split or reach a low-energy cut-off. The starting scale is of the order of the hard scattering scale \( Q_{hard} \), see Equation 1.5). There is, however, no unique prescription for the value of this parameter. It may be tuned to give the best results for a specific application. The definition \( Q_{PS}^2 \equiv 4 Q_{hard}^2 \) will be used in this work. This is the default in the applied parton shower algorithm.

The probability for a parton branch at a certain scale is calculated with perturbative QCD. Calculation of the diagrams in Figure 2.4 gives a differential probability \( \Gamma_a(Q) \, dQ \) for the splitting of parton \( a \) (quark or gluon) in an interval \( dQ \). \( \Gamma \) is proportional to \( \alpha_s \), since each diagram contains one vertex. \( \alpha_s \) is evaluated at a scale related to \( Q \).

The naive branching probability \( \Gamma \) is modified by the probability of having no branch between the production scale of the parton \( (Q_0) \) and scale \( Q \). This modification factor is called the Sudakov form factor:

\[
\Delta_a(Q, Q_0) = e^{-\int_{Q_0}^{Q} dQ' \, \Gamma_a(Q')}
\]  

(2.1)

Including the form factor, the probability distribution for a parton branch at scale \( Q \) is given by:

\[
P_a(Q, Q_0) = \Delta_a(Q, Q_0) \, \Gamma_a(Q)
\]  

(2.2)

Showers starting from the outgoing partons of the hard scattering are called final state showers. A similar method is used to allow splitting of the incoming partons. These initial state showers also start at \( Q_{PS} \) and evolve backwards to a cut-off scale.

For each parton \( b \) in the initial state shower, the probability that it was produced in the splitting of \( a \to bc \) is calculated. In this case, the Sudakov form factor gives the probability that parton \( b \) did not split in the evolution from its branching scale to its production scale. The shower continues with parton \( a \) until the cut-off scale is reached. Parton \( c \) may initiate a final state shower, starting from the scale of the splitting of \( a \to bc \).

A complication in initial state showers is that the incoming partons emerge from the protons. Therefore, the branching probabilities are derived from the QCD evolution equations, which give the rate of change in the PDF for parton \( b \) due to its production. The evolution equations again contain the parton splitting probabilities calculated with the diagrams in Figure 2.4. The result of this procedure is that the PDFs and momentum fractions of partons \( a \) and \( b \) are included in the branching probability.
2.3. MERGING

leads to \( \Gamma_b(x_b, Q) \) and \( \Delta_b(x_b, Q, Q_0) \), which are thus different from \( \Gamma_a(Q) \) and \( \Delta_a(Q, Q_0) \) in final state showers.

The initial state shower reconstructs one of the branching paths that gives an evolution from the cut-off scale to the scale of the hard interaction. Because the branching probabilities are derived from the evolution equations, this is one of the many paths reflected by the proton PDFs. The momentum fraction distributions for the incoming partons after showering are automatically given by the PDFs at the cut-off scale.

An unlimited number of parton branches may occur between the energy scale of matrix element calculation and the cut-off scale, each one introducing a factor \( \alpha_s \). This makes the parton shower algorithm an approximation to all orders in \( \alpha_s \), which is its advantage over the matrix element approach.

Contrary to the matrix element method, the parton shower actually uses the large logarithms that give rise to divergences for tree level matrix elements. Logarithms from different orders in \( \alpha_s \) are summed, which results in a reliable approximation for soft and/or collinear additional partons.

The diagrams from Figure 2.4 represent the lowest order approximation for parton splitting. No higher order splitting processes are calculated in the parton shower. As a result, the parton shower approximation contains only the largest terms in the logarithmic expansion. This is called the leading logarithmic approximation.

The leading logarithmic terms are dominant for emission of soft and collinear partons. However, when minimum parton energies and opening angles increase, the logarithms become smaller and other terms become important. Therefore, the parton shower is less reliable when hard, non-collinear partons are generated.

2.3 Merging Matrix Elements and Parton Shower

In order to obtain reliable results in all regions of additional parton phase space, matrix elements and the parton shower may be combined. The phase space is divided into a hard, non-collinear part and a soft and/or collinear part. Partons in the former are generated with matrix elements and partons in the latter with the parton shower. A merging scheme is applied to connect the two phase space regions without overlaps (double counting) or gaps.

Events with additional partons are generated with weights determined by matrix elements (\( W_{\text{hard}} \)). The strong coupling constant at each vertex is evaluated at the scale of the hard interaction (\( Q_{\text{hard}} \)). A merging scale (\( Q_M \)) is defined, which serves as a cut-off for the additional parton kinematics. This scale is much lower than \( Q_{\text{hard}} \). Partons produced above the merging scale are considered to be hard and non-collinear.

In the merging scheme, events from the matrix element calculation are interpreted as lowest order events with \( n \) parton branches above the merging
scale. Logarithms that normally lead to divergences become part of the parton shower description. This improves the parton shower approximation, because part of the probabilities now contain higher order terms. Branches below the merging scale are generated in a “normal” shower evolution.

To integrate the matrix element events into the parton shower description, a reweighting factor is calculated for each event. The first step of the reweighting procedure is a change in the scale of the strong coupling constant. In the second step, the weight is corrected with a Sudakov form factor.

The higher order matrix element squared is approximately equal to the product of the lowest order matrix element squared and the naive branching probabilities:

$$W_{\text{hard}} \propto |M_{\text{hard}}|^2 \approx |M_0|^2 \prod_{i=1}^{n} \Gamma_{\text{hard},i}$$ \hspace{1cm} (2.3)

Since strong coupling constants in the branching probabilities were evaluated at $Q_{\text{hard}}$ and not at the scales of the branches, the factors $\Gamma_{\text{hard},i}$ are multiplied by $\alpha_s(Q_i)/\alpha_s(Q_{\text{hard}})$. A product of appropriate form factors for the generated configuration of partons is determined for Sudakov reweighting:

$$F_{\text{config}} = \prod_j^{4+2n} \Delta_j(Q_j, Q_{j-1})$$ \hspace{1cm} (2.4)

Sudakov factors $\Delta$ for the incoming and outgoing partons are evaluated at the merging scale.

The weight of the event is now given by:

$$W_n = W_{\text{hard}} F_{\text{config}} \alpha_s(Q_{\text{hard}})^{-n} \prod_{i=1}^{n} \alpha_s(Q_i)$$

$$\approx W_0 P_{\text{config}}$$ \hspace{1cm} (2.5)

Where $W_0$ is the weight of the lowest order matrix element and $P_{\text{config}}$ the probability for adding this configuration of partons to the lowest order event. For $n = 0$, there are no branches and only the Sudakov factor is included. In this case, $P_{\text{config}}$ is the probability for having no branches above the merging scale.

Since the number of partons that can be generated in the matrix element calculation is limited, events with the maximum number of partons ($N$) are made inclusive. For these events, the Sudakov factor is not evaluated at the merging scale, but at the lowest branching scale in the tree. This allows further branches above the merging scale. $P_{\text{config}}$ becomes the probability for this configuration of $n$ partons plus any number of new branches between the lowest branching scale and the merging scale.
2.3. MERGING

The average weight of events with \( n \) partons gives the “cross section” for that parton multiplicity. This number is an approximation of the product of the lowest order cross section and the probability to produce \( n \) partons above the merging scale. The sum for all parton multiplicities approximates the lowest order cross section:

\[
\sum_{k=0}^{N} W_k \approx \sum_{k=0}^{N} \sigma_0 P_k = \sigma_0
\]  

(2.6)

The generated partons are further evolved by the parton shower. For events with less than \( N \) matrix element partons, the algorithm is constrained to produce only branches below the merging scale. For inclusive events, the parton shower is also allowed to add branches between the lowest branching scale and the merging scale.

A priori, there is no prescribed value for the merging scale. There will be a range of values below which the parton shower is still reliable. For an ideal merging scheme, results are independent of the actual value of the merging scale in this range. Several studies show that there often is a scale dependence in current implementations of the merging procedure [22, 23]. The magnitude of this dependence may be used to determine the uncertainty of results obtained with the scheme.

Various merging schemes exist (see reference [24] for a comparison). They differ in definition of the merging and branching scales, determination and application of Sudakov form factors and the starting conditions for the parton shower. In this work, the MLM matching procedure [25, 26] will be used. This algorithm is discussed in Section 5.1.
CHAPTER 2. HIGHER ORDER QCD CORRECTIONS
Chapter 3

Lowest Order Approximation

An analysis of lowest order $t\bar{t}$ production and its fully hadronic decay is presented. LHC events with a proton energy of 7 TeV are generated with Alpgen [19] and two versions of Pythia [21]. At lowest order, results obtained with these generators should be equal for most variables. Distributions are compared and serve both as a consistency check and as reference in higher order simulations.

Pythia events are produced with Pythia 6.4.19 and Pythia 8.1.30. Pythia 8 is a relatively new version of the program, which has been rewritten in C++. Pythia 6 is the older Fortran 77 version. Since the same physics models are implemented in the two programs, no differences are expected at lowest order.

Alpgen 2.1.3 is used to generate the hard scattering and top quark decays. Events at parton level are processed by Pythia 6 to include hadronization and further decays. Generation processes in Alpgen and Pythia are slightly different. The most important difference at lowest order is that Pythia generates $t\bar{t}$ production and top quark decays separately, while Alpgen calculates the full process.

Top quark decays are mediated by the weak interaction, which has a so called $V$–$A$ structure (see for example reference [2]). Due to this structure, the momentum directions of the decay products depend on the direction of the top quark spin. If the directions of the top and antitop spins are correlated, there are also correlations between the momentum directions of quarks from the top decay and quarks from the antitop decay.

These correlations are generated by Alpgen, because all spin effects are included in the full calculation of the $t\bar{t}$ process. In Pythia, however, spin information from the production process is not taken into account in the decay processes. Instead, directions of the top quark spins are chosen independently from uniform distributions and correlations disappear.

The CTEQ6L1 PDF sets (see Section 1.5) are used for all generators. No transverse momentum is given to the incoming partons (primordial $k_T = 0$).
This results in an opposite transverse momentum that is equal in magnitude for the top and antitop. Top quarks and W bosons are produced on shell. The top quark mass ($m_t$) is set to 172.5 GeV/c$^2$ and the W mass ($M_W$) to 80.419 GeV/c$^2$.

Table 3.1 shows the estimated lowest order $t\bar{t}$ cross sections and their statistical errors with these settings. The cross sections are the average result of ten samples of 100,000 events. The quoted errors are the standard deviations of these ten results.

<table>
<thead>
<tr>
<th>generator</th>
<th>$\sigma_{t\bar{t}}$ (pb)</th>
<th>$\sigma_{t\bar{t}-\text{had}}$ (pb)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PYTHIA 6</td>
<td>561.1 ± 0.3</td>
<td>256.3 ± 0.1</td>
</tr>
<tr>
<td>PYTHIA 8</td>
<td>560.6 ± 0.2</td>
<td>256.3 ± 0.2</td>
</tr>
<tr>
<td>ALPGEN</td>
<td>562.0 ± 0.3</td>
<td>249.8 ± 0.1</td>
</tr>
</tbody>
</table>

Table 3.1: Estimated lowest order $t\bar{t}$ production cross sections and their statistical errors. The first number is the cross section before selection of a decay channel. The second number is the cross section for the fully hadronic decay channel.

The $\sigma_{t\bar{t}}$ column lists the inclusive cross sections for all decay channels, which is approximately 560 pb. Differences between the generators are somewhat larger than the statistical errors due to small differences in (default) parameters of the generation processes. For example, ALPGEN uses a slightly different value for $\Lambda_{\overline{MS}}^{(1)}$, which is responsible for a systematic error of about 0.8 pb (see also Section 3.2).

The $\sigma_{t\bar{t}-\text{had}}$ column in Table 3.1 lists the cross sections for the fully hadronic decay channel. For ALPGEN, this is the product of the inclusive value and the lowest order fully hadronic branching ratio ($\frac{4}{9}$, see Section 3.3). Treatment of decays in PYTHIA is more sophisticated. Experimentally determined values for the branching ratios and first order QCD corrections are taken into account. This causes a significant difference of 6.5 pb between the fully hadronic cross sections for ALPGEN and PYTHIA.

For the analysis of the lowest order probability distributions, two of the 100,000-events samples are used. This corresponds to 0.5 fb$^{-1}$ of integrated luminosity\(^1\). This amount of data will be collected in roughly a day at the LHC design luminosity ($10^{34}$ cm$^{-2}$s$^{-1}$) or a few months at low luminosity ($10^{32}$ cm$^{-2}$s$^{-1}$).

