

## Master's Thesis

# Improving Event Reconstruction for Dileptonic Decays of Top Quarks Pairs Using Machine Learning

prepared by

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## **Abstract**

Here the key results of the thesis can be presented in about half a page.

**Keywords:** Physics, Master thesis

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# 1. Introduction

## 2. Theoretical Background

### 2.1. The Standard Model of Particle Physics

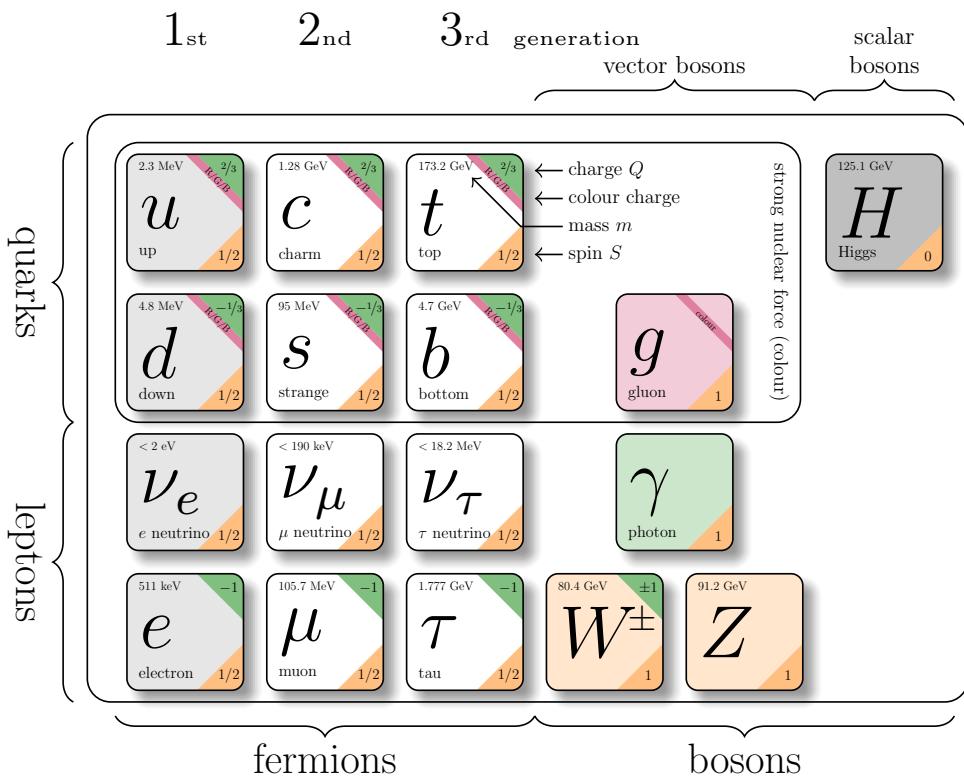


Figure 2.1.: The particles of the Standard Model. Particle properties taken from Ref. [1].

The Standard Model (SM) of particle physics is a quantum field theory describing three of the four fundamental interactions of nature—electromagnetic, weak and strong—and the elementary particles on which they act. It is formulated as a renormalisable, Lorentz-invariant gauge theory with gauge group

$$SU(3)_C \times SU(2)_L \times U(1)_Y,$$

and its structure has been established in a series of seminal works [2–7]. A summary of the particle content is shown in Fig. 2.1.

The elementary particles fall into fermions and bosons. Fermions are spin- $\frac{1}{2}$  fields that constitute matter, organised into three generations of quarks and leptons. Quarks carry colour charge and participate in the strong interaction; leptons do not. Bosons are integer-

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spin gauge fields mediating the fundamental forces: the photon for electromagnetism, the  $W^\pm$  and  $Z$  bosons for the weak interaction, and eight gluons for the strong interaction. The Higgs boson completes the SM and is responsible for electroweak symmetry breaking (EWSB), giving mass to the weak gauge bosons and, through Yukawa couplings, to the fermions. The SM Lagrangian can be written schematically as

$$\mathcal{L}_{\text{SM}} = \mathcal{L}_{\text{gauge}} + \mathcal{L}_{\text{fermion}} + \mathcal{L}_{\text{Yukawa}} + \mathcal{L}_{\text{Higgs}},$$

where the first term contains the gauge kinetic terms and self-interactions, the second describes the fermions and gauge covariant derivatives, the third encodes the Yukawa couplings to the Higgs field, and the last term contains the Higgs potential and EWSB mechanism.

Below, the three interaction sectors are briefly summarised, with emphasis on the aspects relevant for top-quark physics and LHC phenomenology.

### 2.1.1. Electromagnetic Interaction

The electromagnetic interaction is described by quantum electrodynamics (QED), the  $U(1)_{\text{EM}}$  gauge theory that remains after EWSB. Its massless gauge boson, the photon, couples to electric charge and does not self-interact. Because QED is an Abelian theory, its coupling runs only mildly with energy and remains perturbative at all experimentally accessible scales.

### 2.1.2. Weak Interaction

The weak interaction forms, together with electromagnetism, the electroweak theory based on the gauge group  $SU(2)_L \times U(1)_Y$ . The vacuum expectation value of the Higgs field spontaneously breaks the symmetry to  $U(1)_{\text{EM}}$ , giving masses to the weak gauge bosons through the Higgs mechanism [8–10]. The resulting massive  $W^\pm$  and  $Z$  bosons mediate a short-range force.

A defining property of the weak interaction is its *chiral* structure: charged-current interactions couple only to left-handed fermions and right-handed antifermions. This feature, predicted in [11] and confirmed in the Wu experiment [12], leads to maximal parity violation and characteristic angular distributions of weak decay products. The vertex factor of the charged-current interaction is given by

$$\frac{-ig}{2\sqrt{2}}\gamma^\mu(1 - \gamma^5), \quad (2.1)$$

where  $g$  is the weak coupling constant,  $\gamma^\mu$  are the Dirac matrices. The projection operator  $(1 - \gamma^5)$  leads to a coupling exclusively to the left-handed components. Based on this, the left-handed particles are arranged in  $SU(2)_L$  doublets corresponding, while the right-handed particles are singlets.

For quarks, the weak eigenstates  $d', s', b'$  are not identical to their mass eigenstates  $d, s, b$ . This misalignment is described by the Cabibbo-Kobayashi-Maskawa (CKM) matrix [13, 14], which encodes flavour-changing transitions in charged-current interactions.

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### 2.1.3. Strong Interaction

The strong interaction is described by quantum chromodynamics (QCD), a non-Abelian gauge theory with gauge group  $SU(3)_C$ . Quarks carry colour charge, while gluons carry a colour and anticolour index, giving rise to self-interactions through three- and four-gluon vertices. These features lead to two fundamental properties:

**Asymptotic freedom.** The QCD coupling decreases at high momentum transfer [5, 15], allowing perturbative calculations of hard processes such as top-quark pair production. In the high-energy regime of the LHC, quarks and gluons behave as effectively quasi-free particles.

**Confinement.** At low energies the QCD coupling becomes large, preventing coloured states from existing in isolation. Instead, they form colour-neutral bound states—hadrons. The transition from short-distance partons to long-distance hadrons involves nonperturbative dynamics encapsulated through hadronisation models.

A crucial consequence for collider physics is that quarks and gluons produced in hard interactions undergo a cascade of QCD emissions before hadronising into jets. This process is typically described in terms of:

- **Parton distribution functions (PDFs)**, characterising the proton structure and entering via the QCD factorisation theorem [16].
- **Initial- and final-state radiation (ISR/FSR)**, arising from soft and collinear gluon emission.
- **Parton showers**, which resum logarithmically enhanced emissions and are implemented in Monte Carlo generators such as PYTHIA, first developed in [17, 18] and extended in modern formulations [19].
- **Hadronisation models**, such as the Lund string model [20, 21], which describe the confinement-driven formation of hadrons.

These aspects of QCD are essential for the reconstruction of hadronic final states at the LHC and for modelling top-quark production and decay.