Distributions from PYTHIA 8 and ALPGEN are compared to the PYTHIA 6 distribution. All histograms are normalized to the PYTHIA cross section. In addition, the difference between the generators is shown as the (natural) logarithm of the ratio of the distributions. This variable is approximately equal to their relative difference if it is smaller than $\approx 15\%$.

\[1 \quad \int \mathcal{L} \, dt = \frac{N}{\sigma_{t\bar{t}} \cdot \text{Br}(t\bar{t}-\text{had})} = \frac{2 \cdot 10^5}{852 \cdot 10^3 \text{fb} \cdot 0.462} = 0.5 \text{ fb}^{-1}\]
The number of entries in each bin of the histograms is given by a binomial distribution. The generated number of entries ($N$) is an estimate of the mean of this distribution. For most histograms, the number of bins is large (typically of the order of 50), so the probability for an event to end up in a particular bin ($p$) is small. Therefore, the statistical error on the number of entries is estimated by $\sqrt{N(1-p)} \approx \sqrt{N}$. This results in the following error for the plots of the difference ($\ln(N_2/N_1)$):

$$
\Delta N \approx \sqrt{\frac{1}{N_1^2} \Delta N_1^2 + \frac{1}{N_2^2} \Delta N_2^2}
$$

$$
\approx \sqrt{\frac{2}{N}} \quad \text{if } N_2 \approx N_1 \equiv N
$$

With a total of 200,000 entries, the average bin content is approximately $200,000/50 = 4000$. Therefore, statistical fluctuations in the plots of the difference are of order 0.02.

Analysis of the generated events requires an algorithm to cluster particles into jets. Also coordinates and directions of partons and jets should be defined. The jet algorithm and the definition of coordinates in the ATLAS detector are discussed in Section 3.1.

Properties of the $t\bar{t}$ production process at lowest order are studied in Section 3.2. Distributions for the strong coupling constant, the energy scale of the hard scattering and some kinematic properties of the top quarks are compared. Kinematic distributions for the quarks produced in the top decays are discussed in Section 3.3. Properties of the events after hadronization are studied in Section 3.4, where the distributions for kinematic variables of jets at particle level are shown.

### 3.1 Coordinates, Directions and Jets

Positions and directions of particles and jets in the ATLAS detector are specified in a right-handed coordinate system. The origin of the system is the interaction point. The positive $x$ axis points toward the centre of the LHC ring, the positive $y$ axis points upwards and the $z$ axis lies along the beam line.

Directions are given in the spherical coordinates $\phi$ and $\theta$. $\phi$ is defined as the azimuthal angle in the $x$-$y$ plane, measured from the positive $x$ axis. $\theta$ is the polar angle with the positive $z$ axis.

The direction perpendicular to the $z$ axis is called the **transverse direction** and the direction along the $z$ axis the **longitudinal direction**. **Transverse momentum** ($p_T$) is the momentum component of a particle in the transverse plane. **Transverse energy** ($E_T$) is defined as $E \sin \theta$. 
Often, pseudorapidity ($\eta$) is used instead of $\theta$. This quantity is defined as:

$$\eta = \frac{1}{2} \ln \left( \frac{|p| + p_z}{|p| - p_z} \right) = -\ln \left[ \tan \left( \frac{1}{2} \theta \right) \right] \quad (3.3)$$

For particles with only a transverse momentum component, $\theta = 1/2\pi$ and $\eta = 0$. For $|\eta| \lesssim 0.5$, it is approximately equal to $\cos(\theta)$ and to $1/2\pi - \theta$. For particles with vanishing $p_T$, $\eta$ goes to plus or minus infinity.

As a measure of distance between paths of particles or jets $\Delta R$ is used:

$$\Delta R = \sqrt{\Delta \phi^2 + \Delta \eta^2} \quad (3.4)$$

$\Delta \eta$ is approximately invariant under Lorentz transformations in the $z$ direction. This symmetry is exact for massless particles. $\phi$ does not depend on the momentum in the $z$ direction, so $\Delta R$ is also approximately invariant.

In hadron collisions, an asymmetry in the momenta of the incoming partons may give the centre-of-mass system of the interaction a large boost in the $z$ direction. Therefore, the use of $\eta$ gives an advantage, since the dependence of $\Delta R$ on this boost is small.

Properties of particles created in the hadronization process are analysed by clustering them into jets. In simulations, this procedure may also be applied to partons. There are several clustering algorithms, all using their own definition of a jet. In this work, a cone jet algorithm is used.

The cone jet algorithm simulates a calorimeter by dividing the $\phi$–$\eta$ plane in rectangular cells with a given size ($\Delta \phi \times \Delta \eta$). Only cells with $|\eta| < \eta_{clus}$ are considered, so the number of cells is finite ($N_\phi \times N_\eta$).

The energy in a cell is given by the sum of the energies of particles with momenta pointing towards the cell. Masses of particles are not taken into account, so the energy defines also the magnitude of the momentum. The direction of the momentum is defined by the $\phi$ and $\eta$ coordinates of the centre of the cell.

All cells with a momentum vector within a predefined cone are clustered into a jet. This cone is defined by the interaction point and a circle in the $\phi$–$\eta$ plane with radius $R_{clus}$. The centre of the circle coincides with the centre of the cell with the largest transverse energy.

The transverse energy of the jet is given by the sum of the cell transverse energies. If the total $E_T$ is smaller than a given minimum ($E_T^{clus}$), the jet is rejected. The cells of rejected jets are considered to be clustered and removed from the list of remaining cells. The algorithm continues to search the unclustered cells for new jets until there are no cells left with an $E_T$ larger than a given seed energy ($E_{T_{seed}}$).

The jet momentum is given by the vectorial sum of the cell momenta. In general, the magnitudes of the cell momenta are all different. Therefore, the $\phi$ and $\eta$ coordinates of the jet are not necessarily equal to the coordinates of the centre of the jet cone.
3.2. Top Quark Production

Figure 3.1: Incoming parton momentum fraction \( x \) at lowest order: PYTHIA 8 vs PYTHIA 6 (a) and ALPGEN vs PYTHIA 6 (b).

### 3.2 Top Quark Production

Figure 3.1 shows the distribution of the parton momentum fractions \( x \), which are identical for the two incoming partons. This distribution is closely related to the production of additional partons at higher order (see Chapter 4).

The behaviour of the momentum fractions at lowest order is dominantly determined by the invariant mass of the \( t \bar{t} \) pair (see below). As a result, \( x \) is of order 0.02 for the majority of events (see Section 1.5).

Another important variable in the generation of additional partons is the energy scale of the hard scattering \( (\sqrt{Q^2}, \text{Figure 3.2}) \). At lowest order, its distribution is determined by the mass and transverse energy of the top quarks (see Equation 1.5). For most events, the energy scale is close to its minimum value: \( p_T t = 0 \Leftrightarrow \sqrt{Q^2} = m_t c = 173 \text{ GeV}/c \). The mean of the distribution is approximately 210 GeV/c.

The strong coupling constant \( (\alpha_s, \text{Figure 3.3}) \) is a function of the energy scale. This relation is given by Equation 1.1. At the scale of the hard interaction, there are five quark flavours \( (n_f = 5) \) and \( \Lambda_5^{(1)} = 0.165 \text{ GeV}/c \) for the CTEQ6L1 PDFs. The minimum \( Q^2 \) of \( (172 \text{ GeV}/c)^2 \) gives a maximum \( \alpha_s \) of 0.118.

ALPGEN uses a value for \( \Lambda_5^{(1)} \) that is slightly different from the PDF value: 0.167 GeV/c. This makes \( \alpha_s \) the only variable in this section with
Figure 3.2: Energy scale of the hard scattering ($\sqrt{Q^2}$) at lowest order: Pythia 8 vs Pythia 6 (a) and Alpgen vs Pythia 6 (b).

Figure 3.3: Strong coupling constant ($\alpha_s$) at the energy scale of the hard scattering at lowest order: Pythia 8 vs Pythia 6 (a) and Alpgen vs Pythia 6 (b). A difference between Alpgen and Pythia is observed due to different definitions of the parameter $\Lambda_\chi^{(1)}$. 
Figure 3.4: Invariant mass of the $\bar{t}t$ pair ($M_{t\bar{t}}$) at lowest order: PYTHIA 8 vs PYTHIA 6 on a linear scale (a) and on a logarithmic scale (b), ALPGEN vs PYTHIA 6 on a linear scale (c) and on a logarithmic scale (d).
Figure 3.5: The $t\bar{t}$ opening angle in the detector frame ($\cos\theta_{t\bar{t}}^*$) at lowest order: PYTHIA 8 vs PYTHIA 6 (a) and ALPGEN vs PYTHIA 6 (b).

a systematic difference between PYTHIA and ALPGEN. This is apparent in Figure 3.3b, but the effect is small and does not significantly change other distributions.

In Figure 3.4, the invariant mass of the $t\bar{t}$ system ($M_{t\bar{t}}$) is shown. At lowest order, this is also the invariant mass of the incoming partons ($\sqrt{s}$). This variable is sensitive to the relative difference of the top and antitop momenta in the $t\bar{t}$ rest frame.

The $t\bar{t}$ mass is dominated by the large mass of the top quark. Its minimum value is $2m_t = 345$ GeV/$c^2$ (the top and antitop are on shell). Most events are produced close to this threshold. The distribution peaks around 400 GeV/$c^2$ and its mean is approximately 520 GeV/$c^2$.

Figure 3.5 shows the cosine of the opening angle of the top and antitop directions in the detector frame ($\cos\theta_{t\bar{t}}^*$). This variable is included to show how a boost of the $t\bar{t}$ system may affect the top and antitop momenta. When the boost is small, the momenta are nearly opposite and this variable is close to minus one. However, there may be a large difference in incoming parton momenta, which causes a boost in the $z$-direction. At higher order, other boosts may appear when high energy additional partons are produced. Because the change in momentum is in the same direction for top and antitop, their momenta are being aligned and $\cos\theta_{t\bar{t}}^*$ shifts towards plus one.

The distributions show that the effect of $z$-direction boosts is significant. There are peaks at both plus and minus one. Roughly speaking, this
3.2. TOP QUARK PRODUCTION

Figure 3.6: Transverse momentum of the (anti)top quark (p_T) at lowest order: PYTHIA 8 vs PYTHIA 6 (a) and ALPGEN vs PYTHIA 6 (b).

indicates that when there is a significant boost, its effect on the top quark momenta is large. This may be explained by the fact that a large part of the energy of the top quark is given by its mass. A boost adds a term \( \gamma v E_T / c \) to the top and antitop momenta (where \( \gamma \) and \( v \) are the Lorentz parameters of the boost and \( E_T \) the energy of the top quark in the \( t \bar{t} \) rest frame). Because the top quark mass makes \( E_T \) much larger the initial momenta of the top quarks, relatively small boosts may affect the momenta significantly.

The magnitude of the top quark momentum is represented by its transverse component (p_T). This is done because the longitudinal component is highly dependent on the asymmetry between the incoming parton momenta, as the \( \cos \theta_T^* \) distributions show. The top/antitop p_T does not depend on this asymmetry and gives an indication of the magnitude of the momentum created in the hard scattering process.

\( p_T \) is shown in Figure 3.6. Because the top and antitop distributions are identical, they are added. At lowest order, the transverse momentum peaks around 80 GeV/c and its mean is approximately 120 GeV/c.

The direction of the top quarks is represented by their pseudorapidity (\( \eta \)). The \( t \bar{t} \) production process is symmetric around the z-axis, so the \( \phi \) distributions are not shown.

The \( \eta \) distributions are shown in Figure 3.7. The distributions are rather central, with a standard deviation of approximately 1.9 (17° from the \( \pm z \) direction, |p_T/p_z| = 0.31). The distributions peak at approximately \( \pm 1.5 \)
CHAPTER 3. LOWEST ORDER APPROXIMATION

Figure 3.7: Pseudorapidity of the (anti)top quark ($\eta_t$) at lowest order: Pythia 8 vs Pythia 6 (a) and Alpgen vs Pythia 6 (b).

(25°, 0.47).

The dip in the distributions at $\eta = 0$ is caused by the large mass of the top quarks. Like $\cos \theta^*_{tt}$, the top quark pseudorapidity is affected significantly by relatively small boosts. The large longitudinal momentum that results from a boost in the $z$-direction pushes $\eta_t$ away from zero. For objects with an even larger mass, like the $t\bar{t}$ system, this effect is also larger (see Chapters 4 and 5).