## 2.2. Top Quark Physics

The top quark is the heaviest known elementary particle. Its predicted existence arose from the already observed CP-Violation in the kaon system, which required a third generation of quarks to be explained within the SM framework [14]. Furthermore, the discovery of the bottom quark in 1977 [22] implied the existence of its weak isospin partner, the top quark. The top quark was eventually discovered in 1995 by the CDF and DØ collaborations at the TEVATRON collider [23, 24]. Currently, the world average of the top quark mass is measured to be [1]

$$m_t = 172.56 \pm 0.31 \text{ GeV}. \quad (2.2)$$

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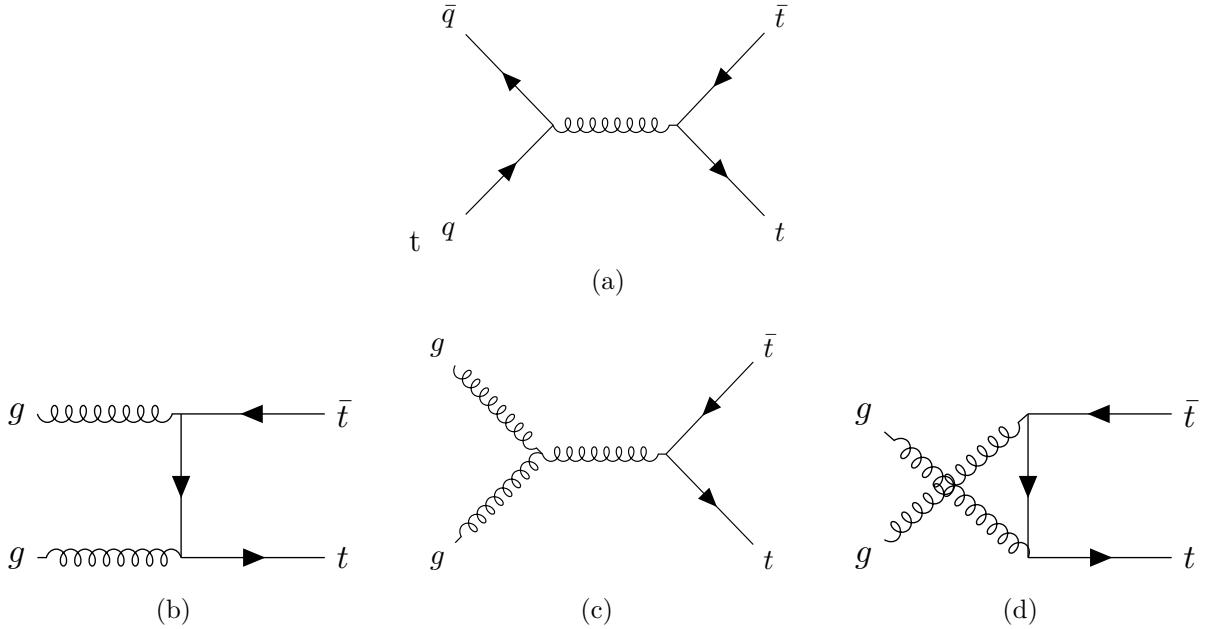


Figure 2.2.: Leading order Feynman diagrams for top quark pair production in (a) quark-antiquark annihilation and (b), (c) & (d) gluon fusion (ggF).

Along with the highest mass, the top quark also has the strongest Yukawa coupling to the Higgs boson, making it interesting for studies of the Higgs mechanism and electroweak symmetry breaking.

Due to its large mass, the top quark also has the shortest lifetime of all quarks, about  $5 \times 10^{-25}$  s [1], which is shorter than the typical hadronisation timescale of  $3 \times 10^{-24}$  s [25]. Therefore, the top is the only quark that decays before it can hadronise, allowing for direct studies of its properties through its decay products.

Notably, the top quark also decays before its spin can decorrelate, preserving spin information in the angular distributions of its decay products [26]. This unique feature enables precise measurements of top quark spin correlations and polarisation. At hadron colliders like the LHC, top quarks are predominantly produced in pairs via the strong interaction. The leading order (LO) Feynman diagrams for top quark pair production are shown in Fig. 2.2. At the LHC, the dominant production mechanism is gluon fusion (ggF). This is due to the high gluon density in the proton at the relevant Bjorken- $x$  values for top quark production.

The CKM matrix element  $V_{tb}$  is close to unity [1], leading to a nearly exclusive decay of the top quark into a  $W$  boson and a  $b$  quark. The  $W$  can subsequently decay either leptonically into a charged lepton and a neutrino, or hadronically into a pair of quarks, with branching ratios of about  $\text{BR}(W \rightarrow \ell\nu) = 1/3$  and  $\text{BR}(W \rightarrow q\bar{q}) = 2/3$ , respectively [1].

Based on these  $W$  decay modes, top quark pair events are categorised into three channels. In the **dileptonic channel**, both  $W$  bosons decay leptonically ( $W^+ \rightarrow \ell^+\nu_\ell$ ,  $W^- \rightarrow \ell^-\bar{\nu}_\ell$ ), resulting in two charged leptons, two neutrinos and two  $b$  quarks in the final state. This channel has a branching ratio of approximately 1/9. The **semileptonic channel**

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occurs when one  $W$  boson decays leptonically and the other hadronically ( $W \rightarrow q\bar{q}'$ ), yielding one charged lepton, one neutrino, four quarks (including two  $b$  quarks) in the final state. This is the most common channel with a branching ratio of about 4/9. Finally, in the **all-hadronic channel**, both  $W$  bosons decay hadronically, producing six quarks (including two  $b$  quarks) in the final state. This channel has the highest branching ratio of approximately 4/9 but suffers from large multijet background contamination, especially in the busy environment of hadron colliders.

### 2.2.1. Dileptonic Decay Channel

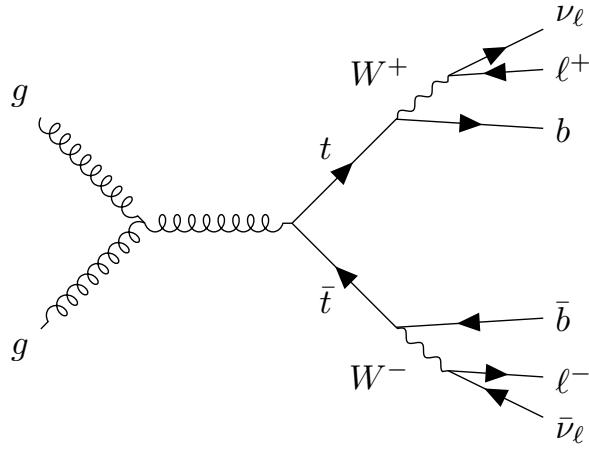


Figure 2.3.: Leading order Feynman diagram for top quark pair production with dileptonic decay.

The dileptonic decay channel, where both  $W$  bosons decay leptonically, has a branching ratio of about 1/9 and results in a final state with two charged leptons, two neutrinos and two  $b$  quarks, as illustrated in Fig. 2.2.1. Due to the lower branching ratio, the dileptonic channel has a smaller event yield compared to the other channels. However, it offers a cleaner signature with reduced background contamination, making it particularly suitable for precision measurements of top quark properties. The presence of two neutrinos in the final state leads to missing transverse energy ( $\cancel{E}_T$ ) in the event, complicating the full reconstruction of the top quark kinematics. Advanced techniques, such as kinematic fitting and multivariate analyses, are often employed to address these challenges and extract maximum information from the dileptonic events.

## 2. Theoretical Background

### Kinematic Constraints

Assuming both  $W$  bosons and top quarks are on-shell, the following kinematic constraints can be applied to the dileptonic decay channel

$$(p_{\ell_1} + p_{\nu_1})^2 = m_W^2, \quad (2.3)$$

$$(p_{\ell_2} + p_{\nu_2})^2 = m_W^2, \quad (2.4)$$

$$(p_{b_1} + p_{\ell_1} + p_{\nu_1})^2 = m_t^2, \quad (2.5)$$

$$(p_{b_2} + p_{\ell_2} + p_{\nu_2})^2 = m_t^2, \quad (2.6)$$

$$(\vec{p}_{\nu_1} + \vec{p}_{\nu_2})_x = \vec{E}_{T_x}, \quad (2.7)$$

$$(\vec{p}_{\nu_1} + \vec{p}_{\nu_2})_y = \vec{E}_{T_y}. \quad (2.8)$$

If one assumes, the neutrinos to be massless, these six equations provide constraints on the six unknown components of the two neutrino momenta. Therefore, additional assumptions or techniques are required to fully reconstruct the event kinematics in the dileptonic channel. Due to the algebraic nature of the constraints, multiple solutions can exist for a given event, leading to ambiguities in the reconstruction [27, 28]. Various methods have been developed to address these challenges, including likelihood-based approaches [29], matrix element methods, and machine learning techniques [30], which aim to optimally utilise the available information and improve the accuracy of the top quark kinematic reconstruction in dileptonic events.