3.3 Top Quark Decay

Relative directions of top quark decay products are studied in the rest frame of the W boson. In this frame, the top and bottom momenta are equal. Momenta of the down-type quark and the up-type quark in the W decay are opposite and equal in magnitude. This is shown in Figure 3.8.

The V-A structure of the top decay tends to align the bottom quark momentum, the down-type quark momentum and the top quark spin. As a result, the cosine of the opening angle between the bottom quark and the down-type quark ($\cos \theta^*_{bd}$ in Figure 3.8) tends to be positive. This is shown in Figure 3.9.

The directions of the quarks in the top decay may be used to study the direction of the top quark spin. The relative direction of the down-type
3.3. TOP QUARK DECAY

Figure 3.8: The top quark decay in the rest frame of the W boson. $\theta_{bd}^{\ast}$ is defined as the opening angle of the bottom quark and the down-type quark in the W decay.

Figure 3.9: The distribution of $\cos\theta_{bd}^{\ast}$ at lowest order: PYTHON 8 vs PYTHON 6 (a) and ALPGEN vs PYTHON 6 (b).
Figure 3.10: $t\bar{t}$ decay in different Lorentz frames. The top and antitop have opposite momenta in the $t\bar{t}$ rest frame (in the middle). Lorentz transformations give the momenta of the decay products in the top rest frame (on the right) and in the antitop rest frame (on the left). $\theta_{\text{dd}}^*$ is defined as the angle between the momentum vector of the down-type antiquark in the decay of the W from the top and the momentum vector of the down-type quark in the decay of the W from the antitop. These vectors are given in the top and antitop rest frames, respectively.

Figure 3.11: The distribution of $\cos \theta_{\text{dd}}^*$ at lowest order: PYTHIA 8 vs PYTHIA 6 (a) and ALPGEN vs PYTHIA 6 (b). A difference between ALPGEN and PYTHIA is observed due to a different treatment of spin correlations.
quarks in the W decays is analysed to demonstrate the relation between the top and antitop spins. To eliminate the dependence on boosts, directions are specified in the top and antitop rest frames. The $t\bar{t}$ centre-of-mass system serves as a common reference frame. This is depicted in Figure 3.10. $\theta^*_{dd}$ is the angle between the down-type quarks in the W decays.

In Pythia, the directions of the top and antitop spins are independent and distributed isotropically. This gives a flat distribution for $\cos \theta^*_{dd}$ (Figure 3.11a). In Alpgen, the relative direction is determined by the $t\bar{t}$ production process. This leads to a small deviation from a flat distribution and thus to a difference with Pythia, which is shown in Figure 3.11b. It appears that the top and antitop spins tend to have the same direction in Alpgen.

Since the masses of the bottom quarks and the quarks from the W decays are small compared to their momenta, their $p_T$ is almost equal to their $E_T$. In the calorimeters, particle energies are measured, so $E_T$ is used for the magnitude of parton and jet momenta.

The energies of the up-type quark and the down-type quark are equal in the rest frame of the W boson (see Figure 3.8). In general, this is changed by a Lorentz transformation to the top quark rest frame, because the quarks have opposite directions. Since the down-type quark tends to have the same direction as the top quark in the W frame, its average energy becomes smaller. The energy of the up-type quark becomes larger on average.

This asymmetry also appears in the $E_T$ distributions in the detector frame. Figure 3.12 shows the transverse energy of the down-type quarks ($E_T^d$). This distribution peaks around 30 GeV and its mean is approximately 50 GeV. The distribution for the up-type quarks ($E_T^u$ in Figure 3.13) has a similar shape, but peaks around 35 GeV and it has a mean of approximately 60 GeV. The relation between the spin of the top quark and the directions of its decay products are taken into account by both Pythia and Alpgen. Therefore, both distributions are equal for all generators.

Because the asymmetry between the up-type and down-type quarks in the W decay is small, there are no observable differences between their pseudorapidity distributions ($\eta_d$ in Figure 3.14 and $\eta_u$ in Figure 3.15). The dip in the top quark pseudorapidity at $\eta = 0$ is absent for the quarks from the top decay, since their masses are small compared to their energies. The standard deviations are 1.5 (25° from the $\pm z$ direction, $|p_T/p_z| = 0.47$).

Figure 3.16 shows the transverse energy of the bottom quark ($E_T^b$). The average energy is larger than for the other quarks, because the bottom comes directly from the $t\rightarrow bW$ decay. The $E_T$ distributions peak around 50 GeV and their averages are approximately 70 GeV. The bottom pseudorapidity ($\eta_b$) is shown in Figure 3.17. These distributions are equal to those of the quarks in the W decay.
CHAPTER 3. LOWEST ORDER APPROXIMATION

Figure 3.12: Transverse energy of the down-type quarks from the W decays ($E_{T_d}$) at lowest order: PYTHIA 8 vs PYTHIA 6 (a) and ALPGEN vs PYTHIA 6 (b).

Figure 3.13: Transverse energy of the up-type quarks from the W decays ($E_{T_u}$) at lowest order: PYTHIA 8 vs PYTHIA 6 (a) and ALPGEN vs PYTHIA 6 (b).
3.3. TOP QUARK DECAY

Figure 3.14: Pseudorapidity of the down-type quarks from the W decays ($\eta_d$) at lowest order: PYTHIA 8 vs PYTHIA 6 (a) and ALPGEN vs PYTHIA 6 (b).

Figure 3.15: Pseudorapidity of the up-type quarks from the W decays ($\eta_u$) at lowest order: PYTHIA 8 vs PYTHIA 6 (a) and ALPGEN vs PYTHIA 6 (b).
Figure 3.16: Transverse energy of the (anti) bottom quark ($E_T$) at lowest order: Pythia 8 vs Pythia 6 (a) and Alpgen vs Pythia 6 (b).

Figure 3.17: Pseudorapidity of the (anti)bottom quark ($\eta_b$) at lowest order: Pythia 8 vs Pythia 6 (a) and Alpgen vs Pythia 6 (b).
3.4 Particle Jets

Parameters of the cone jet algorithm used in this section are listed in Table 3.2. Distributions are shown for particle jets with $E_T > 6$ GeV and $|\eta| < 5$.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
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</tr>
<tr>
<td>$\eta_{clus}$</td>
<td>6</td>
</tr>
<tr>
<td>$E_T^{clus}$</td>
<td>5 GeV</td>
</tr>
<tr>
<td>$E_T^{seed}$</td>
<td>1.5 GeV</td>
</tr>
<tr>
<td>$N_\phi \times N_\eta$</td>
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<td>$\Delta \phi \times \Delta \eta$</td>
<td>0.112 $\times$ 0.120</td>
</tr>
<tr>
<td>cells/cone</td>
<td>37</td>
</tr>
</tbody>
</table>

Table 3.2: Cone jet algorithm parameters for jets at particle level.

Figure 3.18 shows the jet multiplicity. At lowest order, one expects to find roughly one jet for each quark from the $t \bar{t}$ decay. However, the particle topology varies from jet to jet and particles originating from one quark may be spread over an area larger than the cone size. In particular, colour connections between partons may “pull” particles out of the jet cone. It is also possible that the opening angle of two quarks is small and particles from two different quarks end up in the same cone. Therefore, the multiplicity may be larger or smaller than six. The five-jet contribution in Figure 3.18 shows that particles from two quarks merge for a significant number of events with this jet algorithm.

The logarithmic plot of this distribution shows that PYTHIA 8 produces less seven-jet events than PYTHIA 6. The value of the plot of the difference is $-0.7$. The number of events in this bin is approximately 2300. This gives an expected statistical error of order 0.03, so the deviation is significantly larger than the expected statistical fluctuations.

In Figure 3.19, the minimum $\Delta R$ between two jets in the event ($\Delta R_{\text{min}}$) is shown. This variable is expected to be larger than approximately $R_{clus} = 0.4$. It may be smaller, however, because jet cones are allowed to overlap in this relatively simple algorithm.

At higher order, the direction of additional partons may be close to the direction of one of the quarks from the $t \bar{t}$ decay. Therefore, a decrease of the average $\Delta R_{\text{min}}$ is expected at higher order.

At lowest order, there appears to be a difference between PYTHIA 6 and PYTHIA 8 again for $\Delta R_{\text{min}} \lesssim 0.6$. The PYTHIA 6 distribution slightly exceeds the PYTHIA 8 distribution in this region.

Figure 3.20 shows the invariant mass of all jets ($\sqrt{s_{\text{jets}}}$). This variable is approximately equal to the invariant mass of the event. Additional jets from the $t \bar{t}$ production process will increase this invariant mass, so $\sqrt{s_{\text{jets}}}$ is sensitive to higher order corrections.

At lowest order, $\sqrt{s_{\text{jets}}}$ is approximately equal to the $t \bar{t}$ mass (Figure 3.4).
Figure 3.18: Particle jet multiplicity at lowest order: **Pythia 8 vs Pythia 6** on a linear scale (a) and on a logarithmic scale (b), **Alpgen vs Pythia 6** on a linear scale (c) and on a logarithmic scale (d).
Figure 3.19: Minimum $\Delta R$ between two particle jets ($\Delta R_{\text{min}}$) at lowest order: Pythia 8 vs Pythia 6 (a) and Alpgen vs Pythia 6 (b).

Figure 3.20: Invariant mass of all particle jets ($\sqrt{s_{\text{jets}}}$) at lowest order: Pythia 8 vs Pythia 6 (a) and Alpgen vs Pythia 6 (b).
Figure 3.21: Sum of all particle jet transverse energies ($H_T$) at lowest order: PYTHIA 8 vs PYTHIA 6 (a) and ALPGEN vs PYTHIA 6 (b).

However, not all particles are necessarily assigned to a jet. Therefore, the mean invariant mass of the jets (470 GeV/$c^2$) is smaller than the mean $t\bar{t}$ invariant mass (500 GeV/$c^2$). $\sqrt{s_{\text{jet}}}$ may also be smaller than $2m_t$. Below this value, there is a small difference between PYTHIA 6 and PYTHIA 8 again. PYTHIA 8 produces less events with small invariant mass.

Figure 3.21 shows the scalar sum of the transverse energies for all jets ($H_T$). This variable is sensitive to the energy scale of the event. It is important in Tevatron analyses to separate fully hadronic $t\bar{t}$ events from background events. Six jets or more are produced in regular QCD background events, but the shape of their $H_T$ distribution is different from the $t\bar{t}$ $H_T$ distribution.

Additional jets contribute to $H_T$, so this variable is also sensitive to higher order corrections. At lowest order, it peaks at 300 GeV and its mean value is 350 GeV.

In Figures 3.22 and 3.23, the transverse energies of jets 1 and 6 ($E_{T_{\text{jet}}}$) are shown. The jets are ordered by decreasing $E_T$, so jet 1 is the jet with the largest $E_T$. At lowest order, jet 6 is often the softest jet in the event.

The distribution for jet 1 peaks around 90 GeV and its mean is approximately 110 GeV. This corresponds well to the quark distributions, bearing in mind that jet 1 is always the hardest jet.

The distribution for jet 6 suggests that this jet is below the 6 GeV threshold for part of the events. These events also contribute to the events with
3.4. PARTICLE JETS

Figure 3.22: Transverse energy of the first particle jet ($E_{T1}$) at lowest order: Pythia 8 vs Pythia 6 (a) and Alpgen vs Pythia 6 (b).

Figure 3.23: Transverse energy of the sixth particle jet ($E_{T6}$) at lowest order: Pythia 8 vs Pythia 6 (a) and Alpgen vs Pythia 6 (b).
Figure 3.24: Pseudorapidity of the first particle jet ($\eta_1$) at lowest order: PYTHIA 8 vs PYTHIA 6 (a) and ALPGEN vs PYTHIA 6 (b).

less than six jets in the multiplicity distribution. The PYTHIA 6 distribution is somewhat softer than the PYTHIA 8 distribution.

The pseudorapidity of jets 1 and jet 6 ($\eta_6$) is shown in Figures 3.24 and 3.25. These distributions are very similar to those of the quark pseudorapidity. Because the transverse energy/momentum of jet 1 is much larger than that of jet 6, the momentum of jet 1 is more transverse. Therefore, its pseudorapidity is closer to zero. This makes the distribution for jet 1 narrower than the distribution for jet 6. The standard deviations are 1.3 and 1.7, respectively, compared to 1.5 for the quark distributions.