#### 2.2.2. Spin Correlations in Top Quark Pairs

As before elaborated, the top quark decays before it can hadronise or its spin becomes decorrelate. Therefore, the spin information of the top quark is directly transferred to its decay products. In top quark pair production, the spins of the top and antitop quarks are correlated due to the production mechanism. These spin correlations manifest in the angular distributions of the decay products, providing a unique opportunity to study the spin dynamics of the top quark.

Recent studies at the LHC began to explore quantum entanglement in top quark pairs [31]. Entanglement generally describes a quantum mechanical phenomenon where the quantum states of two or more particles become correlated in such a way that the state of one particle cannot be described independently of the state of the other(s), even when the particles are separated by large distances [32]. This property is expressed as the system having a non-separable density matrix. While a general description of this phenomenon is beyond the scope of this thesis, entanglement can be tested using specific criterions. One such criterion is the *Peres-Horodecki criterion* [33, 34], which states that if the partial transpose of the density matrix of a bipartite system has at least one negative eigenvalue, then the system is entangled. Considering top quark pairs as a bipartite system of two spin- $\frac{1}{2}$  particles (qubits), this criterion can be applied to test for entanglement in their spin states.

In Ref. [35] it was proposed to measure entanglement in top quark pairs produced at the LHC by analysing the angular distributions of their decay products, specifically the charged leptons in the dileptonic decay channel. The study showed that by measuring

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the opening angle between the two leptons, one can construct an observable sensitive to the entanglement of the top quark spins. Due to the kinematics of the top quark pair production, the entanglement is expected to be more pronounced in certain regions of phase space, particularly at high invariant masses of the top quark pair system. One particular region of interest is the so-called *threshold region*, where the top quark pair is produced with low relative velocity. In this region, the top quark is produced as a spin singlet state in about  $\sim 80\%$  of the cases, leading to a strong entanglement signature [36]. The ATLAS collaboration has recently reported the first experimental evidence of quantum correlations consistent with entanglement in top quark pairs [31].

### 2.2.3. Top Quark Pair Bound State Effects

Even though the top quark decays before it can hadronise, near the production threshold of top quark pairs, the strong interaction between the top and antitop quarks can lead to the formation of transient bound states, coined as toponium [36–38]. These bound state effects can influence the production cross section and kinematic distributions of top quark pairs near threshold. The CMS collaboration has recently observed an excess in the invariant mass distribution of top quark pairs near threshold, consistent with the presence of toponium bound state effects [39]. The Modelling of these effects is based on non-relativistic QCD (NRQCD) calculations, which account for the strong interaction dynamics between the top and antitop quarks in the near-threshold region [40, 41]. Understanding and accurately modelling these bound state effects is crucial for precision measurements of top quark properties and for searches for new physics in top quark pair production.

This study is also investigating the threshold region of top quark pair production and makes use of angular correlations between the decay products as a probe of the underlying dynamics, including potential bound state effects.

# 3. Machine Learning in High Energy Physics

Since this work focuses on improving the event reconstruction of dileptonic  $t\bar{t}$  decays using machine learning techniques, this chapter provides an overview of the fundamental concepts and methodologies employed in machine learning.

## 3.1. Supervised Learning

Machine learning can be broadly categorized into supervised and unsupervised learning. In supervised learning, the model is trained on a labeled dataset, where each input data point is associated with a corresponding target output. The goal of the model is to learn a mapping from inputs to outputs, enabling it to make accurate predictions on unseen data.

### 3.1.1. Monte Carlo Training Data

In high energy physics, supervised learning is commonly performed by training models on simulated datasets. The way the Monte Carlo Event modelling is performed in particle physics, makes it naturally suited for supervised learning tasks.

Events are usually simulated using a cascade of different programs, each simulating a different state of the event. First the hard scattering process is simulated using matrix element generators like MADGRAPH [42] or POWHEG [43]. These programs calculate the probabilities of different particle interactions based on the underlying physics theories, such as the Standard Model. Using these probabilities, they generate events that represent the initial state of the particles after the collision. The possible kinematic phase space is sampled according to these probabilities, resulting in a set of particles with specific momenta and energies. This type of event variables is often referred to as *parton-level*.

Next, the parton showering and hadronization processes are simulated using programs like PYTHIA [19]. Parton showering models the emission of additional particles from the initial partons, while hadronization simulates the formation of hadrons from quarks and gluons. These processes are crucial for accurately modelling the final state particles observed in detectors.

Finally, detector simulation programs like GEANT4 [44] are used to simulate the interaction of particles with the detector material, producing realistic detector responses. This includes simulating the energy deposits in calorimeters, hits in tracking detectors, and other relevant signals.

While the actual detector response is simulated using complex detector simulation soft-

### 3. Machine Learning in High Energy Physics

ware, for many machine learning applications, a simplified representation of the detector response is sufficient. This can involve smearing the particle momenta and energies according to the detector resolution, applying efficiency corrections, and simulating the effects of pile-up.

This is because, for the reconstruction of the physics objects, such as jets, leptons, and missing transverse energy, highly sophisticated algorithms are used that already take into account the detector effects (Note, that these algortihms may also be machine learning based,). Therefore, the input features for machine learning models can often be derived directly from these reconstructed objects, rather than relying on the raw detector signals. The reconstructed object event variables are called *reco-level*.

#### 3.1.2. Training

During the training phase, the model is presented with a set of input features derived from the reco-level event variables, along with their corresponding target outputs, which are typically derived from the parton-level event variables. The model learns to map the input features to the target outputs by minimizing a loss function that quantifies the difference between the predicted and true values. Common loss functions include mean squared error for regression tasks and cross-entropy loss [45] for classification tasks. The training process involves iteratively updating the model's parameters using an optimization algorithm to minimize the loss function.

#### 3.1.3. Validation and Testing

To evaluate the performance of the trained model, it is essential to validate and test it on independent datasets that were not used during training. This helps to assess the model's generalization capabilities and ensures that it can make accurate predictions on unseen data. Common evaluation metrics include accuracy, precision, recall, F1-score for classification tasks, and mean absolute error or R-squared for regression tasks.

## 3.2. Neural Networks

Inspired by the structure and function of the human brain, neural networks are composed of interconnected nodes.

# 4. Experimental Setup

## 4.1. The LHC

The Large Hadron Collider (LHC) at CERN is a synchrotron designed to accelerate protons and lead nuclei. This work focuses on the proton-proton collisions during Run 2. During Run 2 from 2015 to 2018, the LHC operated at a centre of mass energy of  $\sqrt{s} = 13 \text{ TeV}$  with an integrated luminosity of  $\mathcal{L}_{int} \approx 140 \text{ fb}^{-1}$  [46].

After completion of Run 3 in Dec. 2025 and an operational pause, the LHC will operate with increased luminosity as the High-Luminosity Large Hadron Collider (HL-LHC). During this phase, it is planned to accumulate data with an integrated luminosity of  $\mathcal{L} = 3 \text{ ab}^{-1}$  [47].

## 4.2. The Detector

The ATLAS detector is a general-purpose particle detector at the LHC at CERN. It can roughly be separated into three elements: the inner detector, the calorimeter and the muon spectrometer [48].

### 4.2.1. The Coordinate System

The interaction point marks the origin of the ATLAS coordinate system. The  $z$ -axis is orientated along the beamline, the  $x$ -axis points towards the centre of the LHC and the  $y$ -axis points upwards.

Using this convention several kinematic variables are defined. One of which is the transverse momentum defined as

$$p_T = \sqrt{p_x^2 + p_y^2} \quad (4.1)$$

Because of the cylindrical shape of the ATLAS detector and the cylindrical symmetry of the interactions, the azimuthal angle is used as another variable. The polar angle relative to the  $z$ -axis can be used to define the pseudorapidity which can also be expressed in terms of the momentum

$$\eta = -\ln(\tan(\frac{\theta}{2})) = \ln\left(\frac{|\vec{p}| + p_z}{|\vec{p}| - p_z}\right). \quad (4.2)$$

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In the ultra-relativistic limit  $m \ll |\vec{p}|$  the pseudorapidity is equal to the rapidity defined as

$$y = \frac{1}{2} \ln\left(\frac{E + p_z}{E - p_z}\right). \quad (4.3)$$

These variables are convenient for the usage in the ATLAS experiment because  $p_T$ ,  $\phi$ , and differences of  $\eta$  are invariant under Lorentz-boost along the  $z$ -axis.