For some of the variables in this section, differences between PYTHIA 6 and PYTHIA 8 are larger than expected from statistical fluctuations. These deviations are due to small changes in the simulation of hadronization.

The distributions suggest that the particles in PYTHIA 6 jets are distributed more broadly than in PYTHIA 8 jets. This would result in more particles outside the initial jet cone, which makes the PYTHIA 6 jets softer. This can be seen from the distributions of the invariant mass, $H_T$ and the sixth jet, which differ slightly for small values.

The particles outside the initial jet cone may form an extra jet. This would result in the larger contribution of seven-jet events for PYTHIA 6. The direction of the extra jet would be very close to the direction of the initial jet. This can be seen from the distribution of the minimum $\Delta R$ between jets, which is smaller for PYTHIA 6.
3.5 Summary

At lowest order Pythia 6, Pythia 8 and Alpgen give almost the same results for $t\bar{t}$ production. The estimated cross section with the CTEQ6L1 PDF sets is approximately 560 pb (Table 3.1). There is a variation of 0.3 per cent between the generators due to differences in (default) parameter settings. One of these differences also appears in the distribution of the strong coupling constant, which has a slightly larger value in Alpgen (Figure 3.3b). Shapes of other distributions (Figures 3.1 through 3.7) are the same for the three generators.

In the top quark decays, there are differences between Pythia and Alpgen. Different branching ratios are applied, which leads to a variation of three per cent in the estimated cross section for the fully hadronic channel (Table 3.1). Furthermore, Pythia calculates $t\bar{t}$ production and the top quark decays separately, without taking account of the correlation between the top and antitop spins. This correlation is included in Alpgen. As a result, differences appear in the distributions of the angles between top and antitop decay products (Figure 3.11b). Other distributions (Figures 3.9 and 3.12 through 3.17) are unaffected by the absence of spin correlations in Pythia.

A difference between the two Pythia versions appears in the simulation of hadronization. The analysis of particle jets suggests that Pythia 6...
distributes particles more broadly than PYTHIA 8. Most likely, this is due to differences in (default) settings of parameters in the hadronization algorithms.
Chapter 4

Comparing Matrix Elements and Parton Shower

Higher order QCD corrections in the $t\bar{t}$ production process will modify distributions for all variables from the lowest order approximation in Chapter 3. Simulations that include higher orders will demonstrate how much each distribution is affected. The matrix element and parton shower methods (described in Chapter 2) are compared for emissions of hard, non-collinear additional partons. It is expected that matrix elements provide a better description of this region of phase space than a parton shower.

Top–antitop events with a fixed number ($n$) of hard, non-collinear additional partons are studied. This region of phase space is defined by three parameters that specify the minimum energy scale for parton emissions. Infrared divergences are avoided by requiring a minimum transverse energy for additional partons. A minimum $\Delta R$ between them and a maximum pseudorapidity avoid collinearities.

These parameters may also be used to define cone jets at parton level (see Section 3.1). $E_T^{\text{clus}}$ is set to the minimum transverse energy, $\eta_{\text{clus}}$ to the maximum pseudorapidity and $R_{\text{clus}}$ to the minimum $\Delta R$. With this definition, each additional parton from $t\bar{t} + n$-parton matrix elements will result a separate parton level jet. The cone jet parameters are listed in Table 4.1.

<table>
<thead>
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<th>$R_{\text{clus}}$</th>
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Table 4.1: Cone jet algorithm parameters for jets at parton level.
Matrix element events are generated with Alpgen. Additional partons have a minimum transverse momentum ($p_T^{\text{min}}$) of 85 GeV/c, a maximum pseudorapidity ($\eta_{\text{max}}$) of 2.6 and a minimum $\Delta R$ ($R_{\text{min}}$) of 0.6. These parameters differ slightly from the cone jet parameters to assure complete coverage of the phase space above the minimum jet scale. Events with jets below this scale are rejected.

The jet algorithm may also be applied to events from the parton shower. Because there are no (hard) cuts on parton momenta, the resulting jets will often consist of more than one parton. In general, collinear partons within these jets are the result of branches at a low energy scale. They originate from hard, non-collinear partons, produced at a high energy scale. A large part of the jet kinematics is determined by these original partons, which are also described by the higher order matrix elements.

Parton shower events are generated with Pythia 6. A full shower evolution is performed and events with one and with two jets are selected. Since the quarks in the top decays give rise to final state showers, kinematic properties of decay products are affected by the parton shower. These showers also lead to production of additional jets in the $t\bar{t}$ decay process, which are not generated by Alpgen. Therefore, analysis of the top quark decays and jets at particle level is postponed to Chapter 5.

Samples of 200,000 events with one and with two additional jets are analysed. Distributions are normalized to the lowest order approximation of the $n$-parton cross sections calculated by Alpgen. These cross sections are listed in Table 4.2. The table also shows the products of the lowest order $t\bar{t}$ cross section and the fractions of $n$-jet events from the parton shower.

<table>
<thead>
<tr>
<th>$n$</th>
<th>$\sigma_{t\bar{t}+n\text{-parton}}$ (pb)</th>
<th>$\sigma_{t\bar{t}+n\text{-jet}}$ (pb)</th>
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<td>42.7</td>
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</tr>
<tr>
<td>3</td>
<td>0.8</td>
<td>0.6</td>
</tr>
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<td>$\geq 3$</td>
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<td>total</td>
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<td>256.8</td>
</tr>
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</table>

Table 4.2: Tree level matrix element and parton shower approximations for $t\bar{t} + n$-jet cross sections.

### 4.1 Effects of Soft/Collinear Partons

Obviously, the comparability of the parton shower and matrix element approaches is limited. Kinematics of the $t\bar{t}$ pair and hard, non-collinear jets are affected by emissions of soft and collinear partons. These emissions are
4.2 Kinematic Distributions

The difference between the matrix element and parton shower approaches becomes immediately clear from the parton momentum fractions ($x$). Fig-

![Figure 4.1: Additional parton jet multiplicity with $E_{\text{clus}} = 6$ GeV and $\eta_{\text{clus}} = 6$: ALPGEN vs PYTHIA for the one-jet sample (a) and for the two-jets sample (b). The lack of soft/collinear additional partons from matrix elements causes a large difference between ALPGEN and PYTHIA.](image)

generated by the parton shower, but not by matrix elements. This complication will be dealt with in Chapter 5, where soft and collinear partons are added to matrix element events by the parton shower.

The effect of soft and collinear emissions is demonstrated by constructing jets below the hard, non-collinear energy scale. The cone jet algorithm is applied on events from the one-jet and two-jet samples, but now with $E_{\text{clus}} = 6$ GeV, $\eta_{\text{clus}} = 6$ and $R_{\text{clus}} = 0.7$.

Figure 4.1 shows the jet multiplicities for these soft/collinear jets. The parton shower generates jets which are not present in the $t\bar{t} + n$-parton matrix element sample. It produces an average of four jets in the one-jet sample and five jets in the two-jet sample, while exactly one and two jets are produced by matrix elements.

The magnitude of contributions from soft/collinear parton shower jets is shown in Figure 4.2. The (scalar) sum of transverse energies ($H_T$) for additional jets is plotted for the one-jet sample (4.2a) and the two-jet sample (4.2b). Significant differences between the two approaches are present in these distributions. The average difference in $H_T$ is approximately $100$ GeV for the one-jet sample and approximately $120$ GeV for the two-jet sample.

For comparison, the $H_T$ distributions for hard, non-collinear jets ($E_{\text{clus}} = 100$ GeV and $\eta_{\text{clus}} = 2.5$) are shown in Figure 4.3. Distributions for matrix elements and the parton shower are very similar. This jet definition will be used Section 4.2.
CHAPTER 4. MATRIX ELEMENTS VS PARTON SHOWER

Figure 4.2: Sum of all additional jet transverse energies ($H_T$) with $E_{\text{clus}} = 6$ GeV and $\eta_{\text{clus}} = 6$: ALPGEN vs PYTHIA for the one-jet sample (a) and for the two-jets sample (b). The lack of soft/collinear additional partons from matrix elements causes a large difference between ALPGEN and PYTHIA.

Figure 4.3: Sum of all additional jet transverse energies ($H_T$) with $E_{\text{clus}} = 100$ GeV and $\eta_{\text{clus}} = 2.5$: ALPGEN vs PYTHIA for the one-jet sample (a) and for the two-jets sample (b).

ures 4.4a and 4.4b show their distributions from the matrix element calculation. For ALPGEN, these are the momentum fractions of the incoming partons. PYTHIA, however, runs the parton shower algorithm after calculating the lowest order $t\bar{t}$ production process. The parton shower may produce parton branches from which a matrix element parton originates. This results in “new” incoming partons with larger momentum fractions. These are shown in Figures 4.4c and 4.4d.

Production of a $t\bar{t}$ pair with additional jets requires a larger invariant mass than lowest order $t\bar{t}$ production. One way of obtaining this mass is increasing $x$. This can be seen in Figures 4.4a and 4.4b, where the momentum fractions are larger for ALPGEN than for PYTHIA. The PYTHIA distributions are essentially the same as at lowest order (Figure 3.1 on page 39). The effect is stronger for the two-jet events than for the one-jet events.
In parton shower language, the higher ALPGEN momentum fractions are the result of “evolution” from the hard scattering energy scale to the minimum scale for hard, non-collinear partons. The incoming partons in PYTHIA still have the scale of the hard scattering, which is associated to smaller values of $x$. The fractions become much larger for PYTHIA than for ALPGEN after parton shower evolution to the cut-off scale, which is much lower than the hard, non-collinear scale. This is shown in Figures 4.4c and 4.4d.

The energy scale of the hard scattering ($\sqrt{Q^2}$) is shown in Figure 4.5. In the PYTHIA calculation, there are no additional partons and $Q^2$ is equal to the sum of the squared masses and transverse momenta of the top quarks (see Equation 1.5 on page 16). In ALPGEN, also the squares of the additional jet transverse momenta are added.

The PYTHIA distributions are almost the same as the lowest order distributions (Figure 3.2 on page 40). Additional partons push the energy scale to higher values for ALPGEN. The minimum energy scale is shifted due to
the minimum energy of the extra jets.

Since the strong coupling constant is a function of the energy scale (Equation 1.1 on page 11), the effect of additional partons in ALPGEN is also reflected by the $\alpha_s$ distributions (Figure 4.6). Note that the parton shower evolves the PYTHIA events to a lower energy scale, resulting in an even higher $\alpha_s$ at parton branches.

Despite the differences in the generation process, properties of partons and parton jets are quite similar for ALPGEN and PYTHIA. Figure 4.7 shows the $t\bar{t}$ invariant mass ($M_{t\bar{t}}$). This variable is dominated by the large mass of the top quark, which makes its distributions remarkably similar to the lowest order distributions (Figure 3.4 on page 41). This indicates that the production of additional partons is dominated by emissions from the incoming partons. This process affects the kinematics of the $t\bar{t}$ centre-of-mass system (see below), but the effect on the relative momenta of the top and antitop quarks is small.

The ALPGEN distributions still peak at 400 GeV/$c^2$. However, the means shift to somewhat larger values due to parton emissions that do affect the relative momenta of the top and antitop quarks. The ALPGEN mean with one parton is approximately 550 GeV/$c^2$ (520 GeV/$c^2$ at lowest order) and with two partons approximately 570 GeV/$c^2$.

Soft/collinear parton emissions from the parton shower seem to have an observable effect on the $t\bar{t}$ mass. The peaks in the PYTHIA distributions are shifted to the right. The smaller PYTHIA contribution at large invariant mass makes the means somewhat smaller than the ALPGEN means: 540 GeV/$c^2$ with one jet and 565 GeV/$c^2$ with two jets.

Some new variables are introduced at higher order. The $t\bar{t}$ system obtains a transverse momentum, which balances the transverse component of
4.2. KINEMATIC DISTRIBUTIONS

Figure 4.6: Strong coupling constant ($\alpha_s$) at the energy scale of the hard scattering: ALPGEN vs PYTHIA, the one-jet sample (a) and the two-jets sample (b). These distributions reflect the differences between the matrix element and parton shower approaches.

The total additional jet momentum. The distribution of $p_T^{\bar{t}\bar{t}}$ is shown in Figure 4.8. The distribution for ALPGEN with one jet is roughly equal to the jet $E_T$ (see below) and $H_T$ (Figure 4.3) distributions. Because the momentum cut-off for jets is a minimum transverse energy (100 GeV) and not a minimum transverse momentum, there is a small number of events below $p_T^{\bar{t}\bar{t}} = 100$ GeV/c.

Because of production of soft partons in the parton shower, the $\bar{t}\bar{t}$ $p_T$ for PYTHIA with one jet may be smaller than 100 GeV/c. This affects the distribution around 100 GeV/c and makes the effect of the additional jet $p_T$ on the $\bar{t}\bar{t}$ $p_T$ less pronounced. From the logarithmic plot on the right, it appears that the parton shower overestimates the contribution of high-$p_T$ jets.

When more than one jet is produced, the additional jet $p_T$s may balance each other and a sharp cut-off in the $\bar{t}\bar{t}$ $p_T$ is absent. Only a small effect due to the jet $E_T$ cut-off is observed in the two-jet ALPGEN distribution at 200 GeV/c. This also results in a smaller difference between ALPGEN and PYTHIA. As in the one-jet distributions, the PYTHIA contribution from high-$p_T$ $\bar{t}\bar{t}$ pairs is larger than for ALPGEN.

Since the $p_T$ of the $\bar{t}\bar{t}$ pair is finite at higher order, so is the $\bar{t}\bar{t}$ pseudo-rapidity ($\eta_{\bar{t}\bar{t}}$, Figure 4.9). The standard deviation of both the distributions for one jet is 1.9. The distributions also peak at approximately this value.

The large invariant mass of the $\bar{t}\bar{t}$ pair results in an even larger dip at $\eta = 0$ than for the top quarks at lowest order (Figure 3.7 at page 44). Because the parton shower creates more $\bar{t}\bar{t}$ pairs with a large transverse momentum than ALPGEN, the PYTHIA dip is slightly less pronounced. PYTHIA events with a transverse momentum below 100 GeV/c are responsible for another difference for one-jet events around $\eta = 4$, where the PYTHIA distribution
Figure 4.7: Invariant mass of the $t\bar{t}$ pair ($M_{t\bar{t}}$): Alpgen vs Pythia, the one-jet sample on a linear scale (a) and on a logarithmic scale (b), the two-jets sample on a linear scale (c) and on a logarithmic scale (d).
4.2. KINEMATIC DISTRIBUTIONS

Figure 4.8: Transverse momentum of the tū pair ($p_{Ttū}$): ALPGEN vs PYTHIA, the one-jet sample on a linear scale (a) and on a logarithmic scale (b), the two-jets sample on a linear scale (c) and on a logarithmic scale (d). The ALPGEN distributions are clearly affected by the energy cut-off for additional partons.
dominates again.

With two jets, the average $t\bar{t}$ transverse momentum is larger than with one jet. This reduces the effect of the large invariant mass and pushes the distributions towards $\eta = 0$. Also with two jets the parton shower produces more $t\bar{t}$ pairs at high-$p_T$, which results in a difference between Pythia and Alpgen.

The transverse momentum of the top and antitop quarks ($p_T$) is shown in Figure 4.10. The one-jet and two-jet distributions are similar to the lowest order distributions (Figure 3.6 at page 43), but the average transverse momentum is higher. The parton shower seems to overestimate the production of high-$p_T$ top quarks, like it does for the $t\bar{t}$ pair.

The distributions have a broad peak around 110–130 GeV/$c$. With $t\bar{t}$ + one jet, the mean is 165 GeV/$c$ for Alpgen and 175 GeV/$c$ for Pythia. With two jets, the means are 200 GeV/$c$ and 210 GeV/$c$, respectively.

Because of the high top/antitop transverse momenta, the dips in the lowest order pseudorapidity distributions (Figure 3.7 at page 44) almost vanish when hard, non-collinear additional jets are produced ($\eta_h$, Figure 4.11). The standard deviations are approximately 1.6 with one jet and 1.5 with two jets.

Figure 4.12 shows the transverse energy of the hardest additional jet ($E_{T1}$). Pythia distributions are harder again. The mean values for the one-jet distributions are 190 GeV for Alpgen and 210 GeV for Pythia. The two-jet means are 265 GeV for Alpgen and 300 GeV for Pythia.

Figure 4.9: Pseudorapidity of the $t\bar{t}$ pair ($\eta_{t\bar{t}}$): Alpgen vs Pythia, the one-jet sample (a) and the two-jets sample (b).
### 4.2. Kinematic Distributions

![Graphs](image)

Figure 4.10: Transverse momentum of the (anti)top quark ($p_T$): ALPGEN vs PYTHIA, the one-jet sample (a) and the two-jets sample (b).

![Graphs](image)

Figure 4.11: Pseudorapidity of the (anti)top quark ($\eta$): ALPGEN vs PYTHIA, the one-jet sample (a) and the two-jets sample (b).
Figure 4.12: Transverse energy of the first additional parton jet ($E_{T1}$): ALPGEN vs PYTHIA, the one-jet sample (a) and the two-jets sample (b).

Figure 4.13: Pseudorapidity of the first additional parton jet ($\eta_1$): ALPGEN vs PYTHIA, the one-jet sample (a) and the two-jets sample (b).
4.2. KINEMATIC DISTRIBUTIONS

Figure 4.14: Kinematics of the second additional parton jet in the two-jets sample: ALPGEN with merging vs PYTHIA, (a) transverse energy ($E_T$) and (b) pseudorapidity ($\eta$).

The difference in transverse momentum is also observed in the pseudorapidity of additional jets ($\eta_1$, Figure 4.13). Distributions are more central for PYTHIA. The difference in the one-jet distributions is smaller than in the two-jet distributions.

The transverse momentum of the second additional jet in the two-jets sample ($E_{T2}$) is shown in Figure 4.14a. This jet is much softer than the first jet: The mean value of the $E_T$ distribution is 155 GeV for ALPGEN and 160 GeV for PYTHIA. This is also softer than the jet in the one-jet sample.

The difference between the PYTHIA and ALPGEN second jet $E_T$ distributions is much smaller than it was for the $E_T$ of the first jet. However, the pseudorapidity distributions ($\eta_2$, Figure 4.14b) show deviations that are similar to those in the distributions of the first jet $\eta$.

Figure 4.15 shows the $\Delta R$ between the additional jets ($\Delta R_{12}$) in the two-jets sample. The size of the jet cone ($R_{clus}$) gives a cut-off at $\Delta R_{12} = 0.7$. The ALPGEN jets consist of one parton, which gives a sharp cut-off. Parton shower jets may consist of multiple partons. Because $\Delta R_{ij}$ is the distance between the sums of their momenta and not the distance between the centre of the jet cones, a small number of events ends up below $\Delta R_{12} = 0.7$ for PYTHIA. The additional jet $\Delta R$ tends to be larger for ALPGEN than for the parton shower. The mean values are 2.5 and 2.4, respectively.

The only top quark decay distributions shown in this chapter are those
Figure 4.15: $\Delta R$ between the first and second additional parton jet ($\Delta R_{12}$) in the two-jets sample: ALPGEN vs PYTHIA.

Figure 4.16: $\cos \theta_{q_2i}$: ALPGEN vs PYTHIA, the one-jet sample (a) and the two-jets sample (b). The different treatment of spin correlations still appears in these distributions, although the effect is much smaller than at lowest order.
of \( \cos \theta^*_\text{dd} \) (Figure 4.16). \( \cos \theta^*_\text{dd} \) is calculated with the directions of the down-type quarks before they radiate gluons in final state showers (see also Figure 3.10 on page 46). The asymmetry in the ALPGEN distributions is smaller than it was in the lowest order distribution (Figure 3.11 on page 46). With two additional jets, it almost vanishes.

Apparently, the correlation between the top and antitop spins becomes smaller with additional partons. This can be explained by the fact that the additional partons carry spin and therefore modify the top quark spins. The more partons are produced, the more spin configurations become available in which the top quark spins are not necessarily aligned.

### 4.3 Summary

Differences between simulating higher order QCD corrections with tree-level matrix elements and a parton shower become apparent in the properties of the hard scattering. Distributions of parton momentum fractions (Figure 4.4), the energy scale (Figure 4.5), and the strong coupling constant (Figure 4.6) differ significantly.

A consequence of these differences appears in distributions that are sensitive to properties of soft/collinear additional partons. These partons are generated by the parton shower, but not by the matrix elements. This is apparent in the \( t \bar{t} p_T \) distributions (Figure 4.8), which show the effects of the energy cut-off in ALPGEN. Soft/collinear additional partons give also rise to jets that are not present in ALPGEN (Figures 4.1 and 4.2).

It is harder to determine the origin of the differences in the kinematic properties of the top quarks and the additional hard, non-collinear jets (Figures 4.7 and 4.10 through 4.15). These could be due to the lack of soft and collinear partons in the matrix element method as well. However, they could also be a result of the difference between matrix elements and the parton shower in the treatment of hard, non-collinear parton emissions.

A repeating feature is that \( E_T/p_T \) distributions are harder and pseudorapidity distributions are more central for the parton shower. This is the case for the top quarks (Figures 4.10 and 4.11) and additional jets (Figures 4.12, 4.13 and 4.14), but also for the \( t \bar{t} \) pair (Figures 4.8 and 4.9). These differences are further investigated in Chapter 5, where soft and collinear partons are added to the matrix element events with the parton shower.
Chapter 5

Merging Matrix Elements and Parton Shower

Results from Chapter 4 show that the lack of soft and collinear additional partons in tree level matrix element calculations has significant consequences for $t\bar{t}$ production. This chapter describes how the matrix element and parton shower approaches can be merged in order to describe both hard and soft additional partons (see also Section 2.3).

Again, matrix element events are generated with ALPGEN and parton shower events with PYTHIA 6. The merging scheme that was designed to combine ALPGEN matrix elements and a parton shower is the MLM matching procedure [25, 26]. This algorithm is described in Section 5.1.

Results of applying the merging scheme on the ALPGEN samples from Chapter 4 are discussed in Section 5.2. Distributions are compared with those from the parton shower and with the original ALPGEN distributions. Only the one-jet and two-jet samples are analysed, like in Chapter 4.

The minimum energy scale for additional partons in Chapter 4 is rather high. This avoids divergences, which makes the ALPGEN matrix element calculation more reliable. Such a high scale is not recommended for merging, since the parton shower may already be unreliable in this region of phase space. In Section 5.3, results from merging at a lower scale are compared with results from the parton shower. Samples that contain all parton multiplicities are used in this analysis.

5.1 The MLM Matching Procedure

In the MLM matching procedure, separating the two phase space regions and reweighting with a Sudakov form factor are performed simultaneously. This is achieved by allowing the parton shower to add partons in the full phase space and then either to accept or to reject an event. Events are
accepted if all parton jets above the merging scale originate from additional partons created by ALPGEN. If the parton shower adds hard, non-collinear jets or if it changes the direction of the original ALPGEN jets too much, the event is rejected.

The fraction of events that is accepted for each point in phase space is an estimate of the probability for having no parton emissions between the energy scale of the hard scattering and the merging scale. In parton shower language, this fraction is an approximation of the Sudakov factor. Reducing the event density has the same effect as reducing the weight, so the acceptance/rejection procedure also handles Sudakov reweighting.

Energy scales of parton branches in the merging process are defined by the transverse energy, the pseudorapidity and the $\Delta R$ of the created partons. The merging scale is defined by the parameters that are used in Chapter 4 to divide the phase space: $E_T^{clus}$, $\eta^{clus}$ and $R^{clus}$. Additional partons are generated by ALPGEN with $c p_T^{part} > c p_T^{min} \leq E_T^{clus}$, $|\eta^{part}| < \eta^{max} \geq \eta^{clus}$ and $\Delta R^{part} \geq R^{min} \leq R^{clus}$. This minimum scale for ALPGEN may be lower than the merging scale to assure complete coverage of the phase space.

Reweighting of $\alpha_s$ is performed in two steps. First, matrix element weights are calculated with the same value for the coupling constant for all “parton branches”. This $\alpha_s$ is evaluated at the lowest scale of all “branches”.

In the second step, events are reweighted with the ratios of the coupling constants at the actual “branching” scales and the coupling constant at the lowest scale. These factors are always smaller than one, because $\alpha_s$ increases with decreasing energy scale. The first and second step together result in the reweighting factor for $\alpha_s$ in Equation 2.5 on page 32.

Reweighting in step two is again a procedure in which events are accepted or rejected. In this case, a random number is drawn from a uniform distribution between zero and one. An event is accepted if its reweighting factor is larger than or equal to the random number.