##### 4.2.2. The Inner Detector

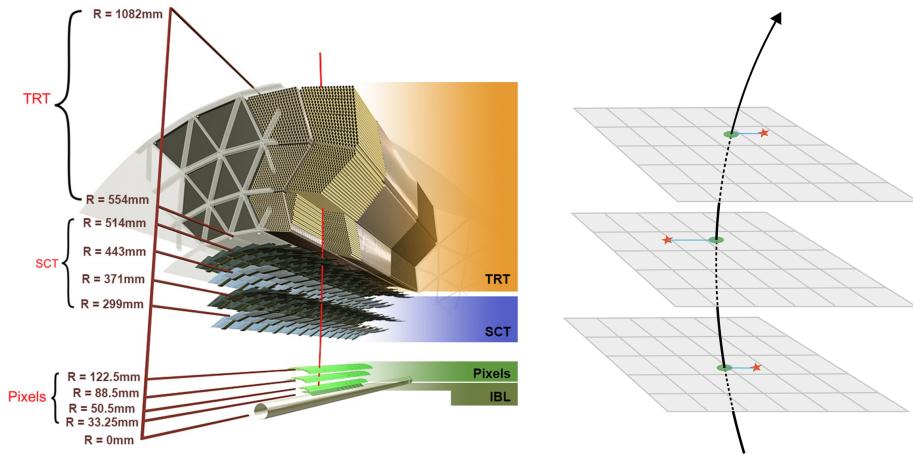


Figure 4.1.: Schematic cross section of the inner detector of the ATLAS detector (© CERN).

The inner detector (ID) is the innermost part of the ATLAS detector. It is used for tracking charged particles, particle identification, and primary and secondary vertexing [48]. The ID consists of three different sub-detectors. Their rough structure is depicted in Figure 4.2.2. The ID is encapsulated with a solenoid magnet providing a 2 T axial magnetic field on the inside of the ID. The magnetic field is crucial to measure the momentum of a charged particle. The transverse momentum is measured as the curvature of the particle's track due to the Lorentz force.

The detector part closest to the beam pipe is the pixel detector. It consists of 1744 modules arranged in three barrel layers. Each module hosts 47232 silicon pixels with a size of  $50 \times 400 \mu\text{m}^2$ . The pixels are semiconductor trackers used to detect the traversing of charged particles.

The following part of the detector is the semiconductor tracker (SCT). It consists of 4088 modules arranged in four layers to guarantee four position measurements of charged particles. Each module consists of four silicon sensors. The sensors offer a  $17 \mu\text{m}$  resolution in-plane lateral and  $580 \mu\text{m}$  in-plane longitudinal.

The outermost part of the inner detector is the transition radiation tracker (TRT). It consists of polyimide drift (straw) tubes with a 4 mm diameter that are arranged in a 528 mm thick cylindrical layer around the beam pipe. The straw tubes are interleaved with fibres for the readout. The transition radiation tracker utilizes the transition light

#### 4. Experimental Setup

emitted by charged particles traversing the interface between two media with different indices of refraction. The TRT offers a measurement of charged particles and electron identification.

##### 4.2.3. Calorimeter

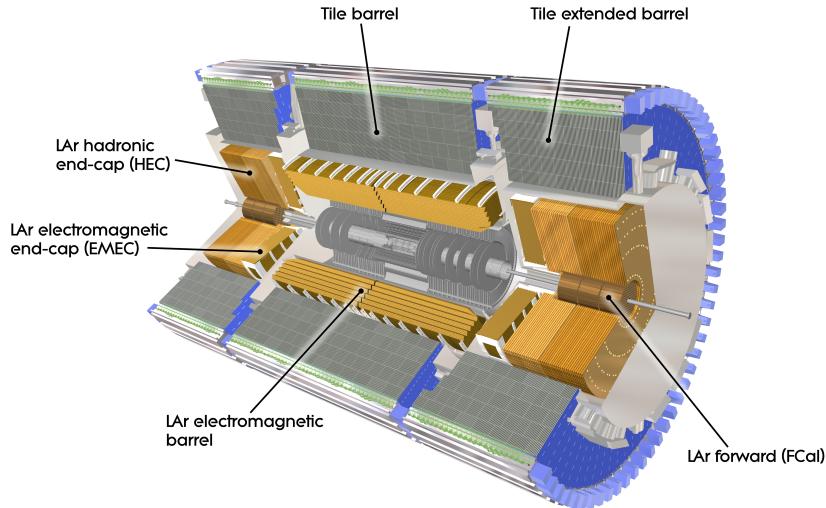


Figure 4.2.: Computer generated image of the ATLAS calorimeter (© CERN).