The quotes around the word “branch” refer to the fact that the ALPGEN partons are not produced in an actual shower evolution. A tree-like structure is constructed by applying a $k_T$ clustering algorithm on the incoming and outgoing partons from the matrix element calculation. In this algorithm, $k_T$ is a measure of distance between two partons in momentum space. This variable is used as the energy scale of the “branch” from which the two partons originated. The definition of this scale is different from the $E_T/\eta/\Delta R$ definition that is used in the rest of the merging scheme:

$$k_T = (\Delta y^2 + \Delta \phi^2) \min \left( p_T^2, p_T^{final} \right)$$ For two final state partons (5.1a) $$k_T = p_T^{final}$$ For an initial and a final state parton (5.1b)

The quantity $y$ is the rapidity of a parton. The definition of rapidity is similar to the definition of pseudorapidity in Equation 3.3 on page 38. Only $|p|$ is replaced by $E$ in this expression.
5.1. THE MLM MATCHING PROCEDURE

Clustering of partons starts with the combination of the two partons with the smallest $k_T$ (lowest scale). One new, branching parton is formed, which may be combined with remaining partons. $\alpha_s$ is calculated at the scale $Q^2 = k_T$ for each branch. The process continues until $n$ branches are constructed. This leaves the two initial state partons and the two final state partons of the “lowest order process”.

After the first step of the $\alpha_s$ reweighting, events have different weights and the event density is equal for every point in phase space. It would be preferable if the event density were proportional to the weight. In that case, only events with significant contributions would have to be considered in the rest of the generation process, which saves computing time. For this reason, events are unweighted.

The event density at each phase space point is decreased by multiplying with an unweighting factor, which is a number between zero and one. The weight at that point is increased by dividing by the same factor. The unweighting factor is the ratio of the original weight and the maximum weight in the accessible phase space. Therefore, all weights become equal to this maximum weight.

Like reweighting, unweighting is an acceptance/rejection process. A random number is drawn from a uniform distribution between zero and one for every event. The event is accepted if the unweighting factor is larger than or equal to the random number.

The cross section for the generated process is calculated by averaging event weights before unweighting. This number is adjusted in the Sudakov and $\alpha_s$ reweighting procedures, which gives the fraction of the lowest order cross section for the generated parton multiplicity (see Section 2.3).

Unweighting provides an additional advantage for the estimation of the ratio of the reweighted and original cross sections. If the reweighting procedure is performed on unweighted events, the estimate of this ratio becomes the average reweighting factor of all events before reweighting. The average reweighting factor is in turn estimated by the fraction of accepted events.

The generation, unweighting and reweighting processes are implemented in the MLM algorithm as follows:

1. $N + 1$ samples of events with hard, non-collinear additional partons are generated with ALPGEN. Each sample has a different additional parton multiplicity ($n = 0, \ldots, N$). $N \leq 6$ for ALPGEN. The sample with $n = 0$ contains the lowest order $t\bar{t}$ production process.

2. The $k_T$ clustering algorithm is applied on the events from Step 1 to find the $k_T$ of the “branch” with the lowest energy scale for each event. The event weight is multiplied by the factor $\left[\alpha_s(k_{T_{\text{low}}})/\alpha_s(Q^2_{\text{hard}})\right]^n$.

3. Events are unweighted relative to the maximum weight after the reweighting of Step 2.
4. The $k_T$ clustering algorithm is applied on events accepted in Step 3 to find the value of $k_T$ for each “branch”. The reweighting factor $\alpha_s(k_{T_{\text{low}}})^{-n} \prod_{i=1}^{n} \alpha_s(k_T_i)$ is calculated and events are reweighted. The cross section is multiplied by the average reweighting factor of all events before reweighting.

5. The parton shower algorithm is applied on events that were accepted in Step 3. Parton jets are constructed with a cone jet algorithm, using the parameters that define the merging scale: $E^{\text{clus}}_T$, $\eta_{\text{clus}}$ and $R_{\text{clus}}$.

6. The jet at the smallest distance $\Delta R$ is selected for each additional ALPGEN parton, in order of descending parton $p_T$. If $\Delta R$ is within the matching radius ($R_{\text{match}} = 1.5 \cdot R_{\text{clus}}$), the jet is matched to the parton. The selected jet is removed from the list of jets, whether it is matched or not. This assures that each jet is matched to at most one parton. If a jet is found for all partons, the event is matched. Unmatched events are rejected.

7. If there are no extra parton shower jets in a matched event, the event is accepted. Matched events from exclusive samples ($n < N$) are rejected if there are extra jets. Extra jets are allowed in matched events from the inclusive sample ($n = N$), but only if their $E_T$ is smaller than the $E_T$ of the softest matched jet.

8. The “cross section” from Step 4 is multiplied by the ratio of the number of accepted events in Steps 6 and 7 and the number of accepted events in Step 4. The sum of the resulting “cross sections” for all samples is an approximation of the lowest order $t \bar{t}$ production cross section.

9. Samples with accepted events are combined into a fully inclusive sample. The relative weight of the samples is determined by the “cross sections” calculated in Step 8.

5.2 Merging at a High Energy Scale

The MLM matching procedure is applied on the ALPGEN samples from Chapter 4. The merging scale is set equal to the scale that defined hard, non-collinear partons in the comparison of ALPGEN and the PYTHIA parton shower. Therefore, the merged one-jet and two-jet samples can be compared with the parton shower samples from Chapter 4 again.

Parameters of the matching procedure are the cone jet algorithm parameters shown in Table 4.1 on page 59. With these parameters, the merging scale is defined by $E^{\text{clus}}_T = 100$ GeV, $\eta_{\text{clus}} = 2.5$ and $R_{\text{clus}} = 0.7$. ALPGEN generates additional partons with $p_T^{\text{min}} = 85$ GeV/$c$, $\eta_{\text{max}} = 2.6$ and $R_{\text{min}} = 0.6$. 
5.2. MERGING AT A HIGH ENERGY SCALE

This value of the merging scale is chosen to make ALPGEN predictions for additional partons reliable, so the merging corrections to additional jet kinematics are expected to be small. Variables that depend on the properties of soft/collinear partons will be affected. The ALPGEN distributions for these variables are expected to be much closer to the parton shower distributions than they are in Chapter 4.

Samples with four different jet multiplicities are generated. Table 5.1 shows the merging and parton shower approximations for the lowest order $t\bar{t}$ cross section and its distribution over the different jet multiplicities.

<table>
<thead>
<tr>
<th>$n$</th>
<th>ALPGEN with merging $\sigma_{t\bar{t}+n\text{-}jet}$ (pb)</th>
<th>PYTHIA 6 shower $\sigma_{t\bar{t}+n\text{-}jet}$ (pb)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>222.4</td>
<td>219.3</td>
</tr>
<tr>
<td>1</td>
<td>32.8</td>
<td>32.0</td>
</tr>
<tr>
<td>2</td>
<td>4.2</td>
<td>4.8</td>
</tr>
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<td>$\geq 3$</td>
<td>0.6</td>
<td>0.7</td>
</tr>
<tr>
<td>total</td>
<td>260.0</td>
<td>256.8</td>
</tr>
</tbody>
</table>

Table 5.1: Approximations for the lowest order $t\bar{t}$ cross section from merging and the parton shower with $E_{T}^{clus} = 100$ GeV, $\eta_{clus} = 2.5$ and $R_{clus} = 0.7$.

The total merging cross section is four per cent higher than the expected value of 250 pb (see also Table 3.1 on page 36). Such a difference indicates that the performance of the merging scheme is not optimal. This may be due to imperfections in the scheme or to its current parameters, which will be further investigated in Section 5.3.

The distribution of the cross section over the jet multiplicities is different for merging and the parton shower. The relative contributions of the zero-jet and one-jet samples are somewhat higher with merging and the relative contributions from the two-jet and inclusive three-jet samples somewhat lower.

5.2.1 Effects of Soft/Collinear Partons

The effect of soft/collinear partons is demonstrated in Chapter 4 with distributions for parton jets defined by $E_{T}^{clus} = 6$ GeV and $\eta_{clus} = 6$ (Figures 4.1 and 4.2 on pages 61 and 62). The parton shower produces on average four of these jets in the one-jet sample and five in the two-jet sample, while ALPGEN produces only the hard, non-collinear jets. This results in much higher values of $H_{T}$ for the parton shower.

Figure 5.1 compares the multiplicity of these soft and collinear jets for ALPGEN after merging and the parton shower. On average, merging produces more jets: five in the one-jet sample and six in the two-jet sample.
Figure 5.1: Additional parton jet multiplicity with $E_{\text{clus}} = 6$ GeV and $\eta_{\text{clus}} = 6$: ALPGEN with merging vs PYTHIA for the one-jet sample (a) and for the two-jets sample (b). ALPGEN vs PYTHIA 6 (b).

Figure 5.2: Sum of all additional jet transverse energies ($H_T$) with $E_{\text{clus}} = 6$ GeV and $\eta_{\text{clus}} = 6$: ALPGEN with merging vs PYTHIA for the one-jet sample (a) and for the two-jets sample (b).

Figure 5.3: Sum of all additional jet transverse energies ($H_T$) with $E_{\text{clus}} = 100$ GeV and $\eta_{\text{clus}} = 2.5$: ALPGEN with merging vs PYTHIA for the one-jet sample (a) and for the two-jets sample (b).
5.2. Merging at a High Energy Scale

Shapes of the $H_T$ distributions for soft/collinear jets (Figure 5.2) are very similar for merging and the parton shower. This is also still true for the $H_T$ of hard, non-collinear jets (Figure 5.3), for which the ALPGEN distributions before and after merging are roughly the same (compare with Figure 4.3 on page 62).

5.2.2 Kinematic Distributions

Figure 5.4 shows the parton momentum fractions before and after shower evolution (compare with Figure 4.4 page 63). Merging does not have a significant effect on the momentum fractions of the hard scattering. These distributions are essentially the same as in Chapter 4. Shower evolution in the merging procedure did affect the ALPGEN distributions for the incoming partons. These are now very similar to the parton shower distributions.
Figure 5.5: Invariant mass of the $t\bar{t}$ pair ($M_{t\bar{t}}$): ALPGEN with merging vs PYTHIA, the one-jet sample on a linear scale (a) and on a logarithmic scale (b), the two-jets sample on a linear scale (c) and on a logarithmic scale (d).
Figure 5.6: Transverse momentum of the $\tau\tau$ pair ($p_T^{\tau\tau}$): ALPGEN with merging vs PYTHIA, the one-jet sample on a linear scale (a) and on a logarithmic scale (b), the two-jets sample on a linear scale (c) and on a logarithmic scale (d).
The invariant mass of the $t\bar{t}$ pair is affected by a small amount (Figure 5.5, compare with Figure 4.7 on page 66). The ALPGEN contribution at large invariant mass becomes smaller, which enhances the difference with the parton shower for masses close to $2m_t$.

The transverse momentum of the $t\bar{t}$ pair is sensitive to soft and non-collinear jets, as was shown in Figure 4.8 on page 67. The lack of ALPGEN events below 100 GeV/c in the one-jet sample is corrected by the merging procedure (see Figure 5.6a). The difference between ALPGEN and the parton shower for high-$p_T$ $t\bar{t}$ pairs (Figure 5.6b) is enhanced by merging. This also results in a larger difference between 70 and 230 GeV/c, since the distributions are normalized to the same cross section.

Similar effects are present in the two-jet $t\bar{t}$ $p_T$ distributions (Figures 5.6c and 5.6d). There is no longer a “bump” in the ALPGEN distribution at 200 GeV/c. The merging distribution dominates below 300 GeV/c, the parton shower distribution above 300 GeV/c.

The $t\bar{t}$ pseudorapidity distributions (Figure 5.7, compare with Figure 4.9 on page 68) also show the effects of merging. There are no longer sharp dips in the one-jet ALPGEN distribution around $\eta = 4$, because there are now events below $p_T = 100$ GeV/c. For $\eta > 4$, the merging distribution is still smaller than the parton shower distribution. This may be correlated to the dominance of the merging $p_T$ at small values. The ALPGEN result for the two-jet sample is nearly the same as before merging.

Figure 5.7: Pseudorapidity of the $t\bar{t}$ pair ($\eta_{t\bar{t}}$): ALPGEN with merging vs PYTHIA, the one-jet sample (a) and the two-jets sample (b).
Figure 5.8: Transverse momentum of the (anti)top quark ($p_T$): ALPGEN with merging vs PYTHIA, the one-jet sample (a) and the two-jets sample (b).

Figure 5.9: Pseudorapidity of the (anti)top quark ($\eta$): ALPGEN with merging vs PYTHIA, the one-jet sample (a) and the two-jets sample (b).
Figure 5.10: Transverse energy of the first additional parton jet ($E_T$): ALPGEN with merging vs PYTHIA, the one-jet sample (a) and the two-jets sample (b).

Figure 5.11: Pseudorapidity of the first additional parton jet ($\eta_1$): ALPGEN with merging vs PYTHIA, the one-jet sample (a) and the two-jets sample (b).
Figure 5.12: Kinematics of the second additional parton jet in the two-jets sample: ALPGEN with merging vs PYTHIA, (a) transverse energy ($E_T$) and (b) pseudorapidity ($\eta$).

The $p_T$ distributions of the (anti)top quark (Figure 5.8) become softer in the merging procedure as well (compare with Figure 4.10 on page 69). This increases the difference between ALPGEN and the parton shower. The (anti)top pseudorapidity distributions do not change (Figure 5.9 and Figure 4.11 on page 69).

Also the $E_T$ spectra of the additional parton jets (Figures 5.10 and 5.12a) become somewhat softer (compare with Figures 4.12 on page 70 and 4.14a on page 71). This appears to be correlated to the change in the additional jet pseudorapidity (Figures 5.11 and 5.12b, compared with Figure 4.13 on page 70 and Figure 4.14b on page 71). The $\eta$ distributions become more central. This most likely results from correction of the collinear divergence for $|\eta| \to \infty$, which may still affect the ALPGEN distributions at this merging scale.

Figure 5.13 shows the $\Delta R$ between the additional partons in the two-jet sample (compare with Figure 4.15 on page 72). The merging distribution is still smaller than the parton shower distribution for $\Delta R < 1.2$ and larger between 3.1 and 5. However, the dominance of the ALPGEN distribution for large $\Delta R$ is smaller after merging. This may be correlated to the smaller values for the pseudorapidity of the additional jets.
5.3 Merging at Lower Energy Scales

A larger part of the additional parton phase space is described by higher order matrix elements when the merging scale is lowered. For the analysis of the full $t\bar{t}$ production and decay process, a new scale is defined by $E_T^{\text{clus}} = 36$ GeV, $\eta_{\text{clus}} = 5.0$ and $\Delta R_{\text{clus}} = 0.4$. ALPGEN additional partons are generated with $p_T^{\text{min}} = 30$ GeV, $\eta_{\text{max}} = 5.0$ and $\Delta R_{\text{min}} = 0.4$. This choice is based on the parameters used in references [24] and [25], where the MLM matching procedure is studied by its authors. Table 5.2 lists the resulting parameters of the cone jet algorithm.

The approximation of the lowest order $t\bar{t}$ cross section and its distribution over the samples with different jet multiplicity is shown in Table 5.3. Similar features are observed as for a high merging scale. The cross section after merging is overestimated by six per cent. Merging contributions from the zero-jet and one-jet samples are higher than for the parton shower, while the contributions from the two-jet and three-jet samples are lower.

The difference between the lowest order ALPGEN and merging cross sections has become larger for the lower merging scale. This may be explained by the fact that more additional partons are generated by ALPGEN and less by the parton shower, which enhances effects of merging.

Other studies confirm this dependence on the merging scale, although decreasing $R_{\text{clus}}$ seems to result in a lower cross section. Table 5.4 lists the cross sections for different scales. These observations indicate that the
5.3. MERGING AT LOWER ENERGY SCALES

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Table 5.2: Cone jet algorithm parameters for hard, non-collinear jets at parton level.

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<th>PYTHIA 6 shower</th>
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<tr>
<td></td>
<td>LO: 249.8</td>
<td>LO: 256.3</td>
</tr>
</tbody>
</table>

Table 5.3: Approximations for the lowest order $t\overline{t}$ cross section from merging and the parton shower with $E_T^{\text{clus}} = 36$ GeV, $\eta_{\text{clus}} = 5.0$ and $R_{\text{clus}} = 0.4$.

<table>
<thead>
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<th>$\eta_{\text{clus}}$</th>
<th>$\Delta R_{\text{clus}}$</th>
<th>$\sigma$ (pb)</th>
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<td>0.4</td>
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Table 5.4: The dependence of the approximation for the lowest order $t\overline{t}$ cross section on the merging scale.
Figure 5.14: Invariant mass of the $t\bar{t}$ pair ($M_{t\bar{t}}$): ALPGEN with merging vs PYTHIA on a linear scale (a) and on a logarithmic scale (b).

Figure 5.15: Transverse momentum of the $t\bar{t}$ pair ($p_{T,t}$): ALPGEN with merging vs PYTHIA on a linear scale (a) and on a logarithmic scale (b).
overestimation of the cross section is not due to the choice of the scale. It may well be an imperfection of the merging scheme in combination with the applied parton shower algorithm. The choice of values for parameters in these algorithms may also affect the performance of the scheme.

### 5.3.1 Top Quark Production

Figure 5.14 shows the invariant mass of the $t\bar{t}$ pair for merging and the parton shower. The distributions are almost the same as at lowest order (Figure 3.4 on page 41). Alpgen produces slightly more $t\bar{t}$ pairs with a small mass, as it does with one or two hard, non-collinear jets (Figure 5.5 on page 82). However, this effect is much smaller for the fully inclusive sample. The largest contribution comes from the zero-jets sample, which contains only soft/collinear jets.

Figure 5.15 shows the transverse momentum of the $t\bar{t}$ pair. The $t\bar{t}$ transverse momentum (Figure 5.15) is predominantly determined by the contribution from soft/collinear additional jets. Its distribution peaks around $5\text{ GeV/c}$ and the average $p_T$ is $60\text{ GeV/c}$. Effects from hard, non-collinear jets make the merging distribution smaller than the parton shower distribution at high $p_T$.

These features also appear in the $t\bar{t}$ pseudorapidity distribution (Figure 5.16). It is much wider than the one-jet and two-jet distributions (Figure 5.7 on page 84). Due to the difference at high $p_T$, the parton shower produces slightly more $t\bar{t}$ pairs around $\eta = 0$. 

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$\text{Figure 5.16: Pseudorapidity of the } t\bar{t} \text{ pair (}\eta_{t\bar{t}}\text{): ALPGEN with merging vs PYTHIA.}$
Figure 5.17: Kinematics of the (anti)top quark: ALPGEN with merging vs PYTHIA, (a) transverse energy ($E_T$) and (b) pseudorapidity ($\eta$).

The distribution of the top/antitop $p_T$ (Figure 5.17a) is almost the same as at lowest order (Figure 3.6 on page 43). The familiar dominance of the parton shower at high $p_T$ is present again. Also the top/antitop pseudorapidity (Figure 5.17b) is very similar to its lowest order distribution (Figure 3.7 on page 44). The parton shower distribution is slightly more central, like the $t\bar{t}$ $\eta$ distribution from the parton shower.

For the analysis of additional partons, two different jet definitions are applied. Distributions are shown for jets above the merging scale ($E_T^{\text{clus}} = 36$ GeV, $\eta_{\text{clus}} = 5$) and for jets with $E_T^{\text{clus}} = 6$ GeV and $\eta_{\text{clus}} = 6$. Multiplicities for both definitions are shown in Figure 5.18.

Figure 5.18a shows that an average of three jets above the low jet scale is produced. The multiplicity is slightly larger for merging than for the parton shower. The average for jets above the merging scale is 0.6 (Figure 5.18b). Note that the one-jet contribution is larger for merging than for the parton shower, while its contribution for other multiplicities is smaller.

The transverse energy of the first low-scale jet is shown in Figures 5.19a and 5.19b. This distribution reveals another dependence on the merging scale. The plots of the difference between ALPGEN and PYTHIA show a discontinuity at the merging $E_T^{\text{clus}}$ (36 GeV). The ALPGEN contribution above this value suddenly becomes larger than the parton shower contribution. Studies with other merging scales show that this discontinuity shifts with the merging $E_T^{\text{clus}}$. 
A similar effect appears in the distributions of the transverse energies of the second, third (Figure 5.20a/5.20b) and fourth jet (Figure 5.21a/5.21b). A difference is that the ALPGEN spectrum suddenly drops below the parton shower spectrum for these jets.

This dependence on the merging scale may be correlated to the dominance of events with one jet in Figure 5.18b. These events come from the one-jet sample, which gives the largest contribution to the $E_T$ spectrum of the first jet above the merging $E_T^{\text{clus}}$. Below this value, the spectrum is determined by parton shower contributions from other samples.

The observed mismatch may be the result of an overestimation of the one-jet weights. Since the one-jet sample contains parton shower jets below the merging scale, this could also lead to discontinuities in the $E_T$ distributions for the other jets. The one-jet contribution to the merging cross section may be responsible for the difference with the lowest order cross section.

Above an $E_T$ of 36 GeV, distributions for jets above the merging scale (Figures 5.19c/5.19d, 5.20c/5.20d and 5.21c/5.21d) are almost equal to the distributions for low-scale jets. This indicates that most jets with $5 < \eta < 6$ have an $E_T$ below 36 GeV. For the first jet, the parton shower dominates again at high $p_T$. For the third and fourth jet, the difference between ALPGEN and the parton shower seems to level out. This is expected for the fourth jet, since it is not generated by ALPGEN.

Figure 5.18: Additional parton jet multiplicity: ALPGEN with merging vs PYTHIA, jets above the low jet scale (a) and jets above the merging scale (b).
Figure 5.19: Transverse energy of the first additional parton jet ($E_T$): ALPGEN with merging vs PYTHIA, jets above the low jet scale on a linear scale (a) and on a logarithmic scale (b), jets above the merging scale on a linear scale (c) and on a logarithmic scale (d). The plots of the difference between ALPGEN and PYTHIA reveal a discontinuity at the merging $E_T^{\text{clust}}$. 
5.3. MERGING AT LOWER ENERGY SCALES

Figure 5.20: Transverse energy of the third additional parton jet ($E_{T3}$): ALPGEN with merging vs PYTHIA, jets above the low jet scale on a linear scale (a) and on a logarithmic scale (b), jets above the merging scale on a linear scale (c) and on a logarithmic scale (d). The plots of the difference between ALPGEN and PYTHIA reveal a discontinuity at the merging $E_T^{\text{plus}}$. 
Figure 5.21: Transverse energy of the fourth additional parton jet ($E_{T4}$): ALPGEN with merging vs PYTHIA, jets above the low jet scale on a linear scale (a) and on a logarithmic scale (b), jets above the merging scale on a linear scale (c) and on a logarithmic scale (d). The plots of the difference between ALPGEN and PYTHIA reveal a discontinuity at the merging $E_T^{\text{clus}}$. 
5.3. MERGING AT LOWER ENERGY SCALES

Figure 5.22: Pseudorapidity of the first additional parton jet ($\eta_1$): ALPGEN with merging vs PYTHIA, jets above the low jet scale (a) and jets above the merging scale (b).

Although the parton shower generates more high-$p_T$ jets, the pseudorapidity distributions for the low-scale jets (Figures 5.22a, 5.23a and 5.24a) are more central for ALPGEN. The slightly larger ALPGEN jet multiplicity results in more events around $\eta = 0$.

Also the pseudorapidity distributions for jets above the merging scale (Figures 5.22b, 5.23b and 5.24b) are more central for ALPGEN. The larger parton shower jet multiplicity for events with more than one jet has an obvious effect on the pseudorapidity of the third and fourth jet. It results in more parton shower events than ALPGEN events in these histograms.

The $\Delta R$ distribution for the first two low-scale jets (Figure 5.25a) is very similar for merging and parton shower. However, this distribution changes for jets above the merging scale (Figure 5.25b). Its shape becomes more similar to the distributions for the one-jet and two-jet samples in Section 5.2 (Figure 5.13 on page 88). ALPGEN produces more events above $\Delta R = 2.5$ and less events below $\Delta R = 1$. 
Figure 5.23: Pseudorapidity of the third additional parton jet ($\eta_3$): ALPGEN with merging vs PYTHIA, jets above the low jet scale (a) and jets above the merging scale (b).

Figure 5.24: Pseudorapidity of the fourth additional parton jet ($\eta_4$): ALPGEN with merging vs PYTHIA, jets above the low jet scale (a) and jets above the merging scale (b).
5.3. MERGING AT LOWER ENERGY SCALES

Figure 5.25: $\Delta R$ between the first and second additional parton jet ($\Delta R_{12}$): ALPGEN with merging vs PYTHIA, jets above the low jet scale (a) and jets above the merging scale (b).