The calorimeters are the detector layers following the inner detectors. Its structure is divided into the Electromagnetic calorimeter (ECal) and the hadronic calorimeter (HCal).

##### Electromagnetic Calorimeter

The ECal is used for the energy and position measurement of electric charged particles and photons. It utilizes bremsstrahlung and pair production to create a cascade of charged particles which are measured. It offers full azimuthal coverage and is equipped with end caps in the longitudinal direction of the beam pipe. The ATLAS ECal is a sampling calorimeter operating with lead as the passive and liquid Argon as the active medium. The innermost part of the ECal is a presampler which detects if the particle started showering before reaching the ECal.

##### Hadronic Calorimeter

The HCal measures the energy and position of baryons and mesons through strong interactions with the nuclei. In the range of  $|\eta| < 1.7$  it is a sampling calorimeter with steel as the passive and scintillators as the active medium. For the end cap, liquid Argon is deployed as the active medium. The HCal works with the same principle as the ECal but offers less precise measurements.

#### *4. Experimental Setup*

In the range of  $3.1 < |\eta| < 4.9$  ECal and HCal are substituted with the forward calorimeters (FCal) which are made up of three modules to fulfil the function of both calorimeters. In combination with the FCal a total range of  $|\eta| < 4.9$  is covered by the calorimeters. A computer-generated image of the structure of the different calorimeters used in the ATLAS detector is shown in Figure 4.2.3.

#### **4.2.4. Muon Spectrometer**

The muon spectrometer is the outermost part of the ATLAS detector. Its purpose is to detect charged particles exiting the calorimeters and measure their momentum in the range of  $|\eta| < 2.7$ . A detector dedicated to the measurement of muons is necessary because their mass makes them minimal ionizing particles in the energy range of the LHC collisions. The amount of energy loss due to bremsstrahlung is not sufficient to develop showers necessary to measure their energy. The muons' transverse momenta can be measured in the ID. Like the inner detector, the muon spectrometer utilizes a magnetic field to conduct a measurement of the particle's momentum. In the muon spectrometer, however, a solenoid magnet is used to allow for the measurement of the muon's momentum along a different direction. Combining the measurements, one obtains full knowledge of the muons four-momentum. Further, does the high rate of stopped electrons and hadrons in the calorimeters enable a high specificity in the muon detection.

#### **4.2.5. Trigger System**

With a bunch spacing of 25 ns [46] collisions happen at a rate of 40 MHz. Each collision involves up to hundreds of particles. To reduce the data to a feasible amount, triggers are employed to filter less interesting events. Different layers of triggers operate either at the hardware or software level. The L1 trigger is a hardware level trigger and acts as the first filter for the events. It makes decisions in less than 2.5  $\mu$ s. The subsequent L2 trigger is a software level trigger and makes decisions in less than 200  $\mu$ s. Combined the trigger system reduces the event rate from 40 MHz to 1000 Hz which are then stored at the CERN data centre.

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# Danksagung

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**Erklärung** nach §17(9) der Prüfungsordnung für den Bachelor-Studiengang Physik und den Master-Studiengang Physik an der Universität Göttingen: Hiermit erkläre ich, dass ich diese Abschlussarbeit selbstständig verfasst habe, keine anderen als die angegebenen Quellen und Hilfsmittel benutzt habe und alle Stellen, die wörtlich oder sinngemäß aus veröffentlichten Schriften entnommen wurden, als solche kenntlich gemacht habe. Darüberhinaus erkläre ich, dass diese Abschlussarbeit nicht, auch nicht auszugsweise, im Rahmen einer nichtbestandenen Prüfung an dieser oder einer anderen Hochschule eingereicht wurde.

Göttingen, den 8. Dezember 2025

(Siemen Henning Aulich)