5.3.2 Top Quark Decay

Both in merging and parton shower events, final state showers emerge from the quarks in the top decays. For the analysis of the decays, momenta of quarks before radiation of additional gluons are used.

In Figure 5.26a, the distribution of $\cos \theta_{bd}^*$ is shown. It is almost the same as at lowest order (Figure 3.9 on page 45). Only for values close to $\cos \theta_{bd}^* = -1$, the parton shower contribution is slightly exceeding the merging contribution. Apparently, the parton shower affects the properties of the top quark decays and enables the production of more down-type quarks at $180^\circ$ from the bottom quark.

Also the distributions of $\cos \theta_{dd}^*$ (Figure 5.26b) are quite similar to the lowest order distributions (Figure 3.11 on page 46). The large effect from additional jets above the high merging scale (Figure 4.16 on page 72) is almost absent in the fully inclusive sample. Therefore, there is a difference between ALPGEN and PYTHIA due to spin correlations again (see Section 3.3).

Figure 5.27a shows the transverse energy of the bottom quarks. The merging distribution is roughly the same as at lowest order (Figure 3.16 on page 50). The parton shower distribution is somewhat larger at high $E_T$ due to higher order corrections in the $t\bar{t}$ production process. Both pseudorapidity distributions (Figure 5.27b) are the same as at lowest order (Figure 3.17 on...
Figure 5.26: Angles in the $t\bar{t}$ decay: ALPGEN with merging vs PYTHIA, $\cos \theta_{b_{d}}^*$ (a) and $\cos \theta_{d_{d}}^*$ (b). A difference between ALPGEN and PYTHIA in $\theta_{d_{d}}^*$ is observed due to a different treatment of spin correlations.

Figure 5.27: Kinematics of the bottom quarks: ALPGEN with merging vs PYTHIA, (a) transverse energy ($E_{T_{b}}$) and (b) pseudorapidity ($\eta_{b}$).
5.3. MERGING AT LOWER ENERGY SCALES

5.3.3 Particle Jets

The cone jet parameters for the analysis of particles jets are the same as at lowest order (Table 3.2 on page 51, $E_{\text{clus}}^{\text{jet}} = 5$ GeV, $\eta_{\text{clus}} = 6$, $R_{\text{clus}} = 0.4$). Distributions are shown for jets with a transverse energy larger than 6 GeV.

Figure 5.28 shows the jet multiplicity distribution. The average increases from six jets at lowest order (Figure 3.18 on page 52) to nine jets. The merging distribution dominates for large jet multiplicities. This is probably due to a similar dominance for large parton jet multiplicities (Figure 5.18).

Figure 5.29 shows the minimum $\Delta R$ between the jets in an event. As expected, the average value of $\Delta R_{\text{min}}$ is much smaller than at lowest order (Figure 3.19 on page 53). Additional jets may be collinear with each other and with the jets from the $t \bar{t}$ decay. $\Delta R_{\text{min}}$ is slightly larger for ALPGEN than for PYTHIA.

The larger jet multiplicity at higher order results in larger values for the $H_T$ of all jets (Figure 5.30 compared to Figure 3.21 on page 54). Due to the additional jets, the parton shower distribution is larger than the ALPGEN distribution at high $H_T$. This results in an average $H_T$ of 430 GeV for PYTHIA and 420 GeV for ALPGEN.

The $E_T$ distribution of the first particle jet (Figure 5.31a) is somewhat broader than at lowest order (Figure 3.22 on page 55). However, this effect...
Figure 5.29: Minimum $\Delta R$ between two particle jets ($\Delta R_{\text{min}}$): ALPGEN with merging vs PYTHIA.

Figure 5.30: Sum of all particle jet transverse energies ($H_T$): ALPGEN with merging vs PYTHIA.
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Figure 5.31: Kinematics of the first particle jet: ALPGEN with merging vs PYTHIA, (a) transverse energy ($E_{T1}$) and (b) pseudorapidity ($\eta_1$).

Figure 5.32: Kinematics of the sixth particle jet: ALPGEN with merging vs PYTHIA, (a) transverse energy ($E_{T6}$) and (b) pseudorapidity ($\eta_6$).
is relatively small, which indicates that the first jet often originates from the \( t\bar{t} \) decay. Its pseudorapidity distribution (Figure 5.31b) is the same as at lowest order (Figure 3.24 on page 56).

Figure 5.32a shows the \( E_T \) of the sixth jet. This jet often originates from additional partons, which makes higher order effects larger than for the first jet. The average \( E_T \) shifts from 20 GeV at lowest order (Figure 3.23 on page 55) to 25 GeV. A smaller fraction of events ends up below the threshold of 6 GeV. Additional jets cause a high-\( E_T \) difference between ALPGEN and PYTHIA for this jet as well.

The pseudorapidity of the sixth jet (Figure 5.32b) is less central than at lowest order (Figure 3.25 on page 57). This is the result of the broader \( \eta \) distributions for additional jets (Figures 5.22a, 5.23a and 5.24a), compared to the quarks from the \( t\bar{t} \) decay (Figures 3.14, 3.15 and 3.17 on pages 49 and 50).

5.4 Summary

Results in this chapter show that the lack of soft/collinear additional partons from tree level matrix elements may be compensated by applying a merging scheme. In this case, the MLM matching procedure adds these partons to ALPGEN matrix element events with the PYTHIA parton shower. This procedure leads to comparable ALPGEN and parton shower distributions for momentum fractions (Figures 5.4c and 5.4d), additional jet multiplicities (Figures 5.1 and 5.18a) and transverse momenta of \( t\bar{t} \) pairs (Figures 5.6 and 5.15). These distributions differ significantly without applying the merging scheme (see Chapter 4).

Merging has only a small effect on the kinematics of hard, non-collinear jets, provided that the energy scale that is used to define this region of phase space is high enough. The merging distributions for these partons (Figures 5.10 through 5.13) are very similar to those without merging in Chapter 4 (Figures 4.12 through 4.15).

As a test of the quality of a merging scheme, its dependence on the merging energy scale may be analysed. For a perfect scheme, there will be no such dependence. It is shown (Table 5.4) that the approximation of the \( t\bar{t} \) cross section after merging varies with the merging scale. There is also a discontinuity in the \( E_T \) spectra of additional jets at the merging \( E_{\text{clus}}^T \) (Figures 5.19 through 5.21). Apparently, imperfections in the correction of the weights of ALPGEN events have observable consequences.

Results in Chapter 4 show a difference between additional partons from ALPGEN and jets from the PYTHIA parton shower at high \( E_T \). ALPGEN produces less jets in this region of phase space than the parton shower. This is also observed after merging. It seems to be a featuring difference between ALPGEN and the virtuality ordered parton shower of PYTHIA 6.
Kinematic properties of the top quarks and their decay products are only modestly affected by higher order corrections in the $t\bar{t}$ production process (see Sections 5.3.1 and 5.3.2). Effects on particle jets are larger, since additional jets are produced at higher order (Section 5.3.3). The average jet multiplicity increases (Figure 5.28), the $\Delta R$ between jets becomes smaller (Figure 5.29) and also $E_T$ and $\eta$ distributions are affected by additional jets (Figures 5.30 through 5.32). The high $E_T/p_T$ difference between Alpgen and the parton shower for additional parton jets also appears in the transverse energy and momentum distributions of the top quarks, their decay products and particle jets.
Production of $t\bar{t}$ pairs and their fully hadronic decays are studied at lowest order (Chapter 3) and with higher order QCD corrections (Chapter 5). Results show that (without cuts) corrections have only a modest effect on kinematics of the top quarks and their decay products. However, additional partons produced in higher order processes do affect the properties of jets.

Jets are analysed with a cone algorithm. They are defined by a cone size of 0.4, a minimum energy of 6 GeV and a maximum (absolute) pseudorapidity of 6. At lowest order, the average particle jet multiplicity is six. These jets originate from the quarks in the top and antitop decays.

Including higher order corrections, an average of nine particle jets is produced. The additional jets may come from corrections to both the production and decay processes. However, analysis of additional partons in the production process shows that an average of three additional parton jets is generated. Although not each of these jets gives rise to a separate particle jet, this indicates that additional particle jets predominantly originate from higher orders in $t\bar{t}$ production.

Two methods for simulating higher order QCD corrections in the $t\bar{t}$ production process are compared. In the first, higher order matrix elements are calculated at tree level. This gives only reliable results when additional partons are hard and non-collinear. The Monte Carlo event generator *Alpgen* is used to generate matrix element events.

In the second approach, the lowest order matrix element is convoluted with a parton shower. This is a good approximation for soft/collinear additional partons, but the shower algorithm is expected to be less reliable when additional partons are hard and non-collinear. The virtuality ordered parton shower implementation of *Pythia* 6 is applied.

First, results from *Alpgen*, *Pythia* 6 and a third generator (*Pythia* 8) are compared at lowest order (Chapter 3). Differences between *Alpgen* and *Pythia* are found in the treatment of spin correlations in the top and antitop decays. This was expected, since *Pythia* calculates $t\bar{t}$ production and the top quark decays separately, without taking these correlations into account. *Alpgen* calculates the complete $t\bar{t}$ production and decay process and thus includes the relation between spins of the top and the antitop. Some small differences between the two *Pythia* versions appear in the simulation of...
CHAPTER 5. MERGING

hadronization. These are most likely due to differences in (default) settings.

Only minor differences are found in the $t\bar{t}$ production process at lowest order. This enables a fair higher order comparison of ALPGEN matrix elements and the PYTHIA 6 parton shower. ALPGEN is restricted to produce only additional partons above an energy scale defined by $E_T > 100$ GeV, $|\eta| < 2.5$ and $\Delta R > 0.7$. Results from both methods are comparable, although distributions of some variables clearly show the lack of soft/collinear additional partons from matrix elements (Chapter 4). For instance, the energy cut-off for additional partons is clearly visible in the $p_T$ distribution of the $t\bar{t}$ pair.

To obtain reliable results for both hard and soft additional partons, the matrix element and parton shower methods are combined by applying a merging scheme. The MLM matching procedure is used to connect the two regions of phase space, avoiding double counting and gaps. Higher order matrix elements are integrated into the parton shower by applying Sudakov form factors and adjusting the value of the strong coupling constant. This enables the use of matrix elements at a much lower energy scale for additional partons.

A dependence on the merging energy scale is observed in both the estimated cross section and the additional jet $E_T$ distributions. Such a dependence implies that there is a systematic uncertainty in the merging description. This is due to uncertainties in the approximation of the Sudakov factors and strong coupling constants.

The minimum energy scale for hard, non-collinear additional ALPGEN partons in Chapter 4 is used as merging scale in Section 5.2. Events with one and with two hard, non-collinear jets are studied. Results show that soft/collinear partons are successfully added to ALPGEN events with the parton shower. Since the value for the energy scale was chosen to make matrix element results reliable, kinematic distributions of additional partons above this scale are not affected much by merging. However, pseudorapidity distributions become somewhat more central. This may indicate that this scale is still too low to use matrix element events without merging.

Both with and without merging, the parton shower generates more additional jets at high transverse energy than ALPGEN. This is also observed (Section 5.3) for events with all jet multiplicities obtained by merging at a much lower energy scale ($E_T > 36$ GeV, $|\eta| < 5$, $\Delta R > 0.4$). However, the pseudorapidity of additional jets in these events is more central for ALPGEN. These observations indicate that the total jet energies are larger for the parton shower, which results in larger transverse energies.

This difference also affects distributions of other variables presented in Chapter 5. The parton shower generates harder $E_T/p_T$ distributions for the $t\bar{t}$ pair, top quarks, quarks from the top decays and particle jets.

Other parton shower implementations may give different results than the virtuality ordered shower in PYTHIA 6. Moreover, the performance of par-
ton shower algorithms is controlled by a number of parameters, which may be tuned to obtain an optimal description of experimental data. Different parameter settings may result in smaller or larger differences with matrix elements. Although it is to be expected that matrix elements provide a better description of high-$E_T$ additional jets in $t\bar{t}$ production, this can only be confirmed by experimental results.

Initially, $t\bar{t}$ data from the LHC may be compared to simulations with the purpose of calibrating calorimeters for high-$E_T$ jets. In such an analysis, the observed differences between ALPGEN matrix elements and the PYTHIA parton shower provide an estimate of the systematic uncertainty in the theoretical description and the jet energy scale.
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